

# StatLib---Applied Statistics algorithms

The Royal Statistical Society has been publishing algorithms in its journal Applied Statistics since 1968. As of 1989, there are over 250 of them. Most are in Fortran, though a few were in Algol, and some recent ones have been in Pascal. The book - Applied Statistics Algorithms by Griffiths, P. and Hill, I.D., Ellis Horwood: Chichester (1985) contains translations of several algorithms from Algol to Fortran. A few of the other algorithms have been supplied in Fortran translations, though a few are in Algol or Pascal. The index which follows indicates which algorithms are not in Fortran.

The full source code is published in the journal. Those available here have been transcribed manually, mainly within CSIRO Division of Mathematics & Statistics, or have been supplied directly by the authors or by the RSS Algorithms Editor. In some cases, later corrections or improvements published in Applied Statistics, have been incorporated.

It is the policy of the editors of the algorithms section of Applied Statistics that algorithms do not use double precision. Many of the algorithms here have been converted to double precision, though users should be careful to check what precision is used. Many of the algorithms require the use of other algorithms, particularly functions for the gamma function and the normal distribution function. Where such functions or subroutines are required, an appropriate comment has been added to the algorithm.

In a few cases, alternative algorithms from other sources have been added. For instance, three algorithms are included in the file for as66 for calculating the area under the normal curve, and an alternative random number generator is provided in the file for as183. The Applied Statistics algorithm for Nelder-Mead simplex minimization (AS 47) does not include the fitting of a quadratic surface; the CSIRO/ Rothamsted implementation which does this is included with AS 47.

Users must consult the original journal articles for details of the calling arguments; they are not included with these algorithms.

\*\*\* Warning. In some cases, there are different arguments (usually more) in the Griffiths & Hill versions of these algorithms. Users should check this.

It has been assumed that the user will be using a Fortran-77 compiler, so functions such as alog and amin1 have been converted to their generic forms (log and min). This simplifies conversion of code between single and double precision. Also all constants in the code, such as 1.0, 0.d0, etc., have been replaced with one, zero, etc., and these are defined in either data or parameter statements. Many of the algorithms have been entered in lower case, which is not acceptable in Fortran, though most compilers accept it.

Some of the algorithms need machine-dependant constants. The user should check this. In most cases, these have been set for compilers which allow a range of floating-point numbers from about  $10^{*(-37)}$  to  $10^{*(+37)}$ , though most modern compilers allow a much wider range

in double precision.

No guarantee is given that the algorithms have been entered correctly, or that they perform as claimed in the journal.

To obtain an algorithm, send an E-mail request of the form: send index from apstat send 207 from apstat to statlib@lib.stat.cmu.edu

The Royal Statistical Society holds the copyright to these routines, but has given its permission for their distribution provided that no fee is charged.

The full collection of Applied Statistics algorithms is very large. Please only request those algorithms which you need. Requesting large numbers of algorithms places a great strain on the StatLib system and the underlying mail networks.

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As of the end of 1997 the Applied Statistics journal does NOT accept algorithms

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## **Listing of available Applied Statistics algorithms**

- No.                      Brief description (volume number/year in brackets)
- [3](#)                         Student's t-distribution. (17/1968) See also AS 27.
- [5](#)                         The non-central t-distribution. (17/1968) See also AS 243.
- [6](#)                         Cholesky decomposition of a symmetric +ve definite matrix. (17/1968)
- [7](#)                         Inversion of a symmetric matrix stored in triangular form. (17/1968)
- [13](#)                        Minimum spanning tree. (18/1969) See also AS 40.
- [14](#)                        Printing the minimum spanning tree. (18/1969)
- [15](#)                        Single-linkage cluster analysis. (18/1969)
- [22](#)                        Calculate treatment effects in a complete factorial experiment for any numbers of levels of factors using the extended Yate's method. (19/1970)

- [27](#)  
Upper tail area under Student's t-distribution. (19/1970) See also AS 3.
- [30](#)  
Half-normal plotting. (19/1970)
- [32](#)  
The incomplete gamma integral. (19/1970) See also AS 239.
- [34](#)  
Update inverse of symmetric banded matrix. (19/1970)
- [38](#)  
Calculate R-squared for all possible regression subsets using the Gauss-Jordan method. (20/1971) See also AS 268.
- [40](#)  
Update a minimum spanning tree. (20/1971)
- [41](#)  
Updates corrected sums of squares and products matrices. (20/1971) See also AS 240.
- [45](#)  
Histogram plotting. (20/1971)
- [46](#)  
Gram-Schmidt orthogonalization. (20/1971)
- [47](#)  
Nelder & Mead simplex method of unconstrained minimization without requiring derivatives. Does not include the quadratic surface fitting part of the algorithm. A CSIRO/Rothamsted version of the algorithm, which does include fitting a quadratic surface, is also included. (20/1971) (Updated, 20/Dec/93)
- [51](#)  
Log-linear fit for contingency tables. (21/1972) See also AS 160.
- [52](#)  
Calculation of sums of powers (up to 4) of deviations from the mean. (21/1972)
- [53](#)  
Wishart variate generator. (21/1972)
- [57](#)  
Printing multi-dimensional tables. (22/1973)
- [58](#)  
Allocates observations to clusters to minimize within-cluster sum of squares. (22/1973) See also AS 136.
- [60](#)

Eigenvalues/vectors of a symmetric matrix. (22/1973)

[62](#)

Distribution of the Mann-Whitney U statistic. (22/1973)

[63](#)

Incomplete beta function. (22/1973) See also TOMS algorithm 708. TOMS algorithms are available from netlib.

[64](#)

Inverse of the incomplete beta function ratio. (22/1973) The file here is actually the Griffiths & Hill version of AS 109.

[65](#)

Expands structure formula to a list of binary integers. This is actually remark R82 which replaces the original AS65. (39/1990)

[66](#)

The normal distribution function. Two other algorithms (not from Applied Statistics) have also been included. (22/1973)

[75](#)

Algorithms for least-squares calculation using square-root free planar rotations (Morven Gentleman's package). (23/1974)

[76](#)

An integral useful in calculating noncentral t and bivariate normal probabilities. (23/1974)

[77](#)

Calculate exact null distribution of the largest root of a beta matrix. (23/1974)

[78](#)

The mediancentre (i.e. the median in a multi-dimensional space). (23/1974) See also AS 143.

[83](#)

Complex discrete fast Fourier transform. (24/1975)

[84](#)

Measures of multivariate skewness and kurtosis. (24/1975)

[88](#)

Generate all  $nCr$  combinations by simulating nested Fortran DO-loops. (Jane Gentleman's routines). (24/1975) See also AS 172.

[89](#)

Tail probabilities for Spearman's rho. (24/1975)

[91](#)

Percentage points of the chi-squared distribution. (24/1975)

- [93](#)  
Calculates frequency distribution for the Ansari-Bradley test statistic. (25/1976) A routine has been added to return the distribution function.
- [95](#)  
Maximum likelihood estimation of scale and location parameters from grouped data. User's distribution function. (25/1976)
- [96](#)  
Finding 'nice' scales for graphs. (25/1976)
- [97](#)  
Real discrete fast Fourier transform. Series length must be a power of 2. (25/1976) See also AS 117 and AS 176.
- [99](#)  
Fitting Johnson curves by moments. (25/1976)
- [100](#)  
Normal-Johnson and Johnson-Normal transformations. (25/1976)
- [103](#)  
Psi or digamma function. (25/1976)
- [107](#)  
Calculate operating characteristics and average sampling number for a general class of sequential sampling plans. (26/1977)
- [108](#)  
Multiple linear regression minimizing the sum of absolute errors. (26/1977) See also AS 238 (in Pascal).
- [109](#)  
Inverse of the incomplete beta function. (26/1977)
- [110](#)  
LP-Norm fit of straight line by extension of Schlossmacher. (26/1977)
- [111](#)  
Percentage points of the normal distribution. (26/1977) See also AS 241.
- [114](#)  
Compute the numerator of certain ordinal measures of association (Kendall's tau, Somer's d, Goodman and Kruskal's gamma) when the data are ordered categories. (26/1977)
- [116](#)  
Calculate the tetrachoric correlation and its standard errors. (26/1977)
- [117](#)

Fast Fourier transform for series of any length using the CHIRP algorithm. (26/1977)

[121](#)

Trigamma function. (27/1978)

[123](#)

Distribution function of mixtures of beta distributions. (27/1978)

[125](#)

Maximum likelihood estimation for censored exponential survival data with covariates. (27/1978)

[126](#)

Distribution function of the range for the normal distribution. (27/1978)

[127](#)

Generation of random orthogonal matrices. (27/1978)

[128](#)

Computes approximate covariance matrix for normal order statistics. (27/1978)

[132](#)

Simple regression minimizing the sum of absolute deviations. (27/1978)

[133](#)

Finding the global maximum or minimum of a function of 1 variable. (27/1978)

[134](#)

Generate random beta variates for  $\alpha < 1$  and  $\beta > 1$ . (28/1979)

[135](#)

Min-Max (L-infinity) estimates for linear multiple regression. (28/1979)

[136](#)

A K-means clustering algorithm. (28/1979)

[138](#)

Maximum likelihood estimates of the mean and standard deviation of the normal distribution with censored or confined observations. (28/1979)

[139](#)

Maximum likelihood estimation in a linear model from confined and censored normal data. (28/1979)

[140](#)

Clustering the nodes of a directed graph. (28/1979)

[141](#)

Inversion of a symmetric matrix ignoring a specified row/column. (28/1979)

[142](#)

Exact tests of significance in binary regression. (28/1979)

[143](#)

Calculates the median centre. (28/1979)

[145](#)

Exact distribution of the largest multinomial frequency. (28/1979)

[147](#)

Incomplete gamma function. (29/1980) See also AS 239.

[148](#)

Removal of bias in the jackknife procedure. (This is actually ASR 62) (29/1980)

[149](#)

Amalgamation of means in the case of simple ordering ('Up-and-Down Blocks' algorithm for isotonic regression). (29/1980)

[150](#)

Computes estimate of spectrum of a point process using a centered moving average of the periodogram of the counting process. (29/1980)

[151](#)

Smoothed spectral estimate for bivariate point processes. (29/1980)

[152](#)

Cumulative hypergeometric probabilities. (This is actually AS R77) (29/1980, revised in 38/1989)

[153](#)

Distribution of weighted sum of squares of normal variables. (29/1980) Pan's procedure for the tail probabilities of the Durbin-Watson statistic.

[154](#)

Exact maximum likelihood estimation of autoregressive-moving average models by Kalman filtering. (29/1980) See also AS 182.

[155](#)

Distribution function of a linear combination of non-central chi- squared random variables. (29/1980) See also AS 204. This is a Fortran translation supplied by the author.

[157](#)

The runs-up and runs-down tests. (30/1981)

[158](#)

Calculation of probabilities for inferences under simple order restrictions. (30/1981) See also AS 198.

[159](#)

Generate random 2-way table with given marginal totals. (30/1981)

[160](#)

Partial and marginal association in multi-dimensional contingency tables. (30/1981)

[161](#)

Critical regions of an unconditional non-randomized test of homogeneity in  $2 \times 2$  contingency tables. (30/1981)

[162](#)

Multivariate Conditional Logistic Analysis of Stratum-matched Case-control Studies. (30/1981) Includes a Fortran version of CACM algorithm 382 for generating all combinations of M out of N items.

[163](#)

A Givens Algorithm for Moving from one Linear Model to another without Going back to the Data. (30/1981)

[164](#)

Least squares subject to linear constraints. (30/1981)

[165](#)

Discriminant analysis of categorical data. (30/1981)

[166](#)

Calculates the entanglement matrix for a specified design. (30/1981)

[167](#)

Calculates efficiencies of estimation and their generalized inverse. (30/1981)

[168](#)

Calculates 'neat' values for plotting scales. (30/1981)

[169](#)

Produces scatter plots. (30/1981)

[170](#)

Computation of probability and non-centrality parameter of a non- central chi-square distribution. (30/1981)

[171](#)

Fisher's exact variance test for the Poisson distribution. (31/1982)

[172](#)

Generates indices for simulated nested DO-loops. Actually converts (either way) between a single index and a vector of subscripts. (31/1982)

[173](#)

Generates design matrix for balanced factorial experiments. (31/1982)

[174](#)

Multivariate rank sum test and median test. (31/1982)

[175](#)



Cramer-Wold factorization of self-reciprocal polynomials as the product of two polynomials. (31/1982)

[176](#)

Kernel density estimation using the fast Fourier transform. (31/1982) Also contains an alternative set of routines for density estimation.

[177](#)

Expected values of normal order statistics. (31/1982)

[178](#)

Gauss-Jordan sweep operator with multi-collinearity detection. (31/1982)

[179](#)

Enumeration of all permutations of multi-sets with fixed repetition numbers. (31/1982)

[180](#)

Linear rank estimate of the standard deviation after symmetric trimming. (31/1982)

181

Withdrawn. See R94 below

[182](#)

Finite-sample prediction from ARIMA processes. (31/1982) Uses AS 154.

[183](#)

The Wichmann & Hill random number generator. An alternative is also provided. (31/1982)

[184](#)

Non-central studentized maximum and related multiple-t probabilities. (31/1982)

[185](#)

Backward elimination procedure to find best-fitting log-linear models for contingency tables. (31/1982) Uses AS 51.

[186](#)

Discrete Fast Fourier Transform with data permutation. Series length must be a power of 2. (31/1982)

[187](#)

Derivatives of the incomplete gamma integral. (31/1982)

[188](#)

Estimation of the order of dependence in sequences. (32/1983)

[189](#)

Maximum likelihood estimation for the beta binomial distribution. (32/1983)

[190](#)

Distribution function & its inverse, for the studentized range. (32/1983)

[191](#)

Approximate likelihood calculation for ARMA and seasonal ARMA models. Includes a routine for the Banachiewicz (or modified Cholesky) factorization  $A = LDL'$ . (32/1983)

[192](#)

Calculate approximate percentage points using Pearson curves and the first three or four moments. (32/1983)

[193](#)

The Knuth spectral test for congruential random number generators. (32/1983)

[194](#)

Test of goodness of fit of ARMA models. (32/1983)

[195](#)

Multivariate normal probabilities for a rectangular region in N- dimensional space. A version which calls IMSL routines is also included. (33/1984) See AS 251 for a special case.

[196](#)

Conditional multivariate logistic analysis of stratified case-control studies. (33/1984)

[197](#)

Likelihood function for an ARMA process. (33/1984)

[198](#)

Calculation of level probabilities for order-restricted inference. (33/1984)

[199](#)

Branch and bound algorithm to find the subset which maximizes a quadratic form. (33/1984)

[200](#)

Approximate the sum of squares of normal score. (33/1984)

[201](#)

Combine predictions about a statistic based on the orderings of a set of means with an F-test of differences between the means. (33/1984)

[202](#)

Data-based nonparametric hazard estimation. (33/1984)

[203](#)

Maximum likelihood estimation of mixtures of distributions (normal, exponential, Poisson and binomial). (33/1984) See also AS221. This is a translation from Algol into Fortran.

[204](#)

Distribution of a sum of non-central chi-squared variables. (33/1984) Translation from Algol into Pascal.

[205](#)

Enumeration of all  $R \times C$  contingency tables with given row and column totals, and calculation of hypergeometric probability for each table. (33/1984)

[206](#)

Isotonic regression in two independent variables. (33/1984)

[207](#)

Fit a generalized log-linear model. (33/1984)

[208](#)

Fit multivariate logistic model by the method of moments. (34/1985)

[209](#)

The distribution function of skewness and kurtosis. (34/1985)

[210](#)

Fit 5-parameter Johnson SB curves by moments. (34/1985)

[211](#)

The F-G diagonalization algorithm. (34/1985) Modifications in ASR 71 & ASR 74 have been added to the file.

[212](#)

Fitting the exponential curve by least squares. (34/1985)

[213](#)

Generation of correlation matrices with specified eigenvalues. (34/1985)

[214](#)

Calculation of Monte Carlo confidence intervals. (34/1985)

[215](#)

Maximum likelihood estimation of the parameters of the generalized extreme-value distribution. (34/1985). Updated on [15/Nov/99]

[216](#)

Maximum likelihood fitting when model contains a linear part and auxiliary parameters. (34/1985)

[217](#)

Computation of the Dip statistic to test for unimodality. (34/1985)

[218](#)

Elements of the Fisher information matrix for the smallest extreme-value distribution, also allows for censored data. (35/1986)

[219](#)

Height balanced trees. (35/1986)

[220](#)

Operating characteristics of James-Stein and Efron-Morris estimation. (35/1986)

[221](#)

Maximum likelihood estimation of a mixing distribution. (35/1986)

[222](#)

Resistant smoothing using the fast Fourier transform. (36/1987)

[223](#)

Optimum ridge parameter selection. (36/1987)

[224](#)

Combining component designs to form a design with several orthogonal blocking factors. (36/1987)

[225](#)

Minimizing linear inequality-constrained Mahalanobis distances. (36/1987)

[226](#)

Cumulative probabilities for the non-central beta distribution. (36/1987)

[227](#)

Generate all possible N-bit binary codes. (36/1987)

[228](#)

Finding I-projections (maximizing cross-entropy) subject to a finite set of linear inequality constraints. (36/1987)

[229](#)

Quantile regression. (36/1987)

[230](#)

Distribution of customers in M/G/m queues using an approximation due to Hokstad. (36/1987)

[231](#)

Distribution of a noncentral chi-squared variable with non-negative degrees of freedom. (36/1987) In Pascal.

[232](#)

Computation of population and sample correlation and partial correlation matrices in MARMA(p,q) time series. (37/1988)

[233](#)

Branch and bound algorithm for feature subset selection. (37/1988)

[234](#)

Approximating the percentage points of simple linear rank statistics with Cornish-Fisher expansions. (37/1988)

[235](#)

Tally frequencies of distinct real values. (37/1988)

[236](#)

Recursive enumeration of RxC tables for exact likelihood evaluation. (37/1988) In Pascal.

[237](#)

The corner method for identifying autoregressive moving average models. (37/1988)

[238](#)

Recursive procedure for the L1-norm fitting of a straight line. (37/1988) In Pascal.

[239](#)

Incomplete gamma function. (37/1988)

[240](#)

Updating the inverse of corrected sums of squares and products. (37/1988)

[241](#)

Inverse normal - more accurate than AS 111. (37/1988)

[242](#)

The exact likelihood of a vector autoregressive moving average model. (38/1989)

[243](#)

Cumulative distribution function of the non-central t-distribution. (38/1989)

[244](#)

Decomposability and collapsibility for log-linear models. (38/1989) In Pascal.

[245](#)

Log of the gamma function. (38/1989) The file includes a slower but more accurate algorithm which is not an AS algorithm.

[246](#)

Repeated measurements analysis of variance with unknown autoregressive parameter. (38/1989)

[247](#)

Updating the sufficient configurations for fitting ZPA (zero partial association) models to multi-dimensional contingency tables. (38/1989) In Pascal.

[248](#)

Empirical distribution function goodness-of-fit tests for the uniform, normal and exponential distributions. (38/1989)

[249](#)

Mean and covariance estimation for the truncated multivariate normal distribution. (38/1989)

[250](#)

Test the equality of dispersion matrices using methods due to Puri & Sen (distribution-free) and Anderson (normal distribution). (38/1989)

[251](#)

Multivariate normal probability integrals with product correlation structure. (38/1989)

[252](#)

Generating classes for log-linear models. (39/1990)

[253](#)

Maximum likelihood estimation of the RC(M) association model. (39/1990)

[254](#)

Fit mixture of normal distributions to grouped & truncated data. (39/1990)

[255](#)

Fitting two-way tables by means for rows, columns and cross-term. (39/1990) In *Algol*.

[256](#)

Distribution of a quadratic form in normal variables. (39/1990) In *Pascal*.

[257](#)

Isotonic regression for umbrella orderings. (39/1990)

[258](#)

Average run lengths for cumulative sum schemes. (39/1990)

[259](#)

Extending confidence intervals by the Robbins-Monro search process. (39/1990)

[260](#)

Distribution function of the square ( $R^2$ ) of the sample multiple- correlation coefficient. (40/1991)

[261](#)

Quantiles of the distribution of square ( $R^2$ ) of the sample multiple- correlation coefficient. (40/1991)

[262](#)

The Wei-Lachin two-sample test, the generalized Wilcoxon test and the log-rank test for incomplete multivariate observations with censoring. (40/1991)

[263](#)

Construction of irredundant test sets. (40/1991)

[264](#)

Printing of bit patterns. (40/1991)

[265](#)

Waiting time distribution for the G/G/1 queue using the Fast Fourier transform. (40/1991)

[266](#)

Maximum likelihood estimation of the parameters of the Dirichlet distribution. (40/1991)

[267](#)

Calculate lower bound for the probability of correct selection of a subset containing the best populations from a set of populations. (40/1991)

[268](#)

Calculates statistics for all possible subset regressions using an orthogonal decomposition. (40/1991)

[269](#)

Calculates the Cornish-Fisher adjustment to distribution functions (from the normal distribution function) using higher cumulants. (41/1992)

[270](#)

Maximum likelihood fitting of a 'key' density function, e.g. normal distribution, multiplied by a series in Hermite polynomials. (41/1992)

[271](#)

Optimal (smallest mis-classification probability) joint classification procedure. (41/1992) See also AS 276.

[272](#)

Produce character Box-plots using supplied quartiles. (41/1992)

[273](#)

Compare the least-squares fit of two subsets of regression variables using Spjøtvoll's method. (41/1992)

[274](#)

Least squares algorithms to supplement those of Gentleman in AS 75. (41/1992)

[274-90](#)

Algorithm 274, translated into Fortran 90.

[275](#)

Non-central chi-squared distribution function, number of degrees of freedom must be positive but not necessarily integer. (41/1992)

[276](#)

Optimal combinatoric classification for two normal classes. (41/1992) See also AS 271.

[277](#)

The Oja bivariate median. (41/1992)

[278](#)

The distribution of quadratic forms of multivariate generalized Student variables. (41/1992)

[279](#)

P-values for the generalized/alternative Durbin-Watson statistic with arbitrary lag using a Cholesky transformation method. (42/1993)

[280](#)

The power function for Fisher's exact test. (42/1993)

[281](#)

Scaling and rounding regression coefficients to force them to be integers. (42/1993)

[282](#)

High breakdown regression and multivariate estimation. (42/1993)

[283](#)

Rapid computation of the permutation paired and grouped t-tests. (42/1993) In ANSI Standard C.

[284](#)

Null distribution of a statistic for testing sphericity and additivity: a Jacobi polynomial expansion. (42/1993)

[285](#)

Calculate multivariate normal probabilities using Monte Carlo methods for a general region defined by a user-supplied function. (42/1993)

[286](#)

Estimation of parameters when there are errors in both the predictor variables and the dependant variable using least squares with a general model (includes implicit non-linear regression). (42/1993)

[287](#)

Adaptive rejection sampling (to generate random variables) from log-concave density functions. (42/1993)

[288](#)

P-value calculation for the generalized two-sample Smirnov tests. The tests are conditional on ties in the pooled sample. (43/1994)

[289](#)

Convolves hypergeometric distributions generated by several 2x2 tables (43/1994)

[290](#)

Generate a grid of variance ratios for contour plotting of confidence regions for a pair of parameters in non-linear regression. (43/1994)

[291](#)

Calculates overlap capability of subsequence SSEQ of length L. (43/1994)

[292](#)

Computes Fisher information matrix elements for time (type I) or failure (type II)



censored units from the smallest extreme value (sev), largest extreme value (lev), normal or logistic distribution. (43/1994)

[293](#)

Convolves conditional distributions generated by several  $2 \times K$  tables (43/1994)

[294](#)

Pascal program for ....?

[295](#)

Heuristic algorithm to pick  $N$  rows of  $X$  out of NCAND to maximize the determinant of  $X'X$ , using the Fedorov exchange algorithm. (43/1994)

[R94](#)

calculates Shapiro-Wilk normality test and P-value for sample sizes  $3 \leq n \leq 5000$ . Handles censored or uncensored data. Corrects AS 181, which was found to be inaccurate for  $n > 50$ . (Uses function POLY in [AS 181](#)) by Patrick Royston (44/1995)

[R96](#)

Interval for trapezoidal rule integration to limit error using moment generating function bound for weighted sum of chi-squared(1) random variables.

[297](#)

Nonparametric regression using ultraspherical polynomials.

[298](#)

Hybrid minimization routine using simulated annealing and any local minimizer supplied by the user.

[300](#)

Efficient algorithm for determining a simulated percentile point with a fixed degree of accuracy.

[301](#)

Computes the logarithms of  $F1$ ,  $P(H)$  and  $P(H')$ .

[302](#)

Subroutine to compute a multiple isotonic regression for umbrella ordering with known peak.

[303](#)

Generation of ordered multinomial frequencies. Given integers  $N$  ( $N \geq 0$ ) and  $K$  ( $K \geq 1$ ), generates all possible integer arrays  $NI$  of size  $K$ , whose elements are non-negative, non-decreasing and sum to  $N$ .

[304](#)

Fisher's non-parametric randomization test for two small independent random samples.

[305](#)

Compute the ARL of a CUSUM mean chart with linear drift.

[306](#)

Calculation of a BIB product operation on any two matrices.

[307](#)

Calculation of the simplicial depth and the halfspace depth

[310](#)

Computes the cumulative distribution function of a non-central beta random variable.

[314](#)

Inverts matrix with contents subject to modulo arithmetic.

[319](#)

A program to implement a quasi-newton method. Using new algorithm Varmet July 1994

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N.B. This library was maintained by Alan Miller, CSIRO Division of Mathematics and Statistics, Clayton, Victoria 3169. E-mail: alan@mel.dms.csiro.au Phone: (03)542-2266 or (03)542-2253 (Secretary) FAX: (03)542-2474

Recent algorithms are provided by "T.R.Hopkins" <T.R.Hopkins@ukc.ac.uk>. The StatLib collection of Applied Statistics Algorithms is maintained by Pantelis Vlachos, vlachos@stat.cmu.edu.

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## Credit where credit is due

If you use an algorithm, dataset, or other information from StatLib, please acknowledge both StatLib and the original contributor of the material.

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Last modified: Mon Nov 15 17:25:32 EST 1999 by [Pantelis Vlachos](#)

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CSTART OF AS 3
      REAL FUNCTION PROBST(T, IDF, IFAULT)
C
C      ALGORITHM AS 3  APPL. STATIST. (1968) VOL.17, P.189
C
C      STUDENT T PROBABILITY (LOWER TAIL)
C
      REAL A, B, C, F, G1, S, FK, T, ZERO, ONE, TWO, HALF, ZSQRT, ZATAN
C
C      G1 IS RECIPROCAL OF PI
C
      DATA ZERO, ONE, TWO, HALF, G1
      $      /0.0, 1.0, 2.0, 0.5, 0.3183098862/
C
      ZSQRT(A) = SQRT(A)
      ZATAN(A) = ATAN(A)
C
      IFAULT = 1
      PROBST = ZERO
      IF (IDF .LT. 1) RETURN
      IFAULT = 0
      F = IDF
      A = T / ZSQRT(F)
      B = F / (F + T ** 2)
      IM2 = IDF - 2
      IOE = MOD(IDF, 2)
      S = ONE
      C = ONE
      F = ONE
      KS = 2 + IOE
      FK = KS
      IF (IM2 .LT. 2) GOTO 20
      DO 10 K = KS, IM2, 2
      C = C * B * (FK - ONE) / FK
      S = S + C
      IF (S .EQ. F) GOTO 20
      F = S
      FK = FK + TWO
10 CONTINUE
20 IF (IOE .EQ. 1) GOTO 30
   PROBST = HALF + HALF * A * ZSQRT(B) * S
   RETURN
30 IF (IDF .EQ. 1) S = ZERO
   PROBST = HALF + (A * B * S + ZATAN(A)) * G1
   RETURN
      END
CEND OF AS 3
```

```

CSTART OF AS 5
      REAL FUNCTION PRNCST(ST, IDF, D, IFAULT)
C
C      ALGORITHM AS 5  APPL. STATIST. (1968) VOL.17, P.193
C
C      COMPUTES LOWER TAIL AREA OF NON-CENTRAL T-DISTRIBUTION
C
      REAL ST, D, G1, G2, G3, ZERO, ONE, TWO, HALF, EPS, EMIN, F,
$      A, B, RB, DA, DRB, FMKM1, FMKM2, SUM, AK, FK, FK1,
$      ALNORM, TFN, ALOGAM, ZSQRT, ZEXP
C
      CONSTANTS - G1 IS 1.0 / SQRT(2.0 * PI)
C                  G2 IS 1.0 / (2.0 * PI)
C                  G3 IS SQRT(2.0 * PI)
C
      DATA G1, G2, G3 /0.3989422804, 0.1591549431, 2.5066282746/
      DATA ZERO, ONE, TWO, HALF,      EPS, EMIN
$      /0.0, 1.0, 2.0, 0.5, 1.0E-6, 12.5/
C
      ZSQRT(A) = SQRT(A)
      ZEXP(A) = EXP(A)
C
      F = IDF
      IF (IDF .GT. 100) GOTO 50
      IFAULT = 0
      IOE = MOD(IDF, 2)
      A = ST / ZSQRT(F)
      B = F / (F + ST ** 2)
      RB = ZSQRT(B)
      DA = D * A
      DRB = D * RB
      SUM = ZERO
      IF (IDF .EQ. 1) GOTO 30
      FMKM2 = ZERO
      IF (ABS(DRB) .LT. EMIN) FMKM2 = A * RB * ZEXP(-HALF * DRB ** 2)
$      * ALNORM(A * DRB, .FALSE.) * G1
      FMKM1 = B * DA * FMKM2
      IF (ABS(D) .LT. EMIN)
$      FMKM1 = FMKM1 + B * A * G2 * ZEXP(-HALF * D ** 2)
      IF (IOE .EQ. 0) SUM = FMKM2
      IF (IOE .EQ. 1) SUM = FMKM1
      IF (IDF .LT. 4) GOTO 20
      IFM2 = IDF - 2
      AK = ONE
      FK = TWO
      DO 10 K = 2, IFM2, 2
      FK1 = FK - ONE
      FMKM2 = B * (DA * AK * FMKM1 + FMKM2) * FK1 / FK
      AK = ONE / (AK * FK1)
      FMKM1 = B * (DA * AK * FMKM2 + FMKM1) * FK / (FK + ONE)
      IF (IOE .EQ. 0) SUM = SUM + FMKM2
      IF (IOE .EQ. 1) SUM = SUM + FMKM1
      AK = ONE / (AK * FK)
      FK = FK + TWO
10 CONTINUE
20 IF (IOE .EQ. 0) GOTO 40
30 PRNCST = ALNORM(DRB, .TRUE.) + TWO * (SUM + TFN(DRB, A))
      RETURN
40 PRNCST = ALNORM(D, .TRUE.) + SUM * G3
      RETURN
C

```

```
C          NORMAL APPROXIMATION - K IS NOT TESTED AFTER THE TWO CALLS
C          OF ALOGAM, BECAUSE A FAULT IS IMPOSSIBLE WHEN F EXCEEDS 100
C
50 IFAULT = 1
   A = ZSQRT(HALF * F) * ZEXP(ALOGAM(HALF * (F - ONE), K)
$   - ALOGAM(HALF * F, K)) * D
   PRNCST = ALNORM((ST - A) / ZSQRT(F * (ONE + D ** 2)
$   / (F - TWO) - A ** 2), .FALSE.)
   RETURN
   END
CEND OF AS 5
```

C This file contains AS6 and the enhanced version ASR44. See AS7 also.

C  
C

SUBROUTINE CHOL (A,N,NN,U,NULLTY,IFAU)LT)

C  
C

Algorithm AS6, Applied Statistics, vol.17, (1968)

C  
C

Given a symmetric matrix order n as lower triangle in a( )  
calculates an upper triangle, u( ), such that uprime \* u = a.  
a must be positive semi-definite. eta is set to multiplying  
factor determining effective zero for pivot.

C  
C

arguments:-

C  
C

a() = input, a +ve definite matrix stored in lower-triangular  
form.

C

n = input, the order of a

C

nn = input, the size of the a and u arrays n\*(n+1)/2

C

u() = output, a lower triangular matrix such that u\*u' = a.  
a & u may occupy the same locations.

C

nullty = output, the rank deficiency of a.

C

ifault = output, error indicator

C

= 1 if n < 1

C

= 2 if a is not +ve semi-definite

C

= 3 if nn < n\*(n+1)/2

C

= 0 otherwise

C

C\*\*\*\*\*

C

DOUBLE PRECISION A(NN),U(NN),ETA,ETA2,X,W,ZERO

C

C

The value of eta will depend on the word-length of the  
computer being used. See introductory text.

C

DATA ETA,ZERO/1.D-9,0.0D0/

C

IFAU)LT=1

IF (N.LE.0) RETURN

IFAU)LT=3

IF (NN.LT.N\*(N+1)/2) RETURN

IFAU)LT=2

NULLTY=0

J=1

K=0

ETA2=ETA\*ETA

II=0

C

C

Factorize column by column, icol = column no.

C

DO 80 ICOL=1,N

II=II+ICOL

X=ETA2\*A(II)

L=0

KK=0

C

C

IROW = row number within column ICOL

C

DO 40 IROW=1,ICOL

KK=KK+IROW

K=K+1

W=A(K)

M=J

```

      DO 10 I=1,IROW
        L=L+1
        IF (I.EQ.IROW) GO TO 20
        W=W-U(L)*U(M)
        M=M+1
10     CONTINUE
20     IF (IROW.EQ.ICOL) GO TO 50
        IF (U(L).EQ.ZERO) GO TO 30
        U(K)=W/U(L)
        GO TO 40
30     IF (W*W.GT.ABS(X*A(KK))) RETURN
        U(K)=ZERO
40     CONTINUE
50     IF (ABS(W).LE.ABS(ETA*A(K))) GO TO 60
        IF (W.LT.ZERO) RETURN
        U(K)=SQRT(W)
        GO TO 70
60     U(K)=ZERO
        NULLTY=NULLTY+1
70     J=J+ICOL
80     CONTINUE
        IFAULT=0
        END
C
C
C
C
SUBROUTINE SUBCHL (A,B,N,U,NULLTY,IFAUULT,NDIM,DET)
C
C   REMARK ASR 44  APPL. STATIST. (1982) VOL. 31, NO. 3
C
C   A revised and enhanced version of
C   ALGORITHM AS 6  APPL. STATIST. (1968) VOL. 17, NO. 2
C
C   Given a symmetric matrix of order N as lower triangle in A(),
C   calculates an upper triangle, U(), such that U'U = the sub-matrix
C   of A whose rows and columns are specified in the integer array
C   B().
C   U() may coincide with A().  A() must be +ve semi-definite.
C   ETA is set to multiplying factor determining effective zero for
C   a pivot.
C   NULLTY is returned as number of effective zero pivots.
C   IFAUULT is returned as 1 if N <= 0, 2 if A() is not +ve semi-
C   definite, otherwise 0 is returned.
C
DOUBLE PRECISION A(NDIM),U(NDIM),DET
INTEGER B(N)
C
C   Local variables
C
DOUBLE PRECISION ETA,ONE,ZERO,W,ETA2
C
C   The value of ETA below will depend upon the word length of the
C   computer being used.
C
DATA ETA/1.D-14/,ONE/1.D0/,ZERO/0.D0/
C
IFAUULT=1
IF (N.LE.0) GO TO 90
IFAUULT=2
NULLTY=0

```

```
DET=ONE
J=1
K=0
ETA2=ETA*ETA
DO 80 ICOL=1,N
  IJ=B(ICOL)*(B(ICOL)-1)/2
  II=IJ+B(ICOL)
  X=ETA2*A(II)
  L=0
  DO 40 IROW=1,ICOL
    KK=B(IROW)*(B(IROW)+1)/2
    K=K+1
    JJ=IJ+B(IROW)
    W=A(JJ)
    M=J
    DO 10 I=1,IROW
      L=L+1
      IF (I.EQ.IROW) GO TO 20
      W=W-U(L)*U(M)
      M=M+1
10    CONTINUE
20    IF (IROW.EQ.ICOL) GO TO 50
    IF (U(L).EQ.ZERO) GO TO 30
    U(K)=W/U(L)
    GO TO 40
30    IF (W*W.GT.ABS(X*A(KK))) GO TO 90
    U(K)=ZERO
40    CONTINUE
50    IF (ABS(W).LE.ABS(ETA*A(KK))) GO TO 60
    IF (W.LT.ZERO) GO TO 90
    U(K)=SQRT(W)
    GO TO 70
60    U(K)=ZERO
    NULLTY=NULLTY+1
70    J=J+ICOL
    DET=DET*U(K)*U(K)
80  CONTINUE
C
  IFAULT=0
90  RETURN
END
```



c This file contains AS7 and an enhanced alternative - ASR44. See also AS6.

c  
c

```
subroutine syminv(a, n, nn, c, w, nullty, ifault)
```

c  
c Algorithm AS7, Applied Statistics, vol.17, 1968, p.198.

c  
c Forms in c( ) as lower triangle, a generalised inverse  
c of the positive semi-definite symmetric matrix a( )  
c order n, stored as lower triangle.

c  
c arguments:-

c a( ) = input, the symmetric matrix to be inverted, stored in  
c lower triangular form  
c n = input, order of the matrix  
c nn = input, the size of the a and c arrays n\*(n+1)/2  
c c( ) = output, the inverse of a (a generalized inverse if c is  
c singular), also stored in lower triangular.  
c c and a may occupy the same locations.  
c w( ) = workspace, dimension at least n.  
c nullty = output, the rank deficiency of a.  
c ifault = output, error indicator  
c = 1 if n < 1  
c = 2 if a is not +ve semi-definite  
c = 3 if nn < n\*(n+1)/2  
c = 0 otherwise

c\*\*\*\*\*

c  
c double precision a(nn), c(nn), w(n), x, zero, one

c  
c data zero, one /0.0d0, 1.0d0/

c  
c cholesky factorization of a, result in c

c  
c call chol(a, n, nn, c, nullty, ifault)  
c if(ifault.ne.0) return

c  
c invert c & form the product (cinv)'\*cinv, where cinv is the inverse  
c of c, row by row starting with the last row.  
c irow = the row number, ndiag = location of last element in the row.

c  
c irow=n  
c ndiag=nn  
10 l=ndiag  
c if (c(ndiag) .eq. zero) goto 60  
c do 20 i=irow,n  
c w(i)=c(l)  
c l=l+i  
20 continue  
c icol=n  
c jcol=nn  
c mdiag=nn  
30 l=jcol  
c x=zero  
c if(icol.eq.irow) x=one/w(irow)  
c k=n  
40 if(k.eq.irow) go to 50  
c x=x-w(k)\*c(l)  
c k=k-1  
c l=l-1

```

        if(l.gt.mdiag) l=l-k+1
        go to 40
50     c(l)=x/w(irow)
        if(icol.eq.irow) go to 80
        mdiag=mddiag-icol
        icol=icol-1
        jcol=jcol-1
        go to 30
60     do 70 j=irow,n
            c(l)=zero
            l=l+j
70     continue
80     ndiag=nddiag-irow
        irow=irow-1
        if(irow.ne.0) go to 10
        return
        end

c
c
c
c
        subroutine subinv(a, nm, b, n, c, w, nullty, ifault, ndim, det)
        implicit double precision (a-h,o-z)

c
c     Remark asr 44.1    Appl. Statist. (1982) Vol.31, No.3
c
c     A revised and enhanced version of
c     algorithm as7, applied statistics, vol.17, 1968.
c
c     Forms in c() as lower triangle, a generalised inverse
c     of a sub-matrix of the positive semi-definite symmetric
c     matrix a() of order n, stored as lower triangle.
c     c() may co-incide with a().  nullty is returned as the nullity
c     of a().  ifault is returned as 1 if n.lt.1, 2 if the
c     submatrix is not positive semi-definite, 3 if the elements
c     of b are inadmissible, otherwise zero.
c     w() is a work array of length at least n that is allocated by
c     the calling routine.
c
c     arguments:-
c     a()      = input, the symmetric matrix to be inverted, stored in
c               lower triangular form
c     nm       = input, the order of a
c     n        = input, order of the sub-matrix to be inverted
c     b        = input, an array containing the numbers of rows and
c               columns of a() to be included.
c     c()      = output, the inverse of a (a generalized inverse if c is
c               singular), also stored in lower triangular.
c               c and a may occupy the same locations.
c     w()      = workspace, dimension at least n.
c     nullty   = output, the rank deficiency of a.
c     ifault   = output, error indicator
c               = 1 if n < 1
c               = 2 if the submatrix of a is not +ve semi-definite
c               = 3 if elements of b are inadmissible
c               = 0 otherwise
c
c     Auxiliary routine required: SUBCHL from ASR44 (see AS6)
c
c*****
c

```

```
dimension a(ndim),c(ndim),w(n)
integer b(n)
data zero/0.0d0/, one/1.0d0/
c
  ifault = 3
  if (n .gt. nm) return
  if (b(1) .lt.1 .or. b(1) .gt. nm-n+1) return
  if (n .eq. 1) goto 19
  do 18 i = 2, n
    if (b(i) .le. b(i-1) .or. b(i) .gt. nm-n+i) return
18  continue
19  nrow=n
  ifault=1
  if(nrow.le.0) go to 100
  ifault=0
c
c  Cholesky factorization of a, result in c
c
  call subchl(a,b,nrow,c,nullty,ifault,ndim,det)
  if(ifault.ne.0) go to 100
c
c  invert c & form the product (cinv)'*cinv, where cinv is the inverse
c  of c, row by row starting with the last row.
c  irow = the row number, ndiag = location of last element in the row.
c
  nn=nrow*(nrow+1)/2
  irow=nrow
  ndiag=nn
10  if(c(ndiag).eq.zero) go to 60
  l=ndiag
  do 20 i=irow,nrow
    w(i)=c(l)
    l=l+i
20  continue
  icol=nrow
  jcol=nn
  mdiag=nn
30  l=jcol
  x=zero
  if(icol.eq.irow) x=one/w(irow)
  k=nrow
40  if(k.eq.irow) go to 50
  x=x-w(k)*c(l)
  k=k-1
  l=l-1
  if(l.gt.mdiag) l=l-k+1
  go to 40
50  c(l)=x/w(irow)
  if(icol.eq.irow) go to 80
  mdiag=mdiag-icol
  icol=icol-1
  jcol=jcol-1
  go to 30
60  l=ndiag
  do 70 j=irow,nrow
    c(l)=zero
    l=l+j
70  continue
80  ndiag=ndiag-irow
  irow=irow-1
  if(irow.ne.0) go to 10
```

```
100  return  
      end
```

```
CSTART OF AS 13
      SUBROUTINE PRTREE(N, M, A, DLARGE, D, B, C, IFAULT)
C
C      ALGORITHM AS 13  APPL. STATIST. (1969) VOL.18, P.103
C
C      COMPUTES THE MINIMUM SPANNING TREE OF A DISTANCE MATRIX
C
      REAL D(M), C(N), AM, DIST, DLARGE
      INTEGER B(N)
      LOGICAL A(N)
      IFAULT = 1
      IF (N .LT. 2) RETURN
      IFAULT = 2
      IF (N * (N - 1) / 2 .NE. M) RETURN
      IFAULT = 0
C
C      A(I) IS .FALSE. IF I IS ALREADY ASSIGNED TO
C      THE TREE (INITIALLY CONSISTING OF NO. 1 ONLY),
C      OR .TRUE. OTHERWISE
C
      DO 10 I = 2, N
      A(I) = .TRUE.
      B(I) = 0
      C(I) = DLARGE
10  CONTINUE
      J = 1
      DO 40 I = 2, N
      AM = DLARGE
      DO 30 K = 2, N
      IF (.NOT. A(K)) GOTO 30
      IF (J .GT. K) L = (J - 1) * (J - 2) / 2 + K
      IF (J .LE. K) L = (K - 1) * (K - 2) / 2 + J
      DIST = D(L)
      IF (DIST .GE. C(K)) GOTO 20
      C(K) = DIST
      B(K) = J
20  IF (AM .LE. C(K)) GOTO 30
      AM = C(K)
      NEXT = K
30  CONTINUE
      J = NEXT
      A(J) = .FALSE.
40  CONTINUE
      RETURN
      END
CEND OF AS 13
```

```
CSTART OF AS 14
      SUBROUTINE MTP(N, B, C, HIST, ROUTE, XPRINT)
C
C      ALGORITHM AS 14  APPL. STATIST. (1969) VOL.18, P.105
C
C      THIS SUBROUTINE ENABLES THE MINIMUM SPANNING TREE TO BE
C      DRAWN RAPIDLY WITHOUT HAVING TO SEARCH FOR END POINTS,
C      AND IS ESPECIALLY USEFUL WHEN N EXCEEDS 100. THE OUTPUT
C      OF SUBROUTINE PRTREE IS USED
C
      INTEGER B(N), HIST(N), ROUTE(N)
      REAL C(N)
      DO 10 I = 1, N
10  HIST(I) = 0
      DO 20 I = 2, N
      J = B(I)
      HIST(J) = HIST(J) + 1
20  CONTINUE
      ROUTE(1) = 1
      J = 1
      K = 1
C
C      ROUTE(J) IS THE CURRENT END POINT AND IF HIST(ROUTE(I))
C      IS NOT ZERO A FURTHER LINE CAN BE FOUND. HIST(I) MUST
C      BE NON-ZERO INITIALLY BECAUSE THE TREE IS CONNECTED
C
      DO 80 I = 2, N
30  IF (HIST(K) .NE. 0) GOTO 40
      J = J - 1
      K = ROUTE(J)
      GOTO 30
40  HIST(K) = HIST(K) - 1
      DO 50 M = 2, N
      IF (K .EQ. B(M)) GOTO 60
50  CONTINUE
60  CALL XPRINT(J, K, M, C(M))
      J = J + 1
      ROUTE(J) = M
      K = M
      B(M) = -B(M)
80  CONTINUE
      DO 90 I = 2, N
90  B(I) = IABS(B(I))
      RETURN
      END
CEND OF AS 14
```

```
CSTART OF AS 15
  SUBROUTINE SLINK(N, N1, N20, DELTA, B, C, DLARGE,
  $  G, H, X, W1, W2, GROUPE, TOPP, PRINTX, IFAULT)
C
C      ALGORITHM AS 15  APPL. STATIST. (1969) VOL.18, P.106
C
C      PERFORMS SINGLE LINKAGE CLUSTERING. INFORMATION IS
C      SUPPLIED BY SUBROUTINE PRTREE, IN ARRAYS B AND C.
C      POINTS ARE LISTED IN SORTED ORDER IN ARRAY G, AND THE
C      CORRESPONDING ARRAY H MARKS THE LAST MEMBER OF EACH
C      CLUSTER WITH A 1, OTHERWISE THE ENTRY IS 0. THE ARRAY
C      X STORES CODE NUMBERS FOR OUTPUT OF THE DENDROGRAM
C
C      INTEGER P, Q, R, S, T, U, V, W, B(N), G(N), H(N),
  $  X(N20), W1(N1), W2(N1)
  REAL DELTA, C(N), DLARGE, D, LEVEL, ONE, ZINT
C
  DATA ONE /1.0/
C
  ZINT(D) = AINT(D)
C
  IFAULT = 1
  IF (N1 .NE. N + 1) RETURN
  IF (N20 .NE. 20 * N) RETURN
  IFAULT = 0
C
C      CLUSTERING STARTS AT THE FIRST INTEGRAL MULTIPLE OF
C      DELTA WHICH IS GREATER THAN D, THE SHORTEST LINK OF
C      THE MINIMUM SPANNING TREE
C
  D = C(2)
  IF (N .LT. 3) GOTO 15
  DO 10 I = 3, N
10 IF (D .GT. C(I)) D = C(I)
15 DO 20 I = 1, N
  G(I) = I
  H(I) = 1
  X(I) = 3
20 CONTINUE
  P = 0
  LEVEL = DELTA * (ONE + ZINT(D / DELTA))
C
C      FOR EACH LINK IN ARRAY C THAT IS SHORTER THAN LEVEL,
C      TWO CLUSTERS ARE AMALGAMATED. THE AMALGAMATION
C      INVOLVES A REORDERING OF ARRAYS G AND H AND REMOVAL
C      OF THE END-OF-CLUSTER MARKER FROM THE EARLIER
C      CLUSTER. LINKS ONCE USED ARE INCREASED BY DLARGE TO
C      PREVENT RE-USE
C
30 P = P + 1
  DO 150 I = 2, N
  IF (C(I) .GE. LEVEL) GOTO 150
  J = B(I)
  C(I) = C(I) + DLARGE
  K = I
  DO 40 M = 1, N
  IF (G(M) .EQ. J) Q = M
  IF (G(M) .EQ. K) R = M
40 CONTINUE
  IF (Q .LE. R) GOTO 50
  M = R
```

```
      R = Q
      Q = M
50 DO 60 S = Q, N
      IF (H(S) .NE. 0) GOTO 70
60 CONTINUE
70 T = R
80 T = T - 1
      IF (T .LT. 1) GOTO 90
      IF (H(T) .EQ. 0) GOTO 80
90 T = T + 1
      H(S) = 0
      L = 0
      DO 100 R = T, N
      L = L + 1
      W1(L) = G(R)
      W2(L) = H(R)
      IF (H(R) .NE. 0) GOTO 110
100 CONTINUE
110 W = S + 1
      M = T
      L = R + 1
120 M = M - 1
      IF (M .LT. W) GOTO 130
      L = L - 1
      G(L) = G(M)
      H(L) = H(M)
      GOTO 120
130 U = R - T + 1
      L = W - 1
      DO 140 M = 1, U
      L = L + 1
      G(L) = W1(M)
      H(L) = W2(M)
140 CONTINUE
150 CONTINUE
      CALL GROUPE(L, N, G, H)
      W = N * P
      U = 0
      V = 0
      K = 0
C
C      DENDROGRAM INDICATORS ARE NOW COMPILED AND STORED
C      IN X. POINTS ARE EXAMINED IN THE ORDER DEFINED BY
C      THE ARRAY G. S IS THE CORRESPONDING ENTRY ON THE
C      PREVIOUS ITERATION, U = 0 FOR THE FIRST MEMBER OF
C      A CLUSTER, V = 1 WHEN AMALGAMATIONS OCCUR, FROM
C      THE LAST MEMBER OF THE FIRST COMPONENT CLUSTER
C      UNTIL THE LAST MEMBER OF THE AMALGAMATED CLUSTER.
C      K IS THE TOTAL NUMBER OF CLUSTERS
C
      DO 160 I = 2, N
160 K = K + H(I)
      IF (P .GT. 19) GOTO 270
      DO 260 I = 1, N
      J = G(I)
      L = J + W - N
      S = X(L)
      IF (U .NE. 0) GOTO 190
      IF (H(I) .NE. 1) GOTO 170
      T = 3
      GOTO 250
```



```
170 IF (S .NE. 3) GOTO 180
    T = 1
    U = 1
    V = 1
    GOTO 250
180 T = 0
    U = 1
    GOTO 250
190 IF (H(I) .NE. 1) GOTO 210
    IF (V .NE. 0) GOTO 200
    T = 3
    U = 0
    GOTO 250
200 T = 2
    U = 0
    V = 0
    GOTO 250
210 IF (S .LT. 2 .OR. S .GT. 3) GOTO 230
    IF (V .NE. 0) GOTO 220
    T = 1
    U = 1
    V = 1
    GOTO 250
220 T = 5
    U = 1
    GOTO 250
230 IF (V .NE. 0) GOTO 240
    T = 0
    U = 1
    GOTO 250
240 T = 4
250 L = J + W
    X(L) = T
260 CONTINUE
270 LEVEL = LEVEL + DELTA
    IF (K .NE. 1) GOTO 30
    CALL TOPP
    DO 280 I = 1, N
280 CALL PRINTX(I, G, N, P, X, N20)
    RETURN
    END
CEND OF AS 15
```

```

SUBROUTINE YATES (Y, LEVS, KODE, NFAC, X, EXTR)
C
C   ALGORITHM  AS 22 APPL.STATIST. (1969) VOL.18, NO.3
C
C   Yates algorithm for general complete factorial experiments.
C   Computes  Y = (IL..X..IR).Y
C
C   where  . denotes ordinary matrix product
C          .. direct matrix product
C          IL unit matrix of order NLFT
C          IR unit matrix of order NRGT
C          Y( ) multi-way table stored as a vector
C          X( ) a square matrix stored as a vector
C
C   INTEGER LEVS(*), KODE, NFAC
C   REAL Y(*), X(*), EXTR(*)
C
C   Local variables
C
C   INTEGER NLFT, NRGT, ILEV, NLEV, JUMP, ILFT, IRGT, JUMPHO, IEL,
*         JEL, JUMPER
C
C   NLFT = 1
C   NRGT = 1
C   DO 3 ILEV = 1, NFAC
C     IF (ILEV - KODE .LT. 0) THEN
C       NLFT = NLFT * LEVS(ILEV)
C     ELSE IF (ILEV - KODE .GT. 0) THEN
C       NRGT = NRGT * LEVS(ILEV)
C     END IF
C 3 CONTINUE
C   NLEV = LEVS(KODE)
C   JUMP = 0
C
C   Loop over left unit matrix
C
C   DO 7 ILFT = 1, NLFT
C     JUMP = JUMP + 1
C
C   Loop over right unit matrix
C
C   DO 6 IRGT = 1, NRGT
C     JUMPHO = JUMP
C     JUMP = JUMP - NRGT
C
C   Extract vector elements for linear combination
C
C   DO 4 ILEV = 1, NLEV
C     JUMP = JUMP + NRGT
C     EXTR(ILEV) = Y(JUMP)
C 4 CONTINUE
C   JUMP = JUMPHO - NRGT
C   ILEV = 0
C
C   Begin matrix by vector product.
C   Loop over the various contrasts.
C
C   DO 5 IEL = 1, NLEV
C     JUMP = JUMP + NRGT
C     Y(JUMP) = 0.0
C
C

```

```
C      Form linear combination.
C
      DO 5 JEL = 1, NLEV
        ILEV = ILEV + 1
        Y(JUMP) = Y(JUMP) + X(ILEV) * EXTR(JEL)
5     CONTINUE
      JUMPER = JUMP
      JUMP = JUMPHO + 1
6     CONTINUE
      JUMP = JUMPER
7     CONTINUE
C
      RETURN
      END
```

```

REAL FUNCTION STUDNT (T, DOFF, IFAULT)
C
C   ALGORITHM AS 27  APPL. STATIST. VOL.19, NO.1
C
C   Calculate the upper tail area under Student's t-distribution
C
C   Translated from Algol by Alan Miller
C
C   INTEGER IFAULT
C   REAL T, DOFF
C
C   Local variables
C
C   REAL V, X, TT, TWO, FOUR, ONE, ZERO, HALF
C   REAL A1, A2, A3, A4, A5, B1, B2,
C   *   C1, C2, C3, C4, C5, D1, D2,
C   *   E1, E2, E3, E4, E5, F1, F2,
C   *   G1, G2, G3, G4, G5, H1, H2,
C   *   I1, I2, I3, I4, I5, J1, J2
C   LOGICAL POS
C   DATA TWO /2.0/, FOUR /4.0/, ONE /1.0/, ZERO /0.0/, HALF /0.5/
C   DATA A1, A2, A3, A4, A5 /0.09979441, -0.581821, 1.390993,
C   *   -1.222452, 2.151185/, B1, B2 /5.537409, 11.42343/
C   DATA C1, C2, C3, C4, C5 /0.04431742, -0.2206018, -0.03317253,
C   *   5.679969, -12.96519/, D1, D2 /5.166733, 13.49862/
C   DATA E1, E2, E3, E4, E5 /0.009694901, -0.1408854, 1.88993,
C   *   -12.75532, 25.77532/, F1, F2 /4.233736, 14.3963/
C   DATA G1, G2, G3, G4, G5 /-9.187228E-5, 0.03789901, -1.280346,
C   *   9.249528, -19.08115/, H1, H2 /2.777816, 16.46132/
C   DATA I1, I2, I3, I4, I5 /5.79602E-4, -0.02763334, 0.4517029,
C   *   -2.657697, 5.127212/, J1, J2 /0.5657187, 21.83269/
C
C   Check that number of degrees of freedom > 4.
C
C   IF (DOFF .LT. TWO) THEN
C     IFAULT = 1
C     STUDNT = - ONE
C     RETURN
C   END IF
C
C   IF (DOFF .LE. FOUR) THEN
C     IFAULT = DOFF
C   ELSE
C     IFAULT = 0
C   END IF
C
C   Evaluate series.
C
C   V = ONE / DOFF
C   POS = (T .GE. ZERO)
C   TT = ABS(T)
C   X = HALF * (ONE +
C   *   TT * (((A1 + V * (A2 + V * (A3 + V * (A4 + V * A5)))) /
C   *   (ONE - V * (B1 - V * B2)))) +
C   *   TT * (((C1 + V * (C2 + V * (C3 + V * (C4 + V * C5)))) /
C   *   (ONE - V * (D1 - V * D2)))) +
C   *   TT * (((E1 + V * (E2 + V * (E3 + V * (E4 + V * E5)))) /
C   *   (ONE - V * (F1 - V * F2)))) +
C   *   TT * (((G1 + V * (G2 + V * (G3 + V * (G4 + V * G5)))) /
C   *   (ONE - V * (H1 - V * H2)))) +
C   *   TT * ((I1 + V * (I2 + V * (I3 + V * (I4 + V * I5)))) /

```

```
*      (ONE - V * (J1 - V * J2)) ) ) ) ) ** (-8)
```

```
IF (POS) THEN
```

```
  STUDNT = X
```

```
ELSE
```

```
  STUDNT = ONE - X
```

```
END IF
```

```
C
```

```
RETURN
```

```
END
```

```

SUBROUTINE HNPLLOT (NTITLE,OBS,N)
C
C      Algorithm as 30 j.r.statist.soc. c. (1970) vol.19. no.2.
C
C      Half-normal plotting
C
DIMENSION OBS(*), A(6), B(4), P(100), NTITLE(20)
DIMENSION OUT(101), XPR(11), D(100), YPR(6)
CHARACTER*1 OUT,DOT,BLANK,PLUS
10  FORMAT (1H1,20A4,///)
20  FORMAT (1H ,F11.4,101A1)
30  FORMAT (1H ,11X,1H.)
40  FORMAT (1H ,F11.4,101H.....
1.....)
50  FORMAT (1H ,11X,101H. . . . .)
1 . . . . .)
60  FORMAT (1H ,8X,F6.2,F7.2,F8.2,F8.2,F11.2,F10.2,F11.2,F7.2,16X,
1 F5.2,12X,F5.2)
70  FORMAT (1H ,11X,101A1)
80  FORMAT (1H ,F11.4,1H.)
C
C      Set iwrite equal to the output device number (system dependent)
C
DATA IWRITE/6/
C
C      set constants for probability scale, and for printing
C
DATA A(1),A(2),A(3),A(4),A(5),A(6)/1.048,-0.8559,0.363,0.108392,
1 0.328117,1.253314/
DATA B(1),B(2),B(3),B(4)/-0.001416,-0.039811,-0.6256,0.401703/
DATA XPR(1),XPR(2),XPR(3),XPR(4),XPR(5),XPR(6),XPR(7),XPR(8),
1XPR(9),XPR(10)/50.0,60.0,70.0,80.0,90.0,95.0,98.0,99.0,99.9,99.99/
DATA DOT,BLANK,PLUS/'. ',' ','+'/'
C
OUT(1)=DOT
C
C      Sort data into ascending order
C
DO 100 I=1,N
DO 100 J=I,N
IF (OBS(J)-OBS(I)) 90,100,100
90  TEMP=OBS(I)
OBS(I)=OBS(J)
OBS(J)=TEMP
100 CONTINUE
C
C      Calculate scales for the axes (the x-axis is assumed to be
C      100 units long, and the y-axis 50 units long
C
XSCALE=0.03719
OBSMAX=OBS(N)
KOUNT=0
110 IF (OBSMAX.GT.100.0) GO TO 120
IF (OBSMAX.GE.10.0) GO TO 130
OBSMAX=OBSMAX*10.0
KOUNT=KOUNT-1
GO TO 110
120 OBSMAX=OBSMAX/10.0
KOUNT=KOUNT+1
GO TO 110
130 IF (AMOD(OBSMAX,5.0).EQ.0) GO TO 140

```

```

OBSMAX=(AINT(OBSMAX/5.0)+1.0)*5.0
140  OBSMAX=OBSMAX*(10.0**KOUNT)
YSCALE=OBSMAX/50.0
YPR(1)=OBSMAX
YPR(6)=0.0
OBSMAX=OBSMAX/5.0
DO 150 I=2,5
150  YPR(I)=YPR(I-1)-OBSMAX
C
C      Calculate positioning of points on probability scale
C
X=50.0/(2.0*FLOAT(N))
P(1)=50.0+X
DO 160 K=2,N
160  P(K)=P(K-1)+2.0*X
DO 200 K=1,N
W=0.02*P(K)-1.0
IF (P(K).GT.95.5) GO TO 180
W2=W*W
D(K)=A(1)
DO 170 I=2,6
170  D(K)=D(K)*W2+A(I)
D(K)=D(K)*W
GO TO 200
180  Z=LOG(1.0-W)
D(K)=B(1)
DO 190 I=2,4
190  D(K)=D(K)*Z+B(I)
200  CONTINUE
WRITE (IWRITE,10) (NTITLE(I),I=1,20)
L=N
QR=YSCALE/1000.0
C
C      Print output line by line, except for the last one, with the
C      scale value printed on every tenth line
C
DO 280 I=1,50
C
C      Calculate position on vertical scale, and which points - of
C      those not yet printed - exceed this value
C
PR=YPR(1)-FLOAT(I-1)*YSCALE-QR
IF (OBS(L).LT.PR) GO TO 260
C
C      Set output array to blanks
C
DO 210 IX=2,101
210  OUT(IX)=BLANK
C
C      Calculate position of point on probability scale and put print
C      symbol in appropriate array element. Repeat for further points
C      at this value, and print line of output
C
220  JP=(D(L)/XSCALE)+1.0
OUT(JP)=PLUS
L=L-1
IF (L.EQ.0) GO TO 230
IF (OBS(L).GE.PR) GO TO 220
230  IF (MOD(I-1,10).NE.0) GO TO 240
I1=((I-1)/10)+1
WRITE (IWRITE,20) YPR(I1),(OUT(I2),I2=1,101)

```

```
GO TO 250
240 WRITE (IWRITE,70) (OUT(I2),I2=1,101)
C
C   If all points have been printed, or points remain after all
C   lines have been printed (except the last) leave the main loop
C   and complete the printing elsewhere
C
250 IF (L.GT.0) GO TO 280
    IF (I.GE.50) GO TO 320
    IL=I+1
    GO TO 290
260 IF (MOD(I-1,10).NE.0) GO TO 270
    I1=((I-1)/10)+1
    WRITE (IWRITE,80) YPR(I1)
    GO TO 280
270 WRITE (IWRITE,30)
280 CONTINUE
    GO TO 320
C
C   Complete printing when all points have already been output
C
290 DO 310 I=IL,50
    IF (MOD(I-1,10).NE.0) GO TO 300
    I1=((I-1)/10)+1
    WRITE (IWRITE,80) YPR(I1)
    GO TO 310
300 WRITE (IWRITE,30)
310 CONTINUE
320 IF (L.LE.0) GO TO 350
C
C   Print last line, including the probability axis and any
C   remaining points
C
DO 330 IX=2,101
330 OUT(IX)=OUT(1)
340 JP=(D(L)/XSCALE)+1.0
    OUT(JP)=PLUS
    L=L-1
    IF (L.GT.0) GO TO 340
    WRITE (IWRITE,20) YPR(6),(OUT(I2),I2=1,101)
    GO TO 360
350 WRITE (IWRITE,40) YPR(6)
C
C   Print probability scale
C
360 WRITE (IWRITE,50)
    WRITE (IWRITE,60) (XPR(IP),IP=1,10)
    RETURN
END
```



```
double precision function gamain (x,p,g,ifault)
implicit double precision (a-h,o-z)
```

```
c
c      Algorithm AS 32 J.R. Statist. Soc. C. (1970) Vol.19 No. 3
c      Algorithm AS 239 is recommended as an alternative.
c
c      Computes incomplete gamma ratio for positive values of
c      arguments x and p.  G must be calculated and should be equal
c      to ln(gamma(p)).  Algorithm AS 245 may be used for this.
c      ifault=1 if p.le.0 else 2 if x.lt.0 else 0.
c      Uses series expansion if p.gt.x or x.le.1, otherwise
c      continued fraction approximation.
c
c      Revised to incorporate the recommendations of Rice & Das,
c      Appl. Statist., 34, 326, 1985, and of Cran, Appl. Statist.,
c      38, 423, 1989.
```

```
dimension pn(6)
data zero/0.0d0/, one/1.0d0/, uflo/1.0d-37/, two/2.0d0/
data acu/1.0d-8/, oflo/1.0d37/
```

```
c
g=alngam(p)
```

```
c      Define accuracy and initialize
```

```
c
gin=zero
ifault=0
```

```
c      Test for admissibility of arguments
```

```
c
if (p.le.zero) ifault=1
if(x.lt.zero) ifault=2
if (ifault .gt. 0 .or. x .eq. zero) go to 50
arg=p*log(x)-x-g
if(arg.lt.log(uflo)) then
  ifault=3
  go to 50
end if
factor=exp(arg)
if(x.gt.one .and. x.ge.p) goto 30
```

```
c      Calculation by series expansion
```

```
c
gin=one
term=one
rn=p
20 rn=rn+one
term=term*x/rn
gin=gin+term
if(term.gt.acu) goto 20
gin=gin*factor/p
goto 50
```

```
c      Calculation by continued fraction
```

```
c
30 a=one-p
b=a+x+one
term=zero
pn(1)=one
pn(2)=x
pn(3)=x+one
```

```
pn(4)=x*b  
gin=pn(3)/pn(4)
```

c

```
32 a=a+one  
   b=b+two  
   term=term+one  
   an=a*term  
   do 33 i=1,2  
33 pn(i+4)=b*pn(i+2)-an*pn(i)  
   if(pn(6).eq.zero) goto 35  
   rn=pn(5)/pn(6)  
   dif=abs(gin-rn)  
   if(dif.gt.acu) goto 34  
   if(dif.le.acu*rn) goto 42  
34 gin=rn  
35 do 36 i=1,4  
36 pn(i)=pn(i+2)  
   if(abs(pn(5)).lt.oflo) goto 32  
   do 41 i=1,4  
41 pn(i)=pn(i)/oflo  
   goto 32  
42 gin=one-factor*gin  
50 gamain=gin  
   return  
   end
```

```
      SUBROUTINE BANINV(N, K, SIGMA, S, G)
C
C   ALGORITHM AS 34 APPL. STATIST. (1970) VOL.19, NO.3
C
C   Update inverse of symmetric banded matrices
C
      INTEGER N, K
      DOUBLE PRECISION SIGMA(N), S(N), G(N)
C
C   Local variables
C
      INTEGER I, J, INDX, M, JJ, MM, NN
      DOUBLE PRECISION B, C, CG, U, V, ZERO, ONE
      DATA ZERO /0.D0/, ONE /1.D0/
C
C   Form C
C
      C = S(1)
      I = N
      DO 1 J = 2, K
         C = C - S(J) * G(I)
         I = I - 1
1 CONTINUE
      C = ONE / C
C
C   Form SIGMA at N+1
C
      INDX = 0
      M = N * (N+1) / 2
      DO 2 J = 1, N
         CG = C * G(J)
         M = M + 1
         SIGMA(M) = -CG
         DO 2 JJ = 1, J
            INDX = INDX + 1
            SIGMA(INDX) = SIGMA(INDX) + CG * G(JJ)
2 CONTINUE
      SIGMA(M+1) = C
C
C   Form G at N+1
C
      B = ZERO
      DO 4 J = 2, K
4 B = B + S(J) * G(J-1)
      NN = N / 2
      M = N - 2 * NN
      B = B * C
      U = G(1)
      G(1) = -B
      DO 5 J = 1, NN
         MM = N - J + 1
         G(MM+1) = G(MM) + B * U
         V = G(J+1)
         G(J+1) = U + B * G(MM)
         U = V
5 CONTINUE
      IF (M .EQ. 0) GO TO 7
      G(NN+2) = U + B * U
7 RETURN
      END
```

```
      SUBROUTINE NEXTGJ(A, IA, K, IWK)
C
C   A FORTRAN translation of Garside's algorithm AS38, but without
C   checks and with only the upper triangle of the SSP-matrix stored.
C   Array IWK must contain (K-1) zeroes initially.
C
      DOUBLE PRECISION A(IA)
      INTEGER IWK(K)
C
C   Local variables
C
      DOUBLE PRECISION ONE, AA, AIP
      DATA ONE/1.D0/
C
      IP = K-1
C
C   IREM = 1 if a variable is being removed from the model,
C   = 0 if it is being added.
C
      10 IREM = IWK(IP)
C
C   Pivot variable no. IP in or out of the model.
C
      IPP = (IP-1)*(K+K+2-IP)/2 + 1
      IJ = IPP+K+1-IP
      AA = -A(IPP)
      A(IPP) = AA
      AA = ONE/AA
      IP1 = IP+1
      DO 30 I = IP1, K
        IPP = IPP+1
        AIP = A(IPP)*AA
        IPJ = IPP
        DO 20 J = I, K
          A(IJ) = A(IJ) + AIP*A(IPJ)
          IJ = IJ+1
          IPJ = IPJ+1
        20 CONTINUE
      30 CONTINUE
C
C   Change the indicator in array IWK for variable IP.
C   If variable was deleted, move onto the next lower numbered
C   variable, otherwise return.
C
      IWK(IP) = 1-IREM
      IF(IREM.EQ.0) RETURN
      IP = IP-1
      IF(IP.GT.0) GO TO 10
C
      RETURN
      END
```

```

SUBROUTINE MSTUPD(KN, KI, DK, DIST, NUM, IREF, IPUSH)
C
C   ALGORITHM AS 40  APPL. STATIST. (1971) VOL.20, NO.2
C
C   This subroutine updates the minimal spanning tree of KN points,
C   defined by KI(J) being the point nearest to J on the chain leading
C   from J to the point KN and DK(J) being the length link J to KI(J),
C   with the new point (KN+1) whose distances from the points of the
C   original M.S.T. are given in the array DIST.
C   The update version of the M.S.T. is left in the arrays KI and DK
C   suitable for re-entry to the subroutine with the next point.
C   A working space of three arrays NUM, IREF and IPUSH, each at least
C   of size KN, is required.
C
C   INTEGER KN, KI(KN), NUM(KN), IREF(KN), IPUSH(KN)
C   REAL DK(KN), DIST(KN)
C
C   KT = KN - 1
C   IP = 0
C
C   If J = IREF(I) > 0 it refers to link J to KI(J), while if < 0 it
C   refers to the link from point (KN+1) to (-J).
C
C   DO 1 I = 1, KN
C       IREF(I) = -I
1 CONTINUE
C
C   NUM(I) holds the number of links pointing to I.  Hence I is an end
C   point if NUM(I) = 0.
C
C   DO 2 I = 1, KT
C       K = KI(I)
C       NUM(K) = NUM(K) + 1
2 CONTINUE
C
C   Start of algorithm
C   NUM(I) = 1 if the link I to KI(I) is included in the new M.S.T.
C   otherwise it is 0 or < 0.
C
C   DO 3 NI = 1, KT
C       IF (NUM(NI) .NE. 0) GO TO 3
C       I = NI
31  J = KI(I)
C       IF (DIST(I) .GT. DK(I)) GO TO 34
C       IF (DK(I) .GE. DIST(J)) GO TO 32
C       IREF(J) = I
C       DIST(J) = DK(I)
32  IF (IREF(I) .GT. 0) GO TO 33
C       IP = IP + 1
C       IPUSH(IP) = -IREF(I)
C       GO TO 36
33  K = IREF(I)
C       NUM(K) = 1
C       GO TO 36
34  IF (DIST(I) .GE. DIST(J)) GO TO 35
C       IREF(J) = IREF(I)
C       DIST(J) = DIST(I)
35  NUM(I) = 1
36  NUM(J) = NUM(J) - 1
C       IF (NUM(J) .NE. 0) GO TO 3
C       I = J

```

```
        NUM(I) = -1
        GO TO 31
3 CONTINUE
C
    K = -IREF(KN)
    IF (K .GE. 0) GO TO 42
    K = -K
    NUM(K) = 1
C
C    KI is updated so that all the chains point towards (KN+1).
C
41 K = IPUSH(IP)
    IP = IP - 1
42 KT = KN + 1
    X = DIST(K)
43 KP = KI(K)
    KI(K) = KT
    Y = DK(K)
    DK(K) = X
    X = Y
    KT = K
    K = KP
    IF (NUM(KT) .GT. 0) GO TO 43
    IF (IP .NE. 0) GO TO 41
C
    RETURN
    END
```

```
subroutine dssp(x,xmean,xssp,wt,sumwt,nvar,nunit,ifault)
c
c      Algorithm AS 41 j.r.statist.soc.c. (1971) vol. 20 no.2
c
c      This subroutine updates the mean vector xmean (length nvar)
c      and the matrix of corrected sums of squares and products xssp
c      (length nvar(nvar+1)/2, stored by lower triangle), when a
c      data vector x (length nvar) with weight wt is either included
c      (wt.gt.0) or excluded (wt.lt.0).  sumwt is the current sum of
c      weights on entry and the updated sum on exit and nunit is
c      the current and updated sample size.  ifault=0 indicates normal
c      exit,  ifault=1 indicates zero or negative value of sumwt,
c      ifault=2 indicates zero or negative nunit, ifault=3 indicates
c      nvar.lt.1.  Note that x, xmean, xssp, wt and sumwt are double
c      precision and must be declared as such in the calling program.
c
dimension x(*), xmean(*), xssp(*)
double precision x, xmean, xssp, wt, sumwt, b, c, co
data co/0.0d0/
c
c      Check variates, weights and sample size
c
      ifault = 0
      if(nvar.lt.1) goto 103
      if(wt)107,100,106
107 nunit = nunit-1
      go to 105
106 nunit = nunit+1
105 sumwt = sumwt+wt
      if(sumwt.le.co) go to 101
      k = 0
      b = wt/sumwt
      if(nunit-1)102,120,110
c
c      Update means and ssp for sample size greater than 1
c
110 c = wt-b*wt
      do 111 i = 1,nvar
         x(i) = x(i)-xmean(i)
         xmean(i) = xmean(i)+b*x(i)
         do 111 j = 1,i
            k = k+1
            xssp(k) = xssp(k)+c*x(i)*x(j)
111 continue
      return
c
c      Initialise means and ssp for sample size = 1
c
120 do 121 i = 1,nvar
      if(wt.lt.co) goto 122
      xmean(i) = x(i)
      goto 123
122 xmean(i) = xmean(i)+b*(x(i)-xmean(i))
123 x(i) = co
      do 121 j = 1,i
         k = k+1
         xssp(k) = co
121 continue
      return
c
c      Set fault indicators
```

c

```
103 ifault = ifault+1
102 ifault = ifault+1
101 ifault = ifault+1
100 return
    end
```



```
CSTART OF AS 45
  SUBROUTINE HISTGM(IWRITE, IWIDTH, FREQ, DAT, NN, MM,
  $ LENG, IND, IFAULT)
C
C      ALGORITHM AS 45  APPL. STATIST. (1971) VOL.20, P.332
C
C      GIVEN A VECTOR OF FREQUENCIES, OR A VECTOR OF RAW DATA,
C      A HISTOGRAM IS PLOTTED SHOWING THE FREQUENCY DISTRIBUTION
C
  DIMENSION IOUT(28), OUT(28), DAT(NN), FREQ(MM)
  INTEGER FREQ, SCALE
  LOGICAL IND
C
  DEFINE CHARACTERS FOR PRINTING, AND MAGNITUDE OF
  SMALLEST ACCEPTABLE NUMBER.
C
  DATA IBLANK, ISTAR, IDASH /1H , 1H*, 1H-/
  DATA ETA /1.0E-38/
C
1  FORMAT(6H EACH , A1, 8H EQUALS , I4, 7H POINTS /)
2  FORMAT(1H , I8, 3X, 28(4X, A1))
3  FORMAT(12H INTERVAL  ), 14(F8.3, 2X))
4  FORMAT(12H MID-POINTS), 5X, 14(F8.3, 2X))
5  FORMAT(24H0THE PRINTED VALUES MUST/ 22H BE MULTIPLIED BY 10**, I3)
6  FORMAT(12H0FREQUENCY  , 28I5)
7  FORMAT(1H , 120A1)
8  FORMAT(16H CELLS COMBINED,, I3, 3H AT / 21H A TIME, TO FIT WIDTH)
C
  CHECK INPUT PARAMETERS AND TYPE OF INPUT
C
  IFAULT = 0
  IF (MM .GT. 28 .OR. IWIDTH .LT. 26) IFAULT = 1
  M = MM
  N = NN
  K = (IWIDTH - 15) / 5
  IF (M .GT. K .AND. IND) M = K
  LENGTH = LENG - 10
  IF (LENGTH .LE. 0) IFAULT = 2
  IF (IFAILT .NE. 0) RETURN
  FM = M
  IF (IND) GOTO 15
  IF (M .LE. K) GOTO 120
  KEY = M / K
  IF (K * KEY .NE. M) KEY = KEY + 1
  L = 1
  DO 10 I = 1, K
  IOUT(I) = 0
  DO 10 J = 1, KEY
  IOUT(I) = IOUT(I) + FREQ(L)
  L = L + 1
  IF (L .GT. M) GOTO 12
10 CONTINUE
12 M = I
  DO 14 I = 1, M
14 FREQ(I) = IOUT(I)
  WRITE (IWRITE, 8) KEY
  GOTO 120
C
  DEFINE A SUITABLE SCALE
C
15 DO 20 I = 1, M
```

```
20 FREQ(I) = 0
   XMIN = DAT(1)
   XMAX = XMIN
   DO 30 I = 2, N
   DT = DAT(I)
   IF (DT .LT. XMIN) XMIN = DT
   IF (DT .GT. XMAX) XMAX = DT
30 CONTINUE
   IF (XMAX - XMIN .GE. ETA * FM) GOTO 35
   IFAULT = 3
   RETURN
35 KEY = 1
   KOUNT = 0
40 R = XMAX - XMIN
   B = XMIN
50 IF (R .GT. 1.0) GOTO 60
   KOUNT = KOUNT + 1
   R = R * 10.0
   GOTO 50
60 IF (R .LE. 10.0) GOTO 70
   KOUNT = KOUNT - 1
   R = R / 10.0
   GOTO 60
70 IF (KEY .GT. 2) GOTO 80
   TK = 10.0 ** KOUNT
   B = B * TK
   IF (B .LT. 0.0 .AND. B .NE. AINT(B)) B = B - 1.0
   B = AINT(B) / TK
   R = (XMAX - B) / FM
   KOUNT = 0
   KEY = KEY + 2
   GOTO 50
80 STEP = AINT(R)
   IF (STEP .NE. R) STEP = STEP + 1.0
   IF (R .LT. 1.5) STEP = STEP - 0.5
   STEP = STEP / 10.0 ** KOUNT
   IF (KEY .EQ. 4) GOTO 90
   IF (XMAX - XMIN .GT. 0.8 * FM * STEP) GOTO 90
   KOUNT = 1
   KEY = 2
   GOTO 40
90 XMIN = B
   C = STEP * AINT(B / STEP)
   IF (C .LT. 0.0 .AND. C .NE. B) C = C - STEP
   IF (C + FM * STEP .GE. XMAX) XMIN = C
C
C   CALCULATE FREQUENCIES FOR EACH INTERVAL
C
   DO 110 I = 1, N
   J = (DAT(I) - XMIN) / STEP + 1.0
   FREQ(J) = FREQ(J) + 1
110 CONTINUE
C
C   PRINT FREQUENCY VECTOR
C
120 WRITE (IWRITE, 6) (FREQ(I), I = 1, M)
   LINE = M * 5 + 15
   WRITE (IWRITE, 7) (IDASH, I = 1, LINE)
C
C   FIND LARGEST FREQUENCY AND SCALE IF NECESSARY
C
```

```
      MAX = 0
      DO 130 I = 1, M
      IF (FREQ(I) .GT. MAX) MAX = FREQ(I)
130 CONTINUE
      SCALE = 1
      DIV = 1.0
      IF (MAX .LE. LENGTH) GOTO 140
      SCALE = (MAX + LENGTH - 1) / LENGTH
      WRITE (IWRITE, 1) ISTAR, SCALE
      DIV = 1.0 / FLOAT(SCALE)
C
C      CLEAR OUTPUT TO BLANKS
C
140 DO 150 I = 1, M
150 IOUT(I) = IBLANK
C
C      FOR EACH LINE OF PRINT, PLACE OUTPUT CHARACTERS IN
C      THEIR APPROPRIATE POSITIONS IN THE OUTPUT VECTOR
C
      MAX = FLOAT(MAX) * DIV + 0.5
      DO 170 I = 1, MAX
      K = MAX + 1 - I
      DO 160 J = 1, M
      INDEX = FLOAT(FREQ(J)) * DIV + 0.5
      IF (INDEX .EQ. K) IOUT(J) = ISTAR
160 CONTINUE
      L = K * SCALE
C
C      PRINT LINE OF FREQUENCIES
C
      WRITE (IWRITE, 2) L, (IOUT(J), J = 1, M)
170 CONTINUE
      WRITE (IWRITE, 7) (IDASH, I = 1, LINE)
      IF (.NOT. IND) RETURN
C
C      COMPUTE INTERVAL MID-POINTS AND SCALE IF NECESSARY
C
      K = 0
      XMIN = XMIN + STEP * 0.5
      XMAX = XMIN + STEP * FLOAT(M - 1)
      XM = AMIN1(ABS(XMIN), ABS(XMAX))
      IF (XM .LT. ETA) XM = XM + STEP
180 IF (XM .GE. 0.1) GOTO 190
      K = K + 1
      XM = XM * 10.0
      GOTO 180
190 XM = AMAX1(XMAX, -XMIN)
200 IF (XM .LT. 1000.0) GOTO 210
      K = K - 1
      XM = XM / 10.0
      GOTO 200
210 TK = 10.0 ** K
      STEP = STEP * TK
      OUT(1) = XMIN * TK
      DO 220 I = 2, M
220 OUT(I) = OUT(I - 1) + STEP
C
C      PRINT INTERVAL MID-POINTS
C
      WRITE (IWRITE, 3) (OUT(J), J = 1, M, 2)
      WRITE (IWRITE, 4) (OUT(J), J = 2, M, 2)
```

```
      K = -K  
      IF (K .NE. 0) WRITE (IWRITE, 5) K  
      RETURN  
      END  
CEND OF AS 45
```

```
subroutine gmsmod (x,n,m,v,c,d,nullty)
```

```
c
c   Algorithm AS 46 Applied Statistics (J.R.Statist.Soc C),
c   (1971) Vol.20, No.3
c
c   Expresses the n*m matrix x as the product of the n*m matrix v
c   and the m*m upper unit triangular matrix c. v-transpose.v is
c   a diagonal matrix and is returned in d. nullty is the nullity
c   of d. v may coincide with x.
c
c   double precision x(*),v(*),c(*),d(*)
c   double precision w0, w1, w2, w3, eta
c   double precision test, zero, one
c
c   data eta/1.0d-12/, zero/0.0d0/, one/1.0d0/
c
c   nullty=0
c   ic=0
c   i1=-n
c   do 70 icol=1,m
c     i1=i1+n
c     w0=zero
c     i2=i1
c     do 10 irow=1,n
c       i2=i2+1
c       w1=x(i2)
c       v(i2)=w1
10    w0=w0+w1*w1
c     i3=0
c     i4=0
c     do 70 icolw=1,icol
c       i2=i1
c       w2=zero
c       do 20 irow=1,n
c         i2=i2+1
c         i3=i3+1
c         w3=v(i2)
c         w1=v(i3)
20    w2=w2+w1*w3
c       if(icolw.lt.icol) goto 30
c       test=w2/w0
c       if(test.ge.eta) goto 25
c       do 21 irow=1,n
c         i4=i4+1
21    v(i4)=zero
c       i4=i4-n
c       nullty=nullty+1
c       w2=zero
25    d(icol)=w2
c       i4=i4+n
c       w1=one
c       goto 60
30    w1=zero
c       w3=d(icolw)
c       if(w3.eq.zero) goto 40
c       w1=w2/w3
40    i2=i1
c       do 50 irow=1,n
c         i2=i2+1
c         i4=i4+1
50    v(i2)=v(i2)-w1*v(i4)
```

```
60      ic=ic+1
        c(ic)=w1
70 continue
   return
end
```

```
c This file contains two versions of the Nelder & Mead simplex algorithm
c for function minimization. The first is that published in the journal
c of Applied Statistics. This does not include the fitting of a quadratic
c surface, which provides the only satisfactory method of testing whether
c a minimum has been found. The search for a minimum is liable to
c premature termination.
c The second version is one which has been developed jointly by CSIRO and
c Rothamsted, and does include the quadratic-surface fitting.
```

```
c
c
c      subroutine nelmin(fn, n, start, xmin, ynewlo, reqmin, step,
c      #      konvge, kcount, icount, numres, ifault)
c      implicit double precision (a-h,o-z)
```

```
c
c      Simplex function minimisation procedure due to Nelder+Mead(1965),
c      as implemented by O'Neill(1971, Appl.Statist. 20, 338-45), with
c      subsequent comments by Chambers+Ertel(1974, 23, 250-1), Benyon(1976,
c      25, 97) and Hill(1978, 27, 380-2)
```

```
c
c      Algorithm AS 47 Applied Statistics (J.R. Statist. Soc. C),
c      (1971) Vol.20, No. 3
```

```
c
c      The Nelder-Mead Simplex Minimisation Procedure
```

```
c
c      Purpose :: To find the minimum value of a user-specified
c                function
```

```
c
c      Formal parameters ::
```

```
c
c      fn      :      : The name of the function to be minimized.
c      n      : input : The number of variables over which we are
c                  :      : minimising
c      start  : input : Array; Contains the coordinates of the
c                  :      : starting point.
c                  :      : output : The values may be overwritten.
c      xmin   : output : Array; Contains the coordinates of the
c                  :      : minimum.
c      ynewlo : output : The minimum value of the function.
c      reqmin : input  : The terminating limit for the variance of
c                  :      : function values.
c      step   : input  : Array; Determines the size and shape of the
c                  :      : initial simplex. The relative magnitudes of
c                  :      : its n elements should reflect the units of
c                  :      : the n variables.
c      konvge : input  : The convergence check is carried out every
c                  :      : konvge iterations.
c      kcount : input  : Maximum number of function evaluations.
c      icount : output : Function evaluations performed
c      numres : output : Number of restarts.
c      ifault : output : 1 if reqmin, n, or konvge has illegal value;
c                  :      : 2 if terminated because kcount was exceeded
c                  :      : without convergence;
c                  :      : 0 otherwise.
```

```
c
c      All variables and arrays are to be declared in the calling
c      program as double precision.
```

```
c
c      Auxiliary algorithm :: The double precision function
c      subprogram fn(a) calculates the function value at point a.
```

```
c      a is double precision with n elements.
c
c
c      Reference :: Nelder,J.A. and Mead,R.(1965).  A simplex method
c      for function minimization.  Computer J., Vol.7,308-313.
c
c*****
c
c      double precision start(n), xmin(n), ynewlo, reqmin, step(n),
1     p(20,21), pstar(20), p2star(20), pbar(20), y(21),
2     dn, dnn, z, ylo, rcoeff, ystar, ecoeff, y2star, ccoeff,
3     rq, x, del, fn, one, half, zero, eps
c      external fn
c
c      data rcoeff/1.0d0/, ecoeff/2.0d0/, ccoeff/5.0d-1/
c      data one/1.0d0/, half/0.5d0/, zero/0.0d0/, eps/0.001d0/
c      reflection, extension and contraction coefficients.
c
c      validity checks on input parameters.
c
c      ifault=1
c      if(reqmin .le. zero .or. n .lt. 1 .or. n .gt. 20
#     .or. konvge .lt. 1) return
c      ifault=2
c      icount=0
c      numres=0
c
c      jcount=konvge
c      dn=float(n)
c      nn=n+1
c      dnn=float(nn)
c      del=one
c      rq=reqmin*dn
c
c      construction of initial simplex.
c
c      10 do 20 i=1,n
c      20 p(i,nn)=start(i)
c         y(nn)=fn(start)
c         do 40 j=1,n
c            x=start(j)
c            start(j)=start(j)+step(j)*del
c            do 30 i=1,n
c      30     p(i,j)=start(i)
c            y(j)=fn(start)
c            start(j)=x
c      40 continue
c         icount=icount+nn
c
c      simplex construction complete
c
c      find highest and lowest y values.  ynewlo (=y(ihi) ) indicates
c      the vertex of the simplex to be replaced.
c
c      43 ylo=y(1)
c         ilo=1
c         do 47 i=2,nn
c            if(y(i).ge.ylo) goto 47
c            ylo=y(i)
c            ilo=i
c      47 continue
```



```
50 ynewlo=y(1)
   ihi=1
   do 70 i=2,nn
     if(y(i) .le. ynewlo) goto 70
     ynewlo=y(i)
     ihi=i
70 continue
c
c   calculate pbar,the centroid of the simplex vertices
c     excepting that with y value ynewlo.
c
   do 90 i=1,n
     z=zero
     do 80 j=1,nn
80    z=z+p(i,j)
     z=z-p(i,ihl)
     pbar(i)=z/dn
90 continue
c
c   reflection through the centroid
c
   do 100 i=1,n
100  pstar(i)=pbar(i) + rcoeff * (pbar(i) - p(i,ihl))
     ystar=fn(pstar)
     icount=icount+1
     if (ystar.ge.ylo) goto 140
c
c   successful reflection,so extension
c
   do 110 i=1,n
110  p2star(i)=pbar(i) + ecoeff * (pstar(i)-pbar(i))
     y2star=fn(p2star)
     icount=icount+1
c
c   check extension
c
   if(y2star .ge. ystar) goto 133
c
c   retain extension or contraction.
c
   do 130 i=1,n
130  p(i,ihl)=p2star(i)
     y(ihl)=y2star
     goto 230
c
c   retain reflection
c
133 do 137 i=1,n
137  p(i,ihl)=pstar(i)
     y(ihl)=ystar
     goto 230
c
c   no extension
c
140 l=0
     do 150 i=1,nn
       if (y( i).gt.ystar) l=l+1
150  continue
     if (l.gt.1) goto 133
     if (l.eq.0) goto 170
c
```

```
c      contraction on the reflection side of the centroid.
c
c      do 160 i=1,n
160  p2star(i) = pbar(i) + ccoeff * (pstar(i) - pbar(i))
      y2star = fn(p2star)
      icount=icount+1
      if(y2star .le. ystar) goto 182
c
c      retain reflection
c
c      do 165 i=1,n
165  p(i,ihi)=pstar(i)
      y(ihi)=ystar
      goto 230
c
c      contraction on the y(ihi) side of the centriod.
c
c      170 do 180 i=1,n
180  p2star(i)=pbar(i) + ccoeff * (p(i,ihi) - pbar(i))
      y2star=fn(p2star)
      icount=icount+1
      if (y2star .gt. y(ihi)) goto 188
c
c      retain contraction
c
c      182 do 185 i=1,n
185  p(i,ihi) = p2star(i)
      y(ihi)=y2star
      goto 230
c
c      contract whole simplex.
c
c      188 do 200 j=1,nn
      do 190 i=1,n
          p(i,j)=(p(i,j)+p(i,ilo))*half
          xmin(i)=p(i,j)
190  continue
      y(j)=fn(xmin)
200  continue
      icount=icount+nn
      if (icount .gt. kcount) go to 260
      goto 43
c
c      Check if ylo improved
c
c      230 if (y(ihi) .ge. ylo) goto 235
      ylo=y(ihi)
      ilo=ihi
235  jcount=jcount-1
      if(jcount .ne. 0) goto 50
c
c      check to see if minimum reached.
c
c      if (icount.gt.kcount) goto 260
      jcount=konvge
      z=zero
      do 240 i=1, nn
240  z = z+y(i)
      x=z / dnn
      z=zero
      do 250 i=1,nn
```

```
250 z = z+(y(i)-x) ** 2
    if (z .gt. rq) goto 50
c
c    factorial tests to check that ynewlo is a local minimum.
c
260 do 270 i=1,n
270 xmin(i)=p(i,ilo)
    ynewlo=y(ilo)
    if (icount.gt.kcount) return
    do 280 i=1,n
        del=step(i)*eps
        xmin(i)=xmin(i)+del
        z=fn(xmin)
        icount=icount+1
        if (z.lt.ynewlo) goto 290
        xmin(i)=xmin(i)-del-del
        z=fn(xmin)
        icount=icount+1
        if (z.lt.ynewlo) goto 290
        xmin(i)=xmin(i)+del
280 continue
    ifault = 0
    return
c
c    restart procedure
c
290 do 300 i=1,n
300 start(i) = xmin(i)
    del=eps
    numres = numres + 1
    goto 10
end
c
c-----
c
SUBROUTINE MINIM(P,STEP,NOP,FUNC,MAX,IPRINT,STOPCR,NLOOP,IQUAD,
1  SIMP,VAR,FUNCTN,IFAUULT)
C
C    A PROGRAM FOR FUNCTION MINIMIZATION USING THE SIMPLEX METHOD.
C    The minimum found will often be a local, not a global, minimum.
C
C    FOR DETAILS, SEE NELDER & MEAD, THE COMPUTER JOURNAL, JANUARY 1965
C
C    PROGRAMMED BY D.E.SHAW,
C    CSIRO, DIVISION OF MATHEMATICS & STATISTICS
C    P.O. BOX 218, LINDFIELD, N.S.W. 2070
C
C    WITH AMENDMENTS BY R.W.M.WEDDERBURN
C    ROTHAMSTED EXPERIMENTAL STATION
C    HARPENDEN, HERTFORDSHIRE, ENGLAND
C
C    Further amended by Alan Miller,
C    CSIRO, Division of Mathematics & Statistics
C    Private Bag 10, CLAYTON, VIC. 3168
C
C    ARGUMENTS:-
C    P()      = INPUT, STARTING VALUES OF PARAMETERS
C             OUTPUT, FINAL VALUES OF PARAMETERS
C    STEP()   = INPUT, INITIAL STEP SIZES
C    NOP      = INPUT, NO. OF PARAMETERS, INCL. ANY TO BE HELD FIXED
C    FUNC     = OUTPUT, THE FUNCTION VALUE CORRESPONDING TO THE FINAL
```

```

C          PARAMETER VALUES
C      MAX      = INPUT, THE MAXIMUM NO. OF FUNCTION EVALUATIONS ALLOWED
C      IPRINT   = INPUT, PRINT CONTROL PARAMETER
C                < 0 NO PRINTING
C                = 0 PRINTING OF PARAMETER VALUES AND THE FUNCTION
C                  VALUE AFTER INITIAL EVIDENCE OF CONVERGENCE.
C                > 0 AS FOR IPRINT = 0 PLUS PROGRESS REPORTS AFTER
C                  EVERY IPRINT EVALUATIONS, PLUS PRINTING FOR THE
C                  INITIAL SIMPLEX.
C      STOPCR   = INPUT, STOPPING CRITERION
C      NLOOP    = INPUT, THE STOPPING RULE IS APPLIED AFTER EVERY NLOOP
C                  FUNCTION EVALUATIONS.
C      IQUAD    = INPUT, = 1 IF THE FITTING OF A QUADRATIC SURFACE IS REQUIRED
C                  = 0 IF NOT
C      SIMP     = INPUT, CRITERION FOR EXPANDING THE SIMPLEX TO OVERCOME
C                  ROUNDING ERRORS BEFORE FITTING THE QUADRATIC SURFACE.
C      VAR()    = OUTPUT, CONTAINS THE DIAGONAL ELEMENTS OF THE INVERSE OF
C                  THE INFORMATION MATRIX.
C      FUNCTN   = INPUT, NAME OF THE USER'S SUBROUTINE - ARGUMENTS (P,FUNC)
C                  WHICH RETURNS THE FUNCTION VALUE FOR A GIVEN SET OF
C                  PARAMETER VALUES IN ARRAY P.
C****      FUNCTN MUST BE DECLARED EXTERNAL IN THE CALLING PROGRAM.
C      IFAULT   = OUTPUT, = 0 FOR SUCCESSFUL TERMINATION
C                  = 1 IF MAXIMUM NO. OF FUNCTION EVALUATIONS EXCEEDED
C                  = 2 IF INFORMATION MATRIX IS NOT +VE SEMI-DEFINITE
C                  = 3 IF NOP < 1
C                  = 4 IF NLOOP < 1
C
C      Advice on usage:
C      If the function minimized can be expected to be smooth in the vicinity
C      of the minimum, users are strongly urged to use the quadratic-surface
C      fitting option. This is the only satisfactory way of testing that the
C      minimum has been found. The value of SIMP should be set to at least
C      1000 times the rounding error in calculating the fitted function.
C      e.g. in double precision on a micro- or mini-computer with about 16
C      decimal digit representation of floating-point numbers, the rounding
C      errors in calculating the objective function may be of the order of
C      1.E-12 say in a particular case. A suitable value for SIMP would then
C      be 1.E-08. However, if numerical integration is required in the
C      calculation of the objective function, it may only be accurate to say
C      1.E-05 and an appropriate value for SIMP would be about 0.1.
C      If the fitted quadratic surface is not +ve definite (and the function
C      should be smooth in the vicinity of the minimum), it probably means
C      that the search terminated prematurely and you have not found the
C      minimum.
C
C      N.B. P, STEP AND VAR (IF IQUAD = 1) MUST HAVE DIMENSION AT LEAST NOP
C          IN THE CALLING PROGRAM.
C      THE DIMENSIONS BELOW ARE FOR A MAXIMUM OF 20 PARAMETERS.
C      The dimension of BMAT should be at least NOP*(NOP+1)/2.
C
C****      N.B. This version is in DOUBLE PRECISION throughout
C
C      LATEST REVISION - 11 August 1991
C
C*****
C
C      implicit double precision (a-h, o-z)
C      external FUNCTN
C      DIMENSION P(NOP),STEP(NOP),VAR(NOP)
C      DIMENSION G(21,20),H(21),PBAR(20),PSTAR(20),PSTST(20),AVAL(20),

```

```
1  BMAT(210),PMIN(20),VC(210),TEMP(20)
   DATA ZERO/0.D0/, ONE/1.D0/, TWO/2.D0/, THREE/3.D0/, HALF/0.5D0/
C
C  A = REFLECTION COEFFICIENT, B = CONTRACTION COEFFICIENT, AND
C  C = EXPANSION COEFFICIENT.
C
   DATA A,B,C/1.D0, 0.5D0, 2.D0/
C
C  SET LOUT = LOGICAL UNIT NO. FOR OUTPUT
C
   DATA LOUT/6/
C
C  IF PROGRESS REPORTS HAVE BEEN REQUESTED, PRINT HEADING
C
   IF(IPRINT.GT.0) WRITE(LOUT,1000) IPRINT
1000 FORMAT(' PROGRESS REPORT EVERY',I4,' FUNCTION EVALUATIONS'//,
1  ' EVAL.  FUNC.',15X,'PARAMETER VALUES')
C
C  CHECK INPUT ARGUMENTS
C
   IFAULT=0
   IF(NOP.LE.0) IFAULT=3
   IF(NLOOP.LE.0) IFAULT=4
   IF(IFAULT.NE.0) RETURN
C
C  SET NAP = NO. OF PARAMETERS TO BE VARIED, I.E. WITH STEP.NE.0
C
   NAP=0
   LOOP=0
   IFLAG=0
   DO 10 I=1,NOP
       IF(STEP(I).NE.ZERO) NAP=NAP+1
10  CONTINUE
C
C  IF NAP = 0 EVALUATE FUNCTION AT THE STARTING POINT AND RETURN
C
   IF(NAP.GT.0) GO TO 30
   CALL FUNCTN(P,FUNC)
   RETURN
C
C  SET UP THE INITIAL SIMPLEX
C
30  DO 40 I=1,NOP
40  G(1,I)=P(I)
   IROW=2
   DO 60 I=1,NOP
       IF(STEP(I).EQ.ZERO) GO TO 60
       DO 50 J=1,NOP
50  G(IROW,J)=P(J)
       G(IROW,I)=P(I)+STEP(I)
       IROW=IROW+1
60  CONTINUE
   NP1=NAP+1
   NEVAL=0
   DO 90 I=1,NP1
       DO 70 J=1,NOP
70  P(J)=G(I,J)
       CALL FUNCTN(P,H(I))
       NEVAL=NEVAL+1
       IF(IPRINT.LE.0) GO TO 90
       WRITE(LOUT,1010) NEVAL,H(I),(P(J),J=1,NOP)
```

```
1010  FORMAT(/I4, 2X, G12.5, 2X, 5G12.5, 3(/20X, 5G12.5))
90  CONTINUE
C
C  START OF MAIN CYCLE.
C
C  FIND MAX. & MIN. VALUES FOR CURRENT SIMPLEX (HMAX & HMIN).
C
100  LOOP=LOOP+1
      IMAX=1
      IMIN=1
      HMAX=H(1)
      HMIN=H(1)
      DO 120 I=2,NP1
          IF(H(I).LE.HMAX) GO TO 110
          IMAX=I
          HMAX=H(I)
          GO TO 120
110  IF(H(I).GE.HMIN) GO TO 120
      IMIN=I
      HMIN=H(I)
120  CONTINUE
C
C  FIND THE CENTROID OF THE VERTICES OTHER THAN P(IMAX)
C
      DO 130 I=1,NOP
130  PBAR(I)=ZERO
      DO 150 I=1,NP1
          IF(I.EQ.IMAX) GO TO 150
          DO 140 J=1,NOP
140  PBAR(J)=PBAR(J)+G(I,J)
150  CONTINUE
      DO 160 J=1,NOP
          FNAP = NAP
160  PBAR(J)=PBAR(J)/FNAP
C
C  REFLECT MAXIMUM THROUGH PBAR TO PSTAR,
C  HSTAR = FUNCTION VALUE AT PSTAR.
C
      DO 170 I=1,NOP
170  PSTAR(I)=A*(PBAR(I)-G(IMAX,I))+PBAR(I)
      CALL FUNCTN(PSTAR,HSTAR)
      NEVAL=NEVAL+1
      IF(IPRINT.LE.0) GO TO 180
      IF(MOD(NEVAL,IPRINT).EQ.0) WRITE(LOUT,1010) NEVAL,HSTAR,
1  (PSTAR(J),J=1,NOP)
C
C  IF HSTAR < HMIN, REFLECT PBAR THROUGH PSTAR,
C  HSTST = FUNCTION VALUE AT PSTST.
C
180  IF(HSTAR.GE.HMIN) GO TO 220
      DO 190 I=1,NOP
190  PSTST(I)=C*(PSTAR(I)-PBAR(I))+PBAR(I)
      CALL FUNCTN(PSTST,HSTST)
      NEVAL=NEVAL+1
      IF(IPRINT.LE.0) GO TO 200
      IF(MOD(NEVAL,IPRINT).EQ.0) WRITE(LOUT,1010) NEVAL,HSTST,
1  (PSTST(J),J=1,NOP)
C
C  IF HSTST < HMIN REPLACE CURRENT MAXIMUM POINT BY PSTST AND
C  HMAX BY HSTST, THEN TEST FOR CONVERGENCE.
C
```

```
200 IF(HSTST.GE.HMIN) GO TO 320
    DO 210 I=1,NOP
        IF(STEP(I).NE.ZERO) G(IMAX,I)=PSTST(I)
210 CONTINUE
    H(IMAX)=HSTST
    GO TO 340

C
C   HSTAR IS NOT < HMIN.
C   TEST WHETHER IT IS < FUNCTION VALUE AT SOME POINT OTHER THAN
C   P(IMAX).  IF IT IS REPLACE P(IMAX) BY PSTAR & HMAX BY HSTAR.
C
220 DO 230 I=1,NP1
    IF(I.EQ.IMAX) GO TO 230
    IF(HSTAR.LT.H(I)) GO TO 320
230 CONTINUE

C
C   HSTAR > ALL FUNCTION VALUES EXCEPT POSSIBLY HMAX.
C   IF HSTAR <= HMAX, REPLACE P(IMAX) BY PSTAR & HMAX BY HSTAR.
C
    IF(HSTAR.GT.HMAX) GO TO 260
    DO 250 I=1,NOP
        IF(STEP(I).NE.ZERO) G(IMAX,I)=PSTAR(I)
250 CONTINUE
    HMAX=HSTAR
    H(IMAX)=HSTAR

C
C   CONTRACTED STEP TO THE POINT PSTST,
C   HSTST = FUNCTION VALUE AT PSTST.
C
260 DO 270 I=1,NOP
270 PSTST(I)=B*G(IMAX,I) + (1.d0-B)*PBAR(I)
    CALL FUNCTN(PSTST,HSTST)
    NEVAL=NEVAL+1
    IF(IPRINT.LE.0) GO TO 280
    IF(MOD(NEVAL,IPRINT).EQ.0) WRITE(LOUT,1010) NEVAL,HSTST,
1   (PSTST(J),J=1,NOP)

C
C   IF HSTST < HMAX REPLACE P(IMAX) BY PSTST & HMAX BY HSTST.
C
280 IF(HSTST.GT.HMAX) GO TO 300
    DO 290 I=1,NOP
        IF(STEP(I).NE.ZERO) G(IMAX,I)=PSTST(I)
290 CONTINUE
    H(IMAX)=HSTST
    GO TO 340

C
C   HSTST > HMAX.
C   SHRINK THE SIMPLEX BY REPLACING EACH POINT, OTHER THAN THE CURRENT
C   MINIMUM, BY A POINT MID-WAY BETWEEN ITS CURRENT POSITION AND THE
C   MINIMUM.
C
300 DO 315 I=1,NP1
    IF(I.EQ.IMIN) GO TO 315
    DO 310 J=1,NOP
        IF(STEP(J).NE.ZERO) G(I,J)=(G(I,J)+G(IMIN,J))*HALF
        P(J)=G(I,J)
310 CONTINUE
    CALL FUNCTN(P,H(I))
    NEVAL=NEVAL+1
    IF(IPRINT.LE.0) GO TO 315
    IF(MOD(NEVAL,IPRINT).EQ.0) WRITE(LOUT,1010) NEVAL,H(I),
```

```

1          (P(J),J=1,NOP)
315 CONTINUE
    GO TO 340
C
C   REPLACE MAXIMUM POINT BY PSTAR & H(IMAX) BY HSTAR.
C
320 DO 330 I=1,NOP
      IF(STEP(I).NE.ZERO) G(IMAX,I)=PSTAR(I)
330 CONTINUE
    H(IMAX)=HSTAR
C
C   IF LOOP = NLOOP TEST FOR CONVERGENCE, OTHERWISE REPEAT MAIN CYCLE.
C
340 IF(LOOP.LT.NLOOP) GO TO 100
C
C   CALCULATE MEAN & STANDARD DEVIATION OF FUNCTION VALUES FOR THE
C   CURRENT SIMPLEX.
C
    HSTD=ZERO
    HMEAN=ZERO
    DO 350 I=1,NP1
350 HMEAN=HMEAN+H(I)
      FNP1 = NP1
    HMEAN=HMEAN/FNP1
    DO 360 I=1,NP1
360 HSTD=HSTD+(H(I)-HMEAN)**2
      HSTD=SQRT(HSTD/FLOAT(NP1))
C
C   IF THE RMS > STOPCR, SET IFLAG & LOOP TO ZERO AND GO TO THE
C   START OF THE MAIN CYCLE AGAIN.
C
    IF(HSTD.LE.STOPCR.OR.NEVAL.GT.MAX) GO TO 410
    IFLAG=0
    LOOP=0
    GO TO 100
C
C   FIND THE CENTROID OF THE CURRENT SIMPLEX AND THE FUNCTION VALUE THERE.
C
410 DO 380 I=1,NOP
      IF(STEP(I).EQ.ZERO) GO TO 380
      P(I)=ZERO
      DO 370 J=1,NP1
370 P(I)=P(I)+G(J,I)
        FNP1 = NP1
      P(I)=P(I)/FNP1
380 CONTINUE
    CALL FUNCTN(P,FUNC)
    NEVAL=NEVAL+1
    IF(IPRINT.LE.0) GO TO 390
    IF(MOD(NEVAL,IPRINT).EQ.0) WRITE(LOUT,1010) NEVAL,FUNC,
1 (P(J),J=1,NOP)
C
C   TEST WHETHER THE NO. OF FUNCTION VALUES ALLOWED, MAX, HAS BEEN
C   OVERRUN; IF SO, EXIT WITH IFAULT = 1.
C
390 IF(NEVAL.LE.MAX) GO TO 420
    IFAULT=1
    IF(IPRINT.LT.0) RETURN
    WRITE(LOUT,1020) MAX
1020 FORMAT(' NO. OF FUNCTION EVALUATIONS EXCEEDS ',I5)
    WRITE(LOUT,1030) HSTD

```



```
1030 FORMAT(' RMS OF FUNCTION VALUES OF LAST SIMPLEX =',G14.6)
      WRITE(LOUT,1040)(P(I),I=1,NOP)
1040 FORMAT(' CENTROID OF LAST SIMPLEX =',4(/1X,6G13.5))
      WRITE(LOUT,1050) FUNC
1050 FORMAT(' FUNCTION VALUE AT CENTROID =',G14.6)
      RETURN
C
C CONVERGENCE CRITERION SATISFIED.
C IF IFLAG = 0, SET IFLAG & SAVE HMEAN.
C IF IFLAG = 1 & CHANGE IN HMEAN <= STOPCR THEN SEARCH IS COMPLETE.
C
420 IF(IPRINT.LT.0) GO TO 430
      WRITE(LOUT,1060)
1060 FORMAT(/' EVIDENCE OF CONVERGENCE')
      WRITE(LOUT,1040)(P(I),I=1,NOP)
      WRITE(LOUT,1050) FUNC
430 IF(IFLAG.GT.0) GO TO 450
      IFLAG=1
440 SAVEMN=HMEAN
      LOOP=0
      GO TO 100
450 IF(ABS(SAVEMN-HMEAN).GE.STOPCR) GO TO 440
      IF(IPRINT.LT.0) GO TO 460
      WRITE(LOUT,1070) NEVAL
1070 FORMAT(//' MINIMUM FOUND AFTER',I5,' FUNCTION EVALUATIONS')
      WRITE(LOUT,1080)(P(I),I=1,NOP)
1080 FORMAT(' MINIMUM AT',4(/1X,6G13.6))
      WRITE(LOUT,1090) FUNC
1090 FORMAT(' FUNCTION VALUE AT MINIMUM =',G14.6)
460 IF(IQUAD.LE.0) RETURN
C-----
C
C QUADRATIC SURFACE FITTING
C
      IF(IPRINT.GE.0) WRITE(LOUT,1110)
1110 FORMAT(/' QUADRATIC SURFACE FITTING ABOUT SUPPOSED MINIMUM'/)
C
C EXPAND THE FINAL SIMPLEX, IF NECESSARY, TO OVERCOME ROUNDING
C ERRORS.
C
      NEVAL=0
      DO 490 I=1,NP1
470 TEST=ABS(H(I)-FUNC)
      IF(TEST.GE.SIMP) GO TO 490
      DO 480 J=1,NOP
          IF(STEP(J).NE.ZERO) G(I,J)=(G(I,J)-P(J))+G(I,J)
          PSTST(J)=G(I,J)
480 CONTINUE
      CALL FUNCTN(PSTST,H(I))
      NEVAL=NEVAL+1
      GO TO 470
490 CONTINUE
C
C FUNCTION VALUES ARE CALCULATED AT AN ADDITIONAL NAP POINTS.
C
      DO 510 I=1,NAP
          I1=I+1
          DO 500 J=1,NOP
500 PSTAR(J)=(G(1,J)+G(I1,J))*HALF
          CALL FUNCTN(PSTAR,AVAL(I))
          NEVAL=NEVAL+1
```

```
510 CONTINUE
C
C THE MATRIX OF ESTIMATED SECOND DERIVATIVES IS CALCULATED AND ITS
C LOWER TRIANGLE STORED IN BMAT.
C
A0=H(1)
DO 540 I=1,NAP
  I1=I-1
  I2=I+1
  IF(I1.LT.1) GO TO 540
  DO 530 J=1,I1
    J1=J+1
    DO 520 K=1,NOP
      PSTST(K)=(G(I2,K)+G(J1,K))*HALF
      CALL FUNCTN(PSTST,HSTST)
      NEVAL=NEVAL+1
      L=I*(I-1)/2+J
      BMAT(L)=TWO*(HSTST+A0-AVAL(I)-AVAL(J))
520 CONTINUE
530 CONTINUE
540 CONTINUE
  L=0
  DO 550 I=1,NAP
    I1=I+1
    L=L+I
    BMAT(L)=TWO*(H(I1)+A0-TWO*AVAL(I))
550 CONTINUE
C
C THE VECTOR OF ESTIMATED FIRST DERIVATIVES IS CALCULATED AND
C STORED IN AVAL.
C
DO 560 I=1,NAP
  I1=I+1
  AVAL(I)=TWO*AVAL(I)-(H(I1)+THREE*A0)*HALF
560 CONTINUE
C
C THE MATRIX Q OF NELDER & MEAD IS CALCULATED AND STORED IN G.
C
DO 570 I=1,NOP
570 PMIN(I)=G(1,I)
DO 580 I=1,NAP
  I1=I+1
  DO 580 J=1,NOP
    G(I1,J)=G(I1,J)-G(1,J)
580 CONTINUE
DO 590 I=1,NAP
  I1=I+1
  DO 590 J=1,NOP
    G(I,J)=G(I1,J)
590 CONTINUE
C
C INVERT BMAT
C
CALL SYMINV(BMAT,NAP,BMAT,TEMP,NULLTY,IFFAULT,RMAX)
IF(IFFAULT.NE.0) GO TO 600
IRANK=NAP-NULLTY
GO TO 610
600 IF(IPRINT.GE.0) WRITE(LOUT,1120)
1120 FORMAT('/' MATRIX OF ESTIMATED SECOND DERIVATIVES NOT +VE DEFN.' /
1 ' MINIMUM PROBABLY NOT FOUND' /)
IFFAULT=2
RETURN
```

```
C
C      BMAT*A/2 IS CALCULATED AND STORED IN H.
C
610 DO 650 I=1,NAP
      H(I)=ZERO
      DO 640 J=1,NAP
        IF(J.GT.I) GO TO 620
        L=I*(I-1)/2+J
        GO TO 630
620     L=J*(J-1)/2+I
630     H(I)=H(I)+BMAT(L)*AVAL(J)
640     CONTINUE
650 CONTINUE

C
C      FIND THE POSITION, PMIN, & VALUE, YMIN, OF THE MINIMUM OF THE
C      QUADRATIC.
C
      YMIN=ZERO
      DO 660 I=1,NAP
660     YMIN=YMIN+H(I)*AVAL(I)
      YMIN=A0-YMIN
      DO 670 I=1,NOP
        PSTST(I)=ZERO
        DO 670 J=1,NAP
670     PSTST(I)=PSTST(I)+H(J)*G(J,I)
        DO 680 I=1,NOP
680     PMIN(I)=PMIN(I)-PSTST(I)
        IF(IPRINT.LT.0) GO TO 682
        WRITE(LOUT,1130) YMIN,(PMIN(I),I=1,NOP)
1130    FORMAT(' MINIMUM OF QUADRATIC SURFACE =',G14.6,' AT',
1       4(/1X,6G13.5))
        WRITE(LOUT,1150)
1150    FORMAT(' IF THIS DIFFERS BY MUCH FROM THE MINIMUM ESTIMATED',
1       1X,'FROM THE MINIMIZATION,')
2       ' THE MINIMUM MAY BE FALSE &/OR THE INFORMATION MATRIX MAY BE',
3       1X,'INACCURATE')

C
C      Calculate true function value at the minimum of the quadratic.
C
682    neval = neval + 1
      call functn(pmin, hstar)

C
C      If HSTAR < FUNC, replace search minimum with quadratic minimum.
C
      if (hstar .ge. func) go to 690
      func = hstar
      do 684 i = 1, nop
684    p(i) = pmin(i)
      write(lout, 1140) func
1140    format(' True func. value at minimum of quadratic = ', g14.6/)

C
C      Q*BMAT*Q'/2 IS CALCULATED & ITS LOWER TRIANGLE STORED IN VC
C
690 DO 760 I=1,NOP
      DO 730 J=1,NAP
        H(J)=ZERO
        DO 720 K=1,NAP
          IF(K.GT.J) GO TO 700
          L=J*(J-1)/2+K
          GO TO 710
700     L=K*(K-1)/2+J
```

```
710      H(J)=H(J)+BMAT(L)*G(K,I)*HALF
720      CONTINUE
730      CONTINUE
          DO 750 J=I,NOP
              L=J*(J-1)/2+I
              VC(L)=ZERO
              DO 740 K=1,NAP
740          VC(L)=VC(L)+H(K)*G(K,J)
750      CONTINUE
760 CONTINUE

C
C      THE DIAGONAL ELEMENTS OF VC ARE COPIED INTO VAR.
C
          J=0
          DO 770 I=1,NOP
              J=J+I
              VAR(I)=VC(J)
770      CONTINUE
          IF(IPRINT.LT.0) RETURN
          WRITE(LOUT,1160) IRANK
1160  FORMAT(' RANK OF INFORMATION MATRIX =',I3/
1      ' GENERALIZED INVERSE OF INFORMATION MATRIX:-')
          IJK=1
          GO TO 880
790 CONTINUE
          WRITE(LOUT,1170)
1170  FORMAT('/' IF THE FUNCTION MINIMIZED WAS -LOG(LIKELIHOOD),'/
1      ' THIS IS THE COVARIANCE MATRIX OF THE PARAMETERS'/
2      ' IF THE FUNCTION WAS A SUM OF SQUARES OF RESIDUALS'/
3      ' THIS MATRIX MUST BE MULTIPLIED BY TWICE THE ESTIMATED',
4      ' 1X RESIDUAL VARIANCE'/' TO OBTAIN THE COVARIANCE MATRIX.'/)
          CALL SYMINV(VC,NAP,BMAT,TEMP,NULLTY,IFAUULT,RMAX)

C
C      BMAT NOW CONTAINS THE INFORMATION MATRIX
C
          WRITE(LOUT,1190)
1190  FORMAT(' INFORMATION MATRIX:-'/)
          IJK=3
          GO TO 880

c
c      Calculate correlations of parameter estimates, put into VC.
c
800  IJK=2
          II=0
          IJ=0
          DO 840 I=1,NOP
              II=II+I
              IF(VC(II).GT.ZERO) THEN
                  VC(II)=ONE/SQRT(VC(II))
              ELSE
                  VC(II)=ZERO
              END IF
              JJ=0
              DO 830 J=1,I-1
                  JJ=JJ+J
                  IJ=IJ+1
                  VC(IJ)=VC(IJ)*VC(II)*VC(JJ)
830      CONTINUE
                  IJ=IJ+1
840 CONTINUE
          WRITE(LOUT,1200)
```

```

1200 FORMAT(/' CORRELATION MATRIX:-')
      II=0
      DO 850 I=1,NOP
          II=II+I
          IF(VC(II).NE.ZERO) VC(II)=ONE
850 CONTINUE
      GO TO 880
860 WRITE(LOUT,1210) NEVAL
1210 FORMAT(/' A FURTHER',I4,' FUNCTION EVALUATIONS HAVE BEEN USED'//)
      RETURN

```

c  
c Pseudo-subroutine to print VC if IJK = 1 or 2, or  
c BMAT if IJK = 3.

```

c
880 L=1
890 IF(L.GT.NOP) GO TO (790,860,800),IJK
      II=L*(L-1)/2
      DO 910 I=L,NOP
          I1=II+L
          II=II+I
          I2=MIN(II,I1+5)
          IF(IJK.EQ.3) GO TO 900
          WRITE(LOUT,1230)(VC(J),J=I1,I2)
          GO TO 910
900 WRITE(LOUT,1230)(BMAT(J),J=I1,I2)
910 CONTINUE
1230 FORMAT(1X,6G13.5)
      WRITE(LOUT,1240)
1240 FORMAT(/)
      L=L+6
      GO TO 890
      END

```

SUBROUTINE SYMINV(A,N,C,W,NULLTY,IFAUULT,RMAX)

C  
C ALGORITHM AS7, APPLIED STATISTICS, VOL.17, 1968.

C  
C ARGUMENTS:-

- C A() = INPUT, THE SYMMETRIC MATRIX TO BE INVERTED, STORED IN
- C LOWER TRIANGULAR FORM
- C N = INPUT, ORDER OF THE MATRIX
- C C() = OUTPUT, THE INVERSE OF A (A GENERALIZED INVERSE IF C IS
- C SINGULAR), ALSO STORED IN LOWER TRIANGULAR.
- C C AND A MAY OCCUPY THE SAME LOCATIONS.
- C W() = WORKSPACE, DIMENSION AT LEAST N.
- C NULLTY = OUTPUT, THE RANK DEFICIENCY OF A.
- C IFAUULT = OUTPUT, ERROR INDICATOR
- C = 1 IF N < 1
- C = 2 IF A IS NOT +VE SEMI-DEFINITE
- C = 0 OTHERWISE
- C RMAX = OUTPUT, APPROXIMATE BOUND ON THE ACCURACY OF THE DIAGONAL
- C ELEMENTS OF C. E.G. IF RMAX = 1.E-04 THEN THE DIAGONAL
- C ELEMENTS OF C WILL BE ACCURATE TO ABOUT 4 DEC. DIGITS.

C LATEST REVISION - 18 October 1985

C  
C\*\*\*\*\*  
C

```
        implicit double precision (a-h, o-z)
        DIMENSION A(*),C(*),W(N)
        DATA ZERO/0.D0/, ONE/1.D0/
C
        NROW=N
        IFAULT=1
        IF(NROW.LE.0) GO TO 100
        IFAULT=0
C
C        CHOLESKY FACTORIZATION OF A, RESULT IN C
C
        CALL CHOLA(A,NROW,C, NULLTY, IFAULT, RMAX, W)
        IF(IFAULT.NE.0) GO TO 100
C
C        INVERT C & FORM THE PRODUCT (CINV)'*CINV, WHERE CINV IS THE INVERSE
C        OF C, ROW BY ROW STARTING WITH THE LAST ROW.
C        IROW = THE ROW NUMBER, NDIAG = LOCATION OF LAST ELEMENT IN THE ROW.
C
        NN=NROW*(NROW+1)/2
        IROW=NROW
        NDIAG=NN
10    IF(C(NDIAG).EQ.ZERO) GO TO 60
        L=NDIAG
        DO 20 I=IROW,NROW
            W(I)=C(L)
            L=L+I
20    CONTINUE
        ICOL=NROW
        JCOL=NN
        MDIAG=NN
30    L=JCOL
        X=ZERO
        IF(ICOL.EQ.IROW) X=ONE/W(IROW)
        K=NROW
40    IF(K.EQ.IROW) GO TO 50
        X=X-W(K)*C(L)
        K=K-1
        L=L-1
        IF(L.GT.MDIAG) L=L-K+1
        GO TO 40
50    C(L)=X/W(IROW)
        IF(ICOL.EQ.IROW) GO TO 80
        MDIAG=MDIAG-ICOL
        ICOL=ICOL-1
        JCOL=JCOL-1
        GO TO 30
c
c        Special case, zero diagonal element.
c
60    L=NDIAG
        DO 70 J=IROW,NROW
            C(L)=ZERO
            L=L+J
70    CONTINUE
c
c        End of row.
c
80    NDIAG=NDIAG-IROW
        IROW=IROW-1
        IF(IROW.NE.0) GO TO 10
100    RETURN
```

END

SUBROUTINE CHOLA(A, N, U, NULLTY, IFAULT, RMAX, R)

```

C
C   ALGORITHM AS6, APPLIED STATISTICS, VOL.17, 1968, WITH
C   MODIFICATIONS BY A.J.MILLER
C
C   ARGUMENTS:-
C   A()      = INPUT, A +VE DEFINITE MATRIX STORED IN LOWER-TRIANGULAR
C             FORM.
C   N        = INPUT, THE ORDER OF A
C   U()      = OUTPUT, A LOWER TRIANGULAR MATRIX SUCH THAT U*U' = A.
C             A & U MAY OCCUPY THE SAME LOCATIONS.
C   NULLTY   = OUTPUT, THE RANK DEFICIENCY OF A.
C   IFAULT   = OUTPUT, ERROR INDICATOR
C             = 1 IF N < 1
C             = 2 IF A IS NOT +VE SEMI-DEFINITE
C             = 0 OTHERWISE
C   RMAX     = OUTPUT, AN ESTIMATE OF THE RELATIVE ACCURACY OF THE
C             DIAGONAL ELEMENTS OF U.
C   R()      = OUTPUT, ARRAY CONTAINING BOUNDS ON THE RELATIVE ACCURACY
C             OF EACH DIAGONAL ELEMENT OF U.

```

LATEST REVISION - 18 October 1985

C\*\*\*\*\*

```

C   implicit double precision (a-h, o-z)
C   DIMENSION A(*),U(*),R(N)

```

```

C   ETA SHOULD BE SET EQUAL TO THE SMALLEST +VE VALUE SUCH THAT
C   1.0 + ETA IS CALCULATED AS BEING GREATER THAN 1.0 IN THE ACCURACY
C   BEING USED.

```

```

C   DATA ETA/1.D-16/, ZERO/0.D0/, FIVE/5.D0/

```

```

C   IFAULT=1
C   IF(N.LE.0) GO TO 100
C   IFAULT=2
C   NULLTY=0
C   RMAX=ETA
C   R(1)=ETA
C   J=1
C   K=0

```

```

C   FACTORIZE COLUMN BY COLUMN, ICOL = COLUMN NO.

```

```

C   DO 80 ICOL=1,N
C     L=0

```

```

C   IROW = ROW NUMBER WITHIN COLUMN ICOL

```

```

C     DO 40 IROW=1,ICOL
C       K=K+1
C       W=A(K)
C       IF(IROW.EQ.ICOL) RSQ=(W*ETA)**2
C       M=J

```

```
        DO 10 I=1,IROW
          L=L+1
          IF(I.EQ.IROW) GO TO 20
          W=W-U(L)*U(M)
          IF(IROW.EQ.ICOL) RSQ=RSQ+(U(L)**2*R(I))**2
          M=M+1
10      CONTINUE
20      IF(IROW.EQ.ICOL) GO TO 50
          IF(U(L).EQ.ZERO) GO TO 30
          U(K)=W/U(L)
          GO TO 40
30      U(K)=ZERO
          IF(ABS(W).GT.ABS(RMAX*A(K))) GO TO 100
40      CONTINUE
C
C      END OF ROW, ESTIMATE RELATIVE ACCURACY OF DIAGONAL ELEMENT.
C
50      RSQ=SQRT(RSQ)
          IF(ABS(W).LE.FIVE*RSQ) GO TO 60
          IF(W.LT.ZERO) GO TO 100
          U(K)=SQRT(W)
          R(I)=RSQ/W
          IF(R(I).GT.RMAX) RMAX=R(I)
          GO TO 70
60      U(K)=ZERO
          NULLTY=NULLTY+1
70      J=J+ICOL
80      CONTINUE
          IFAULT=0
C
100     RETURN
        END
```



```
CSTART OF AS 51
  SUBROUTINE LOGLIN(NVAR, DIM, NCON, CONFIG, NTAB, TABLE, FIT,
$   LOCMAR, NMAR, MARG, NU, U, MAXDEV, MAXIT, DEV, NLAST, IFAULT)
C
C   ALGORITHM AS 51  APPL. STATIST. (1972) VOL.21, P.218
C
C   PERFORMS AN ITERATIVE PROPORTIONAL FIT OF THE MARGINAL
C   TOTALS OF A CONTINGENCY TABLE.
C
C   THIS VERSION PERMITS UP TO SEVEN VARIABLES. IF THIS LIMIT
C   IS TOO SMALL, CHANGE THE VALUE OF MAXVAR, AND OF THE
C   DIMENSION IN THE DECLARATION OF CHECK AND ICON - SEE
C   ALSO THE CHANGES NEEDED IN AS 51.1 AND AS 51.2
C
  REAL MARG(NMAR), U(NU), TABLE(NTAB), FIT(NTAB), MAXDEV,
$   DEV(MAXIT), ZERO, X, Y, XMAX
  INTEGER DIM(NVAR), CONFIG(NVAR, NCON), LOCMAR(NCON),
$   POINT, SIZE, ICON(7)
  LOGICAL CHECK(7)
C
  DATA MAXVAR, ZERO /7, 0.0/
C
  IFAULT = 0
  NLAST = 0
C
  CHECK VALIDITY OF NVAR, THE NUMBER OF VARIABLES,
  AND OF MAXIT, THE MAXIMUM NUMBER OF ITERATIONS
C
  IF (NVAR .GT. 0 .AND. NVAR .LE. MAXVAR .AND. MAXIT .GT. 0) GOTO 10
5  IFAULT = 4
  RETURN
C
  LOOK AT TABLE AND FIT CONSTANTS
C
10  SIZE = 1
  DO 30 J = 1, NVAR
  IF (DIM(J) .LE. 0) GOTO 5
  SIZE = SIZE * DIM(J)
30  CONTINUE
  IF (SIZE .LE. NTAB) GOTO 40
35  IFAULT = 2
  RETURN
40  X = ZERO
  Y = ZERO
  DO 60 I = 1, SIZE
  IF (TABLE(I) .LT. ZERO .OR. FIT(I) .LT. ZERO) GOTO 5
  X = X + TABLE(I)
  Y = Y + FIT(I)
60  CONTINUE
C
  MAKE A PRELIMINARY ADJUSTMENT TO OBTAIN THE FIT
  TO AN EMPTY CONFIGURATION LIST
C
  IF (Y .EQ. ZERO) GOTO 5
  X = X / Y
  DO 80 I = 1, SIZE
80  FIT(I) = X * FIT(I)
  IF (NCON .LE. 0 .OR. CONFIG(1, 1) .EQ. 0) RETURN
C
  ALLOCATE MARGINAL TABLES
C
```

```
POINT = 1
DO 150 I = 1, NCON
C
C      A ZERO BEGINNING A CONFIGURATION INDICATES
C      THAT THE LIST IS COMPLETED
C
      IF (CONFIG(1, I) .EQ. 0) GOTO 160
C
C      GET MARGINAL TABLE SIZE. WHILE DOING THIS
C      TASK, SEE IF THE CONFIGURATION LIST CONTAINS
C      DUPLICATIONS OR ELEMENTS OUT OF RANGE.
C
      SIZE = 1
      DO 90 J = 1, NVAR
90 CHECK(J) = .FALSE.
      DO 120 J = 1, NVAR
      K = CONFIG(J, I)
C
C      A ZERO INDICATES THE END OF THE STRING
C
      IF (K .EQ. 0) GOTO 130
C
C      SEE IF ELEMENT VALID
C
      IF (K .GE. 0 .AND. K .LE. NVAR) GOTO 100
95 IFAULT = 1
      RETURN
C
C      CHECK FOR DUPLICATION
C
100 IF (CHECK(K)) GOTO 95
      CHECK(K) = .TRUE.
C
C      GET SIZE
C
      SIZE = SIZE * DIM(K)
120 CONTINUE
C
C      SINCE U IS USED TO STORE FITTED MARGINALS,
C      SIZE MUST NOT EXCEED NU
C
130 IF (SIZE .GT. NU) GOTO 35
C
C      LOCMAR POINTS TO MARGINAL TABLES TO BE PLACED IN MARG
C
      LOCMAR(I) = POINT
      POINT = POINT + SIZE
150 CONTINUE
C
C      GET N, NUMBER OF VALID CONFIGURATIONS
C
      I = NCON + 1
160 N = I - 1
C
C      SEE IF MARG CAN HOLD ALL MARGINAL TABLES
C
      IF (POINT .GT. NMAR + 1) GOTO 35
C
C      OBTAIN MARGINAL TABLES
C
      DO 190 I = 1, N
```

```
      DO 180 J = 1, NVAR
180  ICON(J) = CONFIG(J, I)
      CALL COLLAP(NVAR, TABLE, MARG, LOCMAR(I), NTAB, NMAR, DIM, ICON)
190  CONTINUE
C
C      PERFORM ITERATIONS
C
      DO 220 K = 1, MAXIT
C
C      XMAX IS MAXIMUM DEVIATION OBSERVED BETWEEN
C      FITTED AND TRUE MARGINAL DURING A CYCLE
C
      XMAX = ZERO
      DO 210 I = 1, N
      DO 200 J = 1, NVAR
200  ICON(J) = CONFIG(J, I)
      CALL COLLAP(NVAR, FIT, U, 1, NTAB, NU, DIM, ICON)
      CALL ADJUST(NVAR, FIT, U, MARG, LOCMAR(I), NTAB, NU, NMAR,
      $ DIM, ICON, XMAX)
210  CONTINUE
C
C      TEST CONVERGENCE
C
      DEV(K) = XMAX
      IF (XMAX .LT. MAXDEV) GOTO 240
220  CONTINUE
      IF (MAXIT .GT. 1) GOTO 230
      NLAST = 1
      RETURN
C
C      NO CONVERGENCE
C
230  IFAULT = 3
      NLAST = MAXIT
      RETURN
C
C      NORMAL TERMINATION
C
240  NLAST = K
      RETURN
      END
C
      SUBROUTINE COLLAP(NVAR, X, Y, LOCY, NX, NY, DIM, CONFIG)
C
C      ALGORITHM AS 51.1 APPL. STATIST. (1972) VOL.21, P.218
C
C      COMPUTES A MARGINAL TABLE FROM A COMPLETE TABLE.
C      ALL PARAMETERS ARE ASSUMED VALID WITHOUT TEST.
C
C      IF THE VALUE OF NVAR IS TO BE GREATER THAN 7, THE
C      DIMENSIONS IN THE DECLARATIONS OF SIZE AND COORD MUST
C      BE INCREASED TO NVAR+1 AND NVAR RESPECTIVELY.
C
      INTEGER SIZE(8), DIM(NVAR), CONFIG(NVAR), COORD(7)
C
C      THE LARGER TABLE IS X AND THE SMALLER ONE IS Y
C
      REAL X(NX), Y(NY), ZERO
      DATA ZERO /0.0/
C
C      INITIALISE ARRAYS
```

```
C
    SIZE(1) = 1
    DO 10 K = 1, NVAR
    L = CONFIG(K)
    IF (L .EQ. 0) GOTO 20
    SIZE(K + 1) = SIZE(K) * DIM(L)
10 CONTINUE

C
    FIND NUMBER OF VARIABLES IN CONFIGURATION
C
C
    K = NVAR + 1
20 N = K - 1

C
    INITIALISE Y. FIRST CELL OF MARGINAL TABLE IS
    AT Y(LOCY) AND TABLE HAS SIZE(K) ELEMENTS
C
C
    LOCU = LOCY + SIZE(K) - 1
    DO 30 J = LOCY, LOCU
30 Y(J) = ZERO

C
    INITIALISE COORDINATES
C
C
    DO 50 K = 1, NVAR
50 COORD(K) = 0

C
    FIND LOCATIONS IN TABLES
C
C
    I = 1
60 J = LOCY
    DO 70 K = 1, N
    L = CONFIG(K)
    J = J + COORD(L) * SIZE(K)
70 CONTINUE
    Y(J) = Y(J) + X(I)

C
    UPDATE COORDINATES
C
C
    I = I + 1
    DO 80 K = 1, NVAR
    COORD(K) = COORD(K) + 1
    IF (COORD(K) .LT. DIM(K)) GOTO 60
    COORD(K) = 0
80 CONTINUE
    RETURN
    END

C
    SUBROUTINE ADJUST(NVAR, X, Y, Z, LOCZ, NX, NY, NZ, DIM, CONFIG, D)
C
C
    ALGORITHM AS 51.2 APPL. STATIST. (1972) VOL.21, P.218
C
C
    MAKES PROPORTIONAL ADJUSTMENT CORRESPONDING TO CONFIG.
    ALL PARAMETERS ARE ASSUMED VALID WITHOUT TEST.
C
C
    IF THE VALUE OF NVAR IS TO BE GREATER THAN 7, THE
    DIMENSIONS IN THE DECLARATIONS OF SIZE AND COORD MUST
    BE INCREASED TO NVAR+1 AND NVAR RESPECTIVELY.
C
C
    INTEGER SIZE(8), DIM(NVAR), CONFIG(NVAR), COORD(7)
    REAL X(NX), Y(NY), Z(NZ), D, E, ZERO, ZABS
C
    DATA ZERO /0.0/
```

```
C
      ZABS(E) = ABS(E)
C
      SET SIZE ARRAY
C
      SIZE(1) = 1
      DO 10 K = 1, NVAR
      L = CONFIG(K)
      IF (L .EQ. 0) GOTO 20
      SIZE(K + 1) = SIZE(K) * DIM(L)
10 CONTINUE
C
      FIND NUMBER OF VARIABLES IN CONFIGURATION
C
      K = NVAR + 1
20 N = K - 1
C
      TEST SIZE OF DEVIATION
C
      L = SIZE(K)
      J = 1
      K = LOCZ
      DO 30 I = 1, L
      E = ZABS(Z(K) - Y(J))
      IF (E .GT. D) D = E
      J = J + 1
      K = K + 1
30 CONTINUE
C
      INITIALIZE COORDINATES
C
      DO 40 K = 1, NVAR
40 COORD(K) = 0
      I = 1
C
      PERFORM ADJUSTMENT
C
50 J = 0
      DO 60 K = 1, N
      L = CONFIG(K)
      J = J + COORD(L) * SIZE(K)
60 CONTINUE
      K = J + LOCZ
      J = J + 1
C
      NOTE THAT Y(J) SHOULD BE NON-NEGATIVE
C
      IF (Y(J) .LE. ZERO) X(I) = ZERO
      IF (Y(J) .GT. ZERO) X(I) = X(I) * Z(K) / Y(J)
C
      UPDATE COORDINATES
C
      I = I + 1
      DO 70 K = 1, NVAR
      COORD(K) = COORD(K) + 1
      IF (COORD(K) .LT. DIM(K)) GOTO 50
      COORD(K) = 0
70 CONTINUE
      RETURN
      END
CEND OF AS 51
```

```
CSTART OF AS 52
      SUBROUTINE MOMNTS(X, K, N, S1, S2, S3, S4, IFAULT)
C
C      ALGORITHM AS 52  APPL. STATIST. (1972) VOL.21, P.226
C
C      ADDS A NEW VALUE, X, WHEN CALCULATING A MEAN, AND SUMS
C      OF POWERS OF DEVIATIONS. N IS THE CURRENT NUMBER OF
C      OBSERVATIONS, AND MUST BE SET TO ZERO BEFORE FIRST ENTRY
C
      REAL X, S1, S2, S3, S4, AN, AN1, DX, DX2, ZERO, ONE, TWO,
$      THREE, FOUR, SIX
      DATA ZERO, ONE, TWO, THREE, FOUR, SIX
$      /0.0, 1.0, 2.0, 3.0, 4.0, 6.0/
C
      IF (K .GT. 0 .AND. K .LT. 5 .AND. N .GE. 0) GOTO 10
      IFAULT = 1
      RETURN
10  IFAULT = 0
      N = N + 1
      IF (N .GT. 1) GOTO 20
C
      FIRST ENTRY, SO INITIALISE
C
      S1 = X
      S2 = ZERO
      S3 = ZERO
      S4 = ZERO
      RETURN
C
      SUBSEQUENT ENTRY, SO UPDATE
C
20  AN = N
      AN1 = AN - ONE
      DX = (X - S1) / AN
      DX2 = DX * DX
      GOTO (60, 50, 40, 30), K
30  S4 = S4 - DX * (FOUR * S3 - DX * (SIX * S2 + AN1 *
$      (ONE + AN1 ** 3) * DX2))
40  S3 = S3 - DX * (THREE * S2 - AN * AN1 * (AN - TWO) * DX2)
50  S2 = S2 + AN * AN1 * DX2
60  S1 = S1 + DX
      RETURN
      END
CEND OF AS 52
```

```

SUBROUTINE WSHRT(D, N, NP, NNP, SB, SA)
C
C ALGORITHM AS 53 APPL. STATIST. (1972) VOL.21, NO.3
C
C Wishart variate generator. On output, SA is an upper-triangular
C matrix of size NP * NP (written in linear form, column ordered)
C whose elements have a Wishart(N, SIGMA) distribution.
C
C D is an upper-triangular array such that SIGMA = D'D (see AS 6)
C
C Auxiliary function required: a random no. generator called RAND.
C The Wichmann & Hill generator is included here. It should be
C initialized in the calling program.
C
C INTEGER N, NP, NNP
C REAL D(NNP), SB(NNP), SA(NNP)
C
C Local variables
C
C INTEGER K, NS, I, J, NR, IP, NQ, II
C REAL DF, U1, U2, RN, C
C REAL ZERO, ONE, TWO, NINE
C DATA ZERO /0.0/, ONE /1.0/, TWO /2.0/, NINE /9.0/
C
C K = 1
1 CALL RNORM(U1, U2)
C
C Load SB with independent normal (0, 1) variates
C
C SB(K) = U1
C K = K + 1
C IF (K .GT. NNP) GO TO 2
C SB(K) = U2
C K = K + 1
C IF (K .LE. NNP) GO TO 1
2 NS = 0
C
C Load diagonal elements with square root of chi-square variates
C
C DO 3 I = 1, NP
C   DF = N - I + 1
C   NS = NS + I
C   U1 = TWO / (NINE * DF)
C   U2 = ONE - U1
C   U1 = SQRT(U1)
C
C Wilson-Hilferty formula for approximating chi-square variates
C
C SB(NS) = SQRT(DF * (U2 + SB(NS) * U1)**3)
3 CONTINUE
C
C RN = N
C NR = 1
C DO 5 I = 1, NP
C   NR = NR + I - 1
C   DO 5 J = I, NP
C     IP = NR
C     NQ = (J*J - J) / 2 + I - 1
C     C = ZERO
C     DO 4 K = I, J
C       IP = IP + K - 1

```

```

      NQ = NQ + 1
      C = C + SB(IP) * D(NQ)
4     CONTINUE
      SA(IP) = C
5     CONTINUE
C
      DO 7 I = 1, NP
        II = NP - I + 1
        NQ = NNP - NP
        DO 7 J = 1, I
          IP = (II*II - II) / 2
          C = ZERO
          DO 6 K = I, NP
            IP = IP + 1
            NQ = NQ + 1
            C = C + SA(IP) * SA(NQ)
6         CONTINUE
          SA(NQ) = C / RN
          NQ = NQ - 2 * NP + I + J - 1
7     CONTINUE
C
      RETURN
      END
C
C
      SUBROUTINE RNORM(U1, U2)
C
C     ALGORITHM AS 53.1  APPL. STATIST. (1972) VOL.21, NO.3
C
C     Sets U1 and U2 to two independent standardized random normal
C     deviates.  This is a Fortran version of the method given in
C     Knuth(1969).
C
C     Function RAND must give a result randomly and rectangularly
C     distributed between the limits 0 and 1 exclusive.
C
      REAL U1, U2
      REAL RAND
C
C     Local variables
C
      REAL X, Y, S, ONE, TWO
      DATA ONE /1.0/, TWO /2.0/
C
1     X = RAND()
      Y = RAND()
      X = TWO * X - ONE
      Y = TWO * Y - ONE
      S = X * X + Y * Y
      IF (S .GT. ONE) GO TO 1
      S = SQRT(- TWO * LOG(S) / S)
      U1 = X * S
      U2 = Y * S
      RETURN
      END
```



```
CSTART OF AS 57
  SUBROUTINE TABWRT(TITLE, NT1, NT2, TABLE, NTAB, DIM, NVAR,
$ LOC, COL, DEC, VARNAM, WORDS, CATNAM, MAXCAT, COLLAB,
$ VERT, RESTOR, LINE, SKIP, PAGE, WIDTH, UNIT, IFAULT)
C
C   ALGORITHM AS 57  APPL. STATIST. (1973) VOL.22, P.118
C
C   TABWRT PRINTS MULTIDIMENSIONAL TABLES.
C
C   A TABLE CAN HAVE AT MOST MAXVAR VARIABLES. NOTE THAT
C   SIZE HAS DIMENSION MAXVAR+1 AND COORD HAS DIMENSION MAXVAR
C
C   LOGICAL RESTOR
C   INTEGER DIM(NVAR), COL, LOC(COL), DEC(COL), WORDS, VERT
C   INTEGER SKIP, PAGE, WIDTH, UNIT
C   INTEGER SIZE(8), COORD(7), HOR, DOWN, SPACE, ONEPAG
C
C   ARRAYS CONTAINING DATA AND LABELS
C
C   REAL TITLE(NT1, NT2), TABLE(NTAB), VARNAM(WORDS, NVAR),
$ CATNAM(WORDS, MAXCAT, NVAR), COLLAB(WORDS, COL)
C   REAL OUT(33), CHAR(3)
C   REAL TAB1, TAB2, XLAB1, XLAB2, XLAB3
C
C   VARIABLE FORMATS.
C
C   REAL FMT(15), FMTT(7)
C   DATA FMTT(1),FMTT(2),FMTT(3),FMTT(4),FMTT(5),FMTT(6),FMTT(7)
$   /4H(A1, ,1H      ,2HX,   ,1H      ,1HA   ,1H      ,1H)   /
C
C   DATA FMT(1),FMT(2),FMT(3),FMT(4),FMT(5),FMT(6),FMT(7),FMT(8)
$   /4H(A1,,1H      ,2HX,   ,1H      ,4H(4X,,1H      ,1HA   ,1H      /
C
C   DATA FMT(9),FMT(10),FMT(11),FMT(12),FMT(13),FMT(14),FMT(15)
$   /2H), ,1H      ,1HF    ,1H      ,1H.    ,1H0    ,1H)   /
C
C   CARRIAGE CONTROL.
C
C   DATA CHAR(1), CHAR(2), CHAR(3) /1H , 1H0, 1H1/
C
C   ADJUSTABLE CONSTANTS - SEE INTRODUCTORY TEXT
C
C   DATA LENGTH, MAXVAR /4, 7/
C
C   SET ERROR INDICATOR AND GET SIZES.
C
C   IFAULT = 0
C   IF (NVAR .GT. MAXVAR) GOTO 98
C   SIZE(1) = 1
C   DO 1 I = 1, NVAR
C   COORD(I) = 1
C   IF (DIM(I) .LE. 0) GOTO 2
C   IF (DIM(I) .GT. MAXCAT) GOTO 98
C   SIZE(I + 1) = SIZE(I) * DIM(I)
1 CONTINUE
  I = NVAR + 1
2 N = I - 1
  DOWN = VERT
C
C   ALLOCATE VARIABLES TO HORIZONTAL AND VERTICAL SCALES.
```

```
      IF (DOWN .GT. N) DOWN = N
      IF (DOWN .LT. 1) DOWN = 1
      HOR = N - DOWN
C
C      LABELW IS WIDTH OF LABEL.
C
      LABELW = WORDS * LENGTH + 4
      I = HOR + 1
      K = I
      DO 3 J = 1, I
C
C      GET LINE WIDTH.
C
      LINEW = LABELW * (SIZE(K) + DOWN + 1)
      IF (LINEW .LT. WIDTH) GOTO 4
      K = K - 1
      DOWN = DOWN + 1
3 CONTINUE
C
C      NOTE THAT LINE IS NOT WIDE ENOUGH.
C
      IFAULT = 2
      RETURN
4 HOR = N - DOWN
C
C      SET FORMATS. CONVRT IS AN AUXILIARY
C      INTEGER TO ALPHANUMERIC ROUTINE.
C
      FMFT(2) = CONVRT((WIDTH - LENGTH * NT1) / 2 + 1)
      FMFT(4) = CONVRT(NT1)
      FMFT(6) = CONVRT(LENGTH)
      FMT(8) = FMFT(6)
      I = (WIDTH - LINEW) / 2 + 1
      TAB1 = CONVRT(I)
      TAB2 = CONVRT(I + LABELW * DOWN)
      XLAB1 = CONVRT(DOWN + 1)
      XLAB2 = CONVRT(1)
      FMT(6) = CONVRT(WORDS)
      FMT(12) = CONVRT(LABELW)
C
C      NOW ASCERTAIN VERTICAL SPACE REQUIREMENTS.
C
      SPACE = (COL + 1) * SIZE(N + 1) / SIZE(HOR + 1)
      ONEPAG = SPACE + 2 + HOR + NT2 + NT2 + SKIP
      IF (RESTOR .OR. LINE + ONEPAG .GT. PAGE) LINE = 0
      ICAR = 2
C
C      SEE IF CARRIAGE RESTORE NEEDED
C
      IF (LINE .NE. 0) GOTO 5
      ICAR = 3
      GOTO 7
C
C      SKIP APPROPRIATE NUMBER OF LINES.
C
      5 DO 6 I = 1, SKIP
      6 WRITE (UNIT, 100)
100 FORMAT(1H )
      7 I = LINE + ONEPAG
      IF (I .LE. PAGE) LINE = I
C
```

```
C          SEE HOW MUCH FITS ON A PAGE.
C
      INDEX = N + 1
      K = PAGE - 2 - HOR - NT2 - NT2
      DO 8 I = 1, DOWN
      IF (SPACE .LE. K) GOTO 9
      INDEX = INDEX - 1
      SPACE = SPACE / DIM(INDEX)
8 CONTINUE

C
C          RETURN WITH IFAULT = 2 IF TOO LITTLE SPACE AVAILABLE.
C
      IFAULT = 2
      RETURN

C
C          NOTCH IS UNITS PER PAGE.
C
9 NOTCH = K / SPACE * SIZE(INDEX)
      INC = SIZE(HOR + 1)
      INC1 = INC - 1
      XLAB3 = CONVRT(INC + 1)
      FMT(10) = CONVRT(INC)
      NUM = (SIZE(N + 1) + NOTCH - 1) / NOTCH * NOTCH
      LL = HOR + 1

C
C          SET MARKER.
C
      MARK = 0
      INDEX = WORDS * DOWN

C
C          PRINT A PAGE.
C
      DO 18 I = NOTCH, NUM, NOTCH
      IC = ICAR

C
C          PRINT TITLE.
C
      DO 10 K = 1, NT2
      WRITE (UNIT, FMTT) CHAR(IC), (TITLE(J, K), J = 1, NT1)
      IC = 1
10 CONTINUE

C
C          SKIP TWO LINES.
C
      WRITE (UNIT, 101)
101 FORMAT(1H0)

C
C          PRINT HORIZONTAL LABELS.
C
      IF (HOR .EQ. 0) GOTO 12
      FMT(2) = TAB2
      FMT(4) = XLAB3
      DO 11 K = 1, HOR
      L = HOR - K + 1
      I1 = SIZE(L)
      I2 = SIZE(L + 1)
      I3 = DIM(L)
      WRITE (UNIT, FMT) CHAR(1), (VARNAM(I4, L), I4 = 1, WORDS),
      $ (((CATNAM(I4, I5, L), I4 = 1, WORDS), I6 = 1, I1),
      $ I5 = 1, I3), I7 = I2, INC, I2)
11 CONTINUE
```

```
C
C      VERTICAL LABELS.
C
12 J = 0
   FMT(2) = TAB1
   FMT(4) = XLAB1
   M = N + 1
   DO 13 K = LL, N
   M = M - 1
   DO 13 I1 = 1, WORDS
   J = J + 1
   OUT(J) = VARNAM(I1, M)
13 CONTINUE
   WRITE (UNIT, FMT) CHAR(1), (OUT(J), J = 1, INDEX)
C
C      NOW PRINT BODY OF TABLE.
C
   DO 18 I2 = INC, NOTCH, INC
   J = 0
   M = N + 1
   DO 14 K = LL, N
   M = M - 1
   I3 = COORD(M)
   DO 14 I1 = 1, WORDS
   J = J + 1
   OUT(J) = CATNAM(I1, I3, M)
14 CONTINUE
   I3 = LOC(1) + MARK
   I4 = I3 + INC1
   FMT(2) = TAB1
   FMT(4) = XLAB1
   FMT(14) = CONVRT(DEC(1))
   WRITE (UNIT, FMT) CHAR(2), (OUT(J), J = 1, INDEX),
$ (COLLAB(J, 1), J = 1, WORDS), (TABLE(I5), I5 = I3, I4)
   IF (COL .LE. 1) GOTO 16
   FMT(2) = TAB2
   FMT(4) = XLAB2
   DO 15 I6 = 2, COL
   I3 = LOC(I6) + MARK
   I4 = I3 + INC1
   FMT(14) = CONVRT(DEC(I6))
   WRITE (UNIT, FMT) CHAR(1), (COLLAB(I5, I6), I5 = 1, WORDS),
$ (TABLE(I5), I5 = I3, I4)
15 CONTINUE
16 MARK = MARK + INC
C
C      RESET COORDINATES.
C
   DO 17 I1 = LL, N
   COORD(I1) = COORD(I1) + 1
   IF (COORD(I1) .LE. DIM(I1)) GOTO 18
   COORD(I1) = 1
17 CONTINUE
   RETURN
18 CONTINUE
C
C      ERROR RETURN.
C
98 IFAULT = 1
   RETURN
   END
```

```
C
FUNCTION CONVRT(I)
C
C      ALGORITHM AS 57.1  APPL. STATIST. (1973) VOL.22, P.118
C
C      CONVERT FROM INTEGER TO ALPHANUMERIC.
C      THE NORMAL RANGE FOR CONVRT IS FROM 0 TO 101.
C      ALL INTEGERS TO BE CONVERTED WILL BE WITHIN THIS
C      RANGE IF WIDTH DOES NOT EXCEED 131, LENGTH IS AT
C      LEAST 4, AND MAXVAR DOES NOT EXCEED 7.
C
REAL C(102)
DATA  C(1), C(2), C(3), C(4), C(5) / 1H0, 1H1, 1H2, 1H3, 1H4/
DATA  C(6), C(7), C(8), C(9),C(10) / 1H5, 1H6, 1H7, 1H8, 1H9/
DATA  C(11),C(12),C(13),C(14),C(15) /2H10,2H11,2H12,2H13,2H14/
DATA  C(16),C(17),C(18),C(19),C(20) /2H15,2H16,2H17,2H18,2H19/
DATA  C(21),C(22),C(23),C(24),C(25) /2H20,2H21,2H22,2H23,2H24/
DATA  C(26),C(27),C(28),C(29),C(30) /2H25,2H26,2H27,2H28,2H29/
DATA  C(31),C(32),C(33),C(34),C(35) /2H30,2H31,2H32,2H33,2H34/
DATA  C(36),C(37),C(38),C(39),C(40) /2H35,2H36,2H37,2H38,2H39/
DATA  C(41),C(42),C(43),C(44),C(45) /2H40,2H41,2H42,2H43,2H44/
DATA  C(46),C(47),C(48),C(49),C(50) /2H45,2H46,2H47,2H48,2H49/
DATA  C(51),C(52),C(53),C(54),C(55) /2H50,2H51,2H52,2H53,2H54/
DATA  C(56),C(57),C(58),C(59),C(60) /2H55,2H56,2H57,2H58,2H59/
DATA  C(61),C(62),C(63),C(64),C(65) /2H60,2H61,2H62,2H63,2H64/
DATA  C(66),C(67),C(68),C(69),C(70) /2H65,2H66,2H67,2H68,2H69/
DATA  C(71),C(72),C(73),C(74),C(75) /2H70,2H71,2H72,2H73,2H74/
DATA  C(76),C(77),C(78),C(79),C(80) /2H75,2H76,2H77,2H78,2H79/
DATA  C(81),C(82),C(83),C(84),C(85) /2H80,2H81,2H82,2H83,2H84/
DATA  C(86),C(87),C(88),C(89),C(90) /2H85,2H86,2H87,2H88,2H89/
DATA  C(91),C(92),C(93),C(94),C(95) /2H90,2H91,2H92,2H93,2H94/
DATA  C(96),C(97),C(98),C(99),C(100) /2H95,2H96,2H97,2H98,2H99/
DATA  C(101),C(102)                /3H100,3H101/
J = I + 1
IF (J .LT. 1) J = 1
IF (J .GT. 102) J = 102
CONVRT = C(J)
RETURN
END
CEND OF AS 57
```

```
subroutine clustr (x,d,dev,b,f,e,i,j,n,nz,k)
implicit double precision (a-h,o-z)
c
c Algorithm AS 58 Appl. Statist. (1973) Vol.22, No.1
c
c Given a matrix of i observations on j variables, the
c observations are allocated to n clusters in such a way that the
c within-cluster sum of squares is minimised.
c
integer b(i),e(k)
dimension x(i,j),d(k,j),dev(k),f(i)
data zero/0.0d0/, one/1.0d0/, two/2.0d0/
data big/1.0d10/
c
do 10 ia=1,n
e(ia)=0
10 continue
c
c For each observation, calculate the distance from each cluster
c centre, and assign to the nearest
c
do 40 ic=1,i
f(ic)=zero
da=big
do 30 id=1,n
db=zero
do 20 ie=1,j
dc=x(ic,ie)-d(id,ie)
db=db+dc*dc
if (db.ge.da) go to 30
20 continue
da=db
b(ic)=id
30 continue
ig=b(ic)
e(ig)=e(ig)+1
40 continue
c
c Calculate the mean and sum of squares for each cluster
c
do 50 ix=1,n
dev(ix)=zero
do 50 iy=a1,j
d(ix,iy)=zero
50 continue
do 60 ic=1,i
ig=b(ic)
do 60 ih=1,j
d(ig,ih)=d(ig,ih)+x(ic,ih)
60 continue
do 80 ij=1,j
do 70 ii=1,n
d(ii,ij)=d(ii,ij)/dble(e(ii))
70 continue
do 80 ik=1,i
il=b(ik)
da=x(ik,ij)-d(il,ij)
db=da*da
f(ik)=f(ik)+db
dev(il)=dev(il)+db
80 continue
```

```
      do 85 ik=1,i
        il=b(ik)
        fl=e(il)
        if (fl.ge.two) f(ik)=f(ik)*fl/(fl-one)
85 continue
c
c   Examine each observation in turn to see if it should be
c   reassigned to a different cluster
c
      if (nz.le.0) nz=1
90 iw=0
      do 140 ik=1,i
        il=b(ik)
        ir=il
c
c   If the number of cluster points is less than or equal to the
c   specified minimum, nz, bypass this iteration
c
        if (e(il).le.nz) go to 140
        fl=e(il)
        dc=f(ik)
        do 100 in=1,n
          if (in.eq.il) goto 100
          fm=e(in)
          fm=fm/(fm+one)
          de=zero
          do 95 ip=1,j
            da=x(ik,ip)-d(in,ip)
            de=de + da *da * fm
            if (de.ge.dc) goto 100
95 continue
          dc=de
          ir=in
100 continue
          if (ir.eq.il) goto 140
c
c   Reassignment is made here if necessary
c
        fq=e(ir)
        dev(il)=dev(il)-f(ik)
        dev(ir)=dev(ir)+dc
        e(ir)=e(ir)+1
        e(il)=e(il)-1
        do 110 is=1,j
          d(il,is) = (d(il,is) * fl - x(ik,is)) / (fl-one)
          d(ir,is) = (d(ir,is) * fq + x(ik,is)) / (fq + one)
110 continue
        b(ik) = ir
        do 130 it=1,i
          ij = b(it)
          if (ij.ne.il. and. ij.ne.ir) goto 130
          f(it)=zero
          do 120 iu=1,j
            da = x(it,iu) - d(ij,iu)
            f(it)=f(it) + da * da
120 continue
          fl=e(ij)
          f(it) = f(it)*fl/(fl-one)
130 continue
          iw=iw+1
140 continue
```

```
c
c   Return to calling program if no reassignments were made during
c   this iteration
c
c   if (iw.eq.o) return
c   goto 90
c   end
```



```
      SUBROUTINE TDIAG (N,TOL,A,D,E,Z,MAXDIM,IFAUULT)
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
C
      DIMENSION A(MAXDIM,MAXDIM), D(MAXDIM), E(MAXDIM), Z(MAXDIM,MAXDIM)
      DATA ZERO/0.0/,ONE/1.0/
      DATA ETA/1.0D-37/,EPS/1.0D-14/
C
      Algorithm as 60.1 appl.statist. (1973) vol.22 no.2
C
      reduces real symmetric matrix to tridiagonal form
C
      tol is a machine dependent constant , tol = eta/eps , where
      eta is the smallest positive number representable in the
      computer and eps is the smallest positive number for which
      1+eps.ne.1.
C
      eta=eps*tol
      eps=0.7105427358e-14
      tol=0.3131513063e-293
      precis=1.0e-14
C
      nb
      real constants must be 1e 15 decimal digits
      the range of a real constant is from 1.0e-293 to 1.0e+322
C
      TOL=ETA/EPS
      IFAULT=1
      IF (N.LE.1) RETURN
      IFAULT=0
      DO 10 I=1,N
        DO 10 J=1,I
10      Z(I,J)=A(I,J)
      I=N
      DO 110 I1=2,N
        L=I-2
        F=Z(I,I-1)
        G=ZERO
        IF (L.LT.1) GO TO 30
        DO 20 K=1,L
20      G=G+Z(I,K)**2
30      H=G+F*F
C
      if g is too small for orthogonality to be guaranteed, the
      transformation is skipped
C
      IF (G.GT.TOL) GO TO 40
      E(I)=F
      D(I)=ZERO
      GO TO 100
40      L=L+1
      G=SQRT(H)
      IF (F.GE.ZERO) G=-G
      E(I)=G
      H=H-F*G
      Z(I,I-1)=F-G
      F=ZERO
      DO 80 J=1,L
        Z(J,I)=Z(I,J)/H
        G=ZERO
C
      form element of a * u
```

```
C
      DO 50 K=1,J
50      G=G+Z(J,K)*Z(I,K)
      IF (J.GE.L) GO TO 70
      J1=J+1
      DO 60 K=J1,L
60      G=G+Z(K,J)*Z(I,K)
C
C      form element of p
C
70      E(J)=G/H
      F=F+G*Z(J,I)
80      CONTINUE
C
C      form k
C
      HH=F/(H+H)
C
C      form reduced a
C
      DO 90 J=1,L
      F=Z(I,J)
      G=E(J)-HH*F
      E(J)=G
      DO 90 K=1,J
      Z(J,K)=Z(J,K)-F*E(K)-G*Z(I,K)
90      CONTINUE
      D(I)=H
100     I=I-1
110     CONTINUE
      D(1)=ZERO
      E(1)=ZERO
C
C      accumulation of transformation matrices
C
      DO 160 I=1,N
      L=I-1
      IF (D(I).EQ.ZERO.OR.L.EQ.0) GO TO 140
      DO 130 J=1,L
      G=ZERO
      DO 120 K=1,L
120     G=G+Z(I,K)*Z(K,J)
      DO 130 K=1,L
      Z(K,J)=Z(K,J)-G*Z(K,I)
130     CONTINUE
140     D(I)=Z(I,I)
      Z(I,I)=ONE
      IF (L.EQ.0) GO TO 160
      DO 150 J=1,L
      Z(I,J)=ZERO
      Z(J,I)=ZERO
150     CONTINUE
160     CONTINUE
      RETURN
      END
C
C      SUBROUTINE LRVT (N,PRECIS,D,E,Z,IFault,MAXDIM)
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
C
C      algorithm as 60.2 appl.statist. (1973) vol.22, no.2
```

```
C
C      finds latent roots and vectors of tridiagonal matrix
C
DIMENSION D(MAXDIM), E(MAXDIM), Z(MAXDIM,MAXDIM)
DATA MITS/30/,ZERO/0.0/,ONE/1.0/,TWO/2.0/
C
PRECIS=1.0D-14
IFault=2
IF (N.LE.1) RETURN
IFault=1
N1=N-1
DO 10 I=2,N
10   E(I-1)=E(I)
E(N)=ZERO
B=ZERO
F=ZERO
DO 100 L=1,N
  JJ=0
  H=PRECIS*(ABS(D(L))+ABS(E(L)))
  IF (B.LT.H) B=H
C
C      look for small sub-diagonal element
C
DO 20 M1=L,N
  M=M1
  IF (ABS(E(M)).LE.B) GO TO 30
20  CONTINUE
30  IF (M.EQ.L) GO TO 90
40  IF (JJ.EQ.MITS) RETURN
  JJ=JJ+1
C
C      form shift
C
P=(D(L+1)-D(L))/(TWO*E(L))
R=SQRT(P*P+ONE)
PR=P+R
IF (P.LT.ZERO) PR=P-R
H=D(L)-E(L)/PR
DO 50 I=L,N
50  D(I)=D(I)-H
  F=F+H
C
C      ql transformation
C
P=D(M)
C=ONE
S=ZERO
M1=M-1
I=M
DO 80 I1=L,M1
  J=I
  I=I-1
  G=C*E(I)
  H=C*P
  IF (ABS(P).GE.ABS(E(I))) GO TO 60
  C=P/E(I)
  R=SQRT(C*C+ONE)
  E(J)=S*E(I)*R
  S=ONE/R
  C=C/R
  GO TO 70
```

```
60      C=E(I)/P
      R=SQRT(C*C+ONE)
      E(J)=S*P*R
      S=C/R
      C=ONE/R
70      P=C*D(I)-S*G
      D(J)=H+S*(C*G+S*D(I))
C
C      form vector
C
      DO 80 K=1,N
      H=Z(K,J)
      Z(K,J)=S*Z(K,I)+C*H
      Z(K,I)=C*Z(K,I)-S*H
80      CONTINUE
      E(L)=S*P
      D(L)=C*P
      IF (ABS(E(L)).GT.B) GO TO 40
90      D(L)=D(L)+F
100     CONTINUE
C
C      order latent roots and vectors
C
      DO 130 I=1,N1
      K=I
      P=D(I)
      I1=I+1
      DO 110 J=I1,N
      IF (D(J).LE.P) GO TO 110
      K=J
      P=D(J)
110     CONTINUE
      IF (K.EQ.I) GO TO 130
      D(K)=D(I)
      D(I)=P
      DO 120 J=1,N
      P=Z(J,I)
      Z(J,I)=Z(J,K)
      Z(J,K)=P
120     CONTINUE
130     CONTINUE
      IFAULT=0
      RETURN
      END
```

c AS 62 generates the frequencies for the Mann-Whitney U-statistic.  
c Users are much more likely to need the distribution function.  
c Code to return the distribution function has been added at the end  
c of AS 62 by Alan Miller. Remove the C's in column 1 to activate it.

```
c
      SUBROUTINE UDIST(M, N, FRQNCY, LFR, WORK, LWRK, IFAULT)
c
c      ALGORITHM AS 62  APPL. STATIST. (1973) VOL.22, NO.2
c
c      The distribution of the Mann-Whitney U-statistic is generated for
c      the two given sample sizes
c
c      INTEGER M, N, LFR, LWRK, IFAULT
c      REAL FRQNCY(LFR), WORK(LWRK)
c
c      Local variables
c
c      INTEGER MINMN, MN1, MAXMN, N1, I, IN, L, K, J
c      REAL ZERO, ONE, SUM
c      DATA ZERO /0.0/, ONE /1.0/
c
c      Check smaller sample size
c
c      IFAULT = 1
c      MINMN = MIN(M, N)
c      IF (MINMN .LT. 1) RETURN
c
c      Check size of results array
c
c      IFAULT = 2
c      MN1 = M * N + 1
c      IF (LFR .LT. MN1) RETURN
c
c      Set up results for 1st cycle and return if MINMN = 1
c
c      MAXMN = MAX(M, N)
c      N1 = MAXMN + 1
c      DO 1 I = 1, N1
1  FRQNCY(I) = ONE
c      IF (MINMN .EQ. 1) GO TO 4
c
c      Check length of work array
c
c      IFAULT = 3
c      IF (LWRK .LT. (MN1 + 1) / 2 + MINMN) RETURN
c
c      Clear rest of FREQNCY
c
c      N1 = N1 + 1
c      DO 2 I = N1, MN1
2  FRQNCY(I) = ZERO
c
c      Generate successively higher order distributions
c
c      WORK(1) = ZERO
c      IN = MAXMN
c      DO 3 I = 2, MINMN
c        WORK(I) = ZERO
c        IN = IN + MAXMN
c        N1 = IN + 2
c        L = 1 + IN / 2
```

```
      K = I
C
C   Generate complete distribution from outside inwards
C
      DO 3 J = 1, L
        K = K + 1
        N1 = N1 - 1
        SUM = FRQNCY(J) + WORK(J)
        FRQNCY(J) = SUM
        WORK(K) = SUM - FRQNCY(N1)
        FRQNCY(N1) = SUM
3   CONTINUE
C
4   IFAULT = 0
C
C   Code to overwrite the frequency function with the distribution
C   function.  N.B. The frequency in FRQNCY(1) is for U = 0, and
C   that in FRQNCY(I) is for U = I - 1.
C
      SUM = ZERO
      DO 10 I = 1, MN1
        SUM = SUM + FRQNCY(I)
        FRQNCY(I) = SUM
10  CONTINUE
      DO 20 I = 1, MN1
20  FRQNCY(I) = FRQNCY(I) / SUM
C
      RETURN
      END
```

```
double precision function betain(x, p, q, beta, ifault)
implicit double precision (a-h, o-z)
c
c algorithm as 63 appl. statist. (1973), vol.22, no.3
c
c computes incomplete beta function ratio for arguments
c x between zero and one, p and q positive.
c log of complete beta function, beta, is assumed to be known
c
c logical indx
c
c define accuracy and initialise
c
c data zero/0.0d0/, one/1.0d0/, acu/0.1d-14/
betain=x
c
c test for admissibility of arguments
c
c ifault=1
c if(p.le.zero .or. q.le.zero) return
c ifault=2
c if(x.lt.zero .or. x.gt.one) return
c ifault=0
c if(x.eq.zero .or. x.eq. one) return
c
c change tail if necessary and determine s
c
c psq=p+q
c cx=one-x
c if(p.ge.psq*x) goto 1
c xx=cx
c cx=x
c pp=q
c qq=p
c indx=.true.
c goto 2
1 xx=x
  pp=p
  qq=q
  indx=.false.
2 term=one
  ai=one
  betain=one
  ns=qq+cx*psq
c
c user soper's reduction formulae.
c
c rx=xx/cx
3 temp=qq-ai
  if(ns.eq.0) rx=xx
4 term=term*temp*rx/(pp+ai)
  betain=betain+term
  temp=abs(term)
  if(temp.le.acu .and. temp.le.acu*betain) goto 5
  ai=ai+one
  ns=ns-1
  if(ns.ge.0) goto 3
  temp=psq
  psq=psq+one
  goto 4
c
```

```
c      calculate result
```

```
c      5 betain=betain*exp(pp*log(xx)+(qq-one)*log(cx)-beta)/pp  
      if(indx) betain=one-betain  
      return  
      end
```



```
CSTART OF AS 64/109
      REAL FUNCTION XINBTA(P, Q, BETA, ALPHA, IFAULT)
C
C      ALGORITHM AS 109  APPL. STATIST. (1977) VOL.26, P.111
C      (REPLACING ALGORITHM AS 64  APPL. STATIST. (1973),
C      VOL.22, P.411)
C
C      COMPUTES INVERSE OF INCOMPLETE BETA FUNCTION
C      RATIO FOR GIVEN POSITIVE VALUES OF THE ARGUMENTS
C      P AND Q, ALPHA BETWEEN ZERO AND ONE.
C      LOG OF COMPLETE BETA FUNCTION, BETA, IS ASSUMED TO BE
C      KNOWN.
C
      LOGICAL INDEX
      REAL A, ALPHA, ADJ, BETA, G, H, P, PP, PREV, Q, QQ, R, S,
$      SQ, T, TX, W, Y, YPREV, ZERO, HALF, ONE, TWO, THREE,
$      FOUR, FIVE, SIX, NINE, ACU, LOWER, UPPER, CONST1,
$      CONST2, CONST3, CONST4, BETAIN, ZEXP, ZLOG, ZSQRT
C
      DEFINE ACCURACY AND INITIALIZE
C
      DATA ZERO, HALF, ONE, TWO, THREE, FOUR, FIVE, SIX, NINE
$      /0.0, 0.5, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 9.0/
      DATA ACU, LOWER, UPPER, CONST1, CONST2, CONST3, CONST4
$      /1.0E-14, 0.0001, 0.9999, 2.30753, 0.27061, 0.99229, 0.04481/
C
      ZEXP(A) = EXP(A)
      ZLOG(A) = ALOG(A)
      ZSQRT(A) = SQRT(A)
C
      XINBTA = ALPHA
C
      TEST FOR ADMISSIBILITY OF PARAMETERS
C
      IFAULT = 1
      IF (P .LE. ZERO .OR. Q .LE. ZERO) RETURN
      IFAULT = 2
      IF (ALPHA .LT. ZERO .OR. ALPHA .GT. ONE) RETURN
      IFAULT = 0
      IF (ALPHA .EQ. ZERO .OR. ALPHA .EQ. ONE) RETURN
C
      CHANGE TAIL IF NECESSARY
C
      IF (ALPHA .LE. HALF) GOTO 1
      A = ONE - ALPHA
      PP = Q
      QQ = P
      INDEX = .TRUE.
      GOTO 2
1 A = ALPHA
  PP = P
  QQ = Q
  INDEX = .FALSE.
C
      CALCULATE THE INITIAL APPROXIMATION
C
2 R = ZSQRT(-ZLOG(A * A))
  Y = R - (CONST1 + CONST2 * R) / (ONE + (CONST3 + CONST4 *
$ R) * R)
  IF (PP .GT. ONE .AND. QQ .GT. ONE) GOTO 5
  R = QQ + QQ
```

```
T = ONE / (NINE * QQ)
T = R * (ONE - T + Y * ZSQRT(T)) ** 3
IF (T .LE. ZERO) GOTO 3
T = (FOUR * PP + R - TWO) / T
IF (T .LE. ONE) GOTO 4
XINBTA = ONE - TWO / (T + ONE)
GOTO 6
3 XINBTA = ONE - ZEXP((ZLOG((ONE - A) * QQ) + BETA) / QQ)
GOTO 6
4 XINBTA = ZEXP((ZLOG(A * PP) + BETA) / PP)
GOTO 6
5 R = (Y * Y - THREE) / SIX
S = ONE / (PP + PP - ONE)
T = ONE / (QQ + QQ - ONE)
H = TWO / (S + T)
W = Y * ZSQRT(H + R) / H - (T - S) * (R + FIVE / SIX -
$ TWO / (THREE * H))
XINBTA = PP / (PP + QQ * ZEXP(W + W))
C
C     SOLVE FOR X BY A MODIFIED NEWTON-RAPHSON METHOD,
C     USING THE FUNCTION BETAIN
C
6 R = ONE - PP
T = ONE - QQ
YPREV = ZERO
SQ = ONE
PREV = ONE
IF (XINBTA .LT. LOWER) XINBTA = LOWER
IF (XINBTA .GT. UPPER) XINBTA = UPPER
7 Y = BETAIN(XINBTA, PP, QQ, BETA, IFAULT)
IF (IFAULT .EQ. 0) GOTO 8
IFAULT = 3
RETURN
8 Y = (Y - A) * ZEXP(BETA + R * ZLOG(XINBTA) + T *
$ ZLOG(ONE - XINBTA))
IF (Y * YPREV .LE. ZERO) PREV = SQ
G = ONE
9 ADJ = G * Y
SQ = ADJ * ADJ
IF (SQ .GE. PREV) GOTO 10
TX = XINBTA - ADJ
IF (TX .GE. ZERO .AND. TX .LE. ONE) GOTO 11
10 G = G / THREE
GOTO 9
11 IF (PREV .LE. ACU) GOTO 12
IF (Y * Y .LE. ACU) GOTO 12
IF (TX .EQ. ZERO .OR. TX .EQ. ONE) GOTO 10
IF (TX .EQ. XINBTA) GOTO 12
XINBTA = TX
YPREV = Y
GOTO 7
12 IF (INDEX) XINBTA = ONE - XINBTA
RETURN
END
CEND OF AS 64/109
```

```

SUBROUTINE SFINT(ICODE, LCODE, KPOWER, IORDER, LIMIT,
*   MAXLBP, LISTBP, LENBP, IFAULT)
C
C   AS R82 (REMARK ON AS65) APPL.STATIST. (1990), VOL.39, NO.1
C
C   Expands a structure formula into a list of binary integers
C
INTEGER IFAULT, IORDER, KPOWER, LCODE, LENBP, LIMIT, MAXLBP
INTEGER ICODE(LCODE), LISTBP(MAXLBP)
INTEGER I, IBP, IBS, IJB, ILS, IORD, IORJ, IP, IPRONO, IREL, IRS,
1   J, JB, JBP, JC, JLFAC, JLSUM, JLSYM, JMFAC, JMSUM, JMSYM, JOP, JP,
2   JRFAC, JRSUM, JRSYM, JTFAC, JTSUM, JTSYM, K, LLSUM, M, NPOWER, NS
LOGICAL LCHECK, RCHECK
C
C   Set NBI so that 2**NBI-1 is a large legal positive integer
C
INTEGER NBI
PARAMETER (NBI=31)
C
C   Set codes for K-symbols and L according to number of symbols
C   (PNSYM) and number N of precedence classes (PNPREC), also
C   codes for symbols
C
INTEGER PDOT, PK0, PK2NP1, PK2NP2, PL, PLBRKT, PMINSL, PMINST, PMINUS,
1   PNPREC, PNSYM, PPLUS, PRBRKT, PSLASH, PSTAR, PSTAR2
PARAMETER (PSTAR2=1, PDOT=2, PSLASH=3, PSTAR=4, PPLUS=5, PMINUS=6,
1   PMINSL=7, PMINST=8, PLBRKT=9, PRBRKT=10, PNPREC=5, PNSYM=10,
2   PK0=PNSYM+1, PK2NP1=PK0+2*PNPREC+1, PK2NP2=PK2NP1+1, PL=PK2NP2+1)
C
C   Initialise compact precedence table and set auxiliary
C   quantities
C
INTEGER KILLEG, KOPEN, KCON, KCLOSE
PARAMETER (KILLEG=0, KOPEN=1, KCON=2, KCLOSE=3)
INTEGER IPRTAB(5,5), IENTRY(PNSYM+2*PNPREC+4),
1   IPREC(PNSYM+2*PNPREC+4)
C
DATA IPRTAB /2*0,-1,-1,1, -3,3,3*0, 2*0,3*1, -3,3,3*0, 2*3,3*0/
DATA IENTRY /8*4, 3, 2, 13*1, 5/
DATA IPREC /2, 4, 6, 8, 4*10, 12, 11,
1   0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13/
C
C   LITERAL =   ** . / * + - -/ -* ( ) FACTOR
C   SYMBOL   =   O2 O4 O6 O8 10 10 10 10 ( ) K0 K1 ... K12(=K2N+2) L
C   CODE     =   1 2 3 4 5 6 7 8 9 10 11 12 ... 23 24
C   IENTRY   =   4 4 4 4 4 4 4 4 3 2 1 1 ... 1 5
C   IPREC    =   2 4 6 8 10 10 10 10 12 11 0 1 ... 12 13
C
C-----INITIALISATION-----
C   IORD=highest order of retained terms
C   JC=pointer to next input symbol in icode
C   JB=pointer to top of sum stack LISTBP(1...)
C   JP=pointer to top of symbol stack LISTBP(...MAXLBP) (top.down)
C   containing 3-integer cells (symbol code,pointer to SUM,FAC)
C
IFAULT = 0
LENBP = 0
IORD = LIMIT
IF (IORD.LE.0) IORD = NBI
JC = 0
IF (LCODE) 1001, 999, 10

```

```

10 JB = 0
    JP = MAXLBP + 1
C
C----- SYNTAX ANALYSER -----
C----- Stack limit symbol L and/or next ICODE symbol
C         Stack -input code for factor
C
100 I = PL
    IF (JC.LT.1.OR.JC.GE.LCODE) GOTO 115
110 JC = JC + 1
    I = ICODE(JC)
    IF (I.EQ.0.OR.I.GT.PNSYM) GOTO 1004
115 JP = JP - 3
    IF (JB.GE.JP) GOTO 1002
    LISTBP(JP + 2) = -I
    LISTBP(JP + 1) = 0
    IF (I.LT.0) I = PK0
    LISTBP(JP) = I
    IF (JC.EQ.0) GOTO 110
C
C----- SEARCH FOR PRODUCTION
C         If closing relation between top two stacked symbols scan for
C         matching opening relation to delimit possible rightpart
C
120 IP = JP
    IBS = 0
130 IP = IP + 3
C
C         IREL=relation between leftsymbol at IP and rightsymbol at IP-3
C
    ILS = LISTBP(IP)
    IRS = LISTBP(IP - 3)
    IREL = IPRTAB(IENTRY(ILS), IENTRY(IRS))
    IF (IREL.GE.0) GOTO 140
    IREL = -IREL
    M = IPREC(ILS) - IPREC(IRS)
    IF (IREL.EQ.KOPEN) M = 1 - M
    IF (M.EQ.0) IREL = KCON
    IF (M.GT.0) IREL = KILLEG
C
C         Branch on IBS=0/1 for terminal/earlier relation
C
140 IF (IBS.EQ.1) GOTO 170
C
C         Terminal relation
C
    IF (IREL.EQ.KILLEG) GOTO 1005
    IBS = 1
    IF (IREL - KCLOSE) 100, 130, 100
C
C         Earlier relation
C
170 IF (IREL.NE.KOPEN) GOTO 130
C
C----- IDENTIFY PRODUCTION
C         Leftpart      rightpart      Semantic action      IPRONO
C         K1            K0              load                  1
C         K1            ( K2N+1 )      copy                  2
C         KI            KI OI KI-1 I=2,4,...,2N  dyadic operation 3
C         KI            KI-1          I=1,2,...,2N+1      last two productions
C         K2N+2      L K2N+1 L        are shortcircuited

```

C Identify production, if any, with rightpart matching the NS  
C stacked symbols between the opening and closing relations  
C Copy terminal + rightpart cells  
C

```
NS = (IP - JP - 3) / 3
IF (NS.NE.1.AND.NS.NE.3) GOTO 1005
JTSYM = LISTBP(JP)
JTSM = LISTBP(JP + 1)
JTFAC = LISTBP(JP + 2)
JRSYM = LISTBP(JP + 3)
JRSM = LISTBP(JP + 4)
JRFAC = LISTBP(JP + 5)
IPRONO = 4
IF (NS.EQ.3) GOTO 180
IF (JRSYM.EQ.PK0) IPRONO = 1
GOTO 190
```

```
180 JMSYM = LISTBP(JP + 6)
JMSUM = LISTBP(JP + 7)
JMFAC = LISTBP(JP + 8)
JLSYM = LISTBP(JP + 9)
JLSUM = LISTBP(JP + 10)
JLFAC = LISTBP(JP + 11)
IF (JMSYM.EQ.PK2NP1.AND.JLSYM.EQ.PLBRKT.AND.JRSYM.EQ.PRBRKT)
* IPRONO = 2
I = IPREC(JMSYM)
IF (IENTRY(JMSYM).EQ.4.AND.
* JLSYM.EQ.PK0 + I.AND.JRSYM.EQ.PK0 + I - 1) IPRONO = 3
```

C  
C Branch to semantics section  
C

```
190 GOTO (500, 600, 700, 1005), IPRONO
```

C  
C----- UPDATE STACK  
C Set JRSYM=K-symbol in leftpart. anticipate and shortcircuit  
C chain of 1-symbol productions by promoting JRSYM until it  
C concatenates with a stacked neighbouring symbol  
C

```
200 JRSYM = PK0 + MIN(IPREC(LISTBP(IP)) - 1, IPREC(LISTBP(JP)))
```

C  
C If leftpart=K2N+2 (formula) set LENBP and return  
C else stack terminal + leftpart cells  
C

```
IF (JRSYM.LT.PK2NP2) GOTO 210
LENBP = JB
GOTO 999
```

```
210 JP = IP - 6
LISTBP(JP) = JTSYM
LISTBP(JP + 1) = JTSM
LISTBP(JP + 2) = JTFAC
LISTBP(JP + 3) = JRSYM
LISTBP(JP + 4) = JRSM
LISTBP(JP + 5) = JRFAC
GOTO 120
```

C  
C----- SEMANTICS -----  
C----- LOAD  
C

```
500 IF (JRFAC.GT.KPOWER) THEN
    JRFAC = - MIN(IORD, JRFAC - KPOWER)
ELSE
    IF (JRFAC.GT.NBI) GOTO 1003
```

```

        JRFAC = 2 ** (JRFAC - 1)
    ENDIF
    JRSUM = JB
    JB = JB + 1
    IF (JB.GE.JP) GOTO 1002
    LISTBP(JB) = JRFAC
    GOTO 200
C
C----- COPY
    600 JRSYM = JMSYM
        JRSUM = JMSUM
        JRFAC = JMFAC
        GOTO 200
C
C----- DYADIC OPERATION
C
    700 JOP = JMSYM
        IJB = JB
        LLSUM = JRSUM
        RCHECK = (JOP.EQ.PSTAR2).OR.(JOP.EQ.PSTAR)
        LCHECK = (JOP.EQ.PSLASH).OR.(JOP.EQ.PSTAR)
C
C          ** . / * + - -/ -*
    GOTO (702, 730, 710, 730, 780, 720, 720, 720), JOP
    702 NPOWER = - LISTBP(JRSUM + 1)
        IF(NPOWER.LE.0) GOTO 1005
        JB = JRSUM
        JRFAC = JLFAC
        IF (NPOWER.EQ.1) GOTO 775
        JRSUM = JLSUM
        IJB = LLSUM
        GOTO 730
    710 JB = JRSUM
        IBP = JLFAC
        I = JRSUM
        GOTO 740
    720 JB = JLSUM
C
C          Outer loop over left operand
C
    730 I = JLSUM
    735 I = I + 1
        IF (I.GT.LLSUM) GOTO 770
        IBP = LISTBP(I)
        IF(IBP.LT.0) GOTO 1005
C
C          Inner loop over right operand
C
    740 J = JRSUM
    745 J = J + 1
        IF (J.GT.IJB) GOTO 760
        JBP = LISTBP(J)
        IF(JBP.LT.0) GOTO 1005
        IORJ = IOR(IBP, JBP)
        IF ((JOP.EQ.PMINUS).OR.(JOP.EQ.PMINSL).OR.(JOP.EQ.PMINST))GOTO 750
C
C          ** . / and * only
C
        IF ((LCHECK.AND.(IORJ.EQ.IBP)).OR.
    1      (RCHECK.AND.(IORJ.EQ.JBP)).OR.
    2      (ICNT(IORJ).GT.IORD)) GOTO 745

```

```
        JB = JB + 1
        IF (JB.GE.JP) GOTO 1002
        LISTBP(JB) = IORJ
        GOTO 745
C
C      - -/ and -* only
C
750 IF (IORJ.NE.IBP) GOTO 745
    K = PMINUS
    IF (IBP.EQ.JBP) K = PMINSL
    IF (JOP - K) 735, 745, 735
C
C      End of inner loop
C      Copy integer not deleted in - -/ or -* operation
C
760 IF ((JOP.NE.PMINUS).AND.(JOP.NE.PMINSL).AND.(JOP.NE.PMINST))
    1  GOTO 735
    JB = JB + 1
    LISTBP(JB) = IBP
    GOTO 735
C
C      End of outer loop
C      For . / and * reorder sum and copy omitting repeats
C
770 IF ((JOP.EQ.PMINUS).OR.(JOP.EQ.PMINSL).OR.(JOP.EQ.PMINST))GOTO 790
    IF (JOP.NE.PSTAR2) GOTO 775
    NPOWER = NPOWER - 1
    IF(NPOWER.EQ.1) GO TO 775
    J = IJB
    GO TO 776
775 IF (JOP.NE.PDOT) IJB = JLSUM
    J = JLSUM
776 CALL BISORT(LISTBP, IJB, JB, IORDER)
    IBP = -1
    DO 779 I = IJB + 1, JB
    IF (LISTBP(I).EQ.IBP) GOTO 779
    IBP = LISTBP(I)
    J = J + 1
    LISTBP(J) = IBP
779 CONTINUE
    JB = J
    IF (JOP.NE.PSTAR2) GO TO 790
    IF (NPOWER.EQ.1) GO TO 790
C      For ** form next power
    JRSUM = IJB
    IJB = JB
    GO TO 730
C
C      + merge right with left sum
C
780 JB = JRSUM
    DO 784 J = JRSUM + 1, IJB
    JBP = LISTBP(J)
    DO 782 I = JLSUM + 1, LLSUM
    IF(JBP.EQ.LISTBP(I)) GO TO 784
782 CONTINUE
    JB = JB + 1
    LISTBP(JB) = JBP
784 CONTINUE
C
C      Set JRSUM, JRFAC
```

```
C
  790 JRSUM = JLSUM
      JRFAC = IOR(JLFAC, JRFAC)
      IF ((JOP.EQ.PMINUS).OR.(JOP.EQ.PMINSL).OR.(JOP.EQ.PMINST))
1    JRFAC = JLFAC
      GOTO 200

C
C----- RETURN AND ERROR SETTING -----
C
1005 IFAULT = IFAULT + 1
1004 IFAULT = IFAULT + 1
1003 IFAULT = IFAULT + 1
1002 IFAULT = IFAULT + 1
1001 IFAULT = IFAULT + 1
      LENBP = JC
  999 RETURN
      END
```



```
c This file includes the Applied Statistics algorithm AS 66 for calculating
c the tail area under the normal curve, and two alternative routines which
c give higher accuracy. The latter have been contributed by Alan Miller of
c CSIRO Division of Mathematics & Statistics, Clayton, Victoria. Notice
c that each function or routine has different call arguments.
```

```
c
c
```

```
double precision function alnorm(x,upper)
```

```
c
c Algorithm AS66 Applied Statistics (1973) vol22 no.3
```

```
c Evaluates the tail area of the standardised normal curve
c from x to infinity if upper is .true. or
c from minus infinity to x if upper is .false.
```

```
c
c double precision zero,one,half
c double precision con,z,y,x
c double precision p,q,r,a1,a2,a3,b1,b2,c1,c2,c3,c4,c5,c6
c double precision d1,d2,d3,d4,d5
c logical upper,up
```

```
c*** machine dependent constants
c double precision ltone,utzero
c data zero/0.0d0/, one/1.0d0/, half/0.5d0/
c data ltone/7.0d0/, utzero/18.66d0/
c data con/1.28d0/
c data p/0.398942280444d0/, q/0.39990348504d0/, r/0.398942280385d0/
c data a1/5.75885480458d0/, a2/2.62433121679d0/, a3/5.92885724438d0/
c data b1/-29.8213557807d0/, b2/48.6959930692d0/
c data c1/-3.8052d-8/, c2/3.98064794d-4/, c3/-0.151679116635d0/
c data c4/4.8385912808d0/, c5/0.742380924027d0/, c6/3.99019417011d0/
c data d1/1.00000615302d0/, d2/1.98615381364d0/, d3/5.29330324926d0/
c data d4/-15.1508972451d0/, d5/30.789933034d0/
```

```
c
c up=upper
c z=x
c if(z.ge.zero)goto 10
c up=.not.up
c z=-z
10 if(z.le.ltone.or.up.and.z.le.utzero)goto 20
c alnorm=zero
c goto 40
20 y=half*z*z
c if(z.gt.con) goto 30
```

```
c
c alnorm=half-z*(p-q*y/(y+a1+b1/(y+a2+b2/(y+a3))))
c goto 40
30 alnorm=r*dexp(-y)/(z+c1+d1/(z+c2+d2/(z+c3+d3/(z+c4+d4/(z+c5+d5/
2 (z+c6))))))
40 if(.not.up)alnorm=one-alnorm
c return
c end
```

```
c
c
c SUBROUTINE NORMP(Z, P, Q, PDF)
C
C Normal distribution probabilities accurate to 1.e-15.
C Z = no. of standard deviations from the mean.
C P, Q = probabilities to the left & right of Z. P + Q = 1.
C PDF = the probability density.
```

```
C
```

```

C      Based upon algorithm 5666 for the error function, from:
C      Hart, J.F. et al, 'Computer Approximations', Wiley 1968
C
C      Programmer: Alan Miller
C
C      Latest revision - 30 March 1986
C
      IMPLICIT DOUBLE PRECISION (A-H, O-Z)
      DATA P0, P1, P2, P3, P4, P5, P6/220.20 68679 12376 1D0,
*      221.21 35961 69931 1D0, 112.07 92914 97870 9D0,
*      33.912 86607 83830 0D0, 6.3739 62203 53165 0D0,
*      .70038 30644 43688 1D0, .35262 49659 98910 9D-01/,
*      Q0, Q1, Q2, Q3, Q4, Q5, Q6, Q7/440.41 37358 24752 2D0,
*      793.82 65125 19948 4D0, 637.33 36333 78831 1D0,
*      296.56 42487 79673 7D0, 86.780 73220 29460 8D0,
*      16.064 17757 92069 5D0, 1.7556 67163 18264 2D0,
*      .88388 34764 83184 4D-1/,
*      CUTOFF/7.071D0/, ROOT2PI/2.5066 28274 63100 1D0/
C
      ZABS = ABS(Z)
C
C      |Z| > 37.
C
      IF (ZABS .GT. 37.D0) THEN
        PDF = 0.D0
        IF (Z .GT. 0.D0) THEN
          P = 1.D0
          Q = 0.D0
        ELSE
          P = 0.D0
          Q = 1.D0
        END IF
        RETURN
      END IF
C
C      |Z| <= 37.
C
      EXPNTL = EXP(-0.5D0*ZABS**2)
      PDF = EXPNTL/ROOT2PI
C
C      |Z| < CUTOFF = 10/sqrt(2).
C
      IF (ZABS .LT. CUTOFF) THEN
        P = EXPNTL*(((P6*ZABS + P5)*ZABS + P4)*ZABS + P3)*ZABS +
*          P2)*ZABS + P1)*ZABS + P0)/((((Q7*ZABS + Q6)*ZABS +
*          Q5)*ZABS + Q4)*ZABS + Q3)*ZABS + Q2)*ZABS + Q1)*ZABS +
*          Q0)
C
C      |Z| >= CUTOFF.
C
      ELSE
        P = PDF/(ZABS + 1.D0/(ZABS + 2.D0/(ZABS + 3.D0/(ZABS + 4.D0/
*          (ZABS + 0.65D0))))))
      END IF
C
      IF (Z .LT. 0.D0) THEN
        Q = 1.D0 - P
      ELSE
        Q = P
        P = 1.D0 - Q
      END IF

```

```

RETURN
END

C
C
C
SUBROUTINE NPROB(Z,P,Q,PDF)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)

C
C P, Q = PROBABILITIES TO THE LEFT AND RIGHT OF Z
C FOR THE STANDARD NORMAL DISTRIBUTION.
C PDF = THE PROBABILITY DENSITY FUNCTION
C
C REFERENCE: ADAMS,A.G. AREAS UNDER THE NORMAL CURVE,
C ALGORITHM 39, COMPUTER J., VOL. 12, 197-8, 1969.
C
C LATEST REVISION - 23 JANUARY 1981
C
C*****
C
DATA A0,A1,A2,A3,A4,A5,A6,A7/0.5D0, 0.398942280444D0,
1 0.399903438504D0, 5.75885480458D0, 29.8213557808D0,
2 2.62433121679D0, 48.6959930692D0, 5.92885724438D0/,
3 B0,B1,B2,B3,B4,B5,B6,B7,B8,B9,B10,B11/0.398942280385D0,
4 3.8052D-8, 1.00000615302D0, 3.98064794D-4, 1.98615381364D0,
5 0.151679116635D0, 5.29330324926D0, 4.8385912808D0,
6 15.1508972451D0, 0.742380924027D0, 30.789933034D0,
7 3.99019417011D0/

C
ZABS = ABS(Z)
IF(ZABS.GT.12.7D0) GO TO 20
Y = A0*Z*Z
PDF = EXP(-Y)*B0
IF(ZABS.GT.1.28D0) GO TO 10

C
C Z BETWEEN -1.28 AND +1.28
C
Q = A0-ZABS*(A1-A2*Y/(Y+A3-A4/(Y+A5+A6/(Y+A7))))
IF(Z.LT.0.D0) GO TO 30
P = 1.D0-Q
RETURN

C
C ZABS BETWEEN 1.28 AND 12.7
C
10 Q = PDF/(ZABS-B1+B2/(ZABS+B3+B4/(ZABS-B5+B6/(ZABS+B7-B8/
1 (ZABS+B9+B10/(ZABS+B11))))))
IF(Z.LT.0.D0) GO TO 30
P = 1.D0-Q
RETURN

C
C Z FAR OUT IN TAIL
C
20 Q = 0.D0
PDF = 0.D0
IF(Z.LT.0.D0) GO TO 30
P = 1.D0
RETURN

C
C NEGATIVE Z, INTERCHANGE P AND Q
C
30 P = Q
Q = 1.D0-P

```

RETURN

END

```
      SUBROUTINE INCLUD (NP,NRBAR,WEIGHT,XROW,YELEM,D,RBAR,THETAB,SSERR,
1 IFAULT)
C
C   Algorithm AS 75.1 Appl. Statist. (1974) Vol.23, No.3, p448
C
C   Calling this subroutine updates d, rbar, thetab and sserr
C   by the inclusion of xrow, yelem with specified weight.
C
      DOUBLE PRECISION XROW(NP),D(NP),RBAR(NRBAR),THETAB(NP),WEIGHT,
1 SSERR,CBAR,DI,DPI,SBAR,W,XI,XK,Y,ZERO,YELEM
C
      DATA ZERO/0.0D0/
C
      check input parameters
C
      IFAULT=1
      IF (NP.LT.1.OR.NRBAR.LE.NP*(NP-1)/2) RETURN
      IFAULT=0
C
      W=WEIGHT
      Y=YELEM
      DO 30 I=1,NP
C
C   Skip unnecessary transformations. Test on exact zeros must
C   be used or stability can be destroyed.
C
      IF (W.EQ.ZERO) RETURN
      IF (XROW(I).EQ.ZERO) GO TO 30
      XI=XROW(I)
      DI=D(I)
      DPI=DI+W*XI*XI
      CBAR=DI/DPI
      SBAR=W*XI/DPI
      W=CBAR*W
      D(I)=DPI
      IF (I.EQ.NP) GO TO 20
      NEXTR=(I-1)*(NP+NP-I)/2+1
      IP=I+1
      DO 10 K=IP,NP
          XK=XROW(K)
          XROW(K)=XK-XI*RBAR(NEXTR)
          RBAR(NEXTR)=CBAR*RBAR(NEXTR)+SBAR*XK
          NEXTR=NEXTR+1
10      CONTINUE
20      XK=Y
          Y=XK-XI*THETAB(I)
          THETAB(I)=CBAR*THETAB(I)+SBAR*XK
30      CONTINUE
          SSERR=SSERR+W*Y*Y
      RETURN
      END
C
C
      SUBROUTINE CONFND (NP,NRBAR,J,RBAR,CONTRA,IFAUULT)
C
C   Algorithm AS 75.2 Appl. Statist. (1974) Vol. 23, No. 3, P448
C
C   Calling this subroutine obtains the contrast which could not
C   be estimated if D(j) were assumed to be zero, that is, obtains the
C   linear combination of the first j columns which would be zero. Th
C   obtained by setting the first j-1 elements of contra to the soluti
```

```
C      of the triangular system formed by the first j-1 rows and columns
C      rbar with the first j-1 elements of the jth column as right hand
C      side, setting the jth element of contra to -1, and setting the
C      remaining elements of contra to zero.
C
C      DOUBLE PRECISION RBAR(NRBAR),CONTRA(NP),ZERO,ONE
C
C      DATA ZERO/0.0D0/,ONE/1.0D0/
C
C      check input parameters
C
C      IFAULT=1
C      IF (NP.LT.1.OR.NRBAR.LE.NP*(NP-1)/2) RETURN
C      IFAULT=0
C
C      JM=J-1
C      IF (J.EQ.NP) GO TO 20
C      JP=J+1
C      DO 10 I=JP,NP
10      CONTRA(I)=ZERO
20      CONTRA(J)=-ONE
C      IF (J.EQ.1) RETURN
C      DO 40 IJ=1,JM
C      I=J-IJ
C      NEXTR=(I-1)*(NP+NP-I)/2+1
C      K=NEXTR+J-I-1
C      CONTRA(I)=RBAR(K)
C      IF (I.EQ.JM) GO TO 40
C      IP=I+1
C      DO 30 K=IP,JM
C      CONTRA(I)=CONTRA(I)-RBAR(NEXTR)*CONTRA(K)
C      NEXTR=NEXTR+1
30      CONTINUE
40      CONTINUE
C      RETURN
C      END
C
C
C      SUBROUTINE SSDCMP (NP,D,THETAB,SS,IFAUULT)
C
C      Algorithm AS75.3 Appl. Statist. (1974) Vol.23, No. 3, P448
C
C      Calling this subroutine computes the np components of the sum
C      of squares decomposition from D and thetab.
C
C      DOUBLE PRECISION D(NP),THETAB(NP),SS(NP)
C
C      check input parameters
C
C      IFAULT=1
C      IF (NP.LT.1) RETURN
C      IFAULT=0
C
C      DO 10 I=1,NP
10      SS(I)=D(I)*THETAB(I)**2
C      RETURN
C      END
C
C
C      SUBROUTINE REGRSS (NP,NRBAR,RBAR,THETAB,BETA,IFAUULT)
C
```

```
C      Algorithm AS 75.4  Appl. Statist. (1974), Vol. 23, No. 3, p448
C
C      Calling this subroutine obtains beta by back-substitution in
C      the triangular system rbar and thetab.
C
C      DOUBLE PRECISION RBAR(NRBAR),THETAB(NP),BETA(NP)
C
C      check input parameters
C
C      IFAULT=1
C      IF (NP.LT.1.OR.NRBAR.LE.NP*(NP-1)/2) RETURN
C      IFAULT=0
C
C      DO 20 J=1,NP
C          I=NP-J+1
C          BETA(I)=THETAB(I)
C          NEXTR=(I-1)*(NP+NP-I)/2+1
C          IP=I+1
C          DO 10 K=IP,NP
C              BETA(I)=BETA(I)-RBAR(NEXTR)*BETA(K)
C              NEXTR=NEXTR+1
C          CONTINUE
C      CONTINUE
C      RETURN
C      END
```

```
C
C      SUBROUTINE ANALYZ (MAXP,MAXR,NP,NRBAR,INPUT,OUTPUT,X,DD,THETA,R,
C      1 IFAULT)
```

```
C
C      Algorithm AS 75.5  Appl. Statist. (1974) Vol. 23, P. 448
C
C      This subroutine reads data from channel input and
C      produces least squares variance component analyses on
C      channel output.  The input medium is assumed to
C      contain first a value for the integer np, the number of
C      independent variates, and then a sequence of records
C      containing the rows of x and y together with weights.
C      The number zero (read as a weight) will indicate the end of
C      each data set, and upon reading this an analysis will be
C      produced.  Successive analyses will be done until np,
C      the number of independent variates, is read as zero.
C
C      No need to check the ifault parameter after calling
C      auxiliary routines as parameters have already been
C      checked here.
C
C      INTEGER OUTPUT
C      LOGICAL FIRST
C      DOUBLE PRECISION X(MAXP),DD(MAXP),THETA(MAXP),R(MAXR),ERROR,W,Y,
C      1 ZERO,ONE,EPS,TOL
C
C      DATA ZERO,ONE,EPS,TOL/0.0D0,1.0D0,1.0D-8,1.0D-4/
C
C      input formats
C
C      10  FORMAT (I3)
C      20  FORMAT (F10.6)
C      30  FORMAT (F10.6)
C      40  FORMAT (I3)
C      50  FORMAT (F10.6)
```

```
C
C      output formats
C
60  FORMAT (1H1,I5,18H observations read/19H diagonal matrix is/(1X,
1  5G15.8))
70  FORMAT (21H confounded contrasts)
80  FORMAT (1X,5G15.8)
90  FORMAT (29H sum of squares decomposition/(1X,5G15.8))
100 FORMAT (22H sum of squares error ,G15.8)
110 FORMAT (24H regression coefficients,(1X,5G15.8))
C
C      read np, check its value and initialise arrays
C
      IFAULT=0
120 READ (INPUT,10) NP
      IF (NP.EQ.0) RETURN
      NRBAR=NP*(NP-1)/2
      IF (NP.LT.0.OR.NP.GT.MAXP.OR.NRBAR.GT.MAXR) GO TO 240
      DO 130 K=1,NP
          DD(K)=ZERO
          THETA(K)=ZERO
130  CONTINUE
      DO 140 K=1,NRBAR
140  R(K)=ZERO
      ERROR=ZERO
      N=0
C
C      read weight and check its value
C
150 READ (INPUT,20) W
      IF (W.EQ.ZERO) GO TO 190
      IF (W.GT.ZERO) N=N+1
      IF (W.LT.ZERO) N=N-1
C
C      read the y-value and all corresponding x-values
C
      READ (INPUT,30) Y
      DO 160 K=1,NP
160  X(K)=ZERO
170  READ (INPUT,40) K
      IF (K.LT.0.OR.K.GT.NP) GO TO 250
      IF (K.EQ.0) GO TO 180
      READ (INPUT,50) X(K)
      GO TO 170
180  CALL INCLUD (NP,NRBAR,W,X,Y,DD,R,THETA,ERROR,IFAIL)
      GO TO 150
C
C      begin output
C
190  WRITE (OUTPUT,60) N,(DD(I),I=1,NP)
      FIRST=.TRUE.
      DO 230 J=1,NP
          IF (ABS(DD(J)).GE.EPS) GO TO 230
C
C      confounding discovered
C
      IF (.NOT.FIRST) GO TO 200
      FIRST=.FALSE.
      WRITE (OUTPUT,70)
200  CALL CONFND (NP,NRBAR,J,R,X,IFAIL)
      WRITE (OUTPUT,80) (X(I),I=1,NP)
```



```
C
C      choose resolving constraint
C
      IF (J.EQ.1) GO TO 220
      JM=J-1
      DO 210 K=1,JM
        IF (ABS(X(K)).LE.TOL) GO TO 210
        X(K)=ZERO
        GO TO 220
210    CONTINUE
220    CALL INCLUD (NP,NRBAR,ONE,X,ZERO,DD,R,THETA,ERROR,IFAIL)
230    CONTINUE
      CALL SSDCMP (NP,DD,THETA,X,IFAIL)
      WRITE (OUTPUT,90) (X(I),I=1,NP)
      WRITE (OUTPUT,100) ERROR
      CALL REGRSS (NP,NRBAR,R,THETA,X,IFAIL)
      WRITE (OUTPUT,110) (X(I),I=1,NP)
      GO TO 120

C
C      error returns
C
240  IFAULT=2
      RETURN
250  IFAULT=3
      RETURN
      END
```

C Two versions of algorithm AS 76 are given here; the original with one  
C correction incorporated, and AS R55, also amended. AS R55 requires  
C AS 76. N.B. The accuracy of AS 76 could be increased by using more  
C Gaussian quadrature points, or better, by using Hermite integration.

```
C
  FUNCTION TFN(X, FX)
C
C  ALGORITHM AS 76  APPL. STATIST. (1974) VOL.23, NO.3
C
C  Calculates the T-function of Owen, using Gaussian quadrature.
C  Incorporates correction AS R30 (vol.28, no.1, 1979)
C
  REAL U(5), R(5)
C
  DATA U /0.0744372, 0.2166977, 0.3397048, 0.4325317, 0.4869533/
  DATA R /0.1477621, 0.1346334, 0.1095432, 0.0747257, 0.0333357/
  DATA NG,   TP,   TV1,   TV2,   TV3,   TV4
*   / 5, 0.159155, 1.E-35, 15.0, 15.0, 1.E-5 /
  DATA ZERO, QUART, HALF, ONE, TWO
*   / 0.0, 0.25, 0.5, 1.0, 2.0 /
C
  Test for X near zero
C
  IF (ABS(X) .GE. TV1) GO TO 5
  TFN = TP * ATAN(FX)
  RETURN
C
  Test for large values of abs(X)
C
  5 IF (ABS(X) .GT. TV2) GO TO 10
C
  Test for FX near zero
C
  IF (ABS(FX) .GE. TV1) GO TO 15
  10 TFN = ZERO
  RETURN
C
  Test whether abs(FX) is so large that it must be truncated
C
  15 XS = -HALF * X * X
  X2 = FX
  FXS = FX * FX
  IF (LOG(ONE + FXS) - XS * FXS .LT. TV3) GO TO 25
C
  Computation of truncation point by Newton iteration
C
  X1 = HALF * FX
  FXS = QUART * FXS
  20 RT = FXS + ONE
  X2 = X1 + (XS * FXS + TV3 - LOG(RT)) / (TWO * X1 * (ONE/RT - XS))
  FXS = X2 * X2
  IF (ABS(X2 - X1) .LT. TV4) GO TO 25
  X1 = X2
  GO TO 20
C
  Gaussian quadrature
C
  25 RT = ZERO
  DO 30 I = 1, NG
    R1 = ONE + FXS * (HALF + U(I))**2
    R2 = ONE + FXS * (HALF - U(I))**2
```

```

      RT = RT + R(I) * (EXP(XS * R1) / R1 + EXP(XS * R2) / R2)
30 CONTINUE
      TFN = RT * X2 * TP
C
      RETURN
      END
C
C-----
C
      REAL FUNCTION THA(H1, H2, A1, A2)
C
C      AS R55  APPL. STATIST. (1985) VOL.34, NO.1
C
C      A remark on AS 76
C      Incorporating improvements in AS R80 (Appl. Statist. (1989)
C      vol.38, no.3), and AS R89 (Appl. Statist. (1992) vol.41, no.2).
C
C      Computes T(H1/H2, A1/A2) for any real numbers H1, H2, A1 and A2
C
C      Auxiliary function required: ALNORM (= AS 66) and AS 76
C
      REAL A, ALNORM, A1, A2, G, H, H1, H2, TFN, ABSA, AH, GH, GAH,
*      TWOPI, LAM, EX, C1, C2,
*      AH, ZERO, ONE, TWO, PT3, SEVEN, HALF, SIX, QUART
C
      DATA TWOPI /6.2831853/, ZERO /0.0/, ONE /1.0/, TWO /2.0/,
*      PT3 /0.3/, SEVEN /7.0/, HALF /0.5/, SIX /6.0/, QUART /0.25/
C
      IF (H2 .NE. ZERO) GO TO 1
      THA = ZERO
      RETURN
C
1  H = H1 / H2
   IF (A2 .EQ. ZERO) GO TO 2
   A = A1 / A2
   IF ((ABS(H) .LT. PT3) .AND. (ABS(A) .GT. SEVEN)) GO TO 6
C
C      Correction AS R89
C
      ABSA = ABS(A)
      IF (ABSA .GT. ONE) GO TO 7
      THA = TFN(H, A)
      RETURN
7  AH = ABSA * H
   GH = ALNORM(H, .FALSE.)
   GAH = ALNORM(AH, .FALSE.)
   THA = HALF * (GH + GAH) - GH * GAH - TFN(AH, ONE/ABSA)
   IF (A .LT. ZERO) THA = - THA
   RETURN
C
2  G = ALNORM(H, .FALSE.)
   IF (H .GE. ZERO) GO TO 3
   THA = G / TWO
   GO TO 4
3  THA = (ONE - G) / TWO
4  IF (A1 .GE. ZERO) RETURN
   THA = -THA
   RETURN
C
6  LAM = ABS(A * H)
   EX = EXP(-LAM * LAM / TWO)

```

```
G = ALNORM(LAM, .FALSE.)
C1 = (EX/LAM + SQRT(TWOPI) * (G - HALF)) / (TWOPI)
C2 = ((LAM * LAM + TWO) * EX/LAM**3 + SQRT(TWOPI) * (G - HALF))
*      / (SIX * TWOPI)
AH = ABS(H)
THA = QUART - C1 * AH + C2 * AH**3
THA = SIGN(THA, A)
RETURN
END
```

```

      DOUBLE PRECISION FUNCTION ROY TST(NN1, NN2, NNP, X, IFAULT)
C
C   ALGORITHM AS 77  APPL. STATIST. (1974) VOL.23, NO.3
C
C   A function for the exact null distribution of the largest root
C   of a beta matrix.
C
C   Restrictions:
C     The value of NN2 - NNP - 1 must be an even number.
C     Local storage is sufficient for min(NN1, NNP) at most 10.
C     The number of terms is limited to at most 150,000.
C
      INTEGER ND(10), NP(10), K(56), R, P, PMAX, TERMS
      DOUBLE PRECISION T(10), S(10), A, B, C, CX, CXS, HALF, HCX, ONE,
+ P1, P2, TL, TWO, X, XM, XMM, XMN2, XN1, XN11, ZERO
      LOGICAL C1, C2
      DATA ZERO, HALF, ONE, TWO /0.D0, 0.5D0, 1.D0, 2.D0/
      DATA PMAX, TERMS /10, 150000/
C
C   Check for errors in the parameters.
C   Commence initialisation.
C
      N1 = MAX(NN1, NNP)
      N2 = MIN(NN2, NN1 + NN2 - NNP)
      P = MIN(NN1, NNP)
      IFAULT = 0
      ROY TST = ZERO
      IF (N1 .GT. 0 .AND. N2 .GT. 0 .AND. P .GT. 0 .AND. X .GE. ZERO
+ .AND. X .LE. ONE) GO TO 10
      IFAULT = 1
      RETURN
10  M = (N2 - P - 1) / 2
      IF (M .GE. 0 .AND. M + M .EQ. N2 - P - 1) GO TO 20
      IFAULT = 2
      RETURN
20  P1 = ONE
      P2 = ZERO
      IF (M .EQ. 0) GO TO 160
      A = ONE
      B = M + P
      R = MIN(M, P)
      C = R
      DO 30 J = 1, R
          A = A * B / C
          B = B - ONE
          C = C - ONE
30  CONTINUE
      R = A
      IF (P .LE. PMAX .AND. R .LE. TERMS) GO TO 40
      IFAULT = 3
      RETURN
C
C   Error checks complete; initialisation continues.
C
40  XM = P
      XN11 = N1 - 1
      CX = ONE - X
      P2 = ONE
      DO 50 I = 1, P
          A = -I
          DO 50 J = 1, M

```

```
      A = A + TWO
      P2 = P2 * CX * (XN11 + A) / (XM + A)
50 CONTINUE
S(1) = P2
MP = M * P
MN = MP - 2
IF (MN .LT. 0) GO TO 160
R = 0
L = 0
N = 1
LE = 1
K(1) = M
XMM = P + P + 1 - N1 - N2
XMN2 = P - N2
XN1 = N1
HCX = HALF * CX
CXS = ONE / (CX * CX)
T(1) = ONE
GO TO 80

C
C   Initialisation finished.   Main loop starts here.
C
C   Check if the current partition cannot have a unit part appended.
C
60 C1 = (R .EQ. P)

C
C   Check if the current partition cannot have its last part
C   increased.
C
      C2 = (K(LE) .EQ. K(LE-1))
      IF (C1 .AND. C2) GO TO 150
      IF (C1) GO TO 100
      IF (C2) GO TO 90
      LB = LE - R + 1
      DO 70 I = LB, LE
        J = I + R
        K(J) = K(I)
70 CONTINUE
      S(L+1) = S(L)
      T(L+1) = T(L)

C
C   Signal that a second partition is waiting in the list.
C
      ASSIGN 80 TO NEXT
      GO TO 100
80 ASSIGN 140 TO NEXT
      L = L + 1
      LE = LE + R
90 LE = LE + 1
      R = R + 1
      NP(L) = R
      K(LE) = 0
100 K(LE) = K(LE) + 1
      ND(L) = N

C
C   Use the recurrence formulae for the terms of the current partition
C
      B = 2 * K(LE) - R - 1
      A = K(LE)
      TL = T(L)
      TL = TL * HCX * (XN1 + B) * (XM + B) / (A * (A + A - ONE))
```

```
    JP = R - 1
    IF (JP .EQ. 0) GO TO 130
    LB = LE - JP
    C = R + 2
    DO 120 J = 1, JP
        C = C - ONE
        TL = TL * (ONE - TWO / (TWO * (K(LB) - A) + C))
        LB = LB + 1
120 CONTINUE
130 P1 = P1 + TL
    T(L) = TL
C
C    Check if conjugate partition terms are necessary.
C
    IF (MN .EQ. 0) GO TO NEXT, (80, 140)
    B = B + ONE
    S(L) = S(L) * CXS * (XMN2 + B) * (XM + B) / ((XMM + B) *
+          (XN11 + B))
    P2 = P2 + TL * S(L)
C
C    Check if a second partition has been generated.
C
    GO TO NEXT, (80, 140)
140 N = ND(L) + 1
    R = NP(L)
C
C    Check that the degree of the partition is within limits.
C
    MN = MP - N - N
    IF (MN .GE. 0) GO TO 60
150 L = L - 1
    LE = LE - R
C
C    If L = 0 then list is empty and calculation complete.
C
    IF (L .GT. 0) GO TO 140
C
C    Multiply by the external factor, and return
C
160 ROY TST = (P1 + P2) * X ** (HALF * (N1 * P))
    RETURN
    END
```

```
      SUBROUTINE MEDIAN(X, Y, N, IP, IT, IFAULT)
C
C   ALGORITHM AS 78  APPL. STATIST. (1974) VOL.23, NO.3
C
C   The mediancentre, generalising the median, is the point with
C   minimum total distance from a set of multivariate samples
C
      REAL X(N, IP), Y(IP)
      REAL Z(50), LAMBDA, LEPSI, LEPSR, LEPSD
C
      DOUBLE PRECISION C(50), COMP, D, DD, DELTA, EPSR, EPSD, SLAM,
+   ZERO, ONE
C
      DATA LEPSD /0.0001/, LEPSR / 0.00001/, LEPSI /0.000001/
      DATA ICOUNT /100/, LCOUNT /50/
      DATA ZERO /0.D0/, ONE /1.D0/
C
      Initial settings
C
      IFAULT = 0
      LL = 0
      II = 1
      IF (N .EQ. 1) GO TO 25
      IF (N .LE. 0 .OR. IP .LE. 0) GO TO 5
C
      Calculate the diameter
C
      DIAM = 0.0
      DO 2 I = 2, N
        DO 2 J = 1, I-1
          S = 0.0
          DO 1 K = 1, IP
1          S = S + (X(I,K) - X(J,K))**2
          DIAM = MAX(S, DIAM)
2 CONTINUE
      DIAM = SQRT(DIAM)
      EPSR = LEPSR * DIAM
      EPSI = LEPSI * DIAM
      EPSD = LEPSD * DIAM
C
      Initial median centre = the centroid
C
      U1 = 1.0 / FLOAT(N)
      DO 4 J = 1, IP
        S = 0.0
        DO 3 I = 1, N
3          S = S + X(I,J)
          Y(J) = S * U1
4 CONTINUE
      IT = ICOUNT
      IF (IP .LE. 50) GO TO 6
5 IFAULT = 1
      IT = 0
      RETURN
C
      Main iterative loop
C
6 DO 23 L = 1, ICOUNT
C
      Direction cosines and resultant
C
```



```

CORNER = 0.0
DO 7 J = 1, IP
7 C(J) = ZERO
LL = L
DO 11 I = 1, N
D = ZERO
DO 8 J = 1, IP
8 D = D + (X(I,J) - Y(J))**2
DD = SQRT(D)
IF (DD .GT. EPSD) GO TO 9
CORNER = CORNER + 1.0
II = I
GO TO 11
9 D = ONE / DD
DO 10 J = 1, IP
10 C(J) = C(J) + (X(I,J) - Y(J)) * D
11 CONTINUE
D = ZERO
DO 12 J = 1, IP
12 D = D + C(J)**2
D = SQRT(D)
DD = D

C
C Tests for zero resultant or degenerate solution
C
IF (CORNER .EQ. 0.0) GO TO 13
IF (D .LE. CORNER) GO TO 25
D = D - CORNER
13 IF (D .LE. EPSR) GO TO 24
DD = ONE / DD
DO 14 J = 1, IP
14 C(J) = C(J) * DD

C
C Step by bisection to give zero component at lambda
C
U1 = 0.0
U2 = DIAM
DO 20 LC = 1, LCOUNT
COMP = ZERO
LAMBDA = 0.5 * (U1 + U2)
SLAM = LAMBDA * LAMBDA
DO 15 J = 1, IP
15 Z(J) = Y(J) + LAMBDA * C(J)
DO 17 I = 1, N
DELTA = ZERO
D = SLAM
DO 16 J = 1, IP
XX = X(I,J)
D = D - (XX - Y(J))**2
DELTA = DELTA + (XX - Z(J))**2
16 CONTINUE
DD = SQRT(DELTA)
IF (DD .LT. EPSD) GO TO 21
COMP = COMP - (D + DELTA) / DD
17 CONTINUE
IF (COMP .GT. ZERO) GO TO 18
U2 = LAMBDA
GO TO 19
18 U1 = LAMBDA
19 IF ((U2 - U1) .LE. EPSI) GO TO 21
20 CONTINUE
```

```
C
 21  DO 22 J = 1, IP
 22  Y(J) = Y(J) + C(J) * LAMBDA
 23  CONTINUE
C
 24  IT = LL
     RETURN
 25  IT = -LL
     DO 26 J = 1, IP
 26  Y(J) = X(IT,J)
     RETURN
     END
```

```
      subroutine fastf(xreal, ximag, isize, itype)
c
c      Algorithm AS 83.1 Appl. Statist. (1975) vol.24, no.1
c
c      Radix 4 complex discrete fast Fourier transform with
c      unscrambling of the transformed arrays.
c
      real    xreal(isize), ximag(isize)
c
c      Check for valid transform size.
c
      ii = 4
      do 2 k = 2, 20
        if (ii .eq. isize) go to 4
        if (ii .gt. isize) go to 3
        ii = ii * 2
      2 continue
c
c      If this point is reached a size error has occurred.
c
      3 return
c
c      Call FASTG to perform the transform.
c
      4 call fastg(xreal, ximag, isize, itype)
c
c      Call SCRAM to unscramble the results.
c
      call scram(xreal, ximag, isize, k)
c
      return
      end
c
c
c
      subroutine fastg(xreal, ximag, n, itype)
c
c      Algorithm AS 83.2 Appl. Statist. (1975) vol.24, no.1
c
c      Radix 4 complex discrete fast Fourier transform without
c      unscrambling, suitable for convolutions or other applications
c      which do not require unscrambling.  Called by subroutine
c      FASTF which also does the unscrambling.
c
c
      real    xreal(n), ximag(n)
      data    zero, half, one, one5, two, four
+           /0.0, 0.5, 1.0, 1.5, 2.0, 4.0/
      pi = four * atan(one)
      ifaca = n / 4
      if (itype .eq. 0) return
      if (itype .gt. 0) go to 5
c
c      ITYPE < 0 indicates inverse transform required.
c      Calculate conjugate.
c
      do 4 k = 1, n
      4 ximag(k) = -ximag(k)
c
c      Following code is executed for IFACA = N/4, N/16, N/64, ...
c      until IFACA <= 1.
c
```

```

5 ifcab = ifaca * 4
  z = pi / ifcab
  bcos = -two * sin(z)**2
  bsin = sin(two * z)
  cw1 = one
  sw1 = zero
  do 10 litla = 1, ifaca
    do 8 i0 = litla, n, ifcab
      i1 = i0 + ifaca
      i2 = i1 + ifaca
      i3 = i2 + ifaca
      xs0 = xreal(i0) + xreal(i2)
      xs1 = xreal(i0) - xreal(i2)
      ys0 = ximag(i0) + ximag(i2)
      ys1 = ximag(i0) - ximag(i2)
      xs2 = xreal(i1) + xreal(i3)
      xs3 = xreal(i1) - xreal(i3)
      ys2 = ximag(i1) + ximag(i3)
      ys3 = ximag(i1) - ximag(i3)
      xreal(i0) = xs0 + xs2
      ximag(i0) = ys0 + ys2
      x1 = xs1 + ys3
      y1 = ys1 - xs3
      x2 = xs0 - xs2
      y2 = ys0 - ys2
      x3 = xs1 - ys3
      y3 = ys1 + xs3
      if (litla .eq. 1) then
        xreal(i2) = x1
        ximag(i2) = y1
        xreal(i1) = x2
        ximag(i1) = y2
        xreal(i3) = x3
        ximag(i3) = y3
      else
        xreal(i2) = x1 * cw1 + y1 * sw1
        ximag(i2) = y1 * cw1 - x1 * sw1
        xreal(i1) = x2 * cw2 + y2 * sw2
        ximag(i1) = y2 * cw2 - x2 * sw2
        xreal(i3) = x3 * cw3 + y3 * sw3
        ximag(i3) = y3 * cw3 - x3 * sw3
      end if
    8 continue
  c
  c Calculate a new set of twiddle factors.
  c
  if (litla .lt. ifaca) then
    z = cw1 * bcos - sw1 * bsin + cw1
    sw1 = bcos * sw1 + bsin * cw1 + sw1
    tempr = one5 - half * (z * z + sw1 * sw1)
    cw1 = z * tempr
    sw1 = sw1 * tempr
    cw2 = cw1 * cw1 - sw1 * sw1
    sw2 = two * cw1 * sw1
    cw3 = cw1 * cw2 - sw1 * sw2
    sw3 = cw1 * sw2 + cw2 * sw1
  end if
10 continue
  if (ifaca .le. 1) go to 14
  c
  c Set up the transform split for the next stage.

```

```
c
  ifaca = ifaca / 4
  if (ifaca .gt. 0) go to 5
c
c   Radix 2 calculation, if needed.
c
  if (ifaca .lt. 0) return
  do 13 k = 1, n, 2
    tempr = xreal(k) + xreal(k+1)
    xreal(k+1) = xreal(k) - xreal(k+1)
    xreal(k) = tempr
    tempr = ximag(k) + ximag(k+1)
    ximag(k+1) = ximag(k) - ximag(k+1)
    ximag(k) = tempr
13 continue
14 if (itype .lt. 0) then
c
c   Inverse transform; conjugate the result.
c
  do 16 k = 1, n
16  ximag(k) = -ximag(k)
    return
  end if
c
c   Forward transform
c
  z = one / n
  do 18 k = 1, n
    xreal(k) = xreal(k) * z
    ximag(k) = ximag(k) * z
18 continue
c
  return
  end
c
c
c
c   subroutine scram(xreal, ximag, n, ipow)
c
c   Algorithm AS 83.3 Appl. Statist. (1975) vol.24, no.1
c
c   Subroutine for unscrambling FFT data.
c
  real    xreal(n), ximag(n)
  integer l(19)
  equivalence (l1,l(1)), (l2,l(2)), (l3,l(3)), (l4,l(4)),
+             (l5,l(5)), (l6,l(6)), (l7,l(7)), (l8,l(8)), (l9,l(9)),
+             (l10,l(10)), (l11,l(11)), (l12,l(12)), (l13,l(13)),
+             (l14,l(14)), (l15,l(15)), (l16,l(16)), (l17,l(17)),
+             (l18,l(18)), (l19,l(19))
c
  ii = 1
  itop = 2 ** (ipow - 1)
  i = 20 - ipow
  do 5 k = 1, i
5  l(k) = ii
  l0 = ii
  i = i + 1
  do 6 k = i, 19
    ii = ii * 2
    l(k) = ii
```

```
6 continue
c
  ii = 0
  do 9 j1 = 1, 11, 10
    do 9 j2 = j1, 12, 13
      do 9 j3 = j2, 13, 12
        do 9 j4 = j3, 14, 13
          do 9 j5 = j4, 15, 14
            do 9 j6 = j5, 16, 15
              do 9 j7 = j6, 17, 16
                do 9 j8 = j7, 18, 17
                  do 9 j9 = j8, 19, 18
                    do 9 j10 = j9, 110, 19
                      do 9 j11 = j10, 111, 110
                        do 9 j12 = j11, 112, 111
                          do 9 j13 = j12, 113, 112
                            do 9 j14 = j13, 114, 113
                              do 9 j15 = j14, 115, 114
                                do 9 j16 = j15, 116, 115
                                  do 9 j17 = j16, 117, 116
                                    do 9 j18 = j17, 118, 117
                                      do 9 j19 = j18, 119, 118
                                        j20 = j19
                                        do 9 i = 1, 2
                                          ii = ii + 1
                                          if (ii .lt. j20) then
c
c      J20 is the bit-reverse of II pairwise interchange.
c
                                          tempr = xreal(ii)
                                          xreal(ii) = xreal(j20)
                                          xreal(j20) = tempr
                                          tempr = ximag(ii)
                                          ximag(ii) = ximag(j20)
                                          ximag(j20) = tempr
                                          end if
                                          j20 = j20 + itop
c
c      9 continue
c
      return
      end
```



```

    l = 0
    do 40 j = 1, ip
      do 40 k = 1, j
        l = l + 1
        xm = zero
        do 35 i = 1, n
35      xm = xm + x(j, i) * x(k, i)
        ssq(l) = xm
40 continue
c
c      ssq at this stage contains the sample matrix of corrected sums
c      of squares and products, stored as lower triangle
c
    call syminv (ssq, ip, nn, ssq, work, irank, ifault)
    if (ifault .ne. 0) return
    if (irank .ne. 0) ifault = 1
    irank = ip - irank
    b1 = zero
    b2 = zero
    do 100 i = 1, n
      xm = ssq(1) * x(1, i) ** 2
      m = 1
      do 70 k = 2, ip
        qq = zero
        kk = k - 1
        do 50 l = 1, kk
          m = m + 1
          qq = qq + ssq(m) * x(l, i)
50      continue
        m = m + 1
        xki = x(k, i)
        xm = xm + (ssq(m) * xki + two * qq) * xki
70      continue
        qq = xm ** 2
        b2 = b2 + qq
        b1 = b1 + qq * xm
100 continue
    do 150 i = 2, n
      ii = i - 1
      ss = ssq(1) * x(1, i)
      do 150 j = 1, ii
        xm = ss * x(1, j)
        m = 1
        do 120 k = 2, ip
          xki = x(k, i)
          xkj = x(k, j)
          qq = zero
          qr = zero
          kk = k - 1
          do 110 l = 1, kk
            m = m + 1
            ssqm = ssq(m)
            qq = qq + ssqm * x(l, j)
            qr = qr + ssqm * x(l, i)
110      continue
          qq = qq * xki + qr * xkj
          m = m + 1
          xm = xm + qq + ssq(m) * xki * xkj
120      continue
          b1 = b1 + two * xm ** 3
150 continue
```



```
b1 = b1 * sumwts  
b2 = b2 * sumwts  
return  
end
```

```
subroutine allnr(n, r, j, ifault)
c
c   Algorithm AS 88  Appl. Statist. (1975) Vol.24, No. 3
c
c   When called once, generates all possible combinations
c   from a group of N items.  Each combination (represented in j as
c   r ordered integers between 1 and n) is processed within allnr.
c
c   Parameters:-
c
c   n          integer          input:  The size of the group from which
c                                     the combinations are selected.
c
c   r          integer          input:  The size of each combination.
c
c   j          integer array(r) workspace: Used by allnr to store
c                                     combinations.
c
c   ifault     integer          output: Fault indicator, equal to:
c                                     0 if 1 ≤ R ≤ N;
c                                     1 otherwise.
c
integer r, j(r)
c
ifault = 1
if (r .lt. 1 .or. r .gt. n) return
ifault = 0
kount = 0
nmr = n - r
c
c   Initialize J(1) to lower limit separately, since lower limit for
c   each index depends on lower limit for previous index
c
i = 1
j(1) = 1
c
c   Initialize indices for loops i=1,...,r to lower limits
c
1 if (i .eq. r) goto 3
ip1 = i + 1
do 2 l = ip1, r
2 j(l) = j(l - 1) + 1
c
c   Update the count (kount) of combinations and process the current
c   combination.  The call to Subroutine job may be replaced by
c   statements to process the current combination.
c
3 kount = kount + 1
call job(n, r, j, kount)
c
c   Increment the first possible index (of loop i) among indices of
c   loops R, R-1,...,1
c
i = r
4 if (j(i) .lt. nmr + i) goto 5
i = i - 1
c
c   Return after all indices have achieved their upper limits
c
if (i .le. 0) return
goto 4
```

```
5 j(i) = j(i) + 1  
   goto 1  
   end
```

```
c  
c  
c
```

```
subroutine job (n, r, j, kount)  
integer r, j(r)  
return  
end
```

```

double precision function prho(n, is, ifault)
c
c      Algorithm AS 89   Appl. Statist. (1975) Vol.24, No. 3, P377.
c
c      To evaluate the probability of obtaining a value greater than or
c      equal to is, where is=(n**3-n)*(1-r)/6, r=Spearman's rho and n
c      must be greater than 1
c
c      Auxiliary function required: ALNORM = algorithm AS66
c
c      dimension l(6)
c      double precision zero, one, two, b, x, y, z, u, six,
$   c1, c2, c3, c4, c5, c6, c7, c8, c9, c10, c11, c12
c      data zero, one, two, six /0.0d0, 1.0d0, 2.0d0, 6.0d0/
c      data      c1,      c2,      c3,      c4,      c5,      c6,
$   c7,      c8,      c9,      c10,      c11,      c12/
$   0.2274d0, 0.2531d0, 0.1745d0, 0.0758d0, 0.1033d0, 0.3932d0,
$   0.0879d0, 0.0151d0, 0.0072d0, 0.0831d0, 0.0131d0, 0.00046d0/
c
c      Test admissibility of arguments and initialize
c
c      prho = one
c      ifault = 1
c      if (n .le. 1) return
c      ifault = 0
c      if (is .le. 0) return
c      prho = zero
c      if (is .gt. n * (n * n -1) / 3) return
c      js = is
c      if (js .ne. 2 * (js / 2)) js = js + 1
c      if (n .gt. 6) goto 6
c
c      Exact evaluation of probability
c
c      nfac = 1
c      do 1 i = 1, n
c         nfac = nfac * i
c         l(i) = i
1 continue
c      prho = one / dble(nfac)
c      if (js .eq. n * (n * n -1) / 3) return
c      ifr = 0
c      do 5 m = 1,nfac
c         ise = 0
c         do 2 i = 1, n
c            ise = ise + (i - l(i)) ** 2
2 continue
c         if (js .le. ise) ifr = ifr + 1
c         n1 = n
3          mt = l(1)
c         nn = n1 - 1
c         do 4 i = 1, nn
c            l(i) = l(i + 1)
4          continue
c         l(n1) = mt
c         if (l(n1) .ne. n1 .or. n1 .eq. 2) goto 5
c         n1 = n1 - 1
c         if (m .ne. nfac) goto 3
5          continue
c      prho = dble(ifr) / dble(nfac)
c      return

```

```
c
c      Evaluation by Edgeworth series expansion
c
6 b = one / dble(n)
  x = (six * (dble(js) - one) * b / (one / (b * b) -one) -
$  one) * sqrt(one / b - one)
  y = x * x
  u = x * b * (c1 + b * (c2 + c3 * b) + y * (-c4
$  + b * (c5 + c6 * b) - y * b * (c7 + c8 * b
$  - y * (c9 - c10 * b + y * b * (c11 - c12 * y))))))
c
c      Call to algorithm AS 66
c
prho = u / exp(y / two) + alnorm(x, .true.)
if (prho .lt. zero) prho = zero
if (prho .gt. one) prho = one
return
end
```

```

double precision function ppchi2(p, v, g, ifault)
c
c   Algorithm AS 91   Appl. Statist. (1975) Vol.24, P.35
c
c   To evaluate the percentage points of the chi-squared
c   probability distribution function.
c
c   p must lie in the range 0.000002 to 0.999998,
c   v must be positive,
c   g must be supplied and should be equal to
c   ln(gamma(v/2.0))
c
c   Incorporates the suggested changes in AS R85 (vol.40(1),
c   pp.233-5, 1991) which should eliminate the need for the limited
c   range for p above, though these limits have not been removed
c   from the routine.
c   If IFAULT = 4 is returned, the result is probably as accurate as
c   the machine will allow.
c
c   Auxiliary routines required: PPND = AS 111 (or AS 241) and
c   GAMMAD = AS 239.
c
integer maxit
parameter (maxit = 20)
double precision p, v, g, gammad, ppnd, aa, e, zero, half, one,
$   two, three, six, pmin, pmax, c1, c2, c3, c4, c5, c6, c7,
$   c8, c9, c10, c11, c12, c13, c14, c15, c16, c17, c18, c19,
$   c20, c21, c22, c23, c24, c25, c26, c27, c28, c29, c30,
$   c31, c32, c33, c34, c35, c36, c37, c38, a, b, c, ch, p1, p2,
$   q, s1, s2, s3, s4, s5, s6, t, x, xx
c
c   data          aa,          e,          pmin,          pmax
$   /0.6931471806d0, 0.5d-6, 0.000002d0, 0.999998d0/
c   data zero, half, one, two, three, six
$   /0.0d0, 0.5d0, 1.0d0, 2.0d0, 3.0d0, 6.0d0/
c   data          c1,          c2,          c3,          c4,          c5,          c6,
$   c7,          c8,          c9,          c10,         c11,         c12,
$   c13,         c14,         c15,         c16,         c17,         c18,
$   c19,         c20,         c21,         c22,         c23,         c24,
$   c25,         c26,         c27,         c28,         c29,         c30,
$   c31,         c32,         c33,         c34,         c35,         c36,
$   c37,         c38/
$   0.01d0, 0.222222d0, 0.32d0, 0.4d0, 1.24d0, 2.2d0,
$   4.67d0, 6.66d0, 6.73d0, 13.32d0, 60.0d0, 70.0d0,
$   84.0d0, 105.0d0, 120.0d0, 127.0d0, 140.0d0, 175.0d0,
$   210.0d0, 252.0d0, 264.0d0, 294.0d0, 346.0d0, 420.0d0,
$   462.0d0, 606.0d0, 672.0d0, 707.0d0, 735.0d0, 889.0d0,
$   932.0d0, 966.0d0, 1141.0d0, 1182.0d0, 1278.0d0, 1740.0d0,
$   2520.0d0, 5040.0d0/
c
c   test arguments and initialise
c
ppchi2 = -one
ifault = 1
if (p .lt. pmin .or. p .gt. pmax) return
ifault = 2
if (v .le. zero) return
ifault = 0
xx = half * v
c = xx - one
c

```

```

c      starting approximation for small chi-squared
c
c      if (v .ge. -c5 * log(p)) goto 1
c      ch = (p * xx * exp(g + xx * aa)) ** (one/xx)
c      if (ch .lt. e) goto 6
c      goto 4
c
c      starting approximation for v less than or equal to 0.32
c
1 if (v .gt. c3) goto 3
  ch = c4
  a = log(one-p)
2 q = ch
  p1 = one + ch * (c7+ch)
  p2 = ch * (c9 + ch * (c8 + ch))
  t = -half + (c7 + two * ch) / p1 - (c9 + ch * (c10 +
$ three * ch)) / p2
  ch = ch - (one - exp(a + g + half * ch + c * aa) *
$ p2 / p1) / t
  if (abs(q / ch - one) .gt. c1) goto 2
  goto 4
c
c      call to algorithm AS 111 - note that p has been tested above.
c      AS 241 could be used as an alternative.
c
3 x = ppnd(p, if1)
c
c      starting approximation using Wilson and Hilferty estimate
c
c      p1 = c2 / v
c      ch = v * (x * sqrt(p1) + one - p1) ** 3
c
c      starting approximation for p tending to 1
c
c      if (ch .gt. c6 * v + six)
c      $ ch = -two * (log(one-p) - c * log(half * ch) + g)
c
c      call to algorithm AS 239 and calculation of seven term
c      Taylor series
c
4 do 7 i = 1, maxit
  q = ch
  p1 = half * ch
  p2 = p - gammad(p1, xx, if1)
  if (if1 .eq. 0) goto 5
c
c      ifault = 3
c      return
5 t = p2 * exp(xx * aa + g + p1 - c * log(ch))
  b = t / ch
  a = half * t - b * c
  s1 = (c19 + a * (c17 + a * (c14 + a * (c13 + a * (c12 +
$ c11 * a)))) / c24
  s2 = (c24 + a * (c29 + a * (c32 + a * (c33 + c35 *
$ a)))) / c37
  s3 = (c19 + a * (c25 + a * (c28 + c31 * a))) / c37
  s4 = (c20 + a * (c27 + c34 * a) + c * (c22 + a * (c30 +
$ c36 * a))) / c38
  s5 = (c13 + c21 * a + c * (c18 + c26 * a)) / c37
  s6 = (c15 + c * (c23 + c16 * c)) / c38

```

```
      ch = ch + t * (one + half * t * s1 - b * c * (s1 - b *  
$ (s2 - b * (s3 - b * (s4 - b * (s5 - b * s6))))))  
      if (abs(q / ch - one) .gt. e) goto 6  
7 continue  
      ifault = 4  
c  
6 ppchi2 = ch  
  return  
  end
```



```
c Routine AS 93 returns frequencies. The following short routine calculates
c the distribution function from these frequencies (overwriting them).
c The calling arguments are as for AS 93. The distribution function is
c returned in array A1. The first element in A1 is F(ASTART). N.B. ASTART
c is a real variable.
```

```
c
c      subroutine wprob(test, other, astart, a1, l1, a2, a3, ifault)
c      integer test, other, l1, ifault
c      real astart, a1(l1), a2(l1), a3(l1)
```

```
c
c      Local variables
```

```
c
c      real zero, sum
c      data zero /0.0/
```

```
c
c      call gscale(test, other, astart, a1, l1, a2, a3, ifault)
c      if (ifault .ne. 0) return
```

```
c
c      Scale column of F
```

```
c
c      nrows = 1 + (test * other)/2
c      sum = zero
c      do 10 i = 1, nrows
c         sum = sum + a1(i)
c         a1(i) = sum
10 continue
c      do 20 i = 1, nrows
c      20 a1(i) = a1(i) / sum
```

```
c
c      return
c      end
```

```
c-----
```

```
      SUBROUTINE GSCALE(TEST, OTHER, ASTART, A1, L1, A2, A3, IFAULT)
```

```
C
C      ALGORITHM AS 93 APPL. STATIST. (1976) VOL.25, NO.1
C
C      FROM THE SIZES OF TWO SAMPLES THE DISTRIBUTION OF THE
C      ANSARI-BRADLEY TEST FOR SCALE IS GENERATED IN ARRAY A1.
```

```
C
C      REAL ASTART, A1(L1), A2(L1), A3(L1), AI, ONE, FPOINT
C      INTEGER TEST, OTHER
C      LOGICAL SYMM
C      DATA ONE /1.0/
```

```
C
C      TYPE CONVERSION (EFFECT DEPENDS ON TYPE STATEMENT ABOVE).
```

```
C
C      FPOINT(I) = I
```

```
C
C      CHECK PROBLEM SIZE AND DEFINE BASE VALUE OF THE DISTRIBUTION.
```

```
C
C      M = MIN0(TEST, OTHER)
C      IFAULT = 2
C      IF (M. LT. 0) RETURN
C      ASTART = FPOINT((TEST + 1) / 2) * FPOINT(1 + TEST / 2)
C      N = MAX0(TEST, OTHER)
```

```
C
C      CHECK SIZE OF RESULT ARRAY.
```

```
C
C      IFAULT = 1
```

```
      LRES = 1 + (M * N) / 2
      IF (L1 .LT. LRES) RETURN
      SYMM = MOD(M + N, 2) .EQ. 0
C
C      TREAT SMALL SAMPLES SEPARATELY.
C
      MM1 = M - 1
      IF (M .GT. 2) GOTO 5
C
C      START-UP PROCEDURES ONLY NEEDED.
C
      IF (MM1) 1, 2, 3
C
C      ONE SAMPLE ONLY.
C
      A1(1) = ONE
      GOTO 15
C
C      SMALLER SAMPLE SIZE = 1.
C
      CALL START1(N, A1, L1, LN1)
      GOTO 4
C
C      SMALLER SAMPLE SIZE = 2.
C
      CALL START2(N, A1, L1, LN1)
C
      RETURN IF A1 IS NOT IN REVERSE ORDER.
C
      IF (SYMM .OR. (OTHER .GT. TEST)) GOTO 15
      GOTO 13
C
C      FULL GENERATOR NEEDED
C      SET UP INITIAL CONDITIONS (DEPENDS ON MOD(N, 2)).
C
      NM1 = N - 1
      NM2 = N - 2
      MNOW = 3
      NC = 3
      IF (MOD(N, 2) .EQ. 1) GOTO 6
C
C      SET UP FOR EVEN N.
C
      N2B1 = 3
      N2B2 = 2
      CALL START2(N, A1, L1, LN1)
      CALL START2(NM2, A3, L1, LN3)
      CALL START1(NM1, A2, L1, LN2)
      GOTO 8
C
C      SET UP FOR ODD N.
C
      N2B1 = 2
      N2B2 = 3
      CALL START1(N, A1, L1, LN1)
      CALL START2(NM1, A2, L1, LN2)
C
C      INCREASE ORDER OF DISTRIBUTION IN A1 BY 2
C      (USING A2 AND IMPLYING A3).
C
      CALL FRQADD(A1, LN1, L1OUT, L1, A2, LN2, N2B1)
      LN1 = LN1 + N
```

```
      CALL IMPLY(A1, L1OUT, LN1, A3, LN3, L1, NC)
      NC = NC + 1
      IF (MNOW .EQ. M) GOTO 9
      MNOW = MNOW + 1
C
C      INCREASE ORDER OF DISTRIBUTION IN A2 BY 2 (USING A3).
C
8     CALL FRQADD(A2, LN2, L2OUT, L1, A3, LN3, N2B2)
      LN2 = LN2 + NM1
      CALL IMPLY(A2, L2OUT, LN2, A3, J, L1, NC)
      NC = NC + 1
      IF (MNOW .EQ. M) GOTO 9
      MNOW = MNOW + 1
      GOTO 7
C
C      IF SYMMETRICAL, RESULTS IN A1 ARE COMPLETE.
C
9     IF (SYMM) GOTO 15
C
C      FOR A SKEW RESULT ADD A2 (OFFSET) INTO A1.
C
      KS = (M + 3) / 2
      J = 1
      DO 12 I = KS, LRES
      IF (I .GT. LN1) GOTO 10
      A1(I) = A1(I) + A2(J)
      GOTO 11
10    A1(I) = A2(J)
11    J = J + 1
12    CONTINUE
C
C      DISTRIBUTION IN A1 POSSIBLY IN REVERSE ORDER.
C
      IF (OTHER .LT. TEST) GOTO 15
C
C      REVERSE THE RESULTS IN A1.
C
13    J = LRES
      NDO = LRES / 2
      DO 14 I = 1, NDO
      AI = A1(I)
      A1(I) = A1(J)
      A1(J) = AI
      J = J - 1
14    CONTINUE
C
C      FINAL RESULTS NOW IN A1.
C
15    IFAULT = 0
      RETURN
      END

SUBROUTINE START1(N, F, L, LOU)

C
C      ALGORITHM AS 93.1 APPL. STATIST. (1976) VOL.25, NO.1
C
C      GENERATES A 1,N ANSARI-BRADLEY DISTRIBUTION IN F.
C
      REAL F(L), ONE, TWO
      DATA ONE, TWO /1.0, 2.0/
      LOU = 1 + N / 2
```

```
1      DO 1 I = 1, LOUT
      F(I) = TWO
      IF (MOD(N, 2) .EQ. 0) F(LOUT) = ONE
      RETURN
      END

C
      SUBROUTINE START2(N, F, L, LOUT)

C
C      ALGORITHM AS 93.2 APPL. STATIST. (1976) VOL.25, NO.1
C
C      GENERATES A 2,N ANSARI-BRADLEY DISTRIBUTION IN F.

C
      REAL F(L), ONE, TWO, THREE, FOUR
      DATA ONE, TWO, THREE, FOUR /1.0, 2.0, 3.0, 4.0/

C
      DERIVE F FOR 2, NU, WHERE NU IS HIGHEST EVEN INTEGER
      LESS THAN OR EQUAL TO N.
      DEFINE NU AND ARRAY LIMITS.

C
      NU = N - MOD(N, 2)
      J = NU + 1
      LOUT = J
      LT1 = LOUT + 1
      NDO = LT1 / 2
      A = ONE
      B = THREE

C
      GENERATE THE SYMMETRICAL 2,NU DISTRIBUTION.

C
      DO 1 I = 1, NDO
      F(I) = A
      F(J) = A
      J = J - 1
      A = A + B
      B = FOUR - B
1     CONTINUE
      IF (NU .EQ. N) RETURN

C
      ADD AN OFFSET 1,N DISTRIBUTION INTO F TO GIVE 2,N RESULT.

C
      NU = NDO + 1
      DO 2 I = NU, LOUT
2     F(I) = F(I) + TWO
      F(LT1) = TWO
      LOUT = LT1
      RETURN
      END

C
      SUBROUTINE FRQADD(F1, L1IN, L1OUT, L1, F2, L2, NSTART)

C
C      ALGORITHM AS 93.3 APPL. STATIST. (1976) VOL.25, NO.1
C
C      ARRAY F1 HAS TWICE THE CONTENTS OF ARRAY F2 ADDED INTO IT
C      STARTING WITH ELEMENTS NSTART AND 1 IN F1 AND F2 RESPECTIVELY.

C
      REAL F1(L1), F2(L2), MUL2
      DATA MUL2 /2.0/
      I2 = 1
      DO 1 I1 = NSTART, L1IN
      F1(I1) = F1(I1) + MUL2 * F2(I2)
      I2 = I2 + 1
```

```
1      CONTINUE
      NXT = L1IN + 1
      L1OUT = L2 + NSTART - 1
      DO 2 I1 = NXT, L1OUT
      F1(I1) = MUL2 * F2(I2)
      I2 = I2 + 1
2      CONTINUE
      NSTART = NSTART + 1
      RETURN
      END

C
      SUBROUTINE IMPLY(F1, L1IN, L1OUT, F2, L2, L2MAX, NOFF)
C
C      ALGORITHM AS 93.4 APPL. STATIST. (1976) VOL.25, NO.1
C
C      GIVEN L1IN ELEMENTS OF AN ARRAY F1, A SYMMETRICAL
C      ARRAY F2 IS DERIVED AND ADDED ONTO F1, LEAVING THE
C      FIRST NOFF ELEMENTS OF F1 UNCHANGED AND GIVING A
C      SYMMETRICAL RESULT OF L1OUT ELEMENTS IN F1.
C
      REAL F1(L1OUT), F2(L2MAX), SUM, DIFF
C
C      SET-UP SUBSCRIPTS AND LOOP COUNTER.
C
      I2 = 1 - NOFF
      J1 = L1OUT
      J2 = L1OUT - NOFF
      L2 = J2
      J2MIN = (J2 + 1) / 2
      NDO = (L1OUT + 1) / 2
C
C      DERIVE AND IMPLY NEW VALUES FROM OUTSIDE INWARDS.
C
      DO 6 I1 = 1, NDO
C
C      GET NEW F1 VALUE FROM SUM OF L/H ELEMENTS OF
C      F1 + F2 (IF F2 IS IN RANGE).
C
      IF (I2 .GT. 0) GOTO 1
      SUM = F1(I1)
      GOTO 2
1      SUM = F1(I1) + F2(I2)
C
C      REVISE LEFT ELEMENT OF F1.
C
      F1(I1) = SUM
C
C      IF F2 NOT COMPLETE IMPLY AND ASSIGN F2 VALUES
C      AND REVISE SUBSCRIPTS.
C
      I2 = I2 + 1
      IF (J2 .LT. J2MIN) GOTO 5
      IF (J1 .LE. L1IN) GOTO 3
      DIFF = SUM
      GOTO 4
3      DIFF = SUM - F1(J1)
4      F2(I1) = DIFF
      F2(J2) = DIFF
      J2 = J2 - 1
C
C      ASSIGN R/H ELEMENT OF F1 AND REVISE SUBSCRIPT.
```

```
C
5      F1(J1) = SUM
      J1 = J1 - 1
6      CONTINUE
      RETURN
      END
```

```
      SUBROUTINE CURVE (P, X, N0, N, EPS, MAXITR, MU, SIGMA, ITER,
1     SEMU, SESIG, COVAR, E0, EX, CHISQ, IFAULT)
C
C     ALGORITHM AS 95 APPL. STATIST. (1976) VOL.25, NO.1
C
C     ESTIMATES MU AND SIGMA OF DISTRIBUTION FUNCTION
C     F( (X-MU)/SIGMA ) FROM A GROUPED SAMPLE OF X VALUES.
C     NOTE ON ARRAY SIZES
C     THE ARRAYS IN THE SECOND DIMENSION STATEMENT MUST HAVE
C     MINIMUM SIZE P.  IF P IS TO EXCEED 20, A SUITABLE SIZE
C     MUST BE SET FOR THEM, AND THE IF STATEMENT WHICH CHECKS
C     THE VALUE OF P MUST BE AMENDED.
C
C     Auxiliary routines required: FUNC & DEVIAT (both user-supplied)
C
C     INTEGER P
C     REAL NN, NI, NP, MU, ONE, ZERO
C     DIMENSION X(P), N(P), EX(P)
C     DIMENSION F(20), F1(20), XN(20)
C     DATA RR/1.0E-10/, ONE/1.0/, ZERO/0.0/
C
C     ERROR EXIT IF P TOO SMALL OR TOO LARGE
C
C     IF (P.LT.2 .OR. P.GT.20) GO TO 80
C     IFAULT = 0
C
C     SET FREQUENCIES IN FLOATING POINT
C
C     XN0 = N0
C     NSUM = N0
C     DO 10 I = 1, P
C       XN(I) = N(I)
C       NSUM = NSUM + N(I)
10    CONTINUE
C     K = P - 1
C     XNSUM = FLOAT(NSUM)
C     NP = XN(P)
C
C     ITERATIVE APPROXIMATION
C
C     DO 40 ITER = 1, MAXITR
C
C     COMPUTE VALUES OF DISTRIBUTION AND DENSITY FUNCTIONS,
C     USING CURRENT VALUES OF MU, SIGMA
C
C     DO 20 I = 1, P
20    CALL FUNC ((X(I) - MU)/SIGMA, F(I), F1(I))
C     DM = ONE - F(P)
C
C     TEST FOR SMALL DIVISOR TO AVOID OVERFLOW
C
C     IF (ABS(DM).LT.RR) GO TO 90
C     F1P = F1(P)
C     IF (ABS(F(1)).LT.RR) GO TO 90
C     XI1 = X(1) - MU
C     XP = X(P) - MU
C     R = F1(1)/F(1)
C     S = F1P/DM
C     T = -XN0*R
C     U = NP*S
```

```
A = T + U
B = XI1*T + XP*U
R = F1(1)*R
S = F1P*S
C = R + S
R = XI1*S
S = XP*S
D = R + S
E = XI1*R + XP*S
DO 30 I = 1, K
  FI = F(I)
  FI1 = F(I + 1)
  F1I1 = F1(I + 1)
  F1I = F1(I)
  XI = XI1
  XI1 = X(I + 1) - MU
  NI = XN(I)
  R = FI1 - FI
  IF (ABS(R).LT.RR) GO TO 90
  S = F1I1 - F1I
  U = XI1*F1I1 - XI*F1I
  SR = S/R
  UR = U/R
  A = A - NI*SR
  B = B - NI*UR
  C = C + S*SR
  D = D + S*UR
  E = E + U*UR
30 CONTINUE
DENOM = (C*E - D*D)*XNSUM
C
C COMPUTE ADJUSTMENTS TO MU, SIGMA
C
SIGDEN = SIGMA/DENOM
DMU = (E*A - D*B)*SIGDEN
DSIGMA = (C*B - D*A)*SIGMA*SIGDEN
MU = MU + DMU
SIGMA = SIGMA + DSIGMA
ERR = ABS(DMU) + ABS(DSIGMA)
C
C TEST FOR CONVERGENCE
C
IF (ERR.LT.EPS) GO TO 50
40 CONTINUE
C
C SET FAULT IF LIMIT FOR NUMBER OF ITERATIONS IS
C REACHED, THEN PROCEED
C
IFFAULT = 4
ITER = MAXITR
50 DO 60 I = 1, P
60 CALL FUNC ((X(I) - MU)/SIGMA, F(I), DUM)
C
C COMPUTE VARIANCES AND COVARIANCE OF ESTIMATES
C
SIGDEN = SIGMA*SIGMA/DENOM
VARMU = E*SIGDEN
SIGDEN = SIGMA*SIGDEN
COVAR = -D*SIGDEN
VARSIG = C*SIGMA*SIGDEN
IF (VARMU.LT.ZERO .OR. VARSIG.LT.ZERO) GO TO 100
```



```
      SEMU = SQRT(VARMU)
      SESIG = SQRT(VARSIG)
C
C      COMPUTE EXPECTED FREQUENCIES AND CHI SQUARE
C
      E0 = XNSUM*F(1)
      EP = XNSUM*(ONE - F(P))
      EX(P) = EP
      CHISQ = ((XN0 - E0)**2)/E0 + ((NP - EP)**2)/EP
      DO 70 I = 1, K
          NN = XNSUM*(F(I+1) - F(I))
          CHISQ = CHISQ + ((NN - XN(I))**2)/NN
          EX(I) = NN
70    CONTINUE
      RETURN
C
C      ERROR EXITS
C
80    IFAULT = 1
      RETURN
90    IFAULT = 2
      RETURN
100   IFAULT = 3
      RETURN
      END
C
C
      SUBROUTINE INITL (P, X, N0, N, MU, SIGMA, IFAULT)
C
C      ALGORITHM AS 95.1 APPL. STATIST. (1976) VOL.25, NO.1
C
C      COMPUTES ROUGH LEAST SQUARES ESTIMATES OF MU AND SIGMA
C      ( FOR DEFINITION OF MU AND SIGMA SEE SUBROUTINE CURVE ).
C
      INTEGER P
      REAL MU, ONE, ZERO
      DIMENSION X(P), N(P)
      DATA ONE/1.0/, ZERO/0.0/
C
C      ERROR EXIT IF P TOO SMALL
C
      IFAULT = 1
      IF (P.LT.2) RETURN
      IFAULT = 0
C
C      COMPUTE AND FLOAT SUM OF FREQUENCIES
C
      NSUM = N0
      DO 10 I = 1, P
10    NSUM = NSUM + N(I)
      XNSUM = FLOAT(NSUM)
C
C      ZERO ACCUMULATORS
C
      NPAR = N0
      XBAR = ZERO
      YBAR = ZERO
      SXX = ZERO
      SXY = ZERO
      SW = ZERO
C
```

```
C      COMPUTE WEIGHTED MEANS XBAR, YBAR, AND CORRECTED SUMS
C      OF X*X AND X*Y.
C
      DO 30 I = 1, P
C
C      NULL FREQUENCIES AT EITHER END OF THE RANGE ARE
C      ZERO WEIGHTED
C
      IF (NPAR.EQ.0 .OR. NPAR.EQ.NSUM) GO TO 20
      PROB = FLOAT(NPAR)/XNSUM
      Y = DEVIAT(PROB)
      CALL FUNC (Y, DUMMY, DFY)
      DX = X(I) - XBAR
      DY = Y - YBAR
      W = DFY*DFY/(PROB*(ONE - PROB))
      SW = SW + W
      FAC = W/SW
      XBAR = XBAR + FAC*DX
      YBAR = YBAR + FAC*DY
      FAC = W*DX*(ONE - FAC)
      SXX = SXX + FAC*DX
      SXY = SXY + FAC*DY
20     NPAR = NPAR + N(I)
30     CONTINUE
      SIGMA = SXX/SXY
      MU = XBAR - SIGMA*YBAR
      RETURN
      END
```

```
      SUBROUTINE SCALE(FMN, FMX, N, VALMIN, STEP, VALMAX, IFAULT)
C
C   ALGORITHM AS 96  APPL. STATIST. (1976) VOL.25, NO.1
C
C   Given extreme values FMN, FMX, and the need for a scale with N
C   marks, calculates value for the lowest scale mark (VALMIN) and
C   step length (STEP) and highest scale mark (VALMAX).
C
      REAL FMN, FMX, VALMIN, STEP, VALMAX
      INTEGER N, IFAULT
C
C   Units for step lengths
C
      REAL UNIT(11)
C
C   Local variables
C
      INTEGER NUNIT, I, J
      REAL TOL, ZERO, HALF, ONE, TEN, BIAS, FMAX, FMIN, RN, X, S, RANGE
C
C   Array length unit()
C
      DATA NUNIT /11/
C
C   Local constant, defining effective equality of values.
C
      DATA TOL /5.0E-6/
      DATA ZERO /0.0/, HALF /0.5/, ONE /1.0/, TEN /10.0/
      DATA BIAS /1.0E-4/
      DATA UNIT /1.0, 1.2, 1.6, 2.0, 2.5, 3.0, 4.0, 5.0, 6.0, 8.0,
*         10.0/
C
      FMAX = FMX
      FMIN = FMN
      IFAULT = 1
C
C   Test for valid parameter values
C
      IF (FMAX .LT. FMIN .OR. N .LE. 1) RETURN
      IFAULT = 0
      RN = N - 1
      X = ABS(FMAX)
      IF (X .EQ. ZERO) X = ONE
      IF ((FMAX - FMIN) / X .GT. TOL) GO TO 20
C
C   All values effectively equal
C
      IF (FMAX .LT. ZERO) THEN
         FMAX = ZERO
      ELSE IF (FMAX .EQ. ZERO) THEN
         FMAX = ONE
      ELSE
         FMIN = ZERO
      END IF
C
      20 STEP = (FMAX - FMIN) / RN
         S = STEP
C
C   Find power of 10
C
      25 IF (S .GE. ONE) GO TO 30
```

```
      S = S * TEN
      GO TO 25
30  IF (S .LT. TEN) GO TO 35
      S = S / TEN
      GO TO 30
C
C   Calculate STEP
C
35  X = S - BIAS
      DO 40 I = 1, NUNIT
          IF (X .LE. UNIT(I)) GO TO 45
40  CONTINUE
45  STEP = STEP * UNIT(I) / S
      RANGE = STEP * RN
C
C   Make first estimate of VALMIN
C
      X = HALF * (ONE + (FMIN + FMAX - RANGE) / STEP)
      J = X - BIAS
      IF (X .LT. ZERO) J = J - 1
      VALMIN = STEP * FLOAT(J)
C
C   Test if VALMIN could be zero
C
      IF (FMIN .GE. ZERO .AND. RANGE .GE. FMAX) VALMIN = ZERO
      VALMAX = VALMIN + RANGE
C
C   Test if VALMAX could be zero
C
      IF (FMAX .GT. ZERO .OR. RANGE .LT. -FMIN) RETURN
      VALMAX = ZERO
      VALMIN = -RANGE
      RETURN
      END
```

```
      SUBROUTINE FORRT(X, M)
C
C   ALGORITHM AS 97  APPL. STATIST. (1976) VOL.25, NO. 2
C
C   Forward discrete Fourier transform in one dimension of real
C   data using complex transform subroutine FASTG.
C
C   X = array of real input data, type real, dimension M.
C   M = length of the transform, must be a power of 2.
C   The minimum length is 8, maximum 2**21.
C
C   The result is placed in X as described in the text of the paper.
C
C   Auxiliary routines required: SCRAG (or SCRAM) & FASTG from AS 83,
C   but with SCRAG modified as described on page 168 of the paper for
C   this algorithm.
C
      REAL X(M)
      DATA ZERO/0.0/, QUART/0.25/, HALF/0.5/, ONE/1.0/, ONE5/1.5/,
*     TWO/2.0/, FOUR/4.0/
C
C   Check for valid transform size.
C
      II = 8
      DO 2 K = 3, 21
          IPOW = K
          IF (II .EQ. M) GO TO 3
          II = II * 2
2     CONTINUE
C
C   If this point is reached, an illegal size was specified.
C
      RETURN
3     PIE = FOUR * ATAN(ONE)
C
C   Separate odd and even parts into two halves.
C   First bit reverse the whole array of length M.
C
      CALL SCRAG(X, M, IPOW)
C
C   Next bit reverse the half arrays separately.
C
      N = M / 2
      JPOW = IPOW - 1
      CALL SCRAG(X, N, JPOW)
      CALL SCRAG(X(N+1), N, JPOW)
C
C   Faster alternative to the two lines above to SCRAM.
C       CALL SCRAM(X, X(N+1), N, JPOW)
C
C   Now do the transform.
C
      CALL FASTG(X, X(N+1), N, 1)
C
C   Unscramble the transform results.
C
      CALL SCRAG(X, N, JPOW)
      CALL SCRAG(X(N+1), N, JPOW)
C
C   Faster alternative to the two lines above to SCRAM.
C       CALL SCRAM(X, X(N+1), N, JPOW)
```

```
C
  NN = N / 2
C
C   Now unravel the result; first the special cases.
C
  Z = HALF * (X(1) + X(N+1))
  X(N+1) = HALF * (X(1) - X(N+1))
  X(1) = Z
  NN1 = NN + 1
  NN2 = NN1 + N
  X(NN1) = HALF * X(NN1)
  X(NN2) = -HALF * X(NN2)
  Z = PIE / N
  BCOS = -TWO * (SIN(Z / TWO) **2)
  BSIN = SIN(Z)
  UN = ONE
  VN = ZERO
  DO 4 K = 2, NN
    Z = UN * BCOS + VN * BSIN + UN
    VN = VN * BCOS - UN * BSIN + VN
    SAVE1 = ONE5 - HALF * (Z * Z + VN * VN)
    UN = Z * SAVE1
    VN = VN * SAVE1
    KI = N + K
    L = N + 2 - K
    LI = N + L
    AN = QUART * (X(K) + X(L))
    BN = QUART * (X(KI) - X(LI))
    CN = QUART * (X(KI) + X(LI))
    DN = QUART * (X(L) - X(K))
    XN = UN * CN - VN * DN
    YN = UN * DN + VN * CN
    X(K) = AN + XN
    X(KI) = BN + YN
    X(L) = AN - XN
    X(LI) = YN - BN
4 CONTINUE
  RETURN
  END
C
  SUBROUTINE REVRT(X, M)
C
C   ALGORITHM AS 97.1 APPL. STATIST. (1976) VOL.25, NO. 2
C
C   Inverse discrete Fourier transform in one dimension of real
C   data using complex transform subroutine FASTG.
C
C   X = array of Fourier components as output from subroutine FORRT,
C       type real, dimension M.
C   M = length of the inverse transform, must be a power of 2.
C   The minimum length is 8, maximum 2**21.
C
C   Auxiliary routines required: SCRAG & FASTG from AS 83, but
C   with SCRAG modified as described on page 168 of the paper for
C   this algorithm.
C
  REAL X(M)
  DATA ZERO/0.0/, HALF/0.5/, ONE/1.0/, ONE5/1.5/,
*   TWO/2.0/, FOUR/4.0/
C
```

```
C      Check for valid transform size.
C
      II = 8
      DO 2 K = 3, 21
        IPOW = K
        IF (II .EQ. M) GO TO 3
        II = II * 2
2 CONTINUE

C
C      If this point is reached, an illegal size was specified.
C
      RETURN
3 PIE = FOUR * ATAN(ONE)
      N = M / 2
      NN = N / 2

C
C      Undo the spectrum into that of two interleaved series.
C      First, the special cases.
C
      Z = X(1) + X(N+1)
      X(N+1) = X(1) - X(N+1)
      X(1) = Z
      NN1 = NN + 1
      NN2 = NN1 + N
      X(NN1) = TWO * X(NN1)
      X(NN2) = -TWO * X(NN2)
      Z = PIE / N
      BCOS = -TWO * (SIN(Z / TWO) **2)
      BSIN = SIN(Z)
      UN = ONE
      VN = ZERO
      DO 4 K = 2, NN
        Z = UN * BCOS + VN * BSIN + UN
        VN = VN * BCOS - UN * BSIN + VN
        SAVE1 = ONE5 - HALF * (Z * Z + VN * VN)
        UN = Z * SAVE1
        VN = VN * SAVE1
        KI = N + K
        L = N + 2 - K
        LI = N + L
        AN = X(K) + X(L)
        BN = X(KI) - X(LI)
        PN = X(K) - X(L)
        QN = X(KI) + X(LI)
        CN = UN * PN + VN * QN
        DN = UN * QN - VN * PN
        X(K) = AN - DN
        X(KI) = BN + CN
        X(L) = AN + DN
        X(LI) = CN - BN
4 CONTINUE

C
C      Now do the inverse transform
C
      CALL FASTG(X, X(N+1), N, -1)

C
C      Now undo the order - the half arrays are already bit reversed;
C      bit reverse the whole array.
C
      CALL SCRAG(X, M, IPOW)
      RETURN
```

END

```

C
  subroutine fastg(xreal, ximag, n, itype)
C
C   Algorithm AS 83.2 Appl. Statist. (1975) vol.24, no.1
C
C   Radix 4 complex discrete fast Fourier transform without
C   unscrambling, suitable for convolutions or other applications
C   which do not require unscrambling.  Called by subroutine
C   FASTF which also does the unscrambling.
C
  real    xreal(n), ximag(n)
  data    zero, half, one, one5, two, four
+         /0.0, 0.5, 1.0, 1.5, 2.0, 4.0/
  pi = four * atan(one)
  ifaca = n / 4
  if (itype .eq. 0) return
  if (itype .gt. 0) go to 5
C
C   ITYPE < 0 indicates inverse transform required.
C   Calculate conjugate.
C
  do 4 k = 1, n
4   ximag(k) = -ximag(k)
C
C   Following code is executed for IFACA = N/4, N/16, N/64, ...
C   until IFACA <= 1.
C
5   ifcab = ifaca * 4
   z = pi / ifcab
   bcos = -two * sin(z)**2
   bsin = sin(two * z)
   cw1 = one
   sw1 = zero
   do 10 litla = 1, ifaca
     do 8 i0 = litla, n, ifcab
       i1 = i0 + ifaca
       i2 = i1 + ifaca
       i3 = i2 + ifaca
       xs0 = xreal(i0) + xreal(i2)
       xs1 = xreal(i0) - xreal(i2)
       ys0 = ximag(i0) + ximag(i2)
       ys1 = ximag(i0) - ximag(i2)
       xs2 = xreal(i1) + xreal(i3)
       xs3 = xreal(i1) - xreal(i3)
       ys2 = ximag(i1) + ximag(i3)
       ys3 = ximag(i1) - ximag(i3)
       xreal(i0) = xs0 + xs2
       ximag(i0) = ys0 + ys2
       x1 = xs1 + ys3
       y1 = ys1 - xs3
       x2 = xs0 - xs2
       y2 = ys0 - ys2
       x3 = xs1 - ys3
       y3 = ys1 + xs3
       if (litla .eq. 1) then
         xreal(i2) = x1
         ximag(i2) = y1
         xreal(i1) = x2
         ximag(i1) = y2
         xreal(i3) = x3

```



```
        ximag(i3) = y3
    else
        xreal(i2) = x1 * cw1 + y1 * sw1
        ximag(i2) = y1 * cw1 - x1 * sw1
        xreal(i1) = x2 * cw2 + y2 * sw2
        ximag(i1) = y2 * cw2 - x2 * sw2
        xreal(i3) = x3 * cw3 + y3 * sw3
        ximag(i3) = y3 * cw3 - x3 * sw3
    end if
8    continue
c
c    Calculate a new set of twiddle factors.
c
    if (litla .lt. ifaca) then
        z = cw1 * bcos - sw1 * bsin + cw1
        sw1 = bcos * sw1 + bsin * cw1 + sw1
        tempr = one5 - half * (z * z + sw1 * sw1)
        cw1 = z * tempr
        sw1 = sw1 * tempr
        cw2 = cw1 * cw1 - sw1 * sw1
        sw2 = two * cw1 * sw1
        cw3 = cw1 * cw2 - sw1 * sw2
        sw3 = cw1 * sw2 + cw2 * sw1
    end if
10   continue
    if (ifaca .le. 1) go to 14
c
c    Set up the transform split for the next stage.
c
    ifaca = ifaca / 4
    if (ifaca .gt. 0) go to 5
c
c    Radix 2 calculation, if needed.
c
    if (ifaca .lt. 0) return
    do 13 k = 1, n, 2
        tempr = xreal(k) + xreal(k+1)
        xreal(k+1) = xreal(k) - xreal(k+1)
        xreal(k) = tempr
        tempr = ximag(k) + ximag(k+1)
        ximag(k+1) = ximag(k) - ximag(k+1)
        ximag(k) = tempr
13   continue
14   if (itype .lt. 0) then
c
c    Inverse transform; conjugate the result.
c
        do 16 k = 1, n
16      ximag(k) = -ximag(k)
        return
    end if
c
c    Forward transform
c
    z = one / n
    do 18 k = 1, n
        xreal(k) = xreal(k) * z
        ximag(k) = ximag(k) * z
18   continue
c
    return
```



```
end if  
j20 = j20 + itop
```

```
9 continue  
c  
return  
end
```

```
CSTART OF AS 99
  SUBROUTINE JNSN(XBAR, SD, RB1, BB2, ITYPE, GAMMA, DELTA,
  $ XLAM, XI, IFAULT)
C
C      ALGORITHM AS 99  APPL. STATIST. (1976) VOL.25, P.180
C
C      FINDS TYPE AND PARAMETERS OF A JOHNSON CURVE
C      WITH GIVEN FIRST FOUR MOMENTS
C
  REAL XBAR, SD, RB1, BB2, GAMMA, DELTA, XLAM, XI, TOL,
  $ B1, B2, Y, X, U, W, ZERO, ONE, TWO, THREE, FOUR, HALF,
  $ QUART, ZABS, ZEXP, ZLOG, ZSIGN, ZSQRT
  LOGICAL FAULT
C
  DATA TOL /0.01/
  DATA ZERO, QUART, HALF, ONE, TWO, THREE, FOUR
  $ /0.0, 0.25, 0.5, 1.0, 2.0, 3.0, 4.0/
C
  ZABS(X) = ABS(X)
  ZEXP(X) = EXP(X)
  ZLOG(X) = ALOG(X)
  ZSIGN(X, Y) = SIGN(X, Y)
  ZSQRT(X) = SQRT(X)
C
  IFAULT = 1
  IF (SD .LT. ZERO) RETURN
  IFAULT = 0
  XI = ZERO
  XLAM = ZERO
  GAMMA = ZERO
  DELTA = ZERO
  IF (SD .GT. ZERO) GOTO 10
  ITYPE = 5
  XI = XBAR
  RETURN
10 B1 = RB1 * RB1
  B2 = BB2
  FAULT = .FALSE.
C
  TEST WHETHER LOGNORMAL (OR NORMAL) REQUESTED
C
  IF (B2 .GE. ZERO) GOTO 30
20 IF (ZABS(RB1) .LE. TOL) GOTO 70
  GOTO 80
C
  TEST FOR POSITION RELATIVE TO BOUNDARY LINE
C
30 IF (B2 .GT. B1 + TOL + ONE) GOTO 60
  IF (B2 .LT. B1 + ONE) GOTO 50
C
  ST DISTRIBUTION
C
40 ITYPE = 5
  Y = HALF + HALF * ZSQRT(ONE - FOUR / (B1 + FOUR))
  IF (RB1 .GT. ZERO) Y = ONE - Y
  X = SD / ZSQRT(Y * (ONE - Y))
  XI = XBAR - Y * X
  XLAM = XI + X
  DELTA = Y
  RETURN
50 IFAULT = 2
```

```

        RETURN
    60 IF (ZABS(RB1) .GT. TOL .OR. ZABS(B2 - THREE) .GT. TOL) GOTO 80
C
C     NORMAL DISTRIBUTION
C
    70 ITYPE = 4
        DELTA = ONE / SD
        GAMMA = -XBAR / SD
        RETURN
C
C     TEST FOR POSITION RELATIVE TO LOGNORMAL LINE
C
    80 X = HALF * B1 + ONE
        Y = ZABS(RB1) * ZSQRT(QUART * B1 + ONE)
        U = (X + Y) ** (ONE / THREE)
        W = U + ONE / U - ONE
        U = W * W * (THREE + W * (TWO + W)) - THREE
        IF (B2 .LT. ZERO .OR. FAULT) B2 = U
        X = U - B2
        IF (ZABS(X) .GT. TOL) GOTO 90
C
C     LOGNORMAL (SL) DISTRIBUTION
C
        ITYPE = 1
        XLAM = ZSIGN(ONE, RB1)
        U = XLAM * XBAR
        X = ONE / ZSQRT(ZLOG(W))
        DELTA = X
        Y = HALF * X * ZLOG(W * (W - ONE) / (SD * SD))
        GAMMA = Y
        XI = XLAM * (U - ZEXP((HALF / X - Y) / X))
        RETURN
C
C     SB OR SU DISTRIBUTION
C
    90 IF (X .GT. ZERO) GOTO 100
        ITYPE = 2
        CALL SUFIT(XBAR, SD, RB1, B2, GAMMA, DELTA, XLAM, XI)
        RETURN
    100 ITYPE = 3
        CALL SBFIT(XBAR, SD, RB1, B2, GAMMA, DELTA, XLAM, XI, FAULT)
        IF (.NOT. FAULT) RETURN
C
C     FAILURE - TRY TO FIT APPROXIMATE RESULT
C
        IFAULT = 3
        IF (B2 .GT. B1 + TWO) GOTO 20
        GOTO 40
        END
C
        SUBROUTINE SUFIT (XBAR, SD, RB1, B2, GAMMA, DELTA, XLAM, XI)
C
C     ALGORITHM AS 99.1 APPL. STATIST. (1976) VOL.25, P.180
C
C     FINDS PARAMETERS OF JOHNSON SU CURVE WITH
C     GIVEN FIRST FOUR MOMENTS
C
        REAL XBAR, SD, RB1, B2, GAMMA, DELTA, XLAM, XI, TOL, B1,
$ B3, W, Y, W1, WM1, Z, V, A, B, X, ZERO, ONE, TWO, THREE,
$ FOUR, SIX, SEVEN, EIGHT, NINE, TEN, HALF, ONE5, TWO8,
$ SIXTEN, ZABS, ZEXP, ZLOG, ZSIGN, ZSQRT

```

```

C
DATA TOL /0.01/
DATA ZERO, ONE, TWO, THREE, FOUR, SIX, SEVEN,
$ EIGHT, NINE, TEN, SIXTEN, HALF, ONE5, TWO8
$ /0.0, 1.0, 2.0, 3.0, 4.0, 6.0, 7.0,
$ 8.0, 9.0, 10.0, 16.0, 0.5, 1.5, 2.8/

C
ZABS(X) = ABS(X)
ZEXP(X) = EXP(X)
ZLOG(X) = ALOG(X)
ZSIGN(X, Y) = SIGN(X, Y)
ZSQRT(X) = SQRT(X)

C
B1 = RB1 * RB1
B3 = B2 - THREE

C
W IS FIRST ESTIMATE OF EXP(DELTA ** (-2))

C
W = ZSQRT(TWO * B2 - TWO8 * B1 - TWO)
W = ZSQRT(W-ONE)
IF (ZABS(RB1) .GT. TOL) GOTO 10

C
SYMMETRICAL CASE - RESULTS ARE KNOWN

C
Y = ZERO
GOTO 20

C
JOHNSON ITERATION (USING Y FOR HIS M)

C
10 W1 = W + ONE
WM1 = W - ONE
Z = W1 * B3
V = W * (SIX + W * (THREE + W))
A = EIGHT * (WM1 * (THREE + W * (SEVEN + V)) - Z)
B = SIXTEN * (WM1 * (SIX + V) - B3)
Y = (ZSQRT(A * A - TWO * B * (WM1 * (THREE + W *
$ (NINE + W * (TEN + V))) - TWO * W1 * Z)) - A) / B
Z = Y * WM1 * (FOUR * (W + TWO) * Y + THREE * W1 * W1) ** 2 /
$ (TWO * (TWO * Y + W1) ** 3)
V = W * W
W = ZSQRT(ONE - TWO * (ONE5 - B2 + (B1 *
$ (B2 - ONE5 - V * (ONE + HALF * V))) / Z))
W = ZSQRT(W-ONE)
IF (ZABS(B1 - Z) .GT. TOL) GOTO 10

C
END OF ITERATION

C
Y = Y / W
Y = ZLOG(ZSQRT(Y) + ZSQRT(Y + ONE))
IF (RB1 .GT. ZERO) Y = -Y
20 X = ZSQRT(ONE / ZLOG(W))
DELTA = X
GAMMA = Y * X
Y = ZEXP(Y)
Z = Y * Y
X = SD / ZSQRT(HALF * (W - ONE) * (HALF * W *
$ (Z + ONE / Z) + ONE))
XLAM = X
XI = (HALF * ZSQRT(W) * (Y - ONE / Y)) * X + XBAR
RETURN
END

```

```

SUBROUTINE SBFIT(XBAR, SIGMA, RTB1, B2, GAMMA, DELTA, XLAM,
$ XI, FAULT)

```

```

C
C     ALGORITHM AS 99.2  APPL. STATIST. (1976) VOL.25, P.180
C

```

```

C     FINDS PARAMETERS OF JOHNSON SB CURVE WITH
C     GIVEN FIRST FOUR MOMENTS
C

```

```

REAL HMU(6), DERIV(4), DD(4), XBAR, SIGMA, RTB1, B2, GAMMA,
$ DELTA, XLAM, XI, TT, TOL, RB1, B1, E, U, X, Y, W, F, D,
$ G, S, H2, T, H2A, H2B, H3, H4, RBET, BET2, ZERO, ONE,
$ TWO, THREE, FOUR, SIX, HALF, QUART, ONE5, A1, A2, A3,
$ A4, A5, A6, A7, A8, A9, A10, A11, A12, A13, A14, A15,
$ A16, A17, A18, A19, A20, A21, A22, ZABS, ZLOG, ZSQRT
LOGICAL NEG, FAULT

```

```

C
DATA TT, TOL, LIMIT /1.0E-4, 0.01, 50/
DATA ZERO, ONE, TWO, THREE, FOUR, SIX, HALF, QUART, ONE5
$ /0.0, 1.0, 2.0, 3.0, 4.0, 6.0, 0.5, 0.25, 1.5/
DATA A1, A2, A3, A4, A5, A6,
$ A7, A8, A9, A10, A11, A12,
$ A13, A14, A15, A16, A17, A18,
$ A19, A20, A21, A22
$ /0.0124, 0.0623, 0.4043, 0.408, 0.479, 0.485,
$ 0.5291, 0.5955, 0.626, 0.64, 0.7077, 0.7466,
$ 0.8, 0.9281, 1.0614, 1.25, 1.7973, 1.8,
$ 2.163, 2.5, 8.5245, 11.346/

```

```

C
ZABS(X) = ABS(X)
ZLOG(X) = ALOG(X)
ZSQRT(X) = SQRT(X)

```

```

C
RB1 = ZABS(RTB1)
B1 = RB1 * RB1
NEG = RTB1 .LT. ZERO

```

```

C
C     GET D AS FIRST ESTIMATE OF DELTA
C

```

```

E = B1 + ONE
X = HALF * B1 + ONE
Y = ZABS(RB1) * ZSQRT(QUART * B1 + ONE)
U = (X + Y) ** (ONE / THREE)
W = U + ONE / U - ONE
F = W * W * (THREE + W * (TWO + W)) - THREE
E = (B2 - E) / (F - E)
IF (ZABS(RB1) .GT. TOL) GOTO 5
F = TWO
GOTO 20
5 D = ONE / ZSQRT(ZLOG(W))
IF (D .LT. A10) GOTO 10
F = TWO - A21 / (D * (D * (D - A19) + A22))
GOTO 20
10 F = A16 * D
20 F = E * F + ONE
IF (F .LT. A18) GOTO 25
D = (A9 * F - A4) * (THREE - F) ** (-A5)
GOTO 30
25 D = A13 * (F - ONE)

```

```

C
C     GET G AS FIRST ESTIMATE OF GAMMA
C

```

```

30 G = ZERO
   IF (B1 .LT. TT) GOTO 70
   IF (D .GT. ONE) GOTO 40
   G = (A12 * D ** A17 + A8) * B1 ** A6
   GOTO 70
40 IF (D .LE. A20) GOTO 50
   U = A1
   Y = A7
   GOTO 60
50 U = A2
   Y = A3
60 G = B1 ** (U * D + Y) * (A14 + D * (A15 * D - A11))
70 M = 0

C
C     MAIN ITERATION STARTS HERE
C

80 M = M + 1
   FAULT = M .GT. LIMIT
   IF (FAULT) RETURN

C
C     GET FIRST SIX MOMENTS FOR LATEST G AND D VALUES
C

   CALL MOM(G, D, HMU, FAULT)
   IF (FAULT) RETURN
   S = HMU(1) * HMU(1)
   H2 = HMU(2) - S
   FAULT = H2 .LE. ZERO
   IF (FAULT) RETURN
   T = ZSQRT(H2)
   H2A = T * H2
   H2B = H2 * H2
   H3 = HMU(3) - HMU(1) * (THREE * HMU(2) - TWO * S)
   RBET = H3 / H2A
   H4 = HMU(4) - HMU(1) * (FOUR * HMU(3) - HMU(1) *
$ (SIX * HMU(2) - THREE * S))
   BET2 = H4 / H2B
   W = G * D
   U = D * D

C
C     GET DERIVATIVES
C

   DO 120 J = 1, 2
   DO 110 K = 1, 4
   T = K
   IF (J .EQ. 1) GOTO 90
   S = ((W - T) * (HMU(K) - HMU(K + 1)) + (T + ONE) *
$ (HMU(K + 1) - HMU(K + 2))) / U
   GOTO 100
90 S = HMU(K + 1) - HMU(K)
100 DD(K) = T * S / D
110 CONTINUE
   T = TWO * HMU(1) * DD(1)
   S = HMU(1) * DD(2)
   Y = DD(2) - T
   DERIV(J) = (DD(3) - THREE * (S + HMU(2) * DD(1) - T * HMU(1))
$ - ONE5 * H3 * Y / H2) / H2A
   DERIV(J + 2) = (DD(4) - FOUR * (DD(3) * HMU(1) + DD(1) * HMU(3))
$ + SIX * (HMU(2) * T + HMU(1) * (S - T * HMU(1)))
$ - TWO * H4 * Y / H2) / H2B
120 CONTINUE
   T = ONE / (DERIV(1) * DERIV(4) - DERIV(2) * DERIV(3))

```



```

      U = (DERIV(4) * (RBET - RB1) - DERIV(2) * (BET2 - B2)) * T
      Y = (DERIV(1) * (BET2 - B2) - DERIV(3) * (RBET - RB1)) * T

```

```

C
C
C

```

```

      FORM NEW ESTIMATES OF G AND D

```

```

      G = G - U
      IF (B1 .EQ. ZERO .OR. G .LT. ZERO) G = ZERO
      D = D - Y
      IF (ZABS(U) .GT. TT .OR. ZABS(Y) .GT. TT) GOTO 80

```

```

C
C
C

```

```

      END OF ITERATION

```

```

      DELTA = D
      XLAM = SIGMA / ZSQRT(H2)
      IF (NEG) GOTO 130
      GAMMA = G
      GOTO 140

```

```

130 GAMMA = -G
      HMU(1) = ONE - HMU(1)
140 XI = XBAR - XLAM * HMU(1)
      RETURN
      END

```

```

C

```

```

      SUBROUTINE MOM(G, D, A, FAULT)

```

```

C
C
C
C
C
C

```

```

      ALGORITHM AS 99.3 APPL. STATIST. (1976) VOL.25, P.180

```

```

      EVALUATES FIRST SIX MOMENTS OF A JOHNSON
      SB DISTRIBUTION, USING GOODWIN METHOD

```

```

      REAL A(6), B(6), C(6), G, D, ZZ, VV, RTTWO, RRTPI, W, E, R,
$ H, T, U, Y, X, V, F, Z, S, P, Q, AA, AB, EXPA, EXPB,
$ ZERO, QUART, HALF, P75, ONE, TWO, THREE, ZABS, ZEXP
      LOGICAL L, FAULT

```

```

C

```

```

      DATA ZZ, VV, LIMIT /1.0E-5, 1.0E-8, 500/

```

```

C
C
C
C
C
C
C
C

```

```

      RTTWO IS SQRT(2.0)
      RRTPI IS RECIPROCAL OF SQRT(PI)
      EXPA IS A VALUE SUCH THAT EXP(EXPA) DOES NOT QUITE
      CAUSE OVERFLOW
      EXPB IS A VALUE SUCH THAT 1.0 + EXP(-EXPB) MAY BE
      TAKEN TO BE 1.0

```

```

      DATA RTTWO, RRTPI, EXPA, EXPB
$ /1.414213562, 0.5641895835, 80.0, 23.7/
      DATA ZERO, QUART, HALF, P75, ONE, TWO, THREE
$ /0.0, 0.25, 0.5, 0.75, 1.0, 2.0, 3.0/

```

```

C

```

```

      ZABS(X) = ABS(X)
      ZEXP(X) = EXP(X)

```

```

C

```

```

      FAULT = .FALSE.
      DO 10 I = 1, 6

```

```

10 C(I) = ZERO
      W = G / D

```

```

C
C
C

```

```

      TRIAL VALUE OF H

```

```

      IF (W .GT. EXPA) GOTO 140
      E = ZEXP(W) + ONE

```

```
      R = RTTWO / D
      H = P75
      IF (D .LT. THREE) H = QUART * D
      K = 1
      GOTO 40
C
C      START OF OUTER LOOP
C
20  K = K + 1
      IF (K .GT. LIMIT) GOTO 140
      DO 30 I = 1, 6
30  C(I) = A(I)
C
C      NO CONVERGENCE YET - TRY SMALLER H
C
      H = HALF * H
40  T = W
      U = T
      Y = H * H
      X = TWO * Y
      A(1) = ONE / E
      DO 50 I = 2, 6
50  A(I) = A(I - 1) / E
      V = Y
      F = R * H
      M = 0
C
C      START OF INNER LOOP
C      TO EVALUATE INFINITE SERIES
C
60  M = M + 1
      IF (M .GT. LIMIT) GOTO 140
      DO 70 I = 1, 6
70  B(I) = A(I)
      U = U - F
      Z = ONE
      IF (U .GT. -EXPB) Z = ZEXP(U) + Z
      T = T + F
      L = T .GT. EXPB
      IF (.NOT. L) S = ZEXP(T) + ONE
      P = ZEXP(-V)
      Q = P
      DO 90 I = 1, 6
      AA = A(I)
      P = P / Z
      AB = AA
      AA = AA + P
      IF (AA .EQ. AB) GOTO 100
      IF (L) GOTO 80
      Q = Q / S
      AB = AA
      AA = AA + Q
      L = AA .EQ. AB
80  A(I) = AA
90  CONTINUE
100 Y = Y + X
      V = V + Y
      DO 110 I = 1, 6
      IF (A(I) .EQ. ZERO) GOTO 140
      IF (ZABS((A(I) - B(I)) / A(I)) .GT. VV) GOTO 60
110 CONTINUE
```

```
C
C      END OF INNER LOOP
C
      V = RRTPI * H
      DO 120 I = 1, 6
120  A(I) = V * A(I)
      DO 130 I = 1, 6
      IF (A(I) .EQ. ZERO) GOTO 140
      IF (ZABS((A(I) - C(I)) / A(I)) .GT. ZZ) GOTO 20
130  CONTINUE
C
C      END OF OUTER LOOP
C
      RETURN
140  FAULT = .TRUE.
      RETURN
      END
CEND OF AS 99
```

```
CSTART OF AS 100
      REAL FUNCTION AJV(SNV, ITYPE, GAMMA, DELTA, XLAM, XI, IFAULT)
C
C      ALGORITHM AS 100.1  APPL. STATIST. (1976) VOL.25, P.190
C
C      CONVERTS A STANDARD NORMAL VARIATE (SNV) TO A
C      JOHNSON VARIATE (AJV)
C
      REAL SNV, GAMMA, DELTA, XLAM, XI, V, W, ZERO, HALF, ONE,
$      ZABS, ZEXP, ZSIGN
C
      DATA ZERO, HALF, ONE /0.0, 0.5, 1.0/
C
      ZABS(W) = ABS(W)
      ZEXP(W) = EXP(W)
      ZSIGN(W, V) = SIGN(W, V)
C
      AJV = ZERO
      IFAULT = 1
      IF (ITYPE .LT. 1 .OR. ITYPE .GT. 4) RETURN
      IFAULT = 0
      GOTO (10, 20, 30, 40), ITYPE
C
      SL DISTRIBUTION
C
10  AJV = XLAM * ZEXP((XLAM * SNV - GAMMA) / DELTA) + XI
      RETURN
C
      SU DISTRIBUTION
C
20  W = ZEXP((SNV - GAMMA) / DELTA)
      W = HALF * (W - ONE / W)
      AJV = XLAM * W + XI
      RETURN
C
      SB DISTRIBUTION
C
30  W = (SNV - GAMMA) / DELTA
      V = ZEXP(-ZABS(W))
      V = (ONE - V) / (ONE + V)
      AJV = HALF * XLAM * (ZSIGN(V, W) + ONE) + XI
      RETURN
C
      NORMAL DISTRIBUTION
C
40  AJV = (SNV - GAMMA) / DELTA
      RETURN
      END
C
      REAL FUNCTION SNV(AJV, ITYPE, GAMMA, DELTA, XLAM, XI, IFAULT)
C
C      ALGORITHM AS 100.2  APPL. STATIST. (1976) VOL.25, P.190
C
C      CONVERTS A JOHNSON VARIATE (AJV) TO A
C      STANDARD NORMAL VARIATE (SNV)
C
      REAL AJV, GAMMA, DELTA, XLAM, XI, V, W, C, ZERO, HALF, ONE,
$      ZLOG, ZSQRT
C
      DATA ZERO, HALF, ONE, C /0.0, 0.5, 1.0, -63.0/
C
```

```
      ZLOG(W) = ALOG(W)
      ZSQRT(W) = SQRT(W)
C
      SNV = ZERO
      IFAULT = 1
      IF (ITYPE .LT. 1 .OR. ITYPE .GT. 4) RETURN
      IFAULT = 0
      GOTO (10, 20, 30, 40), ITYPE
C
      SL DISTRIBUTION
C
      10 W = XLAM * (AJV - XI)
         IF (W .LE. ZERO) GOTO 15
         SNV = XLAM * (ZLOG(W) * DELTA + GAMMA)
         RETURN
      15 IFAULT = 2
         RETURN
C
      SU DISTRIBUTION
C
      20 W = (AJV - XI) / XLAM
         IF (W .GT. C) GOTO 23
         W = -HALF / W
         GOTO 27
      23 W = ZSQRT(W * W + ONE) + W
      27 SNV = ZLOG(W) * DELTA + GAMMA
         RETURN
C
      SB DISTRIBUTION
C
      30 W = AJV - XI
         V = XLAM - W
         IF (W .LE. ZERO .OR. V .LE. ZERO) GOTO 35
         SNV = ZLOG(W / V) * DELTA + GAMMA
         RETURN
      35 IFAULT = 2
         RETURN
C
      NORMAL DISTRIBUTION
C
      40 SNV = DELTA * AJV + GAMMA
         RETURN
      END
CEND OF AS 100
```

```
REAL FUNCTION DIGAMA(X, IFAULT)
C
C ALGORITHM AS 103 APPL. STATIST. (1976) VOL.25, NO.3
C
C Calculates DIGAMMA(X) = D( LOG( GAMMA(X))) / DX
C
REAL ZERO, HALF, ONE
C
C Set constants, SN = Nth Stirling coefficient, D1 = DIGAMMA(1.0)
C
DATA ZERO/0.0/, HALF/0.5/, ONE/1.0/
DATA S, C, S3, S4, S5, D1 /1.E-05, 8.5, 8.333333333E-02,
* 8.333333333E-03, 3.96825 3968E-03, -0.57721 56649/
C
C Check argument is positive
C
DIGAMA = ZERO
Y = X
IFault = 1
IF (Y .LE. ZERO) RETURN
IFault = 0
C
C Use approximation if argument <= S
C
IF (Y .LE. S) THEN
  DIGAMA = D1 - ONE / Y
  RETURN
END IF
C
C Reduce to DIGAMA(X + N) where (X + N) >= C
C
1 IF (Y .GE. C) GO TO 2
DIGAMA = DIGAMA - ONE/Y
Y = Y + ONE
GO TO 1
C
C Use Stirling's (actually de Moivre's) expansion if argument > C
C
2 R = ONE / Y
DIGAMA = DIGAMA + LOG(Y) - HALF*R
R = R * R
DIGAMA = DIGAMA - R*(S3 - R*(S4 - R*S5))
RETURN
END
```

```
      SUBROUTINE SEQUAL(BDRY, LBDRY, VEC, LVEC, NSTRD, LNSTRD, NDECNS,  
*      NSTOP, PROBS, IPROB1, IPROB2, TSTEPS, INCS, UNITT, RESULT,  
*      IFAULT)  
C  
C      ALGORITHM AS 107  APPL.STATIST. (1977), VOL.26, NO.1  
C  
C      Calculates the first (M-1) operating characteristics and the  
C      average sampling number, given the parameter, for a general closed  
C      sequential sampling plan with M terminal decisions.  
C  
      INTEGER LBDRY, LVEC, LNSTRD, NSTRD(LNSTRD), NDECNS, NSTOP, IPROB1,  
*      IPROB2, INCS(IPROB2), IFAULT  
      REAL BDRY(LBDRY), VEC(LVEC), PROBS(IPROB2), TSTEPS(IPROB2), UNITT,  
*      RESULT(NDECNS)  
C  
C      Local variables  
C  
      INTEGER NL, NPAIRS, NBDRYS, JJ, N, IBASEC, IBASEL, NPC, NPL, KPC,  
*      L1, L2, J, IT, ITLIM, IBC, KKPC, KNPC, IR, IB, KKPL, KPL,  
*      KNPL, L, K, NS, LL, JPOS  
      LOGICAL FLAG  
      REAL U2, Z, T, TLIM, PN, PXGTH  
      REAL SMALL, ZERO, HALF, ONE  
C  
C      SMALL is a machine-dependent constant used to test that TSTEPS  
C      values divided by UNITT equal INCS values.  
C  
      DATA SMALL /1.E-06/, ZERO /0.0/, HALF /0.5/, ONE /1.0/  
C  
      NL = (LVEC / 2) / NDECNS  
      NPAIRS = NDECNS - 1  
      NBDRYS = 2 * NPAIRS  
C  
C      Test for admissibility of parameters.  
C  
      IFAULT = 1  
      IF (NDECNS .LE. 1) RETURN  
      IFAULT = 2  
      IF (NSTOP .LE. 0) RETURN  
      IFAULT = 3  
      IF (IPROB1 .LE. 0) RETURN  
      IFAULT = 4  
      IF (IPROB2 .LE. IPROB1) RETURN  
      IFAULT = 5  
      IF (LVEC .LE. 0) RETURN  
      IFAULT = 6  
      IF (LNSTRD .LT. NBDRYS) RETURN  
      IFAULT = 7  
      IF (LBDRY .LT. NBDRYS * NSTOP) RETURN  
C  
      U2 = HALF * UNITT  
      Z = UNITT * U2  
      JJ = 2  
C  
C      Test that sampling plan is closed at observation count NSTOP.  
C  
      IFAULT = 10  
      DO 10 N = 1, NPAIRS  
          IF (BDRY(JJ) - BDRY(JJ-1) .GT. Z) GO TO 190  
          JJ = JJ + 2  
10 CONTINUE
```

```
C
C      Test that TSTEPS values divided by UNITT equal INCS values.
C
      IFAULT = 100
      DO 20 N = IPROB1, IPROB2
        T = INCS(N)
        IF (ABS(TSTEPS(N) / UNITT - T) .GT. SMALL) GO TO 190
20 CONTINUE
C
      IFAULT = 0
      IBASEC = 0
      IBASEL = 0
      NPC = 0
      NPL = NPAIRS
      N = NSTOP - 1
      FLAG = .FALSE.
      KPC = 0
      L1 = NPL + 1
      L2 = NPL + NPAIRS
      DO 30 J = L1, L2
30 NSTRD(J) = 0
C
C      Enter backward instruction cycle.
C
40 KPL = KPC
      IF (N .GT. 0) GO TO 50
      FLAG = .TRUE.
      T = ZERO
      GO TO 80
50 KPC = KPC + NBDRYS
      IT = IBASEC
      ITLIM = IT + NL
      IBC = IBASEC
      J = 1
      KKPC = KPC
      KNPC = NPC
C
C      Enter loop through boundary pairs for sample size N.
C
60 KKPC = KKPC + 2
      TLIM = BDRY(KKPC) - U2
      T = BDRY(KKPC-1)
C
C      Enter cycle to compute results for each T in continuation region
C      at sample size N.
C
70 T = T + UNITT
      IF (T .GT. TLIM) GO TO 170
      IT = IT + 1
C
C      Test that number of continuation states does not exceed the limit.
C
      IF (IT .GT. ITLIM) GO TO 180
C
80 DO 90 IR = 1, NPAIRS
90 RESULT(IR) = ZERO
      RESULT(NDECNS) = ONE
      IB = IBASEL
      KKPL = KPL
      KNPL = NPL
      L1 = IPROB1
```



```
C
C   Loop through reachable continuation and stopping regions at
C   sample size (N+1).
C
DO 140 K = 1, NPAIRS
  KKPL = KKPL + 2
  KNPL = KNPL + 1
  NS = NSTRD(KNPL)
  Z = T - BDRY(KKPL-1)
  JJ = Z / UNITT + SIGN(HALF, Z - U2)
  JJ = JJ + IB - 1
  Z = U2 - Z
  PN = ZERO
C
C   Loop through stop region for decision K.
C
DO 100 L = L1, IPROB2
  IF (TSTEPS(L) .GT. Z) GO TO 110
  PN = PN + PROBS(L)
100 CONTINUE
  RESULT(K) = RESULT(K) + PN
  GO TO 150
110 L1 = L
  RESULT(K) = RESULT(K) + PN
  IF (NS .EQ. 0) GO TO 140
  Z = BDRY(KKPL) - T - U2
C
C   Loop through continuation region between decisions K and (K+1).
C
DO 120 LL = L1, IPROB2
  IF (TSTEPS(LL) .GT. Z) GO TO 130
  JPOS = (JJ + INCS(LL)) * NDECNS
  PXGTH = PROBS(LL)
  DO 120 IR = 1, NDECNS
    JPOS = JPOS + 1
    RESULT(IR) = RESULT(IR) + PXGTH * VEC(JPOS)
120 CONTINUE
  GO TO 150
130 IB = IB + NS
  L1 = LL
140 CONTINUE
C
C   Test for completion of calculations.
C
150 IF (FLAG) RETURN
C
C   Store results for (N, T).
C
JPOS = (IT - 1) * NDECNS
DO 160 IR = 1, NDECNS
  JPOS = JPOS + 1
  VEC(JPOS) = RESULT(IR)
160 CONTINUE
  GO TO 70
C
170 KNPC = KNPC + 1
  NSTRD(KNPC) = IT - IBC
  IBC = IT
  J = J + 1
  IF (J .LE. NPAIRS) GO TO 60
C
```

C End of calculations for sample size N.

C

IBASEL = IBASEC

IBASEC = NL - IBASEC

NPL = NPC

N = N - 1

GO TO 40

C

180 IFAULT = 1000

190 IFAULT = IFAULT + N

RETURN

END

```
      SUBROUTINE MSAE(K, N, KPN, IMAX, JMAX, X, XBAR, Y, YBAR, ALPHA, B,  
+  LSAE, IDEP, IFAULT, A, C, IS, NB)
```

```
C  
C  ALGORITHM AS 108  APPL. STATIST. (1977), VOL. 26, NO.1
```

```
C  Computes the minimum sum of absolute errors (MSAE) estimates of  
C  unknown parameters ALPHA, B(1), B(2), ... , B(K) in the linear  
C  regression equation:
```

$$Y(I) = ALPHA + B(1)X(1) + B(2)X(2) + \dots + B(K)X(K)$$

```
C  The regression line passes through the point  
C  ( XBAR(1), XBAR(2), ... , XBAR(K), YBAR ) ,  
C  where these are the mean values of these variables,  
C  though the values of XBAR() and YBAR are input by the user, and  
C  could be any point through which the line is to be forced.  
C  Users should read the criticism of this algorithm on page 378 of  
C  volume 27 of Applied Statistics (1978).  
C  One way to use this algorithm would be to fix the XBAR's, say  
C  equal to the means, but to vary the value of YBAR until the minimum  
C  value of LSAE is found.
```

```
C  An alternative source of Fortran algorithms for this task is:  
C  Gonin, R. and Money, A.H. (1989) Nonlinear Lp-norm estimation,  
C  Dekker: New York.
```

```
C  N.B. The user should check the output values of both IFAULT & IDEP.
```

```
      REAL A(IMAX, JMAX), B(K), C(KPN), X(N, K), XBAR(K), Y(N)  
      INTEGER IS(IMAX), NB(JMAX)  
      LOGICAL DONE  
      REAL SMALL, TOL, ZERO, ONE, TWO  
      REAL LSAE  
      DATA SMALL/-1.E+10/, TOL/1.E-08/, ZERO/0.0/, ONE/1.0/, TWO/2.0/
```

```
C  Check for parameter consistency
```

```
      IFAULT = 0  
      KP1 = K + 1  
      KN = K + N  
      NP1 = N + 1  
      IF (K .GT. N) IFAULT = 1  
      IF (IMAX .NE. NP1) IFAULT = 2  
      IF (JMAX .NE. KP1) IFAULT = 3  
      IF (KPN .NE. KN) IFAULT = 4  
      IF (IFAULT .GT. 0) RETURN
```

```
C  Set up the initial tableau.
```

```
      LCOL = JMAX - 1  
      DO 1 J = 1, JMAX  
1  A(1, J) = ZERO  
      DO 10 I = 1, K  
          B(I) = ZERO  
          C(I) = ZERO  
          NB(I) = I  
10  CONTINUE  
      DO 20 I = KP1, KPN  
20  C(I) = TWO  
      DO 30 J = 1, K  
          DO 30 I = 1, N
```

```

        A(I+1, J) = X(I, J) - XBAR(J)
30 CONTINUE
    DO 40 I = 1, N
        IS(I+1) = I + K
        A(I+1, JMAX) = Y(I) - YBAR
40 CONTINUE
C
C    Determine the variable to leave the basis.
C
50 H = -TOL
    ICAND = 0
    DONE = .TRUE.
    DO 80 I = 2, IMAX
        AA = A(I, JMAX)
        IF (AA .GE. H) GO TO 80
        DONE = .FALSE.
        H = AA
        ICAND = I
80 CONTINUE
    IF (DONE) GO TO 200
C
C    Determine the variable to enter the basis.
C
    JCAND = 0
    RATIO = SMALL
    DO 110 J = 1, LCOL
        IONE = 1
        AA = A(ICAND, J)
        IF (ABS(AA) .LT. TOL) GO TO 110
        RCOST = A(1, J)
        IF (AA .LT. -TOL) GO TO 90
        IONE = -1
        IF (ABS(NB(J)) .GT. K) RCOST = RCOST - TWO
90    R = RCOST / AA
        IF (R .LE. RATIO) GO TO 110
        JCAND = J * IONE
        RATIO = R
        RSAVE = RCOST
110 CONTINUE
C
C    Determine if an ordinary simplex pivot is unnecessary.
C
    IT = IS(ICAND)
    II = ABS(IT)
    CJ = C(II)
    IF (RATIO .GT. -CJ) GO TO 140
    IS(ICAND) = -IS(ICAND)
    DO 130 J = 1, JMAX
        A(1, J) = A(1, J) + CJ * A(ICAND, J)
        A(ICAND, J) = -A(ICAND, J)
130 CONTINUE
    GO TO 50
C
C    Perform ordinary simplex pivot.
C
140 WUN = ONE
    IF (JCAND .GT. 0) GO TO 160
    JCAND = -JCAND
    NB(JCAND) = -NB(JCAND)
    WUN = -ONE
    A(1, JCAND) = RSAVE

```

```
160 PIVOT = A(ICAND, JCAND) * WUN
    DO 170 J = 1, JMAX
170 A(ICAND, J) = A(ICAND, J) / PIVOT
    DO 190 I = 1, IMAX
        IF (I .EQ. ICAND) GO TO 190
        AIJ = A(I, JCAND) * WUN
        IF (AIJ .EQ. ZERO) GO TO 190
        DO 180 J = 1, JMAX
            A(I, J) = A(I, J) - A(ICAND, J) * AIJ
180 CONTINUE
        A(I, JCAND) = -AIJ / PIVOT
190 CONTINUE
    A(ICAND, JCAND) = ONE / PIVOT
    IS(ICAND) = NB(JCAND)
    NB(JCAND) = IT
    GO TO 50

C
C    Compute ALPHA and the vector B containing the slopes.
C
200 ALPHA = YBAR
    DO 220 I = 2, IMAX
        WUN = ONE
        II = IS(I)
        IF (ABS(II) .GT. K) GO TO 220
        IF (II .GT. 0) GO TO 210
        II = -II
        WUN = -ONE
210 B(II) = WUN * A(I, JMAX)
        ALPHA = ALPHA - XBAR(II) * B(II)
220 CONTINUE
    LSAE = -A(1, JMAX)

C
C    Inspect the final solution for dependencies amongst the predictor
C    variables.
C
    IDEP = 1
    DO 300 J = 1, LCOL
        IF (ABS(NB(J)) .GT. K) GO TO 300
        IDEP = 0
    RETURN
300 CONTINUE

C
    RETURN
END
```

```
double precision function xinbta(p,q,beta,alpha,ifault)
implicit double precision (a-h,o-z)
c
c algorithm as 109 appl. statist. (1977), vol.26, no.1
c (replacing algorithm as 64 appl. statist. (1973),
c vol.22, no.3)
c
c Remark AS R83 and the correction in vol40(1) p.236 have been
c incorporated in this version.
c
c Computes inverse of the incomplete beta function
c ratio for given positive values of the arguments
c p and q, alpha between zero and one.
c log of complete beta function, beta, is assumed to be known.
c
c Auxiliary function required: BETAIN = algorithm AS63
c
c logical indx
c
c Define accuracy and initialise.
c SAE below is the most negative decimal exponent which does not
c cause an underflow; a value of -308 or thereabouts will often be
c OK in double precision.
c
c data acu/1.0d-14/
c data SAE/-37.D0/
c data zero/0.0d0/, one/1.0d0/, two/2.0d0/
c data three/3.0d0/, four/4.0d0/, five/5.0d0/, six/6.0d0/
c
c fpu = 10.d0 ** sae
c xinbta = alpha
c
c test for admissibility of parameters
c
c ifault = 1
c if (p.le.zero .or. q.le.zero) return
c ifault = 2
c if (alpha.lt.zero .or. alpha.gt.one) return
c ifault = 0
c if (alpha.eq.zero .or. alpha.eq.one) return
c
c change tail if necessary
c
c if (alpha.le.0.5d0) goto 1
c a = one-alpha
c pp = q
c qq = p
c indx = .true.
c goto 2
1 a = alpha
c pp = p
c qq = q
c indx = .false.
c
c calculate the initial approximation
c
2 r = dsqrt(-dlog(a*a))
c y = r-(2.30753d0+0.27061d0*r)/(one+(0.99229d0+0.04481d0*r)*r)
c if(pp.gt.one .and. qq.gt.one) goto 5
c r = qq+qq
c t = one/(9.0d0*qq)
```

```
t = r*(one-t+y*dsqrt(t))**3
if(t.le.zero) goto 3
t = (four*pp+r-two)/t
if(t.le.one) goto 4
xinbta = one-two/(t+one)
goto 6
3 xinbta = one-dexp((dlog((one-a)*qq)+beta)/qq)
goto 6
4 xinbta = dexp((dlog(a*pp)+beta)/pp)
goto 6
5 r = (y*y-three)/six
s = one/(pp+pp-one)
t = one/(qq+qq-one)
h = two/(s+t)
w = y*dsqrt(h+r)/h-(t-s)*(r+five/six-two/(three*h))
xinbta = pp/(pp+qq*dexp(w+w))
c
c solve for x by a modified newton-raphson method,
c using the function betain
c
6 r = one-pp
t = one-qq
yprev = zero
sq = one
prev = one
if(xinbta.lt.0.0001d0) xinbta = 0.0001d0
if(xinbta.gt.0.9999d0) xinbta = 0.9999d0
IEX = MAX(-5.D0/PP**2 - 1.D0/A**.2 - 13.D0, SAE)
ACU = 10.D0 ** IEX
7 y = betain(xinbta,pp,qq,beta,ifault)
if(ifault.eq.0) goto 8
ifault = 3
return
8 continue
xin = xinbta
y = (y-a)*exp(beta+r*log(xin)+t*log(one-xin))
if(y*yprev.le.zero) prev = max(sq, fpu)
g = one
9 adj = g*y
sq = adj*adj
if(sq.ge.prev) goto 10
tx = xinbta-adj
if(tx.ge.zero .and. tx.le.one) goto 11
10 g = g/three
goto 9
11 if(prev.le.acu) goto 12
if(y*y.le.acu) goto 12
if(tx.eq.zero .or. tx.eq.one) goto 10
if(tx.eq.xinbta) goto 12
xinbta = tx
yprev = y
goto 7
12 if (indx) xinbta = one-xinbta
return
end
```

```

SUBROUTINE LPEST(N, P, X, Y, MAXIT, A, B, SD, R, RATE, IT, NPO,
* IFAULT)

```

```

C
C FORMAL PARAMETERS
C   N       INTEGER       input : the number of points
C   P       REAL          input : p in the Lp norm
C   X       REAL ARRAY (N) input : the observed values x(i)
C   Y       REAL ARRAY (N) input : the observed values y(i)
C   MAXIT   INTEGER       input : maximum allowable number of iterations
C   A       REAL          output : the estimate of alfa
C   B       REAL          output : the estimate of beta
C   SD      REAL          output : the Lp norm
C   R       REAL ARRAY (N) output : the signed residuals
C   RATE    REAL          output : abs(S(k+1)-S(k))/S(k+1), where S(k) is
C                               the Lp norm of the fit on the kth iteration
C   IT      INTEGER       output : the number of iterations
C   NPO     INTEGER       output : the number of the points on the line
C   IFAULT  INTEGER       output :
C                               IFAULT = 0 if the routine converged.
C                               = 1 if return was due to an increase
C                               in the norm.
C                               = 2 if the maximum iterations
C                               specified was less than 2.
C                               = 3 if the weighted sample variance of
C                               x is 0.
C                               = 4 if N given less than 2.
C                               = 5 if convergence has not be achieved

```

```

within
C                               the maximum number of iterations
specified.

```

```

C ALGORITHM AS 110 APPL. STATIST. (1977), VOL.26, NO.1
C LP-NORM FIT OF STRAIGHT LINE BY EXTENSION OF SCHLOSSMACHER
C

```

```

implicit INTEGER (h-n)
implicit REAL (a-g)
implicit REAL (o-z)
REAL X(N), Y(N), R(N)
DATA EPS /1.0E-6/

```

```

C
IF(MAXIT .LT. 2) GOTO 9
IF(N .LT. 2) GOTO 10
IF(AULT = 0
WP = P - 2.0
EPS2 = 2.0 * EPS
SD = 0.0
DO 1 I = 1,N
1 R(I) = 1.0
DO 6 IT = 1, MAXIT
NPO = 0

```

```

C
C CALCULATE A AND B BY LEAST SQUARES ON WEIGHTED DATA,
C USING THE HERRAMAN ALGORITHM.
C OMIT OBSERVATIONS WITH SMALL RESIDUALS.
C

```

```

SW = 0.0
XMEAN = 0.0
YMEAN = 0.0
SSX = 0.0
SPXY = 0.0

```



```
DO 3 I = 1, N
  ABSRI = DABS(R(I))
  IF(ABSRI .LE. EPS) GOTO 2
  W = ABSRI ** WP
  SW = SW + W
  DIV = W / SW
  XI = X(I) - XMEAN
  YI = Y(I) - YMEAN
  XIW = XI * W
  DX = XI * XIW
  DXY = YI * XIW
  SSX = SSX + DX - DX * DIV
  SPXY = SPXY + DXY - DXY * DIV
  XMEAN = XMEAN + XI * DIV
  YMEAN = YMEAN + YI * DIV
  GOTO 3
2
  NPO = NPO + 1
3
  CONTINUE
  IF(SSX .LT. EPS) GOTO 11
  B = SPXY / SSX
  A = YMEAN - B * XMEAN
C
C      FORM RESIDUALS AND TEST CONVERGENCE
C
  SD2 = 0.0
  ISW = 0
  DO 4 I = 1, N
    RES = Y(I) - A - B * X(I)
    ABSRI = DABS(RES)
    IF(DABS(ABSRI - DABS(R(I)))) .GT. EPS2) ISW = 1
    SD2 = SD2 + ABSRI ** P
    R(I) = RES
4
  CONTINUE
  RATE = DABS(SD2 - SD) / SD2
  IF(ISW .EQ. 0) RETURN
  IF(IT .EQ. 1) GOTO 5
C
C      TEST FOR INCREASE IN NORM
C
  IF(SD2 .GT. SD) GOTO 7
5
  SD = SD2
  A2 = A
  B2 = B
6
  CONTINUE
C
  FAILED TO CONVERGE IN MAXIT ITERATIONS
C
  IFAULT = 5
  RETURN
C
C      NORM INCREASED, RESTORE A, B, AND R, THEN RETURN
C
7
  IFAULT = 1
  A = A2
  B = B2
  DO 8 I = 1, N
8
    R(I) = Y(I) - A - B * X(I)
  RETURN
C
C      MAXIT SPECIFIED LESS THAN 2
C
9
  IFAULT = 2
```

```
      RETURN
C
C      N LESS THAN 2
C
10     IFAULT = 4
      RETURN
C
C      VARIANCE OF WEIGHTED X IS ZERO
C
11     IFAULT = 3
      RETURN
      END
```

```
DOUBLE PRECISION FUNCTION PPND(P,IER)
C
C   ALGORITHM AS 111, APPL.STATIST., VOL.26, 118-121, 1977.
C
C   PRODUCES NORMAL DEVIATE CORRESPONDING TO LOWER TAIL AREA = P.
C
C   See also AS 241 which contains alternative routines accurate to
C   about 7 and 16 decimal digits.
C
C   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
DATA SPLIT/0.42D0/
DATA A0,A1,A2,A3/2.50662823884D0,-18.61500062529D0,
1  41.39119773534D0,-25.44106049637D0/, B1,B2,B3,B4/
2  -8.47351093090D0,23.08336743743D0,-21.06224101826D0,
3  3.13082909833D0/, C0,C1,C2,C3/-2.78718931138D0,-2.29796479134D0,
4  4.85014127135D0,2.32121276858D0/, D1,D2/3.54388924762D0,
5  1.63706781897D0/
DATA ZERO/0.D0/, ONE/1.D0/, HALF/0.5D0/
C
C   IER = 0
C   Q = P-HALF
C   IF (ABS(Q).GT.SPLIT) GO TO 10
C
C   0.08 < P < 0.92
C
C   R = Q*Q
C   PPND = Q*(((A3*R + A2)*R + A1)*R + A0)/((((B4*R + B3)*R + B2)*R
1      + B1)*R + ONE)
C   RETURN
C
C   P < 0.08 OR P > 0.92, SET R = MIN(P,1-P)
C
10  R = P
C   IF (Q.GT.ZERO) R = ONE-P
C   IF (R.LE.ZERO) GO TO 20
C   R = SQRT(-LOG(R))
C   PPND = (((C3*R + C2)*R + C1)*R + C0)/((D2*R + D1)*R + ONE)
C   IF (Q.LT.ZERO) PPND = -PPND
C   RETURN
20  IER = 1
C   PPND = ZERO
C   RETURN
C   END
```

```
      SUBROUTINE PANDQ(S, F, R, C, ROWSUM, COLSUM, N, IFAULT)
C
C   ALGORITHM AS 114  APPL. STATIST. (1977) VOL. 26, NO. 2
C
C   Finds the numerator S required by several measures of association.
C
      INTEGER S, R, C, F(R,C), ROWSUM(R), COLSUM(C), N, IFAULT
C
C   Local variables
C
      INTEGER P, Q, FI1, FIJ, I, J, NC, ND
C
      IFAULT = 1
      IF (R .LT. 2 .OR. C .LT. 2) RETURN
      IFAULT = 0
C
      ROWSUM(1) = 0
      DO 10 J = 1, C
         COLSUM(J) = F(1,J)
         ROWSUM(1) = ROWSUM(1) + F(1,J)
10  CONTINUE
      NC = 0
      P = 0
      Q = 0
      DO 20 I = 2, R
         FI1 = F(I,1)
         ND = NC + ROWSUM(I-1) - COLSUM(1)
         Q = Q + FI1 * ND
         NC = COLSUM(1)
         COLSUM(1) = COLSUM(1) + FI1
         ROWSUM(I) = FI1
         DO 15 J = 2, C
            FIJ = F(I,J)
            ND = ND - COLSUM(J)
            Q = Q + FIJ * ND
            P = P + FIJ * NC
            NC = NC + COLSUM(J)
            COLSUM(J) = COLSUM(J) + FIJ
            ROWSUM(I) = ROWSUM(I) + FIJ
15  CONTINUE
20  CONTINUE
      N = NC + ROWSUM(R)
      S = P - Q
      RETURN
      END
```

```
SUBROUTINE TETRA(A, B, C, D, R, SDR, SDZERO, ITYPE, IFAULT)
```

```
C
C     ALGORITHM AS 116 APPL. STATIST. (1977) VOL.26, NO.3
C
C     TO COMPUTE THE TETRACHORIC CORRELATION (R) AND ITS STANDARD
C     ERRORS (SDR AND SDZERO) FROM THE FREQUENCIES OF A 2*2 TABLE
C     (A, B, C AND D)
C     X AND W ARE CONSTANTS USED IN GAUSSIAN QUADRATURE
C
```

```

DIMENSION X(16), W(16)
DATA X(1) /0.9972638618/, X(2) /0.9856115115/, X(3) /0.9647622556/,
1     X(4) /0.9349060759/, X(5) /0.8963211558/, X(6) /0.8493676137/,
2     X(7) /0.7944837960/, X(8) /0.7321821187/, X(9) /0.6630442669/,
3     X(10)/0.5877157572/, X(11)/0.5068999089/, X(12)/0.4213512761/,
4     X(13)/0.3318686023/, X(14)/0.2392873623/, X(15)/0.1444719616/,
5     X(16)/0.0483076657/
DATA W(1) /0.0070186100/, W(2) /0.0162743947/, W(3) /0.0253920653/,
1     W(4) /0.0342738629/, W(5) /0.0428358980/, W(6) /0.0509980593/,
2     W(7) /0.0586840935/, W(8) /0.0658222228/, W(9) /0.0723457941/,
3     W(10)/0.0781938958/, W(11)/0.0833119242/, W(12)/0.0876520930/,
4     W(13)/0.0911738787/, W(14)/0.0938443991/, W(15)/0.0956387201/,
5     W(16)/0.0965400885/
DATA ZERO /0.0/, ONE/1.0/, TWO /2.0/, FOUR /4.0/, SIX /6.0/
DATA HALF /0.5/, TWOPI/6.28318531/, SQT2PI /2.50662827/
DATA RLIMIT /0.9999/, RCUT /0.95/, UPLIM /5.0/
DATA CONST /1E-36/, CHALF /1E-18/
DATA CONV /1E-8/, CITER /1E-6/, NITER /25/

```

```
C
C     INITIALIZATION
C
```

```

R = ZERO
SDZERO = ZERO
SDR = ZERO
ITYPE = 0
IFAULT = 0

```

```
C
C     CHECK IF ANY CELL FREQUENCY IS NEGATIVE
C
```

```

IF (A .LT. ZERO .OR. B .LT. ZERO .OR. C .LT. ZERO
*   .OR. D .LT. ZERO) GOTO 92

```

```
C
C     CHECK IF ANY FREQUENCY IS ZERO AND SET KDELTA
C
```

```

KDELTA = 1
DELTA = ZERO
IF (A .EQ. ZERO .OR. D .EQ. ZERO) KDELTA = 2
IF (B .EQ. ZERO .OR. C .EQ. ZERO) KDELTA = KDELTA + 2

```

```
C
C     KDELTA=4 MEANS TABLE HAS ZERO ROW OR COLUMN, RUN IS TERMINATED
C
```

```

GOTO (4, 1, 2 , 92), KDELTA

```

```
C
C     DELTA IS 0.0, 0.5 OR -0.5 ACCORDING TO WHICH CELL IS ZERO
C
```

```

1 DELTA = HALF
  IF (A .EQ. ZERO .AND. D .EQ. ZERO) R = -ONE
  GOTO 4
2 DELTA = -HALF
  IF (B .EQ. ZERO .AND. C .EQ. ZERO) R = ONE
4 IF (R .NE. ZERO) ITYPE = 3

```

```
C
```

```

C          STORE FREQUENCIES IN  AA, BB, CC AND DD
C
C          AA = A + DELTA
C          BB = B - DELTA
C          CC = C - DELTA
C          DD = D + DELTA
C          TOT = AA + BB + CC + DD
C
C          CHECK IF CORRELATION IS NEGATIVE, ZERO, POSITIVE
C
C          IF (AA * DD - BB * CC) 7, 5, 6
5 ITYPE = 4
C
C          COMPUTE PROBABILITIES OF QUADRANT AND OF MARGINALS
C          PROBAA AND PROBAC CHOSEN SO THAT CORRELATION IS POSITIVE.
C          KSIGN INDICATES WHETHER QUADRANTS HAVE BEEN SWITCHED
C
6 PROBAA = AA / TOT
  PROBAC = (AA + CC) / TOT
  KSIGN = 1
  GOTO 8
7 PROBAA = BB / TOT
  PROBAC = (BB + DD) / TOT
  KSIGN = 2
8 PROBAB = (AA + BB) / TOT
C
C          COMPUTE NORMAL DEVIATES FOR THE MARGINAL FREQUENCIES
C          SINCE NO MARGINAL CAN BE ZERO, IE IS NOT CHECKED
C
C          ZAC = PPND(PROBAC, IE)
C          ZAB = PPND(PROBAB, IE)
C          SS = EXP(-HALF * (ZAC ** 2 + ZAB ** 2)) / TWOPI
C
C          WHEN R IS 0.0, 1.0 OR -1.0, TRANSFER TO COMPUTE SDZERO
C
C          IF (R .NE. ZERO .OR. ITYPE .GT. 0) GOTO 85
C
C          WHEN MARGINALS ARE EQUAL, COSINE EVALUATION IS USED
C
C          IF (A .EQ. D .AND. B .EQ. C) GOTO 60
C
C          INITIAL ESTIMATE OF CORRELATION IS YULES Y
C
C          RR = (SQRT(AA * DD) - SQRT(BB * CC)) ** 2 / ABS(AA * DD - BB * CC)
C          ITER = 0
C
C          IF RR EXCEEDS RCUT, GAUSSIAN QUADRATURE IS USED
C
10 IF (RR .GT. RCUT) GOTO 40
C
C          TETRACHORIC SERIES IS COMPUTED
C
C          INITIALIZATION
C
C          VA = ONE
C          VB = ZAC
C          WA = ONE
C          WB = ZAB
C          TERM = ONE
C          ITERM = 0
C          SUM = PROBAB * PROBAC

```

```
      DERIV = ZERO
      SR = SS
15  IF (ABS(SR) .GT. CONST) GOTO 20
C
C      RESCALE TERMS TO AVOID OVERFLOWS AND UNDERFLOWS
C
      SR = SR / CONST
      VA = VA * CHALF
      VB = VB * CHALF
      WA = WA * CHALF
      WB = WB * CHALF
C
C      FORM SUM AND DERIVATIVE OF SERIES
C
20  DR = SR * VA * WA
      SR = SR * RR / TERM
      COF = SR * VA * WA
C
C      ITERM COUNTS NO. OF CONSECUTIVE TERMS .LT. CONV
C
      ITERM = ITERM + 1
      IF (ABS(COF) .GT. CONV) ITERM = 0
      SUM = SUM + COF
      DERIV = DERIV + DR
      VAA = VA
      WAA = WA
      VA = VB
      WA = WB
      VB = ZAC * VA - TERM * VAA
      WB = ZAB * WA - TERM * WAA
      TERM = TERM + ONE
      IF (ITERM .LT. 2 .OR. TERM .LT. SIX) GOTO 15
C
C      CHECK IF ITERATION CONVERGED
C
      IF (ABS(SUM-PROBAA) .GT. CITER) GOTO 25
C
C      ITERATION HAS CONVERGED, SET ITYPE
C
      ITYPE = TERM
      GOTO 70
C
C      CALCULATE NEXT ESTIMATE OF CORRELATION
C
25  ITER = ITER + 1
C
C      IF TOO MANY ITERATIONS, RUN IS TERMINATED
C
      IF (ITER .GE. NITER) GOTO 93
      DELTA = (SUM - PROBAA) / DERIV
      RRPREV = RR
      RR = RR - DELTA
      IF (ITER .EQ. 1) RR = RR + HALF * DELTA
      IF (RR .GT. RLIMIT) RR = RLIMIT
      IF (RR .LT. ZERO) RR = ZERO
      GOTO 10
C
C      GAUSSIAN QUADRATURE
C
40  IF (ITER .GT. 0) GOTO 41
C
```

```

C      INITIALIZATION, IF THIS IS FIRST ITERATION
C
C      SUM = PROBAB * PROBAC
C      RRPREV = ZERO
C
C      INITIALIZATION
C
C      41 SUMPRV = PROBAB - SUM
C      PROB = BB / TOT
C      IF (KSIGN .EQ. 2) PROB = AA / TOT
C      ITYPE = 1
C
C      LOOP TO FIND ESTIMATE OF CORRELATION
C      COMPUTATION OF INTEGRAL (SUM) BY QUADRATURE
C
C      42 RRSQ = SQRT(ONE - RR ** 2)
C      AMID = HALF * (UPLIM + ZAC)
C      XLEN = UPLIM - AMID
C      SUM = ZERO
C      DO 44 IQUAD = 1, 16
C      XLA = AMID + X(IQUAD) * XLEN
C      XLB = AMID - X(IQUAD) * XLEN
C
C      TO AVOID UNDERFLOWS, TEMPA AND TEMPB ARE USED
C
C      TEMPA = (ZAB - RR * XLA) / RRSQ
C      IF (TEMPA .GE. -SIX) SUM = SUM + W(IQUAD) *
*      EXP(-HALF * XLA ** 2) * ALNORM(TEMPA, .FALSE.)
C      TEMPB = (ZAB - RR * XLB) / RRSQ
C      IF (TEMPB .GE. -SIX) SUM = SUM + W(IQUAD) *
*      EXP(-HALF * XLB ** 2) * ALNORM(TEMPB, .FALSE.)
C      44 CONTINUE
C      SUM = SUM * XLEN / SQT2PI
C
C      CHECK IF ITERATION HAS CONVERGED
C
C      IF (ABS(PROB - SUM) .LE. CITER) GOTO 70
C      ITER = ITER + 1
C
C      IF TOO MANY ITERATIONS, RUN IS TERMINATED
C
C      IF (ITER .GE. NITER) GO TO 93
C
C      ESTIMATE CORRELATION FOR NEXT ITERATION BY LINEAR INTERPOLATION
C
C      RREST = ((PROB - SUM) * RRPREV - (PROB - SUMPRV) * RR)
*      / (SUMPRV - SUM)
C
C      IS ESTIMATE POSITIVE AND LESS THAN UPPER LIMIT
C
C      IF (RREST .GT. RLIMIT) RREST = RLIMIT
C      IF (RREST .LT. ZERO) RREST = ZERO
C      RRPREV = RR
C      RR = RREST
C      SUMPRV = SUM
C
C      IF ESTIMATE HAS SAME VALUE ON TWO ITERATIONS, STOP ITERATION
C
C      IF (RR .EQ. RRPREV) GOTO 70
C      GOTO 42
C

```



```
C          WHEN ALL MARGINALS ARE EQUAL THE COSINE FUNCTION IS USED
C
60 RR = -COS(TWOPI * PROBAA)
   ITYPE = 2
C
C          COMPUTE SDR
C
70 R = RR
   RRSQ = SQRT(ONE - R ** 2)
   IF (KDELTA .GT. 1) ITYPE = -ITYPE
   IF (KSIGN .EQ. 1) GOTO 71
   R = -R
   ZAC = -ZAC
71 PDF = EXP(-HALF * (ZAC ** 2 - TWO * R * ZAC * ZAB + ZAB ** 2)
 * / RRSQ ** 2) / (TWOPI * RRSQ)
   PAC = ALNORM((ZAC - R * ZAB) / RRSQ, .FALSE.) - HALF
   PAB = ALNORM((ZAB - R * ZAC) / RRSQ, .FALSE.) - HALF
   SDR = (AA + DD) * (BB + CC) / FOUR + PAB ** 2 * (AA + CC)
1 * (BB + DD) + PAC ** 2 * (AA + BB) * (CC + DD) + TWO * PAB *
2 PAC * (AA * DD - BB * CC) - PAB * (AA * BB - CC * DD) -
3 PAC * (AA * CC - BB * DD)
   IF (SDR .LT. ZERO) SDR = ZERO
   SDR = SQRT(SDR) / (TOT * PDF * SQRT(TOT))
C
C          COMPUTE SDZERO
C
85 SDZERO = SQRT((AA + BB) * (AA + CC) * (BB + DD) * (CC + DD) / TOT)
 * / (TOT ** 2 * SS)
   IF (R .EQ. ZERO) SDR = SDZERO
   GOTO 99
C
C          ERROR TERMINATIONS
C
92 IFAULT = 1
93 IFAULT = IFAULT + 1
C
99 RETURN
   END
```

```
      subroutine chrft(x, y, wr, wi, isize, lwork, itype, ifault)
c
c      Algorithm AS 117.1 Appl. Statist. (1977) vol.26, no.3
c
c      Code for complex discrete Fourier transform of a sequence of
c      general length by the Chirp-Z transform
c
      real    x(lwork), y(lwork), wr(lwork), wi(lwork)
      data    zero, one/0.0, 1.0/
c
c      Check that ISIZE and LWORK are valid
c
      ifault = 0
      if (isize .lt. 3) ifault = 1
      ii = 4
      do 1 k = 3, 20
         ii = ii * 2
         if (ii .eq. lwork) go to 3
         if (ii .gt. lwork) go to 2
1      continue
c
2      ifault = ifault + 2
3      if (lwork .lt. 2 * isize) ifault = ifault + 4
      if (itype .eq. 0) ifault = ifault + 8
      if (ifault .ne. 0) return
c
c      Multiply by the Chirp function in the time domain
c
      call chrp(x, y, one, isize, lwork, itype)
      npl = isize + 1
      do 4 nn = npl, lwork
         x(nn) = zero
         y(nn) = zero
4      continue
c
c      Fourier transform the chirped series
c
      call fastf(x, y, lwork, 1)
c
c      Convolve by frequency domain multiplication with (wr, wi)
c
      do 5 nn = 1, lwork
         xwi = wi(nn)
         if (itype .lt. 0) xwi = -xwi
         z = x(nn) * wr(nn) - y(nn) * xwi
         y(nn) = x(nn) * xwi + y(nn) * wr(nn)
         x(nn) = z
5      continue
c
c      Inverse Fourier transform
c
      call fastf(x, y, lwork, -1)
c
c      Multiply by Chirp function & gain correction
c
      gc = lwork
      if (itype .gt. 0) gc = gc/isize
      call chrp(x, y, gc, isize, lwork, itype)
c
      return
      end
```

```

subroutine chfor(xray, wr, wi, jsize, lwork, mwork, ifault)
c
c Algorithm AS 117.2 Appl. Statist. (1977) vol.26, no.3
c
c Forward Chirp DFT for real even length input sequence
c
real    xray(lwork), wr(mwork), wi(mwork)
data    zero, quart, half, one, one5, two, four
+       /0.0, 0.25, 0.5, 1.0, 1.5, 2.0, 4.0/
c
c Check for valid JSIZE, LWORK & MWORK
c
c
c   ifault = 0
c   ii = 8
c   do 1 k = 4, 21
c     ii = ii * 2
c     if (ii .eq. lwork) go to 3
c     if (ii .gt. lwork) go to 2
1  continue
2  ifault = 2
3  if (lwork .lt. 2 * jsize) ifault = ifault + 4
c   if (lwork .ne. 2 * mwork) ifault = ifault + 16
c   nn = jsize / 2
c   if (2 * nn .ne. jsize) ifault = ifault + 32
c   if (nn .lt. 3) ifault = ifault + 1
c   if (ifault .ne. 0) return
c   ll = mwork
c
c Split XRAY into even and odd sequences of length n/2 placing
c the even terms in the bottom half of XRAY as dummy real terms
c and odd terms in the top half as dummy imaginary terms.
c
c
c   do 4 i = 1, nn
c     ii = 2 * i
c     m = ll + i
c     xray(m) = xray(ii)
c     xray(i) = xray(ii-1)
4  continue
c
c Perform forward Chirp DFT on even and odd sequences.
c IFA is not tested as possible faults have already been checked.
c
c call chrft(xray, xray(ll+1), wr, wi, nn, ll, 1, ifa)
c
c Reorder the results according to output format.
c First, the unique real terms.
c
c   z = half * (xray(1) + xray(ll+1))
c   xray(nn+1) = half * (xray(1) - xray(ll+1))
c   xray(1) = z
c
c If nn is even, terms at nn/2 + 1 and 3*nn/2 can be calculated
c
c   nnn = nn / 2
c   if (nn .ne. 2 * nnn) go to 5
c   m = nnn + 1
c   xray(m) = half * xray(m)
c   mm = m + ll

```

```

        m = m + nn
        xray(m) = -half * xray(mm)
        go to 6
5      nnn = nnn + 1
c
c      Set up trig functions for calculations of remaining
c      non-unique terms
c
6      z = four * atan(one) / nn
        bcos = -two * (sin(z/two) ** 2)
        bsin = sin(z)
        un = one
        vn = zero
c
c      Calculate & place remaining terms in correct locations.
c
do 7 i = 2, nnn
    z = un * bcos + un + vn * bsin
    vn = vn * bcos + vn - un * bsin
    save1 = one5 - half * (z * z + vn * vn)
    un = z * save1
    vn = vn * save1
    ii = nn + 2 - i
    m = ll + i
    mm = ll + ii
    an = quart * (xray(i) + xray(ii))
    bn = quart * (xray(m) - xray(mm))
    cn = quart * (xray(m) + xray(mm))
    dn = quart * (xray(i) - xray(ii))
    xray(i) = an + un * cn + vn * dn
    xray(ii) = two * an - xray(i)
    j = nn + i
    jj = nn + ii
    xray(j) = bn - un * dn + vn * cn
    xray(jj) = xray(j) - two * bn
7  continue

return
end

subroutine chrev(xray, wr, wi, jsize, lwork, mwork, ifault)
c
c      Algorithm AS 117.3 Appl. Statist. (1977) vol.26, no.3
c
c      Inverse Chirp DFT to give real even length sequence
c
real    xray(lwork), wr(mwork), wi(mwork)
data    zero, half, one, one5, two, four
+       /0.0, 0.5, 1.0, 1.5, 2.0, 4.0/
c
c      Check for valid JSIZE, LWORK & MWORK
c
c
ifault = 0
ii = 8
do 1 k = 4, 21
    ii = ii * 2
    if (ii .eq. lwork) go to 3
    if (ii .gt. lwork) go to 2
1  continue
```

```
2   ifault = 2
3   if (lwork .lt. 2 * jsize) ifault = ifault + 4
   if (lwork .ne. 2 * mwork) ifault = ifault + 16
   nn = jsize / 2
   if (2 * nn .ne. jsize) ifault = ifault + 32
   if (nn .lt. 3) ifault = ifault + 1
   if (ifault .ne. 0) return
   ll = mwork

c
c   Reorder the spectrum; first the unique terms.
c
   z = xray(1) + xray(nn+1)
   xray(ll+1) = xray(1) - xray(nn+1)
   xray(1) = z

c
c   If nn is even then terms nn/2 + 1 and 3*nn/2 + 1 must be
c   reordered.
c
   nnn = nn / 2
   if (nn .ne. 2 * nnn) go to 4
   m = nnn + 1
   xray(m) = two * xray(m)
   mm = m + ll
   m = m + nn
   xray(mm) = -two * xray(m)
   go to 5
4   nnn = nnn + 1

c
c   Set up trig functions for manipulation of remaining terms.
c
5   z = four * atan(one) / nn
   bcos = -two * (sin(z/two) ** 2)
   bsin = sin(z)
   un = one
   vn = zero

c
c   Perform manipulation and reordering of remaining non-unique
c   terms.
c
   do 6 i = 2, nnn
     z = un * bcos + un + vn * bsin
     vn = vn * bcos + vn - un * bsin
     savel = one5 - half * (z * z + vn * vn)
     un = z * savel
     vn = vn * savel
     ii = nn + 2 - i
     j = nn + i
     jj = nn + ii
     an = xray(i) + xray(ii)
     bn = xray(j) - xray(jj)
     pn = xray(i) - xray(ii)
     qn = xray(j) + xray(jj)
     cn = un * pn + vn * qn
     dn = vn * pn - un * qn
     xray(i) = an + dn
     xray(ii) = an - dn
     m = ll + i
     mm = ll + ii
     xray(m) = cn + bn
     xray(mm) = cn - bn
6   continue
```

```
c
c      Do inverse Chirp DFT to give even and odd sequences.
c      IFA is not tested as possible faults have already been checked
c
c      call chrft(xray, xray(ll+1), wr, wi, nn, ll, -1, ifa)
c
c      Interlace the results to produce the required output sequence.
c
c      nnn = nn + 1
c      ii = jsize + 2
c      do 7 i = 1, nn
c          j = nnn - i
c          jj = ll + j
c          m = ii - 2 * i
c          mm = m - 1
c          xray(m) = xray(jj)
c          xray(mm) = xray(j)
7      continue
c
c      return
c      end

subroutine setwt(wr, wi, ksize, kwork, ifault)
c
c      Algorithm AS 117.4 Appl. Statist. (1977) vol.26, no.3
c
c      Subroutine to set up Fourier transformed Chirp function for
c      use by subroutine CHRFT.
c
c      real      wr(kwork), wi(kwork)
c      data      zero, one, four /0.0, 1.0, 4.0/
c
c      Check that KSIZE & KWORK are valid
c
c      ifault = 0
c      if (ksize .lt. 3) ifault = 1
c      ii = 4
c      do 1 k = 3, 20
c          ii = ii * 2
c          if (ii .eq. kwork) go to 3
c          if (ii .gt. kwork) go to 2
1      continue
2      ifault = 2
3      if (kwork .lt. 2 * ksize) ifault = ifault + 4
c      if (ifault .ne. 0) return
c      tc = four * atan(one) / ksize
c
c      Set up bottom segment of Chirp function
c
c      do 4 nn = 1, ksize
c          z = nn - 1
c          z = z * z * tc
c          wr(nn) = cos(z)
c          wi(nn) = sin(z)
4      continue
c
c      Clear the rest
c
c      do 5 nn = ksize+1, kwork
```

```
        wr(nn) = zero
        wi(nn) = zero
5 continue
c
c      Copy to the top segment
c
      do 6 nn = kwork-ksize+2, kwork
        ll = kwork - nn + 2
        wr(nn) = wr(ll)
        wi(nn) = wi(ll)
6 continue
c
c      Fourier transform the Chirp function
c
      call fastf(wr, wi, kwork, 1)

      return
      end

      subroutine chrp(x, y, gc, isize, lwork, itype)
c
c      Algorithm AS 117.5 Appl. Statist. (1977) vol.26, no.3
c
c      Subroutine to multiply time series by Chirp function
c
      dimension x(lwork), y(lwork)
      data      one, four /1.0, 4.0/

      tc = four * atan(one) / isize
      do 3 nn = 1, isize
        z = nn - 1
        z = z * z * tc
        xwr = cos(z)
        xwi = -sin(z)
        if (itype .lt. 0) xwi = -xwi
        z = x(nn) * xwr - y(nn) * xwi
        y(nn) = (x(nn) * xwi + y(nn) * xwr) * gc
        x(nn) = z * gc
3 continue

      return
      end
```

```
double precision function trigam(x, ifault)
implicit double precision (a-h,o-z)
c
c   algorithm as121   Appl. Statist. (1978) vol 27, no. 1
c
c   calculates trigamma(x) = d**2(log(gamma(x))) / dx**2
c
double precision a, b, one, half, b2, b4, b6,b8, x, y, z, zero
data a, b, one, half /1.0d-4, 5.0d0, 1.0d0, 0.5d0/
data zero /0.0d0/
c
c   b2, b4, b6 and b8 are Bernoulli numbers
c
data b2, b4, b6,b8
*/0.16666666667d0, -0.03333333333d0, 0.02380952381, -0.03333333333/
c
c   check for positive value of x
c
trigam = zero
ifault = 1
if (x.le.zero) return
ifault = 0
z = x
c
c   use small value approximation if x .le. a
c
if (z .gt. a) goto 10
trigam = one / (z * z)
return
c
c   increase argument to (x+i) .ge. b
c
10 if (z .ge. b) goto 20
trigam = trigam + one / (z * z)
z = z + one
goto 10
c
c   apply asymptotic formula if argument .ge. b
c
20 y = one / (z * z)
trigam = trigam + half * y +
* (one + y * (b2 + y * (b4 + y * (b6 + y * b8)))) / z
return
end
```



```
C UKC NETLIB DISTRIBUTION COPYRIGHT 1990 RSS
C
  FUNCTION BMIX(X, N, L, Q, ITYPE, IFAULT)
C
C   Algorithm AS 123 (Applied Statistics, 27 (1978), pp. 104-109);
C
C   CALCULATES C.D.F.S OF MIXTURES OF BETA DISTRIBUTIONS.
C
  DIMENSION Q(101)
  LOGICAL SEC, ALT
  PARAMETER (C1=0.636619772368, C2=76.7625)
C
C   C1 = 2.0/PI.  C2 MUST NOT EXCEED LOG (BASE 10) OF LARGEST
C   POSSIBLE FLOATING POINT NUMBER.
C
  BMIX = 0.0
C
C   CHECK FOR ERRORS AND INITIALISE.
C
  IFAULT = 1
  I = L + ITYPE
  IF (N .LE. 0 .OR. N .GE. 101 .OR. I .LE. 1) RETURN
  IFAULT = 2
  XF1 = 1.0 - X
  IF (X .LT. 0.0 .OR. XF1 .LE. 0.0) RETURN
  RX = SQRT(X)
  RXF1 = SQRT(XF1)
  IFAULT = 3
  IF (ITYPE .EQ. 2) GO TO 40
  IF (ITYPE .NE. 1) RETURN
  M = L - 2
  D = M
  E = 1.0
  F = L
  C = (F - 1.0)*XF1
  Z = X
  GO TO 50
40 I = L + N
  M = I - 3
  D = I
  E = -1.0
  F = I - 2
  C = F
  Z = X/XF1
50 IFAULT = 4
  NN = N
  ALT = .FALSE.
  K = -2
  J = N + 1
C
C   CHECK FOR POSSIBILITY OF OVERFLOW.
C
60 A = -F*ALOG10(RXF1)
  IF (A .LT. C2) GO TO 90
  IF (ITYPE .EQ. 1 .OR. ALT) RETURN
  IF (I .LT. 101) GO TO 70
  IFAULT = 5
  RETURN
C
C   IF ITYPE = 2 TRY ALTERNATIVE APPROACH.
C
```

```
70 ALT = .TRUE.
   NN = I
   Z = XF1/X
   XF1 = X
   A = RX
   RX = RXF1
   RXF1 = A
   IF (L .EQ. 0) GO TO 85
   J = N + 2
   K = I + 1
   DO 80 I = J, K
80 Q(I) = 0.0
85 J = 1
   K = 2
   GO TO 60

C
C     MAIN SECTION OF ALGORITHM BEGINS HERE.
C
90 IFAULT = 0
   SEC = .FALSE.
   I = NN
100 A = 0.0
   B = 0.0

C
C     INNER LOOP.
C
110 B = B + Q(J)
   IF (I .LE. 1) GO TO 120
   FI = I
   A = A*Z*(D/FI + E) - B
   I = I - 2
   J = J + K
   GO TO 110
120 IF (.NOT. ALT) GO TO 130
   BMIX = BMIX + B
   A = -A
   B = -B
130 IF (I .EQ. 1) GO TO 140

C
C     COMPLETION OF EVEN CALCULATIONS.
C
   BMIX = BMIX + B + A*RXF1**F
   GO TO 180
140 IF (M .GE. 0) A = B + C*A
   I = M

C
C     OUTER LOOP.
C
150 IF (I .LE. 1) GO TO 160
   FI = I
   A = (A - A/FI)*XF1 + B
   I = I - 2
   GO TO 150

C
C     COMPLETION OF ODD CALCULATIONS.
C
160 A = A*RX
   IF (I .EQ. 0 .OR. I .EQ. -2) GO TO 170
   BMIX = BMIX + C1*(ATAN(RX/RXF1)*B + RXF1*A)
   GO TO 180
170 BMIX = BMIX + A
```

```
180 IF (SEC) RETURN
    SEC = .TRUE.
    I = NN - 1
    J = N
    IF (ALT) J = 2
    GO TO 100
END
```

```
C UKC NETLIB DISTRIBUTION COPYRIGHT 1990 RSS
C
C      SUBROUTINE CVSUR1(N, M, L, MM, U, A, Z, IROWS, ITERS, F, THETA,
*      VAR, CRI1, CRI2, F0, DF1, DF2, DDF1, DDF2, IFAULT)
C
C      ALGORITHM AS 125 APPL. STATIST. (1978) VOL.27, NO.2
C
C      THIS SUBROUTINE USES A NEWTON-RAPHSON ITERATION TO DETERMINE
C      THE MAXIMUM LIKELIHOOD ESTIMATES FOR AN EXPONENTIAL COVARIATE
C      SURVIVAL MODEL.
C
C      as r38 vol 30 no 3 1981 p 355 -- code changes included
C
C      Auxiliary routines required: CHOL = AS6, SYMINV = AS7
C
C      DIMENSION U(N), A(N), Z(IROWS, M), THETA(L), DF1(L), DF2(L),
*      VAR(MM), DDF1(MM), DDF2(MM)
C      PARAMETER (ZERO=0.0, ONE=1.0)
C
C      IFAULT = 3
C      IF (N .LT. 1) GOTO 160
C      IFAULT = 4
C      IF (M .LT. 1) GOTO 160
C
C      FLAST PRERESENTS THE FALUE OF THE LOG LIKELIHOOD FUNCTION
C      FOR THE PREVIOUS ITERATION.
C
C      FLAST = ZERO
C      R = ZERO
C      W = ZERO
C      DO 10 I = 1, N
C         IFAULT = 5
C         AI = A(I)
C         IF (AI .NE. ZERO .AND. AI .NE. ONE) GOTO 160
C
C      R IS THE NUMBER OF UNCENSORED OBSERVATIONS
C      W IS THE TOTAL OBSERVED TIME
C
C      R = R + AI
C      IFAULT = 6
C      IF (U(I) .LT. ZERO) GOTO 160
C      W = W + U(I)
10  CONTINUE
C      IFAULT = 7
C      IF (R .EQ. ZERO) GOTO 160
C      IFAULT = 8
C      IF (W .EQ. ZERO) GOTO 160
C      IFAULT = 9
C      IF (R .LT. FLOAT(L)) GOTO 160
C
C      THETA(L) CONTAINS THE ESTIMATE OF ALPHA,
C      INITIALIZE TO ITS MAXIMUM LIKELIHOOD ESTIMATE
C      VALUE FOR NONCOVARIATE CASE.
C
C      THETA(L) = ALOG(R / W)
C
C      COMPUTE F0, THE MAXIMIZED LOG LIKELIHOOD WHEN
C      ALL BETAS ARE ZERO.
C
C      F0 = -R + R * THETA(L)
C
```

```
C      INITIALIZE AND COMPUTE ZSUM AND STORE IN FIRST
C      M ELEMENTS OF ARRAY VAR.
C
      DO 30 J = 1, M
        THETA(J) = ZERO
        VARJ = ZERO
        DO 20 I = 1, N
          VARJ = VARJ + Z(I, J) * A(I)
20      CONTINUE
        VAR(J) = VARJ
30      CONTINUE
C
      BEGIN ITERATING
C
      DO 60 K = 1, ITERS
        CALL CVSUR2(N, M, L, MM, U, A, R, Z, IROWS, VAR, THETA, F,
*        DF1, DDF1)
C
        DETERMINE WHETHER THE RELATIVE CHANGE IN LOG LIKELIHOODS IS
        LESS THAN CRI1 OR NOT AND SET ICODE1 = 0, 1 ACCORDINGLY.
C
        ICODE1 = 1
        DIFF = F - FLAST
        FCRI1 = FLAST * CRI1
        IF (DIFF .LE. -FCRI1 .AND. DIFF .GE. ZERO) ICODE1 = 0
        FLAST = F
C
        FIND THE CHOLESKY DECOMPOSITION OF DDF1 AND RETURN
        RESULTS IN DDF2.
C
        CALL CHOL(DDF1, L, DDF2, NULLTY, IFAULT)
        IF (IFAUULT .NE. 0) GOTO 160
C
        SOLVE THE LINEAR SYSTEM DDF1 * X = DF1.
        X IS RETURNED IN DF2 AND REPRESENTS THE INCREMENT
        IN THE MLE ESTIMATES.
C
        CALL SOLVE(DDF2, DF2, DF1, L, MM, IER)
        IFAULT = 2
        IF (IER .EQ. 1) GOTO 160
C
        IF ICODE1 = 1, F HAS NOT CONVERGED.
C
        IF (ICODE1 .EQ. 1) GOTO 45
C
        SET ICODE2 = 1 IF THE RELATIVE CHANGE IN ANY THETA
        IS GREATER THAN OR EQUAL TO CRI2 AND 0 OTHERWISE.
C
        ICODE2 = 0
        DO 40 J = 1, L
          IF (ABS(DF2(J)) .GE. ABS(THETA(J)) * CRI2) ICODE2 = 1
40      CONTINUE
C
        FOR CONVERGENCE TO BE REACHED, BOTH THE RELATIVE CHANGE IN
        SUCCESSIVE MLES MUST BE LESS THAN CRI2 AND THE RELATIVE
        CHANGE IN SUCCESSIVE LOG LIKELIHOODS MUST BE LESS THAN CRI1.
C
        IF (ICODE1 .EQ. 0 .AND. ICODE2 .EQ. 0) GOTO 70
C
        CONVERGENCE WAS NOT REACHED.
C
        FIND NEW VALUES OF THETA AND BEGIN NEXT ITERATION.
```

```
C
45      DO 50 J = 1, L
          THETA(J) = THETA(J) + DF2(J)
50      CONTINUE
60      CONTINUE
C
C          CONVERGENCE WAS NOT REACHED IN ITERS ITERATIONS
C
          IFAULT = 1
          GOTO 160
70      ITERS = K
          IFAULT = 0
C
C          CONVERGENCE WAS REACHED IN K ITERATIONS.
C
          CALL CVSUR2(N, M, L, MM, U, A, R, Z, IROWS, VAR,
*          THETA, F, DF2, DDF2)
          CALL SYMINV(DDF2, L, VAR, U, NULLTY, IFAULT)
160     RETURN
        END
C
C
          SUBROUTINE CVSUR2(N,M,L,MM,U,WORK,R,Z,IROWS,ZSUM,THETA,
*          F, DF, DDF)
C
          ALGORITHM AS 125.1 APPL. STATIST. (1978) VOL.27, NO.2
C
          THIS SUBROUTINE CALCULATES THE LOG LIKELIHOOD (F), FIRST
          DERIVATIVE ARRAY (DF), AND (-1)*SECOND DERIVATIVE MATRIX (DDF).
          THE ELEMENTS OF DDF ARE IN SYMMETRIC STORAGE MODE.
C
          DIMENSION U(N), Z(IROWS, M), ZSUM(M), THETA(L), DF(L), DDF(MM),
*          WORK(N)
          PARAMETER (ZERO=0.0)
C
          ETHETA = EXP(THETA(L))
          UEPROD = ZERO
          ZPROD = ZERO
          DO 20 J = 1, M
              ZPROD = ZPROD + THETA(J) * ZSUM(J)
20      CONTINUE
          DO 40 I = 1, N
              WORK(I) = ZERO
C
          CALCULATE LOG LIKELIHOOD
          THETA(1) - THETA(M) CONTAIN BETA ESTIMATES
          THETA(M+1) CONTAINS THE ESTIMATE OF ALPHA.
C
          DO 30 J = 1, M
              WORK(I) = WORK(I) + THETA(J) * Z(I, J)
30      CONTINUE
          WORK(I) = EXP(WORK(I))
          UEPROD = UEPROD + U(I) * WORK(I)
40      CONTINUE
          F = R * THETA(L) + ZPROD - ETHETA * UEPROD
C
          CALCULATE FIRST DERIVATIVE ARRAY DF.
          FROM HERE THROUGH STATEMENT 60, DDF IS USED AS A WORK ARRAY
C
          TERM1 = -ETHETA * UEPROD
          DF(L) = R + TERM1
```

```

DO 60 J = 1, M
  DDF(J) = ZERO
  DO 50 I = 1, N
    DDF(J) = DDF(J) + U(I) * Z(I, J) * WORK(I)
50  CONTINUE
    DDF(J) = -ETHETA * DDF(J)
    DF(J) = ZSUM(J) + DDF(J)
60  CONTINUE
C
C    CALCULATE (-1)*SECOND DERIVATIVE ARRAY DDF
C
KK = (L - 1) * L / 2
DO 70 J = 1, M
  KK = KK + 1
  DDF(KK) = -DDF(J)
70  CONTINUE
  DDF(MM) = -TERM1
  KK = 0
DO 85 J = 1, M
  DO 80 K = 1, J
    KK = KK + 1
    DDF(KK) = ZERO
    DO 75 I = 1, N
      DDF(KK) = DDF(KK) + U(I) * Z(I, J) * Z(I, K) * WORK(I)
75  CONTINUE
      DDF(KK) = ETHETA * DDF(KK)
80  CONTINUE
85  CONTINUE
RETURN
END

C
C
SUBROUTINE SOLVE(A, X, B, N, NN, IFAULT)
C
C    ALGORITHM AS 125.2 APPL. STATIST. (1978) VOL.27, NO.2
C
C    THIS SOLVES THE LINEAR SYSTEM L*(L-TRANSPOSE)*X=B,
C    WHERE L IS A LOWER TRIANGULAR MATRIX WITH POSITIVE
C    DIAGONALS. THE ELEMENTS OF L ARE STORED IN ARRAY A
C    IN THE FOLLOWING ORDER - L(1,1), L(2,1), L(2,2),
C    L(3,1), L(3,2),.....
C    X AND B COULD OCCUPY THE SAME LOCATIONS, BUT THIS IS
C    PROHIBITED BY THE FORTRAN STANDARD (SECTION 8.4.2)
C
PARAMETER (ZERO=0.0)
DIMENSION A(NN), X(N), B(N)
C
C    SOLVE LW = B FOR W AND PUT RESULT IN X.
C
IF (A(1) .LE. ZERO) GOTO 50
X(1) = B(1) / A(1)
IF (N .EQ. 1) GOTO 25
DO 20 J = 2, N
  J1 = (J -1) * J / 2
  SUM = B(J)
  JM1 = J - 1
  DO 10 I = 1, JM1
    I1 = J1 + I
    SUM = SUM - A(I1) * X(I)
10  CONTINUE
    I1 = J1 + J

```

```
        IF (A(I1) .LE. ZERO) GOTO 50
        X(J) = SUM / A(I1)
20      CONTINUE
C
C        SOLVE (L-TRANSPPOSE)*W = X AND PUT RESULT IN X
C
25      X(N) = X(N) / A(NN)
        IF (N .EQ. 1) GOTO 45
        DO 40 JJ = 2, N
          J = N - JJ + 1
          SUM = X(J)
          JP1 = J + 1
          DO 30 I = JP1, N
            I1 = (I - 1) * I / 2 + J
            SUM = SUM - A(I1) * X(I)
30          CONTINUE
          I1 = J * (J + 1) / 2
          X(J) = SUM / A(I1)
40      CONTINUE
45      IFAULT = 0
        RETURN
50      IFAULT = 1
        RETURN
        END
```



```
double precision function rngpi(t, n, ifault)
c
c      Algorithm AS 126  Appl. Statist. (1978) Vol. 27, No. 2
c
c      Computes the probability of the normal range given t, the
c      upper limit of integration, and n, the sample size.
c
c      Auxiliary function required: ALNORM = algorithm AS66
c
c      implicit double precision (a-h,o-z)
c      dimension g(8), h(8)
c
c      data g(1), g(2), g(3), g(4), g(5), g(6), g(7), g(8)
c      */0.4947004675d0, 0.4722875115d0, 0.4328156012d0, 0.3777022042d0,
c      * 0.3089381222d0, 0.2290083888d0, 0.1408017754d0, 0.04750625492d0/
c
c      data h(1), h(2), h(3), h(4), h(5), h(6), h(7), h(8)
c      */0.01357622971d0, 0.03112676197d0, 0.04757925584d0,
c      * 0.06231448563d0,
c      * 0.07479799441d0, 0.08457825969d0, 0.09130170752d0,
c      * 0.09472530523d0/
c
c      data zero, half, two, eight /0.0d0, 0.5d0, 2.0d0, 8.0d0/
c
c      risf(x) = 0.3989422804d0 * exp(-half*x*x) * (alnorm(x, .false.)
c      * - alnorm(x-t, .false.)) ** (n-1)
c
c      ifault = 0
c      rngpi = zero
c      if (t .le. zero .or. n .le. 1) return
c
c      ifault = 0
c      xl = half * t
c      a = half * (eight + xl)
c      b = eight - xl
c      y = zero
c      do 10 i = 1, 8
c      c = b * g(i)
c      y = y + h(i) * (risf(a + c) + risf(a - c))
10 continue
c      rngpi = (two * (alnorm(xl, .false.) - half)) ** n +
c      * two * b * y * n
c      return
c      end
```

```

SUBROUTINE RNORTM(N, NP1, IBCONF, NB, B, NDBI, DBI, ISEED, A,
* CHISQ, FAB, U, W, IFAULT)
C
C     ALGORITHM AS 127 APPL. STATIST. (1978) VOL.27, NO.2
C
C     RNORTM GENERATES ORTHOGONAL MATRICES A FROM A DISTRIBUTION
C     WITH DENSITY FUNCTION DEFINED ON THE GROUP OF ORTHOGONAL
C     MATRICES. WHEN THE INPUT PARAMETER IBCONF = 1 THE
C     MATRICES ARE GENERATED FROM THE INVARIANT HAAR MEASURE.
C
C     Corrections in remark AS R42 (Appl. Statist., vol.31, 1982) have
C     been incorporated.
C
REAL B(NB), DBI(NDBI), A(N, N), CHISQ(N), U(NP1), W(N), FAB, UL,
* WL, WIL, WWIL, T2, HV, HW, ZERO, ONE
C
DATA ZERO /0.0/, ONE /1.0/
C
C     STATEMENT FUNCTIONS FOR DOUBLE PRECISION
C     DOUBLE PRECISION SQRT, SIGN, ABS
C     SQRT(UL) = DSQRT(UL)
C     SIGN(UL, WL) = DSIGN(UL, WL)
C     ABS(UL) = DABS(UL)
C
C     SECTION 1  INITIALIZATION
C     CHECK CONSISTENCY OF INPUT DIMENSIONS
C
IFAULT = 0
IF (N .LT. 1) GOTO 1
IF (NP1 .NE. N + 1) GOTO 1
IF (IBCONF .LT. 1 .OR. IBCONF .GT. 3) GOTO 1
IF (IBCONF .EQ. 1 .AND. (NB .NE. 1 .OR. NDBI .NE. 1)) GOTO 1
IF (IBCONF .EQ. 2 .AND. (NB .NE. N * (N + 1) / 2 .OR. NDBI .NE. N))
* GOTO 1
IF (IBCONF .EQ. 3 .AND. (NB .NE. N * (N + 1) * (2 * N + 1) / 6
* .OR. NDBI .NE. N)) GOTO 1
GOTO 4
C
C     ERROR RETURNS
C
1     IFAULT = 1
RETURN
2     IFAULT = 2
RETURN
C
C     INITIALIZE DENSITY, H(STORED IN A), AND IBSUB
C
4     FAB = ONE
DO 100 I = 1, N
DO 50 J = 1, N
50     A(I, J) = ZERO
A(I, I) = ONE
100    CONTINUE
IBSUB = 0
C
C     CONSTRUCT A ONE COLUMN AT A TIME
C
DO 315 L = 1, N
NP1L = NP1 - L
C
C     SECTION 2

```

```

C          CONSTRUCT U(L...N), UNIFORMLY DISTRIBUTED ON THE SURFACE OF THE
C          (N+1-L)-SPHERE OF RADIUS UL = SQRT(CHISQ(L)).
C
C          CALL NORMAL(U(L), NP1L + 1, ISEED, CHISQ(L))
C          UL = SQRT(CHISQ(L))
C          IF (UL .EQ. ZERO) GOTO 2
C          IF (L .EQ. N) GOTO 301
C
C          SECTION 3
C          CALCULATE W = B*U AND STORE ITS LENGTH IN WL.
C          SIGN OF WL PREVENTS LOSS OF SIGNIFICANCE IN WWIL
C
C          GOTO (215, 220, 225), IBCONF
C
C          B IS IDENTITY
C
C          215 WL = SIGN(UL, U(L))
C          DO 219 J = L, N
C          219 W(J) = U(J)
C          GOTO 229
C
C          DIAGONAL MATRICES B
C
C          220 WL = ZERO
C          DO 221 J = L, N
C             ITEMP = IBSUB + J
C             T2 = B(ITEMP) * U(J)
C             WL = WL + T2 * T2
C             W(J) = T2
C          221 CONTINUE
C          IBSUB = IBSUB + N - L
C          GOTO 228
C
C          FULL MATRICES B
C
C          225 WL = ZERO
C          DO 227 J = L, N
C             T2 = ZERO
C             DO 226 K = L, N
C                ITEMP = IBSUB + K
C                T2 = T2 + B(ITEMP) * U(K)
C          226 CONTINUE
C          IBSUB = IBSUB + NP1L
C          WL = WL + T2 * T2
C          W(J) = T2
C          227 CONTINUE
C          IBSUB = IBSUB - 1
C
C          CALCULATE DENSITY FOR IBCONF = 2 OR 3
C
C          228 WL = SIGN(SQRT(WL), -W(L))
C          FAB = (WL / UL) ** NP1L * DBI(L) * FAB
C          IF (FAB .EQ. ZERO) GOTO 2
C          229 CONTINUE
C
C          SECTION 4
C          PROJECT W ONTO ORTHOGONAL COMPLEMENT OF FIRST L-1
C          COLUMNS OF A, NORMALIZE, AND STORE IN L COLUMN OF A.
C          A(L) = H(L) * W * WIL
C          CALCULATE PROJECTION MATRIX H(L) FOR ORTHOGONAL
C          COMPLEMENT OF FIRST L COLUMNS OF A AND STORE IN LAST

```

```
C      N-L COLUMNS OF A.
C
      LP1 = L + 1
      WIL = ONE / WL
      WWIL = ONE / (WL - W(L))
      DO 250 I = 1, N
        T2 = ZERO
        DO 230 J = L, N
230      T2 = T2 + A(I, J) * W(J)
        HV = T2 * WIL
        HW = (HV - A(I, L)) * WWIL
        A(I, L) = HV
        DO 240 J = LP1, N
240      A(I, J) = A(I, J) - HW * W(J)
250      CONTINUE
C
C      END OF L COLUMN OF MATRIX A
C
C      SECTION 5
C      WHEN L = N ONLY SIGN NEEDS TO BE CHOSEN
C      REMEMBER MATRIX H(N) IS STORED IN N COLUMN OF A.
C
301      IF (U(L) .GT. ZERO) GOTO 315
        DO 310 I = 1, N
310      A(I, L) = -A(I, L)
315      CONTINUE
C
C      FAB = ABS(B(LAST) * DBI(N) * FAB)
C
320      FAB = ABS(FAB)
C
      RETURN
      END
```

```

subroutine covmat(v,n,mdim,v11,ex1,ex2,summ2,ifault)
c
c   Appl. Statist. algorithm as 128 (1978), vol. 27
c   Davis C.S. and Stephens M.A.
c
c   Computes and normalises the David-Johnson approximation
c   for the covariance matrix of normal order statistics.
c
c   Auxiliary function equired: PPND = algorithm AS111
c   N.B. This file also includes ASR72 to calculate v11
c
integer n,mdim,ifault
double precision v(mdim,n),v11,ex1,ex2,summ2
c
c   local integer variables
c
integer i,j,k,ni,nj
c
c   local real variables
c
double precision cnst,dxr,d2xr,d3xr,d4xr,d5xr,dxs,d2xs,
1      d3xs,d4xs,d5xs,pr,ps,qr,rn,rn1,rn2,rn22,rn23,sum,
2      two,xr,xs,zero
c
common /cons/ rn2,rn22,rn23
c
c   initialise constants
c
data zero /0.0d0/,half /0.5d0/, one /1.0d0/ ,two/2.0d0/
c
ifault = 1
if(n .gt. mdim .or. n. lt. 2) return
ifault = 0
rn=n
rn1=rn+one
rn2=rn+two
rn22=rn2*rn2
rn23=rn22*rn2
nhalf1=(n+1) / 2
c
c   the elements of the upper triangle
c   are first computed
c
ni=n
do 50 i=1,nhalf1
  pr=float(i)/rn1
  qr=one-pr
c
c   in function ppnd, xr is computed to satisfy
c   prob(z.lt.pr) = pr, where z is n(0,1)
c
  xr = ppnd(pr, ifault)
  call der(xr,dxr,d2xr,d3xr,d4xr,d5xr)
  do 40 j=i,ni
    if (i .ne. j) goto 30
c
c   if i is equal to j, var(xr) is calculated
c
    v(i,j)=var(dxr,d2xr,d3xr,d4xr,d5xr,pr,qr)
    go to 40
c

```

```
c      if i is not equal to j, cov(xr,xs) is calculated
c
30      ps=float(j)/rn1
        xs=ppnd(ps,ifault)
        call der(xs,dxs,d2xs,d3xs,d4xs,d5xs)
        v(i,j)=cov(dxr,d2xr,d3xr,d4xr,d5xr,pr,qr,
1         dxs,d2xs,d3xs,d4xs,d5xs,ps)
        v(j,i)=v(j,i)
40      continue
        ni=ni-1
50      continue
c
c      By symmetry the other elements of v will now be filled
c
        nj = n
        do 70 i = 2,n
          njm1 = nj - 1
          im1 = i - 1
          do 60 j = nj, n
            v(i,j) = v(im1, njm1)
            im1 = im1 - 1
60          continue
          nj = nj - 1
70          continue
c
c      insert exact values of v(1,1) and v(1,2)
c
        v(1,1)=v11
        v(n,n)=v(1,1)
        v(1,2)=v(1,1)+ex1*(ex1-ex2)-one
        v(2,1)=v(1,2)
        nsub1=n-1
        v(n,nsub1)=v(1,2)
        v(nsub1,n)=v(1,2)
c
c      normalise the first row of v, leaving
c      v(1,1) and v(1,2) fixed
c
        if(n.eq.2) return
        sum=zero
        do 80 j=3,n
          sum=sum+v(1,j)
80      continue
        cnst=(one-v(1,1)-v(1,2))/sum
        nj=n-2
        do 90 j=3,n
          v(1,j)=v(1,j)*cnst
          v(j,1)=v(1,j)
          v(n,nj)=v(1,j)
          v(nj,n)=v(1,j)
          nj=nj-1
90      continue
c
c      normalise rows 2 through n-1 of v
c
        call rwnorm(v,n,mdim,0)
c
c      modify v(2,2) and its equal
c      v(n-1,n-1) so the trace identity is satisfied
c
        sum=zero
```

```

      do 100 k=1,n
        if(k.eq.2.or.k.eq.nsub1) go to 100
        sum=sum+v(k,k)
100  continue
      v(2,2)=half*(float(n)-summ2-sum)
      v(nsub1,nsub1)=v(2,2)
c
c  renormalise rows 2 through n-1 of v,
c  leaving diagonal elements fixed,
c
      call rwnorm(v,n,mdim,1)
      return
      end
c
      subroutine rwnorm(v,n,mdim,id)
c
c  Appl. Statist algorithm as 128.4 (1978), vol. 27
c  Davis C.S. and Stephens M.A.
c
c  Normalises rows of covariance matrix of normal order statistics
c  so that sum of row elements equals one.
c
c  arguments :      v - array (mdim,mdim) containing the covariance
c                   matrix approximation.
c                   n - sample size.
c                   mdim - row dimension of v in the calling program.
c                   id -
c
      integer n,mdim,id
      double precision v(mdim,n)
c
c  local integer variables
c
      integer i,j,k,l,m,ni,nj
c
c  local real variables
c
      double precision cnst,one,small,sum,term,zero
c
      data zero /0.0d0/, small /1.0d-12/, one /1.0d0/
c
      nhalf1 = (n+1)/2
      ni=n-1
      do 75 i=2,nhalf1
c
c  find sums of computed terms in each row
c
          sum=zero
          do 55 j=i,ni
            sum=sum+v(i,j)
55      continue
          if(id .ne.0) sum = sum - v(i,i)
          if(abs(sum).lt.small) go to 75
c
c  normalise rows leaving appropriate elements fixed
c
          k=i-1
          if(id .ne. 0) k = i
          term=zero
          do 60 j=1,k
60      term=term+v(i,j)

```

```

        l=ni+1
        do 65 j=1,n
65         term=term+v(i,j)
           cnst=(one-term)/sum
           m=i
           if(id.ne.0) m=i+1
           nj=n-m+1
           do 70 j=m,ni
              v(i,j)=v(i,j)*cnst
              v(j,i)=v(i,j)
              v(ni,nj)=v(i,j)
              v(nj,ni)=v(i,j)
              nj=nj-1
70          continue
           ni=ni-1
75 continue
        return
        end

c
subroutine der(x,dx,d2x,d3x,d4x,d5x)
c
c   Appl. Statist. algorithm as 128.1 (1978), vol 27.
c   Davis C.S. and Stephens M.A.
c
c   Computes derivatives for the david-johnson approximation to the
c   variances and covariances of normal order statistics.
c
c   arguments : x - real number at which derivative is calculated.
c               dx - first derivative of normal probability integral
c                   evaluated at x.
c               :
c               :
c               :
c               d5x - fifth derivative of normal probability integral
c                   evaluated at x.
c
c   double precision x,dx,d2x,d3x,d4x,d5x
c
c   local real variables
c
c   double precision forty6,one,onept5,rad2pi,seven,six,
1      term,twent4,two,twopi,x2
c
c   initialise constants
c
c   data one /1.0d0/, onept5 /1.5d0/, two /2.0d0/,
1      six /6.0d0/,seven /7.0d0/, twent4 /24.0d0/,
2      forty6 /46.0d0/, rad2pi /2.506628274631d0/,
3      twopi/6.2831853071796d0/
      x2=x*x
      dx=rad2pi*exp(x2/two)
      d2x=twopi*x*exp(x2)
      d3x=twopi*rad2pi*(two*x2+one)*exp(onept5*x2)
      term=twopi*twopi*exp(two*x2)
      d4x=term*x*(six*x2+seven)
      d5x=term*dx*(x2*(twent4*x2+forty6)+seven)
      return
      end

c
double precision function var(dxr,d2xr,d3xr,d4xr,d5xr,pr,qr)
c
c   Appl. Statist. algorithm 128.2 (1978), vol 27
c

```



```

c      Computes David-Johnson approximation for the variance of
c      the rth largest order statistic from the normal dist. for
c      a sample size n.
c
c      arguments : dxr - first derivative of normal probability integral
c                   evaluated at xr.
c                   :
c                   :
c                   :
c                   d5xr - fifth derivative of normal probability integral
c                           evaluated at xr.
c                   pr - expected value of rth largest order statistic
c                           from uniform dist. ( = r/(n+1) r=1,...,n).
c                   qr - 1-pr
c                           n.b. xr is the inverse normal probability integral
c                           of pr.
c
c      double precision dxr,d2xr,d3xr,d4xr,d5xr,pr,qr
c
c      local real variables
c
c      double precision d2xr2,dxr2,fiveth,fourth,half,onept5,prqr,
1      qrmpr,rn2,rn22,rn23,two,three
c
c      common /cons/ rn2,rn22,rn23
c
c      initialise constants
c
c      data fourth /0.25d0/, half /0.5d0/, onept5 /1.5d0/,
1      fiveth /1.6666666667d0/, two /2.0d0/ , three /3.0d0/
c      dxr2=dxr*dxr
c      prqr=pr*qr
c      var=prqr*dxr2/rn2
c
c      to order (n+2)**(-2)
c
c      qrmpr=qr-pr
c      d2xr2=d2xr*d2xr
c      var = var+prqr/rn22*(two*qrmpr*dxr*d2xr+prqr*
1      (dxr*d3xr+half*d2xr2))
c
c      to order (n+2)**(-3)
c
c      var = var+prqr/rn23*(-two*qrmpr*dxr*d2xr+
1      (qrmpr*qrmpr-prqr)*(two*dxr*d3xr+onept5*d2xr2)
2      +prqr*qrmpr*(fiveth*dxr*d4xr+three*d2xr*d3xr)
3      +fourth*prqr*prqr*(dxr*d5xr+two*d2xr*d4xr+
4      fiveth*d3xr*d3xr))
c      return
c      end
c
c      double precision function cov(dxr,d2xr,d3xr,d4xr,d5xr
1      ,pr,qr,dxs,d2xs,d3xs,d4xs,d5xs,ps)
c
c      Appl. statist. algorithm as 128.3 (1978), vol. 27
c      Davis C.S. and Stephens M.A.
c
c      Computes David-Johnson approximation for covariance between rth
c      and sth order statistics from the normal dist. for a sample size n.
c
c      arguments : dxr - first derivative of normal probability integral
c                   evaluated at xr.
c                   :
c                   :
c                   :

```

```

c          d5xr - fifth derivative of normal probability integral
c          evaluated at xr.
c          pr - expected value of rth order statistic from
c          uniform dist. ( = r/(n+1) r=1,...,n ).
c          qr - 1-pr.
c          dxs - first derivative of normal probability integral
c          evaluated at xs.
c          :          :          :
c          d5xs - fifth derivative of normal probability integral
c          evaluated at xs.
c          ps - expected value of sth order statistic from
c          uniform distribution. ( = s/(n+1) s=1,...,n).
c          n.b. xr is the inverse normal probability
c          integral of pr etc.
c
c          double precision dxr,d2xr,d3xr,d4xr,d5xr,pr,qr,dxs,d2xs,
1          d3xs,d4xs,d5xs,ps
c
c          local real variables
c
c          double precision eigth,five6,fourth,half,one,onept5,pr2,
1          prqr,prqs,ps2,psqr,psqs,qr2,qrmpr,qs,qs2,qsmps,
2          rn2,rn22,rn23,term1,term2,term3,term4,term5,
3          three,twelth,two
c
c          common /cons/ rn2,rn22,rn23
c
c          initialise constants
c
c          data twelth /0.08333333333333d0/, eigth /0.125d0/,
1          fourth /0.25d0/, half /0.5d0/,
2          five6 /0.83333333333333d0/, one /1.0d0/,
3          onept5 /1.5d0/, two /2.0d0/, three /3.0d0/
c
c          qs=one-ps
c          prqs=pr*qs
c          cov=prqs*dxr*dxs/rn2
c
c          to order (n+2)**(-2)
c
c          qrmpr=qr-pr
c          qsmps=qs-ps
c          prqr=pr*qr
c          psqs=ps*qs
c          cov = cov+prqs/rn22*(qrmpr*d2xr*dxs+
1          qsmps*dxr*d2xs+half*prqr*d3xr*dxs+
2          half*psqs*dxr*d3xs+half*prqs*d2xr*d2xs)
c
c          to order (n+2)**(-3)
c
c          pr2=pr*pr
c          qr2=qr*qr
c          ps2=ps*ps
c          qs2=qs*qs
c          psqr=ps*qr
c          term1=-d2xr*dxs*qrmpr-qsmps*dxr*d2xs+
1          (qrmpr*qrmpr-prqr)*d3xr*dxs
c          term2=(qsmps*qsmps-psqs)*dxr*d3xs+(onept5*qrmpr*
1          qsmps+half*psqr-two*prqs)*d2xr*d2xs
c          term3=five6*(prqr*qrmpr*d4xr*dxs+psqs*qsmps*dxr*
1          d4xs)+(prqs*qrmpr+half*prqr*qsmps)*d3xr*d2xs

```

```

term4=(prqs*qsmps+half*psqs*qrmp)*d2xr*d3xs+
1      eigth*(pr2*qr2*d5xr*dxs+ps2*qs2*dxr*d5xs)
term5=fourth*(pr2*qr*qs*d4xr*d2xs+pr*ps*qs2*
1      d2xr*d4xs)+twelth*(two*pr2*qs2+three*pr*qr*
2      ps*qs)*d3xr*d3xs
cov = cov+prqs/rn23*(term1+term2+term3+term4+term5)
return
end

```

```

c
double precision function v11(n, ifault)
c
c ASR 72 (Remark on AS 128) Applied Stats. (1988) vol. 37 (1)
c
c Calculates an approximation to the variance of the largest
c normal order statistic.
c

```

```
integer n, ifault
```

```

c
c Local variables
c

```

```

double precision zero, one, a0, a1, a2, a3, a4, a5, a6, x,
+      d0, d1, d2, d3, d4, d5, d6, pt09, c0, c1, c2, c3,
+      c4, c5, c6, c7, c8, c9, mpt15, b0, b1, b2, b3, b4
parameter (mpt15 = -0.15, b0 = -0.934d-4, zero = 0.d0,
+      one = 1.d0,
+      b1 = -0.5950321d0, b2 = 0.0165504d0, b3 = 0.0056975d0,
+      pt09 = 0.091105452691946d0, c0 = 0.7956d-11,
+      c1 = -0.595628869836878d0, c2 = 0.08967827948053d0,
+      c3 = -0.007850066416039d0, c4 = -0.296537314353d-3,
+      c5 = 0.215480033104d-3, c6 = -0.33811291323d-4,
+      c7 = 0.2738431187d-5, c8 = -0.106432868d-6,
+      c9 = 0.1100251d-8, a0 = 0.04619831847696d0,
+      a1 = -0.147930264017706d0, a2 = -0.451288155800301d0,
+      a3 = 0.010055707621709d0, a4 = 0.007412441980877d0,
+      a5 = -0.001143407259055d0, a6 = 0.54428754576d-4,
+      d0 = 0.093256818332708d0, d1 = 1.336952989217635d0,
+      d2 = -1.783195691545387d0, d3 = 0.488682076188729d0,
+      d4 = -0.078737246197474d0, d5 = 0.00662561987806d0,
+      d6 = -0.226486218258d-3, b4 = -0.8531d-3)

```

```

c
v11 = zero
ifault = 1
if (n .lt. 1) return
ifault = 0
if (n .eq. 1) then
v11 = one
return
end if

```

```

c
x = n
if (n .gt. 370) then
x = (x**mpt15 - one) / mpt15
v11 = exp(b0 + x*(b1 + x*(b2 + x*(b3 + x*b4))))
else if (n .le. 100) then
x = (x**pt09 - one) / pt09
v11 = exp(c0 + x*(c1 + x*(c2 + x*(c3 + x*(c4 + x*(c5 + x*
+      (c6 + x*(c7 + x*(c8 + x*c9))))))))))
else if (n .le. 200) then
x = log(a0 + x)
v11 = exp(a1 + x*(a2 + x*(a3 + x*(a4 + x*(a5 + x*a6))))
else

```

```
    x = log(d0 + x)
    v11 = exp(d1 + x*(d2 + x*(d3 + x*(d4 + x*(d5 + x*d6))))
end if
c
return
end
```

```

SUBROUTINE SIMLP(N, X, Y, SAD, ALPHA, BETA, D, ITER, INEXT,
*   IFAULT)
C
C   ALGORITHM AS 132  APPL. STATIST. (1978) VOL.27, NO.3
C
C   SIMPL:   Fit  Y = ALPHA + BETA.X + error
C
REAL X(N), Y(N), D(N)
INTEGER INEXT(N)
DATA ACU/1.0E-06/, BIG/1.0E19/, HALF/0.5/, ZERO/0.0/, ONE/1.0/,
*   TWO/2.0/
C
C   Initial settings
C
IFAULT = 0
ITER = 0
AHALF = HALF + ACU
AONE = AHALF + AHALF
C
C   Determine initial basis
C
D(1) = ZERO
Y1 = Y(1)
IBAS1 = 1
A1 = X(1)
DO 10 I = 2, N
  IF (ABS(A1 - X(I)) .LT. ACU) GO TO 10
  A2 = X(I)
  IBAS2 = I
  Y2 = Y(I)
  GO TO 20
10 CONTINUE
IFAULT = 1
RETURN
C
C   Calculate initial beta value
C
20 DET = ONE / (A2 - A1)
AAAA = (A2 * Y1 - A1 * Y2) * DET
BBBB = (Y2 - Y1) * DET
C
C   Calculate initial D-vector
C
DO 30 I = 2, N
  DDD = Y(I) - (AAAA + BBBB * X(I))
  D(I) = SIGN(ONE, DDD)
30 CONTINUE
TOT1 = ONE
TOT2 = X(IBAS2)
D(IBAS2) = - ONE
DO 40 I = 2, N
  TOT1 = TOT1 + D(I)
  TOT2 = TOT2 + D(I) * X(I)
40 CONTINUE
T = (A2 * TOT1 - TOT2) * DET
IF (ABS(T) .LT. AONE) GO TO 50
DET = - DET
GO TO 70
C
C   Main iterative loop begins
C

```

```

50 T = (TOT2 - A1 * TOT1) * DET
   IF (ABS(T) .LT. AONE) GO TO 160
   IFLAG = 2
   IOUT = IBAS2
   X(IOUT) = A1
   AAA = A1
   BBB = A2
   GO TO 80
60 T = (TOT2 - A2 * TOT1) * DET
   IF (ABS(T) .LT. AONE) GO TO 160
70 IFLAG = 1
   BBB = A1
   AAA = A2
   IOUT = IBAS1
80 RHO = SIGN(ONE, T)
   T = HALF * ABS(T)
   DET = DET * RHO
C
C   Perform partial sort of ratios
C
   INEXT(IBAS1) = IBAS2
   RATIO = BIG
   SUM = AHALF
   DO 120 I = 1, N
     DDD = (X(I) - AAA) * DET
     IF (DDD * D(I) .LE. ACU) GO TO 120
     TEST = (Y(I) - AAAA - BBBB * X(I)) / DDD
     IF (TEST .GE. RATIO) GO TO 120
     J = IBAS1
     SUM = SUM + ABS(DDD)
90   ISAVE = ABS(INEXT(J))
     IF (TEST .GE. D(ISAVE)) GO TO 110
     IF (SUM .LT. T) GO TO 100
     SUBT = ABS((X(ISAVE) - AAA) * DET)
     IF (SUM - SUBT .LT. T) GO TO 100
     SUM = SUM - SUBT
     D(ISAVE) = SIGN(1, INEXT(J))
     INEXT(J) = INEXT(ISAVE)
     GO TO 90
100  J = ISAVE
     ISAVE = ABS(INEXT(J))
     IF (TEST .LT. D(ISAVE)) GO TO 100
110  INEXT(I) = INEXT(J)
     INEXT(J) = SIGN(I, INT(D(I)))
     D(I) = TEST
     IF (SUM .LT. T) GO TO 120
     IIN = ABS(INEXT(IBAS1))
     RATIO = D(IIN)
120 CONTINUE
C
C   Update basic indicators
C
   IIN = ABS(INEXT(IBAS1))
   J = IIN
130 ISAVE = ABS(INEXT(J))
   IF (ISAVE .EQ. IBAS2) GO TO 140
   ZZZ = SIGN(1, INEXT(J))
   TOT1 = TOT1 - ZZZ - ZZZ
   TOT2 = TOT2 - TWO * ZZZ * X(ISAVE)
   D(ISAVE) = - ZZZ
   J = ISAVE

```

```
GO TO 130
140 ZZZ = SIGN(1, INEXT(IBAS1))
TOT1 = TOT1 - RHO - ZZZ
TOT2 = TOT2 - RHO * BBB - ZZZ * X(IIN)
D(IOUT) = - RHO
ITER = ITER + 1
IF (IFLAG .EQ. 1) GO TO 150
X(IBAS2) = A2
IBAS2 = IIN
D(IBAS2) = - ONE
A2 = X(IIN)
Y2 = Y(IIN)
DET = ONE / (A1 - A2)
AAAA = (A1 * Y2 - A2 * Y1) * DET
BBBB = (Y1 - Y2) * DET
GO TO 60
150 IBAS1 = IIN
A1 = X(IIN)
D(IBAS1) = ZERO
Y1 = Y(IIN)
DET = ONE / (A2 - A1)
AAAA = (A2 * Y1 - A1 * Y2) * DET
BBBB = (Y2 - Y1) * DET
GO TO 50
C
C Calculate optimal sum of absolute deviations
C
160 SAD = ZERO
DO 170 I = 1, N
D(I) = Y(I) - (AAAA + BBBB * X(I))
SAD = SAD + ABS(D(I))
170 CONTINUE
ALPHA = AAAA
BETA = BBBB
C
RETURN
END
```

```

SUBROUTINE EXTR(BP,EP,M,N,F,YM,XM,NE,E1,E2,N1,NP,X1,Y1,X2,Y2,
+             IFAULT)
C
C     ALGORITHM AS 133 APPL. STATIST. (1978) VOL.27, NO.3
C
C     OPTIMIZATION OF ONE DIMENSIONAL MULTIMODAL FUNCTIONS
C
C     Auxiliary routines required: The user must provide a real function
C     F(X) to return the value of the function to be minimized.
C     Brent's LOCALM has been added to this routine.
C
C     DIMENSION X1(NP),Y1(NP),X2(NP),Y2(NP)
C     EXTERNAL YL,F
C     REAL LOCALM
C     REAL ONE,TEN,TWENT5,ZERO,SEVEN,SMALL,NINET8,PT99,TWO,THREE,FIVE
C     DOUBLE PRECISION EE1,EE2,EE3,DM17
C
C     COMMON /EXTR1/A,EB,YH,XJ1,XJ2,YJ1,YJ2
C
C     K is a machine-dependant constant. 10(-K) should be set to the
C     smallest number which can be represented in the machine.
C
C     DATA K/37/, EPSL/0.0/
C     DATA ONE/1.0/, TEN/10.0/, TWENT5/25.0/, ZERO/0.0/, SEVEN/7.0/,
+     SMALL/3.0E-4/, NINET8/98.0/, PT99/0.99/, TWO/2.0/, THREE/3.0/,
+     FIVE/5.0/
C
C     K1 = K/3
C     CUND = -2*K
C     CP5 = TEN** (K1-1)
C     CP6 = TEN*CP5
C     CM6 = ONE/CP6
C     CM5 = ONE/CP5
C     DM17 = 10.0D0** (-K+2)
C     CM17 = DM17
C     IFAULT = 0
C     IF (NE.GE.6) GO TO 5
C     IFAULT = 3
C     RETURN
5  N1 = NE
   N2 = N1 + 2
   CM = M
   A = MIN(BP,EP)
   EB = MAX(BP,EP) - A
   EB2 = EB/TWENT5
   IF (EB.GE.CM5 .AND. EB.LE.CP5) GO TO 10
   IFAULT = 1
   RETURN
10 DA = EB/REAL(N1-1)
   N6 = N1 + 3
   DO 20 J = 4,N6
     X1(J) = A
     Y1(J) = F(A)*CM
     A = A + DA
20 CONTINUE
   A = ZERO
   YM = Y1(4)
   XM = X1(4)
C

```



```
C      A IS ESTIMATE OF PARAMETER OF WIENER PROCESS
C      (PARAMETER OF MODEL OF FUNCTION F)
C
DO 30 J = 5,N6
  A = A + (Y1(J)-Y1(J-1))**2
  IF (YM.LE.Y1(J)) GO TO 30
  YM = Y1(J)
  XM = X1(J)
30 CONTINUE
  YH = YM
  A = SQRT(A/EB)*SEVEN
  IF (A.GE.CM6 .AND. A.LE.CP6) GO TO 40
  IFAULT = 2
  RETURN

C
C      A IS EVALUATED.  N5 IS THE NUMBER OF LOCAL OPTIMA
C      COMPUTED WITH ACCURACY E1, E2
C
40 N5 = 0
  DO 50 J = 4,N2
50 Y2(J) = ZERO

C
C      BAYESIAN STEP - FIND INTERVAL OF BIGGEST IMPROVEMENT (J)
C
60 DO 70 J = 4,N2
  IF (Y2(J).GT.ZERO) GO TO 70
  XJ1 = X1(J)
  XJ2 = X1(J+1)
  YJ1 = Y1(J)
  YJ2 = Y1(J+1)
  TL = (XJ2-XJ1)*SMALL
  Y2(J) = LOCALM(XJ1,XJ2,EPSL,TL,YL,X2(J))
70 CONTINUE
80 P1 = Y2(4)
  J = 4
  DO 90 N3 = 5,N2
  IF (Y2(N3).GE.P1) GO TO 90
  J = N3
  P1 = Y2(N3)
90 CONTINUE

C
C      SET UP X1, Y1, X2, Y2 FOR NEXT STEP
C
N4 = N1 - J + 3
N7 = N1 + 4
DO 100 N3 = 1,N4
  N7 = N7 - 1
  X1(N7+1) = X1(N7)
  Y1(N7+1) = Y1(N7)
  X2(N7) = X2(N7-1)
  Y2(N7) = Y2(N7-1)
100 CONTINUE
  X1(J+1) = X2(J)
  Y1(J+1) = F(X2(J))*CM
  N4 = 1
  IF (Y1(J+1).GT.YM) GO TO 110
  YM = Y1(J+1)
  XM = X1(J+1)

C
C      IF NEW EVALUATION IS BETTER THAN YM,
C      X2 AND Y2 WILL BE UPDATED (N4 = 2)
```

```

C
      N4 = 2
110 N1 = N1 + 1
      N2 = N1 + 2
      YH = YM
C
      IF NUMBER OF EVALUATIONS OF F EXCEEDS (N-1) GO TO END
C
      IF (N1.LT.N) GO TO 115
      IFAULT = 4
      GO TO 310
C
      P4 IS PROBABILITY OF EVALUATING
      XM, YM WITH ACCURACY E1, E2
C
115 P4 = ONE
      DO 120 N3 = 4,N2
          IF (Y2(N3).GT.ZERO) GO TO 120
          P1 = -NINETEEN* ((Y1(N3)-YM+E1)/A)* ((Y1(N3+1)-YM+E1)/A)/
+           (X1(N3+1)-X1(N3))
          IF (P1.GT.CUND) P4 = P4* (ONE-EXP(P1))
120 CONTINUE
      IF (P4.GE.PT99) GO TO 310
C
      IF N5 = 0 A IS UPDATED IN EACH FIFTH STEP
C
      DO 130 N3 = 1,N1,5
          IF (N3.EQ.N1) GO TO 140
130 CONTINUE
      GO TO 160
C
140 IF (N5.GT.0) GO TO 160
      A = ZERO
      N4 = 2
      DO 150 N3 = 4,N2
150 A = A + ((Y1(N3+1)-Y1(N3))**2)/ (X1(N3+1)-X1(N3))
      A = SQRT(A/REAL(N1-1))*SEVEN
C
      PREPARATION OF BOUNDS OF X1, Y1 FOR TESTING -
      IS INTERVAL OF LOCAL OPTIMUM FOUND
C
160 X1(3) = (THREE*X1(4)-X1(5))/TWO
      X1(1) = X1(3)
      X1(2) = X1(3)
      X1(N1+4) = (THREE*X1(N1+3)-X1(N1+2))/TWO
      X1(N1+5) = X1(N1+4)
      X1(N1+6) = X1(N1+4)
      NR = N1 + 3
      DO 170 N3 = 1,3
          Y1(N3) = Y1(5)
          NR = NR + 1
          Y1(NR) = Y1(N1+2)
170 CONTINUE
      N7 = MAX(1,J-5)
      N8 = MIN(N1,J+1)
C
      TEST IF INTERVAL OF LOCAL OPTIMUM FOUND
C
      DO 180 N3 = N7,N8
          IF (Y1(N3).GE.Y1(N3+1) .AND. Y1(N3+1).GE.Y1(N3+2) .AND.
+           Y1(N3+2).GT.Y1(N3+3) .AND. Y1(N3+3).LT.Y1(N3+4) .AND.

```

```

+          Y1(N3+4).LE.Y1(N3+5) .AND. Y1(N3+5).LE.Y1(N3+6) .AND.
+          (X1(N3+6)-X1(N3)).LE. (EB/FIVE)) GO TO 200
180 CONTINUE
    IF (N4.EQ.2) GO TO 60
C
C          IF INTERVAL OF LOCAL OPTIMUM IS FOUND GO TO
C          LOCAL OPTIMIZATION, ELSE BAYESIAN STEP
C
    N7 = J + 1
    DO 190 N3 = J,N7
      XJ1 = X1(N3)
      XJ2 = X1(N3+1)
      YJ1 = Y1(N3)
      YJ2 = Y1(N3+1)
      IF ((XJ2-XJ1).LT.EB2 .AND. Y2(N3-1).GT.ZERO .AND.
+        YJ1.LT.YJ2) GO TO 185
      TL = (XJ2-XJ1)*SMALL
      Y2(N3) = LOCALM(XJ1,XJ2,EPSL,TL,YL,X2(N3))
      GO TO 190

185    Y2(N3) = ONE
190 CONTINUE
      IF (Y2(N7+1).GT.ZERO .AND. Y1(N7).GT.Y1(N7+1) .AND.
+        X1(N7+1)-X1(N7).LT.EB2) Y2(N7) = ONE
      IF (Y2(N7).GT.ZERO .AND. Y1(N7-1).GT.Y1(N7) .AND.
+        X1(N7)-X1(N7-1).LT.EB2) Y2(N7-1) = ONE
      GO TO 80
C
C          START OF LOCAL OPTIMIZATION
C
200    N6 = N3 + 5
      DO 210 N7 = N3,N6
210    Y2(N7) = ONE
      N3 = N3 + 3
      N5 = N5 + 1
      N7 = 1
220    EE1 = DBLE(Y1(N3-1)-Y1(N3))
      EE2 = DBLE(X1(N3-1)-X1(N3))
      IF (ABS(EE1).LE.DM17 .OR. ABS(EE2).LE.DM17) GO TO 60
      EE3 = DBLE(TWO* (Y1(N3-1)-Y1(N3+1)))/EE1 -
+        DBLE(TWO* (X1(N3-1)-X1(N3+1)))/EE2
      IF (ABS(EE3).LE.DM17) GO TO 60
      XA = (DBLE(X1(N3-1)+X1(N3))*DBLE(Y1(N3-1)-Y1(N3+1)))/EE1-
+        DBLE(X1(N3-1)-X1(N3+1))*DBLE(X1(N3-1)+X1(N3+1))/EE2)/EE3
      EE1 = DBLE(X1(N3)-XA)
      EE2 = DBLE(X1(N3-1)-XA)
      EE3 = DBLE(Y1(N3-1)-Y1(N3))
      IF (ABS(EE2).GE.DM17) GO TO 230
      P1 = Y1(N3-1)
      GO TO 250

230    EE1 = ONE - (EE1/EE2)**2
      IF (ABS(EE1).GE.DM17) GO TO 240
      IF (EE3.LE.ABS(EE1)*1.0D6) GO TO 240
      P1 = Y1(N3-1) - 1.0E5
      GO TO 250

240    EE3 = EE3/EE1
      P1 = Y1(N3-1) - EE3
250    YA = F(XA)*CM
      P3 = ABS(XA-X1(N7))

```

```
      IF (YA.GE.YM) GO TO 260
      YM = YA
      XM = XA
260  N1 = N1 + 1
      N2 = N1 + 2
      YH = YM
      N7 = N3
      IF (XA.GT.X1(N3)) N7 = N7 + 1
      N6 = N1 - N7 + 3
      N4 = N1 + 3
      DO 290 N8 = 1,N6
          N4 = N4 - 1
          X1(N4+1) = X1(N4)
          Y1(N4+1) = Y1(N4)
          X2(N4) = X2(N4-1)
          Y2(N4) = Y2(N4-1)
290  CONTINUE
      X1(N7) = XA
      Y1(N7) = YA
      Y2(N7) = ONE
      Y2(N7-1) = ONE
      X1(3) = (THREE*X1(4)-X1(5))/TWO
      X1(1) = X1(3)
      X1(2) = X1(3)
      X1(N1+4) = (THREE*X1(N1+3)-X1(N1+2))/TWO
      X1(N1+5) = X1(N1+4)
      X1(N1+6) = X1(N1+4)
      NR = N1 + 3
      DO 300 N8 = 1,3
          Y1(N8) = Y1(5)
          NR = NR + 1
          Y1(NR) = Y1(N1+2)
300  CONTINUE
      IF (N1.LT.N) GO TO 305
      IFAULT = 4
      GO TO 310

305  P2 = ABS(P1-YA)
      IF (P2.LE.E1 .AND. P3.LE.E2 .OR. P2.LE.CM17 .OR.
+     P3.LE.CM17) GO TO 60
      IF (N3.EQ.N7 .AND. Y1(N7).GT.Y1(N7+1) .OR.
+     N3+1.EQ.N7 .AND. Y1(N7).LT.Y1(N7-1)) N3 = N3 + 1
      GO TO 220

310  YM = YM*CM
      RETURN
```

END

C  
C

FUNCTION YL(C)

C  
C  
C  
C  
C

ALGORITHM AS 133.1 APPL. STATIST. (1978) VOL.27, NO.3

-YL IS THE MEAN OF THE IMPROVEMENT

C  
C  
C

REAL VSMALL, ZERO  
COMMON /EXTR1/A,EB,YH,XJ1,XJ2,YJ1,YJ2  
DATA VSMALL/1.0E-17/,ZERO/0.0/

P1 = EB\*VSMALL

```
IF (C-XJ1.LE.P1 .OR. XJ2-C.LE.P1) GO TO 1
P1 = XJ2 - XJ1
P2 = A*SQRT((C-XJ1)* (XJ2-C)/P1)
P1 = (YJ1* (XJ2-C)+YJ2* (C-XJ1))/P1 - YH
P3 = P1/P2
YL = P1*0.65*EXP(-0.443* (0.75+P3)**2) -
+ P2*0.3989*EXP(- (P3**2)/2.0)
RETURN
```

```
1 YL = ZERO
RETURN
```

```
END
```

```
C
C
```

```
REAL FUNCTION LOCALM(A, B, EPS, T, F, X)
```

```
C
C
C
C
C
```

```
Entered from pages 188-190 of 'Algorithms for minimization without
derivatives' by Richard P. Brent, Prentice-Hall, 1973
Comments added from the Algol version on pages 79-80.
```

```
REAL A, B, EPS, T, F, X
EXTERNAL F
```

```
C
C
C
```

```
Local variables
```

```
REAL CONST
REAL SA, SB, D, E, M, P, Q, R, TOL, T2, U, V, W, FU, FV, FW, FX
```

```
C
C
C
```

```
CONST = (3 - sqrt(5))/2
```

```
DATA CONST/0.381966/
```

```
C
```

```
SA = A
SB = B
X = SA + CONST*(SB - SA)
W = X
V = W
E = 0.0
FX = F(X)
FW = FX
FV = FW
```

```
C
C
C
```

```
Main loop
```

```
10 M = 0.5*(SA + SB)
TOL = EPS*ABS(X) + T
T2 = 2.0*TOL
```

```
C
C
C
```

```
Check stopping criterion
```

```
IF (ABS(X-M) .LE. T2-0.5*(SB-SA)) GO TO 190
R = 0.0
Q = R
P = Q
IF (ABS(E) .LE. TOL) GO TO 40
```

```
C
C
C
```

```
Fit parabola
```

```
R = (X - W)*(FX - FV)
Q = (X - V)*(FX - FW)
```

```
      P = (X - V)*Q - (X - W)*R
      Q = 2.0*(Q - R)
      IF (Q .LE. 0.0) GO TO 20
      P = -P
      GO TO 30
20    Q = -Q
30    R = E
      E = D
40    IF (ABS(P) .GE. ABS(0.5*Q*R)) GO TO 60
      IF ((P .LE. Q*(SA-X)) .OR. (P .GE. Q*(SB-X))) GO TO 60
C
C    A parabolic interpolation step
C
      D = P/Q
      U = X + D
C
C    F must not be evaluated too close to A or B
C
      IF ((U-SA .GE. T2) .AND. (SB-U .GE. T2)) GO TO 90
      IF (X .GE. M) GO TO 50
      D = TOL
      GO TO 90
50    D = -TOL
      GO TO 90
C
C    A golden section step
C
60    IF (X .GE. M) GO TO 70
      E = SB - X
      GO TO 80
70    E = SA - X
80    D = CONST*E
C
C    F must not be evaluated too close to X
C
90    IF (ABS(D) .LT. TOL) GO TO 100
      U = X + D
      GO TO 120
100   IF (D .LE. 0.0) GO TO 110
      U = X + TOL
      GO TO 120
110   U = X - TOL
120   FU = F(U)
C
C    Update A, B, V, W and X
C
      IF (FU .GT. FX) GO TO 150
      IF (U .GE. X) GO TO 130
      SB = X
      GO TO 140
130   SA = X
140   V = W
      FV = FW
      W = X
      FW = FX
      X = U
      FX = FU
      GO TO 10
150   IF (U .GE. X) GO TO 160
      SA = U
      GO TO 170
```

```
160 SB = U
170 IF ((FU .GT. FW) .AND. (W .NE. X)) GO TO 180
    V = W
    FV = FW
    W = U
    FW = FU
    GO TO 10
180 IF ((FU .GT. FV) .AND. (V .NE. X) .AND. (V .NE. W)) GO TO 10
    V = U
    FV = FU
    GO TO 10
```

C

```
190 LOCALM = FX
    RETURN
    END
```

```

SUBROUTINE BET1GT(BETAR)
C
C     ALGORITHM AS 134.1 APPL. STATIST. (1979) VOL.28 NO.1
C
C     GENERATES BETA RANDOM VARIABLES
C     WITH 0.0 .LT. ALPHA .LT. 1.0 AND BETA .GT. 1.0
C     BY THE SWITCHING ALGORITHM OF ATKINSON AND WHITTAKER
C
C     The random number call has been changed from RANF(..) to RAND()
C     so that the Wichmann & Hill random number generator, AS 183
C     can be used. To conform with Fortran-77, SAVE instructions have
C     been added.
C
C     REAL ONE
C     DATA ONE/1.0/
C     COMMON /BETCOM/ AM1, BM1, ARECIP, BRECIP, T, R
C     SAVE /BETCOM/
C
1  UVAR = RAND()
   CALL FNE(EVAR)
   IF(UVAR .GT. R) GOTO 3
C
C     WARNING. With some compilers, underflow can occur for small
C     values of alpha in executing the next instruction.
C
   BETAR = T*((UVAR/R)**ARECIP)
   IF(-BM1*LOG(ONE-BETAR) .GT. EVAR) GOTO 1
   RETURN
3  BETAR = ONE - (ONE-T)*(((ONE-UVAR)/(ONE-R))**BRECIP)
   IF(-AM1*LOG(BETAR/T) .GT. EVAR) GOTO 1
   RETURN
END
C
SUBROUTINE TOPT(ALPHA, BETA, IFAULT)
C
C     ALGORITHM AS 134.2 APPL. STATIST. (1979) VOL.28 NO.1
C
C     SETS CONSTANTS FOR BETA VARIABLE GENERATION.
C     TOL IS TOLERANCE FOR ACCEPTING T AS SOLUTION OF GX = 0
C
C     COMMON /BETCOM/ AM1, BM1, ARECIP, BRECIP, T, R
C     SAVE /BETCOM/
C     REAL ZERO, ONE, TWO, TOL
C     DATA ZERO/0.0/, ONE/1.0/, TWO/2.0/, TOL/1.0E-5/
C
C     TEST PARAMETERS AND CALCULATE CONSTANTS
C
   IF(ALPHA .GT. ZERO .AND. ALPHA .LT. ONE) GOTO 1
   IFAULT = 1
   RETURN
1  IF(BETA .GT. ONE) GOTO 2
   IFAULT = 2
   RETURN
2  AM1 = ALPHA - ONE
   TTILDE = AM1/(AM1-BETA)
   IF(ONE-TTILDE*TTILDE .LT. ONE) GOTO 3
   IFAULT = 3
   RETURN
3  BM1 = BETA - ONE
   ARECIP = ONE/ALPHA
   BRECIP = ONE/BETA

```



```
C
C      INITIAL VALUES FOR FALSE POSITION
C
      XA = ZERO
      GA = AM1
      XB = ONE
      GB = BETA
C
C      FALSE POSITION
C
4  X = (XA*GB - XB*GA)/(GB - GA)
   AA = ONE - X
   BT = BETA*X
   GX = BT + AA**BM1*(AM1*AA - BT)
   IF(ABS(GX) .LT. TOL) GOTO 6
   IF(GX*GA .LT. ZERO) GOTO 5
C
C      MODIFICATION
C
      XA = X
      GA = GX
      GB = GB/TWO
      GOTO 4
C
C      MODIFICATION
C
5  XB = XA
   GB = GA
   XA = X
   GA = GX
   GOTO 4
C
C      CALCULATE REMAINING CONSTANTS
C
6  T = X
   R = BT/(BT + ALPHA*AA**BETA)
   RETURN
   END
C
SUBROUTINE FNE(REX)
C
      ALGORITHM AS134.3 APPL. STATIST. (1979) VOL.28 NO.1
C
      GENERATES EXPONENTIAL RANDOM VARIABLES
      BY THE METHOD OF VON NEUMANN
C
      REAL ZERO, ONE
      DATA ZERO/0.0/, ONE/1.0/
      A = ZERO
1  U = RAND()
   UO = U
2  USTAR = RAND()
   IF(U .LT. USTAR) GOTO 3
   U = RAND()
   IF(U .LT. USTAR) GOTO 2
   A = A + ONE
   GOTO 1
3  REX = A + UO
   RETURN
   END
```

```
      SUBROUTINE LFNORM(N, M, NDIM, MDIM, X, Y, BETA, Z, KY, IFAULT)
C
C   ALGORITHM AS 135  APPL. STATIST. (1979) VOL.28, NO. 1
C
C   Min-Max estimates for a linear multiple regression problem
C
      DOUBLE PRECISION X(NDIM, MDIM), Y(NDIM), BETA(MDIM), Z, HILO(20),
+   XRXF(20), XSXF(20), LU(20, 20), ACU, BIG, ZERO, ONE, DEV1,
+   SIGR, SUMXR, DEVIAT, YEST, YDEV, SUMXS, RATIO, TEST, DELTA,
+   DIV, SWING, SAVE, SIGS, TOP, TWO
      INTEGER IBASE(20), SSS, RRR, INDX(20)
      LOGICAL INTL
C
      DATA ACU/1.D-15/, BIG/1.D30/, ZERO/0.D0/, ONE/1.D0/, TWO/2.D0/
C
      IFAULT = 0
      KY = 0
      Z = ZERO
      M1 = M - 1
C
C   Set up initial LU decomposition
C
      DO 10 I = 1, M
10  INDX(I) = I
      INTL = .TRUE.
      KKK = 1
      CALL UPDATE(KKK, X, LU, IBASE, INDX, INTL, N, M, NDIM, MDIM,
+   IFAULT)
      IF (IFAULT .NE. 0) RETURN
      INTL = .FALSE.
      IROW = KKK
C
C   Calculate beta value
C
      K = INDX(1)
      K1 = IBASE(1)
      BETA(K) = Y(K1) / LU(K, 1)
      DO 30 II = 2, M
        K = INDX(II)
        K1 = IBASE(II)
        BETA(K) = Y(K1)
        III = II - 1
        DO 20 I = 1, III
          KK = INDX(I)
          BETA(K) = BETA(K) - LU(KK, II) * BETA(KK)
20      CONTINUE
        BETA(K) = BETA(K) / LU(K, II)
30      CONTINUE
      DO 40 II = 1, M1
        K1 = M - II
        K = INDX(K1)
        DO 40 I = 1, II
          KK = M - I + 1
          K2 = INDX(KK)
          BETA(K) = BETA(K) - LU(K2, K1) * BETA(K2)
40      CONTINUE
C
C   Search for and set first violated constraint as R-th constraint
C
50  IROW = IROW + 1
      IF (IROW .GT. N) RETURN
```

```
    DEV1 = ZERO
    DO 60 I = 1, M
60  DEV1 = DEV1 + X(IROW, I) * BETA(I)
    DEV1 = DEV1 - Y(IROW)
    IF (ABS(DEV1) .LT. ACU) GO TO 50
    SIGR = SIGN(ONE, DEV1)
    RRR = IROW
C
C  Adjust for the R-th constraint
C
    K = INDX(1)
    XRXF(1) = X(RRR, K)
    DO 80 II = 2, M
        K = INDX(II)
        XRXF(II) = X(RRR, K)
        III1 = II - 1
        DO 70 I = 1, III1
70  XRXF(II) = XRXF(II) - LU(K, I) * XRXF(I)
80  CONTINUE
    K = INDX(M)
    XRXF(M) = XRXF(M) / LU(K, M)
    HILO(M) = SIGN(ONE, -SIGR * XRXF(M))
    SUMXR = SIGR - HILO(M) * XRXF(M)
    DO 100 II = 1, M1
        K1 = M - II
        K = INDX(K1)
        DO 90 I = 1, II
            K2 = M - I + 1
            XRXF(K1) = XRXF(K1) - LU(K, K2) * XRXF(K2)
90  CONTINUE
        XRXF(K1) = XRXF(K1) / LU(K, K1)
        HILO(K1) = SIGN(ONE, -SIGR * XRXF(K1))
        SUMXR = SUMXR - HILO(K1) * XRXF(K1)
100 CONTINUE
    Z = ABS(DEV1 / SUMXR)
C
C  Start of main iterative loop.
C  Search for the most violated S-th constraint
C
110 SSS = 0
    DEVIAT = ACU
C
C  Calculate beta value
C
    K = INDX(1)
    K1 = IBASE(1)
    BETA(K) = (Y(K1) + Z * HILO(1)) / LU(K, 1)
    DO 130 II = 2, M
        K = INDX(II)
        K1 = IBASE(II)
        BETA(K) = Y(K1) + Z * HILO(II)
        III1 = II - 1
        DO 120 I = 1, III1
            KK = INDX(I)
            BETA(K) = BETA(K) - LU(KK, II) * BETA(KK)
120  CONTINUE
        BETA(K) = BETA(K) / LU(K, II)
130 CONTINUE
    DO 140 II = 1, M1
        K1 = M - II
        K = INDX(K1)
```

```

        DO 140 I = 1, II
            KK = M - I + 1
            K2 = INDX(KK)
            BETA(K) = BETA(K) - LU(K2, K1) * BETA(K2)
140 CONTINUE
C
C   Calculate residuals
C
        DO 160 I = 1, N
            YEST = ZERO
            DO 150 J = 1, M
150     YEST = YEST + X(I, J) * BETA(J)
            DEVI = ABS(Y(I) - YEST) - Z
            IF (DEVI .LE. DEVIAT) GO TO 160
            YDEV = YEST - Y(I)
            DEVIAT = DEVI
            SSS = I
160 CONTINUE
C
C   Check if at optimum
C
        IF (SSS .EQ. 0) RETURN
C
C   Set up information on the S-th constraint
C
        SIGS = SIGN(ONE, YDEV)
        K = INDX(1)
        XSXF(1) = X(SSS, K)
        DO 180 II = 2, M
            K = INDX(II)
            XSXF(II) = X(SSS, K)
            III = II - 1
            DO 170 I = 1, III
170     XSXF(II) = XSXF(II) - LU(K, I) * XSXF(I)
180 CONTINUE
        K = INDX(M)
        XSXF(M) = XSXF(M) / LU(K, M)
        SUMXS = -SIGS + HILO(M) * XSXF(M)
        DO 200 II = 1, M1
            K1 = M - II
            K = INDX(K1)
            DO 190 I = 1, II
                K2 = M - I + 1
                XSXF(K1) = XSXF(K1) - LU(K, K2) * XSXF(K2)
190     CONTINUE
            XSXF(K1) = XSXF(K1) / LU(K, K1)
            SUMXS = SUMXS + HILO(K1) * XSXF(K1)
200 CONTINUE
C
C   Search for minimum ratio
C
210 KKK = 0
        RATIO = BIG
        DO 220 I = 1, M
            IF (SIGS * SIGN(ONE, XSXF(I)) .NE. HILO(I) .OR.
+           ABS(XSXF(I)) .LT. ACU) GO TO 220
            TEST = ABS(XRXF(I) / XSXF(I))
            IF (TEST .GE. RATIO) GO TO 220
            RATIO = TEST
            KKK = I
220 CONTINUE

```

```
C
C   Check if R-th constraint moves interior
C
C   IF (KKK .NE. 0) GO TO 260
C
C   Process the movement of the R-th constraint
C
C   DELTA = ABS(DEVIAT / SUMXS)
C
C   Calculate the largest tolerable delta
C
C   DIV = ABS(SUMXR) - TWO
C   IF (DIV .LT. ACU) GO TO 240
C   SWING = TWO * Z / DIV
C   IF (SWING .GE. DELTA) GO TO 240
C
C   Switch R and S constraint indicators
C
C   SAVE = SUMXS
C   SUMXS = -SUMXR + SIGR + SIGR
C   SUMXR = -SAVE
C   SAVE = SIGR
C   SIGR = SIGS
C   SIGS = -SAVE
C   DEVIAT = ABS(SUMXS * DELTA) - TWO * Z
C   Z = Z + DELTA
C   DO 230 I = 1, M
C     SAVE = XSXF(I)
C     XSXF(I) = XRXF(I)
C     XRXF(I) = SAVE
230 CONTINUE
C   I = RRR
C   RRR = SSS
C   SSS = I
C   GO TO 210
C
C   Replace the R-th constraint with the S-th constraint
C
C   240 SIGR = SIGS
C     DO 250 I = 1, M
250 XRXF(I) = XSXF(I)
C     SUMXR = -SUMXS
C     Z = Z + DELTA
C     RRR = SSS
C     GO TO 110
C
C   Process the movement of the K-th constraint
C
C   260 DELTA = ABS(XRXF(KKK) * DEVIAT /
C     + (XRXF(KKK) * SUMXS + XSXF(KKK) * SUMXR))
C     TOP = -TWO * Z * XRXF(KKK)
C     DIV = XRXF(KKK) * XRXF(KKK) + HILO(KKK) * SUMXR
C     IF (SIGN(ONE, TOP) .NE. SIGN(ONE, DIV)) GO TO 270
C     IF (ABS(DIV) .LT. ACU) GO TO 270
C     SWING = TOP / DIV
C
C   Check to see if the K-th constraint swings across
C
C   IF (SWING .GE. DELTA) GO TO 270
C   Z = Z + SWING
C   DEVIAT = DEVIAT - SWING *
```

```

+          ABS(SUMXS + XSXF(KKK) * SUMXR / XRXF(KKK))
SUMXR = SUMXR + TWO * HILO(KKK) * XRXF(KKK)
SUMXS = SUMXS - TWO * HILO(KKK) * XSXF(KKK)
HILO(KKK) = -HILO(KKK)
GO TO 210
C
C      Update XRXF and the LU of the current basis
C
270 HILO(KKK) = SIGS
SUMXR = SIGR
XRXF(KKK) = XRXF(KKK) / XSXF(KKK)
SUMXR = SUMXR - HILO(KKK) * XRXF(KKK)
DO 280 I = 1, M
    IF (I .EQ. KKK) GO TO 280
    XRXF(I) = XRXF(I) - XSXF(I) * XRXF(KKK)
    SUMXR = SUMXR - HILO(I) * XRXF(I)
280 CONTINUE
IBASE(KKK) = SSS
C
C      Update LU decomposition
C
CALL UPDATE(KKK, X, LU, IBASE, INDX, INTL, N, M, NDIM, MDIM,
+ IFAULT)
IF (IFAULT .NE. 0) RETURN
Z = Z + DELTA
KY = KY + 1
GO TO 110
END
C
SUBROUTINE UPDATE(KKK, X, LU, IBASE, INDX, INTL, N, M, NDIM,
+ MDIM, IFAULT)
C
C      ALGORITHM AS 135.1 APPL. STATIST. (1979) VOL.28, NO. 1
C
C      Update LU decomposition matrix
C
DOUBLE PRECISION X(NDIM, MDIM), LU(20, 20), ACU, SUBT, PIVOT
INTEGER IBASE(20), INDX(20)
LOGICAL INTL
DATA ACU/1.D-15/
C
IROW = 0
DO 90 II = KKK, M
    IF (INTL) GO TO 10
    IROW = IBASE(II)
    GO TO 20
10  IROW = IROW + 1
    IF (IROW .LE. N) GO TO 20
    IFAULT = 1
    RETURN
20  DO 30 I = 1, M
30  LU(I, II) = X(IROW, I)
C
C      Set up representation of incoming row
C
    IF (II .EQ. 1) GO TO 60
    I11 = II - 1
    DO 50 ICOL = 1, I11
        K = INDX(ICOL)
        SUBT = LU(K, II)
        J = ICOL + 1

```

```
        DO 40 I = J, M
          K = INDX(I)
          LU(K, II) = LU(K, II) - SUBT * LU(K, ICOL)
40      CONTINUE
50      CONTINUE
C
C      Find maximum entry
C
60      PIVOT = ACU
        KK = 0
        DO 70 I = II, M
          K = INDX(I)
          IF (ABS(LU(K, II)) .LE. PIVOT) GO TO 70
          PIVOT = ABS(LU(K, II))
          KK = I
70      CONTINUE
        IF (KK .EQ. 0) GO TO 10
C
C      Switch order
C
        ISAVE = INDX(KK)
        INDX(KK) = INDX(II)
        INDX(II) = ISAVE
C
C      Put into columns of LU one at a time
C
        IF (INTL) IBASE(II) = IROW
        IF (II .EQ. M) GO TO 90
        J = II + 1
        DO 80 I = J, M
          K = INDX(I)
          LU(K, II) = LU(K, II) / LU(ISAVE, II)
80      CONTINUE
90      CONTINUE
        KKK = IROW
        RETURN
        END
```

```

SUBROUTINE KMNS(A, M, N, C, K, IC1, IC2, NC, AN1, AN2, NCP, D,
*   ITRAN, LIVE, ITER, WSS, IFAULT)

```

```

C
C   ALGORITHM AS 136  APPL. STATIST. (1979) VOL.28, NO.1
C
C   Divide M points in N-dimensional space into K clusters so that
C   the within cluster sum of squares is minimized.
C

```

```

INTEGER IC1(M), IC2(M), NC(K), NCP(K), ITRAN(K), LIVE(K)
REAL    A(M,N), D(M), C(K,N), AN1(K), AN2(K), WSS(K), DT(2)
REAL    ZERO, ONE

```

```

C
C   Define BIG to be a very large positive number
C

```

```

DATA BIG /1.E30/, ZERO /0.0/, ONE /1.0/

```

```

C
C   IFAULT = 3
C   IF (K .LE. 1 .OR. K .GE. M) RETURN

```

```

C
C   For each point I, find its two closest centres, IC1(I) and
C   IC2(I).  Assign it to IC1(I).
C

```

```

DO 50 I = 1, M
  IC1(I) = 1
  IC2(I) = 2
  DO 10 IL = 1, 2
    DT(IL) = ZERO
    DO 10 J = 1, N
      DA = A(I,J) - C(IL,J)
      DT(IL) = DT(IL) + DA*DA
10  CONTINUE
  IF (DT(1) .GT. DT(2)) THEN
    IC1(I) = 2
    IC2(I) = 1
    TEMP = DT(1)
    DT(1) = DT(2)
    DT(2) = TEMP
  END IF
  DO 50 L = 3, K
    DB = ZERO
    DO 30 J = 1, N
      DC = A(I,J) - C(L,J)
      DB = DB + DC*DC
      IF (DB .GE. DT(2)) GO TO 50
30  CONTINUE
  IF (DB .LT. DT(1)) GO TO 40
  DT(2) = DB
  IC2(I) = L
  GO TO 50
40  DT(2) = DT(1)
  IC2(I) = IC1(I)
  DT(1) = DB
  IC1(I) = L
50  CONTINUE

```

```

C
C   Update cluster centres to be the average of points contained
C   within them.
C

```

```

DO 70 L = 1, K
  NC(L) = 0
  DO 60 J = 1, N

```



```

60   C(L,J) = ZERO
70   CONTINUE
    DO 90 I = 1, M
      L = IC1(I)
      NC(L) = NC(L) + 1
      DO 80 J = 1, N
80    C(L,J) = C(L,J) + A(I,J)
90   CONTINUE
C
C   Check to see if there is any empty cluster at this stage
C
    DO 120 L = 1, K
      IF (NC(L) .EQ. 0) THEN
        IFAULT = 1
        RETURN
      END IF
      AA = NC(L)
      DO 110 J = 1, N
110   C(L,J) = C(L,J) / AA
C
C   Initialize AN1, AN2, ITRAN & NCP
C   AN1(L) = NC(L) / (NC(L) - 1)
C   AN2(L) = NC(L) / (NC(L) + 1)
C   ITRAN(L) = 1 if cluster L is updated in the quick-transfer stage,
C             = 0 otherwise
C   In the optimal-transfer stage, NCP(L) stores the step at which
C   cluster L is last updated.
C   In the quick-transfer stage, NCP(L) stores the step at which
C   cluster L is last updated plus M.
C
      AN2(L) = AA / (AA + ONE)
      AN1(L) = BIG
      IF (AA .GT. ONE) AN1(L) = AA / (AA - ONE)
      ITRAN(L) = 1
      NCP(L) = -1
120  CONTINUE
      INDX = 0
      DO 140 IJ = 1, ITER
C
C   In this stage, there is only one pass through the data.  Each
C   point is re-allocated, if necessary, to the cluster that will
C   induce the maximum reduction in within-cluster sum of squares.
C
      CALL OPTRA(A, M, N, C, K, IC1, IC2, NC, AN1, AN2, NCP, D,
*           ITRAN, LIVE, INDX)
C
C   Stop if no transfer took place in the last M optimal transfer
C   steps.
C
      IF (INDX .EQ. M) GO TO 150
C
C   Each point is tested in turn to see if it should be re-allocated
C   to the cluster to which it is most likely to be transferred,
C   IC2(I), from its present cluster, IC1(I).  Loop through the
C   data until no further change is to take place.
C
      CALL QTRAN(A, M, N, C, K, IC1, IC2, NC, AN1, AN2, NCP, D,
*           ITRAN, INDX)
C
C   If there are only two clusters, there is no need to re-enter the
C   optimal transfer stage.

```

```
C
      IF (K .EQ. 2) GO TO 150
C
C      NCP has to be set to 0 before entering OPTRA.
C
      DO 130 L = 1, K
130     NCP(L) = 0
140 CONTINUE
C
C      Since the specified number of iterations has been exceeded, set
C      IFAULT = 2. This may indicate unforeseen looping.
C
      IFAULT = 2
C
C      Compute within-cluster sum of squares for each cluster.
C
150 DO 160 L = 1, K
      WSS(L) = ZERO
      DO 160 J = 1, N
          C(L,J) = ZERO
160 CONTINUE
      DO 170 I = 1, M
          II = IC1(I)
          DO 170 J = 1, N
              C(II,J) = C(II,J) + A(I,J)
170 CONTINUE
      DO 190 J = 1, N
          DO 180 L = 1, K
180     C(L,J) = C(L,J) / FLOAT(NC(L))
          DO 190 I = 1, M
              II = IC1(I)
              DA = A(I,J) - C(II,J)
              WSS(II) = WSS(II) + DA*DA
190 CONTINUE
C
      RETURN
      END
C
C      SUBROUTINE OPTRA(A, M, N, C, K, IC1, IC2, NC, AN1, AN2, NCP, D,
*      ITRAN, LIVE, INDX)
C
C      ALGORITHM AS 136.1 APPL. STATIST. (1979) VOL.28, NO.1
C
C      This is the optimal transfer stage.
C
C      Each point is re-allocated, if necessary, to the cluster that
C      will induce a maximum reduction in the within-cluster sum of
C      squares.
C
      INTEGER IC1(M), IC2(M), NC(K), NCP(K), ITRAN(K), LIVE(K)
      REAL    A(M,N), D(M), C(K,N), AN1(K), AN2(K), ZERO, ONE
C
C      Define BIG to be a very large positive number.
C
      DATA BIG /1.0E30/, ZERO /0.0/, ONE/1.0/
C
C      If cluster L is updated in the last quick-transfer stage, it
C      belongs to the live set throughout this stage. Otherwise, at
C      each step, it is not in the live set if it has not been updated
C      in the last M optimal transfer steps.
```

```

C
DO 10 L = 1, K
  IF (ITRAN(L) .EQ. 1) LIVE(L) = M + 1
10 CONTINUE
DO 100 I = 1, M
  INDX = INDX + 1
  L1 = IC1(I)
  L2 = IC2(I)
  LL = L2
C
C   If point I is the only member of cluster L1, no transfer.
C
  IF (NC(L1) .EQ. 1) GO TO 90
C
C   If L1 has not yet been updated in this stage, no need to
C   re-compute D(I).
C
  IF (NCP(L1) .EQ. 0) GO TO 30
  DE = ZERO
  DO 20 J = 1, N
    DF = A(I,J) - C(L1,J)
    DE = DE + DF*DF
20 CONTINUE
  D(I) = DE * AN1(L1)
C
C   Find the cluster with minimum R2.
C
30 DA = ZERO
DO 40 J = 1, N
  DB = A(I,J) - C(L2,J)
  DA = DA + DB*DB
40 CONTINUE
R2 = DA * AN2(L2)
DO 60 L = 1, K
C
C   If  $I \geq \text{LIVE}(L1)$ , then L1 is not in the live set. If this is
C   true, we only need to consider clusters that are in the live set
C   for possible transfer of point I. Otherwise, we need to consider
C   all possible clusters.
C
  IF (I .GE. LIVE(L1) .AND. I .GE. LIVE(L) .OR. L .EQ. L1 .OR.
*   L .EQ. LL) GO TO 60
  RR = R2 / AN2(L)
  DC = ZERO
  DO 50 J = 1, N
    DD = A(I,J) - C(L,J)
    DC = DC + DD*DD
    IF (DC .GE. RR) GO TO 60
50 CONTINUE
  R2 = DC * AN2(L)
  L2 = L
60 CONTINUE
  IF (R2 .LT. D(I)) GO TO 70
C
C   If no transfer is necessary, L2 is the new IC2(I).
C
  IC2(I) = L2
  GO TO 90
C
C   Update cluster centres, LIVE, NCP, AN1 & AN2 for clusters L1 and
C   L2, and update IC1(I) & IC2(I).

```

```

C
70     INDX = 0
       LIVE(L1) = M + I
       LIVE(L2) = M + I
       NCP(L1) = I
       NCP(L2) = I
       AL1 = NC(L1)
       ALW = AL1 - ONE
       AL2 = NC(L2)
       ALT = AL2 + ONE
       DO 80 J = 1, N
           C(L1,J) = (C(L1,J) * AL1 - A(I,J)) / ALW
           C(L2,J) = (C(L2,J) * AL2 + A(I,J)) / ALT
80     CONTINUE
       NC(L1) = NC(L1) - 1
       NC(L2) = NC(L2) + 1
       AN2(L1) = ALW / AL1
       AN1(L1) = BIG
       IF (ALW .GT. ONE) AN1(L1) = ALW / (ALW - ONE)
       AN1(L2) = ALT / AL2
       AN2(L2) = ALT / (ALT + ONE)
       IC1(I) = L2
       IC2(I) = L1
90     CONTINUE
       IF (INDX .EQ. M) RETURN
100    CONTINUE
       DO 110 L = 1, K
C
C     ITRAN(L) = 0 before entering QTRAN.  Also, LIVE(L) has to be
C     decreased by M before re-entering OPTRA.
C
       ITRAN(L) = 0
       LIVE(L) = LIVE(L) - M
110    CONTINUE
C
       RETURN
       END
C
C     SUBROUTINE QTRAN(A, M, N, C, K, IC1, IC2, NC, AN1, AN2, NCP, D,
*     ITRAN, INDX)
C
C     ALGORITHM AS 136.2 APPL. STATIST. (1979) VOL.28, NO.1
C
C     This is the quick transfer stage.
C     IC1(I) is the cluster which point I belongs to.
C     IC2(I) is the cluster which point I is most likely to be
C     transferred to.
C     For each point I, IC1(I) & IC2(I) are switched, if necessary, to
C     reduce within-cluster sum of squares.  The cluster centres are
C     updated after each step.
C
       INTEGER IC1(M), IC2(M), NC(K), NCP(K), ITRAN(K)
       REAL    A(M,N), D(M), C(K,N), AN1(K), AN2(K), ZERO, ONE
C
C     Define BIG to be a very large positive number
C
       DATA BIG /1.0E30/, ZERO /0.0/, ONE /1.0/
C
C     In the optimal transfer stage, NCP(L) indicates the step at which
C     cluster L is last updated.  In the quick transfer stage, NCP(L)

```

```
C      is equal to the step at which cluster L is last updated plus M.
C
C      ICOUN = 0
C      ISTEP = 0
10 DO 70 I = 1, M
C      ICOUN = ICOUN + 1
C      ISTEP = ISTEP + 1
C      L1 = IC1(I)
C      L2 = IC2(I)
C
C      If point I is the only member of cluster L1, no transfer.
C
C      IF (NC(L1) .EQ. 1) GO TO 60
C
C      If ISTEP > NCP(L1), no need to re-compute distance from point I to
C      cluster L1. Note that if cluster L1 is last updated exactly M
C      steps ago, we still need to compute the distance from point I to
C      cluster L1.
C
C      IF (ISTEP .GT. NCP(L1)) GO TO 30
C      DA = ZERO
C      DO 20 J = 1, N
C      DB = A(I,J) - C(L1,J)
C      DA = DA + DB*DB
20 CONTINUE
C      D(I) = DA * AN1(L1)
C
C      If ISTEP >= both NCP(L1) & NCP(L2) there will be no transfer of
C      point I at this step.
C
30 IF (ISTEP .GE. NCP(L1) .AND. ISTEP .GE. NCP(L2)) GO TO 60
C      R2 = D(I) / AN2(L2)
C      DD = ZERO
C      DO 40 J = 1, N
C      DE = A(I,J) - C(L2,J)
C      DD = DD + DE*DE
C      IF (DD .GE. R2) GO TO 60
40 CONTINUE
C
C      Update cluster centres, NCP, NC, ITRAN, AN1 & AN2 for clusters
C      L1 & L2. Also update IC1(I) & IC2(I). Note that if any
C      updating occurs in this stage, INDX is set back to 0.
C
C      ICOUN = 0
C      INDX = 0
C      ITRAN(L1) = 1
C      ITRAN(L2) = 1
C      NCP(L1) = ISTEP + M
C      NCP(L2) = ISTEP + M
C      AL1 = NC(L1)
C      ALW = AL1 - ONE
C      AL2 = NC(L2)
C      ALT = AL2 + ONE
C      DO 50 J = 1, N
C      C(L1,J) = (C(L1,J) * AL1 - A(I,J)) / ALW
C      C(L2,J) = (C(L2,J) * AL2 + A(I,J)) / ALT
50 CONTINUE
C      NC(L1) = NC(L1) - 1
C      NC(L2) = NC(L2) + 1
C      AN2(L1) = ALW / AL1
C      AN1(L1) = BIG
```

```
IF (ALW .GT. ONE) AN1(L1) = ALW / (ALW - ONE)
AN1(L2) = ALT / AL2
AN2(L2) = ALT / (ALT + ONE)
IC1(I) = L2
IC2(I) = L1
```

```
C
C   If no re-allocation took place in the last M steps, return.
C
```

```
60  IF (ICOUN .EQ. M) RETURN
70  CONTINUE
    GO TO 10
    END
```

```

      SUBROUTINE EM(N, X1, X2, P, XMEAN, XSIGMA, E1, E2, MAXITS,
*      COV, NOBS, K, IFAULT)
C
C      ALGORITHM AS 138 APPL. STATIST. (1979) VOL.28, NO.2
C
C      COMPUTE THE MAXIMUM LIKELIHOOD ESTIMATES OF THE MEAN
C      AND STANDARD DEVIATION OF A SINGLE NORMAL POPULATION,
C      THE DATA MAY CONTAIN CENSORED OR CONFINED OBSERVATIONS.
C
      DIMENSION X1(N), X2(N), COV(2, 2)
      INTEGER P(N), NOBS(4)
C
      DATA C /0.39894228/, ONEPLS /1.0001/, TOL /0.00001/,
*      TOLL /0.00001/
C
      IFAULT = -2
      IF (N .LT. 2) RETURN
C
      INITIALIZE COUNTERS
C
      K = 0
      SUM = 0.0
      SUM2 = 0.0
      SUMG = 0.0
      SUMG2 = 0.0
      IP = 0
      IQ = 0
      IR = 0
      IS = 0
C
      EXACTLY SPECIFIED OBSERVATIONS ARE REMOVED,
      THE REMAINING DATA PACKED INTO FIRST PART OF ARRAY X
C
      IFAULT = -4
      DO 200 I = 1, N
      IPT = P(I)
      IF (IPT .EQ. 0) GOTO 100
      IF (IPT .EQ. 2 .AND. ABS(X1(I) - X2(I)) .LE. ABS(X1(I) * TOLL))
*      GOTO 100
C
      OBSERVATION NOT EXACTLY SPECIFIED
C
      IS = IS + 1
      P(IS) = IPT
      X1(IS) = X1(I)
C
      HANDLE GROUPED DATA
C
      IF (IPT .NE. 2) GOTO 50
      IQ = IQ + 1
      IF (X1(I) .GT. X2(I)) RETURN
      X2(IS) = X2(I)
      XTEMP = 0.5 * (X1(I) + X2(I))
      SUMG = SUMG + XTEMP
      SUMG2 = SUMG2 + XTEMP ** 2
      GOTO 200
C
      ACCUMULATE NUMBER OF OBSERVATIONS CENSORED ON THE RIGHT
C
50      IF (IPT .EQ. 1) IR = IR + 1
      GOTO 200
C

```

```
C          HANDLE EXACTLY-SPECIFIED OBSERVATIONS
C
100      IP = IP + 1
        XTEMP = X1(I)
        SUM = SUM + XTEMP
        SUM2 = SUM2 + XTEMP ** 2
200      CONTINUE
C
C          INITIAL PASS THROUGH DATA COMPLETED
C
        NOBS(1) = IP
        NOBS(2) = IR
        NOBS(3) = N - IP - IR - IQ
        NOBS(4) = IQ
        RIM = IP + IQ
        IF (IP .EQ. N) GOTO 230
        IF (XSIGMA .GT. 0.0) GOTO 350
        IF (RIM .GT. ONEPLS) GOTO 250
C
C          AT MOST ONE OBSERVATION HAS BEEN EXACTLY
C          SPECIFIED OR CONFINED
C
        XMEAN = 1.0
        XSIGMA = 1.0
        GOTO 350
C
C          ALL OBSERVATIONS EXACTLY SPECIFIED
C
230      XMEAN = SUM / RIM
        XSIGMA = SQRT((SUM2 - RIM * XMEAN ** 2) / RIM)
        COV(1, 1) = XSIGMA ** 2 / RIM
        COV(2, 2) = COV(1, 1) * 0.5
        COV(1, 2) = 0.0
        COV(2, 1) = 0.0
C
C          NORMAL RETURN
C
240      IFAULT = 0
        RETURN
C
C          OBTAIN INITIAL ESTIMATES
C
250      XMEAN = (SUM + SUMG) / RIM
        XSIGMA = SQRT((SUM2 + SUMG2 - RIM * XMEAN ** 2) / RIM)
C
C          INITIALIZE BEFORE STARTING FIRST ITERATION
C
350      RP = IP
        RN = N
C
C          START OF ITERATION CYCLE,
C          ESTIMATE CONDITIONAL EXPECTATION OF CONFINED AND
C          CENSORED OBSERVATIONS
C
        IFAULT = -3
400      TS = SUM
        SUMG2 = SUM2
        TD = RP
        DO 610 I = 1, IS
        YS = (X1(I) - XMEAN) / XSIGMA
        IF (P(I) - 1) 500, 450, 550
```



```
C
C      OBSERVATION CENSORED ON THE RIGHT
C
450  CALL RMILLS(YS, F, TOL)
      W = XMEAN + XSIGMA * F
      TD = TD + F * (F - YS)
      GOTO 600

C
C      OBSERVATION CENSORED ON THE LEFT
C
500  CALL RMILLS(-YS, F, TOL)
      W = XMEAN - XSIGMA * F
      TD = TD + F * (F + YS)
      GOTO 600

C
C      CONFINED OBSERVATION.
C      USE MILLS RATIO RECIPROCAL TO COMPUTE PROBABILITY
C      INTEGRALS THAT ARE REQUIRED,
C      AS IN ORIGINAL ALGORITHM ASSUMING X1(I) IS
C      NEVER GREATER THAN X2(I) FOR CONFINED OBSERVATIONS
C
550  YN = EXP(-0.5 * YS ** 2) * C
      CALL RMILLS(YS, F, TOL)
      YQ = YN / F
      YSU = (X2(I) - XMEAN) / XSIGMA
      YNU = EXP(-0.5 * YSU ** 2) * C
      CALL RMILLS(YSU, FU, TOL)
      YQU = YNU / FU
      YD = YQ - YQU

C
C      IF INTEGRAL NOT EQUAL TO ZERO, CARRY ON
C
      IF (YD .LT. TOLL) RETURN
      A = (YN - YNU) / YD
      W = XMEAN + XSIGMA * A
      TD = TD + (A ** 2 + (YSU * YNU - YS * YN) / YD)

C
600  TS = TS + W
      SUMG2 = SUMG2 + W ** 2
610  CONTINUE
C
C      CALCULATE NEW ESTIMATES
C
      XNEW = TS / RN
      YNEW = SQRT((SUMG2 + RN * XMEAN ** 2 - 2.0 * TS * XMEAN) / TD)
      K = K + 1
      IF (ABS(XNEW - XMEAN) .LT. E1 .AND. ABS(YNEW - XSIGMA) .LT. E2)
*      GOTO 700
      IF (K .GE. MAXITS) GOTO 650
      XMEAN = XNEW
      XSIGMA = YNEW
      GOTO 400

C
C      MAXIMUM NUMBER OF ITERATIONS EXCEEDED
C
650  IFAULT = -1
      COV(1, 1) = 0.0
      COV(2, 2) = 0.0
      COV(1, 2) = XNEW - XMEAN
      COV(2, 1) = YNEW - XSIGMA
      RETURN
```

```
C
C      CONVERGENCE OBTAINED
C
700   XMEAN = XNEW
      XSIGMA = YNEW
      XSIG2 = XSIGMA ** 2
C
C      CALCULATE VARIANCE-COVARIANCE MATRIX
C
      X11 = RP
      X12 = (SUM - RP * XMEAN) / XSIGMA
      X22 = RP + (SUM2 + RP * XMEAN ** 2 - 2.0 * SUM * XMEAN) / XSIG2
      DO 800 I = 1, IS
      YS = (X1(I) - XMEAN) / XSIGMA
      IF (P(I) - 1) 740, 710, 770
710   CALL RMILLS(YS, F, TOL)
C
C      OBSERVATION CENSORED ON THE RIGHT
C
      FL = F * (F - YS)
730   X11 = X11 + FL
      FL = FL * YS
      X12 = X12 + FL
      FL = FL * YS
      X22 = X22 + FL
      GOTO 800
C
740   CALL RMILLS(-YS, F, TOL)
C
C      OBSERVATION CENSORED ON THE LEFT
C
      FL = F * (F + YS)
      GOTO 730
C
770   CALL RMILLS(YS, F, TOL)
C
C      OBSERVATION CONFINED BETWEEN 2 FINITE LIMITS
C
      YN = EXP(-0.5 * YS ** 2) * C
      YQ = YN / F
      YSU = (X2(I) - XMEAN) / XSIGMA
      CALL RMILLS(YSU, FU, TOL)
      YNU = EXP(-0.5 * YSU ** 2) * C
      YQU = YNU / FU
      YD = YQ - YQU
      A = (YN - YNU) / YD
      B = (YNU * YSU - YN * YS) / YD
      X11 = X11 + A ** 2 + B
      B1 = (YS ** 2 * YN - YSU ** 2 * YNU) / YD
      X12 = X12 - A * B - B1
      B1 = (YS ** 3 * YN - YSU ** 3 * YNU) / YD
      X22 = X22 - B1 + B ** 2
800   CONTINUE
      CONST = XSIG2 / (X11 * X22 - X12 * X12)
      COV(1, 1) = CONST * X22
      COV(2, 2) = CONST * X11
      COV(1, 2) = -CONST * X12
      COV(2, 1) = COV(1, 2)
      GOTO 240
      END
C
```

```
      SUBROUTINE RMILLS(X, FUNC, TOL)
C
C      ALGORITHM AS 138.1 APPL. STATIST. (1979) VOL.28 NO.2
C
C      COMPUTE THE RECIPROCAL OF MILLS RATIO
C
DATA FPI /1.2533141/, FPII /0.7978846/
C
      FUNC = 0.0
      IF (X .LT. -10.0) RETURN
      FUNC = FPII
      Y = ABS(X)
      IF (Y .LT. 0.000001) RETURN
      SGN = 1.0
      IF (X .LT. 0.0) SGN = -1.0
      IF (Y .GT. 2.0) GOTO 100
      S = 0.0
      A = 1.0
      T = Y
      R = Y
      B = Y ** 2
40     A = A + 2.0
      S = T
      R = R * B / A
      T = T + R
      IF (R .GT. TOL) GOTO 40
      FUNC = 1.0 / (FPI * EXP(0.5 * B) - SGN * T)
      RETURN
100    A = 2.0
      B1 = Y
      S = Y
      A1 = Y ** 2 + 1.0
      A2 = Y * (A1 + 2.0)
      B2 = A1 + 1.0
      T = A2 / B2
140   A = A + 1.0
      A0 = A1
      A1 = A2
      A2 = Y * A1 + A * A0
      B0 = B1
      B1 = B2
      B2 = Y * B1 + A * B0
      R = S
      S = T
      T = A2 / B2
      IF (T - R .GT. TOL .OR. T - S .GT. TOL) GOTO 140
      FUNC = T
      IF (SGN .LT. 0.0) FUNC =
*     T / (2.0 * FPI * EXP(0.5 * Y ** 2) * T - 1.0)
      RETURN
      END
```

```

      program t_as139
c
c      Test AS139
c
      IMPLICIT NONE
      INTEGER n, p(100), m, mplone, rowx, colx, lenw, lenwrk, maxits,
*          ifault, i, il, j
      PARAMETER (n=100, m=5, mplone=m+1, rowx=n, colx=m, lenw=mplone+n,
*          lenwrk=m*n, maxits=25)
      DOUBLE PRECISION y, y1(n), y2(n), x(rowx, colx), w(lenw),
*          vcov(lenwrk), work(lenwrk), alpha(mplone), tol(mplone),
*          temp, se(m)
      REAL rand, randn
      INTEGER IX, IY, IZ
      COMMON /RANDC/ IX, IY, IZ
c
c      Generate artificial data
c
      WRITE(*, *)'Enter 3 integers for random number seeds: '
      READ(*, *) ix, iy, iz

      DO i = 1, n
          x(i, 1) = 1.0
          x(i, 2) = i/10
          x(i, 3) = MOD(i, 10)
          x(i, 4) = x(i, 2) + rand() - 0.5
          x(i, 5) = x(i, 3) + rand() - 0.5
          y = x(i, 1) + x(i, 2) + x(i, 3) + x(i, 4) + x(i, 5) + randn()

          temp = rand()
          IF (temp .LT. 0.1) THEN
              p(i) = 1
              y1(i) = INT(y)
          ELSE IF (temp .LT. 0.2) THEN
              p(i) = -1
              y1(i) = INT(y) + 1
          ELSE IF (temp .LT. 0.3) THEN
              p(i) = 2
              y1(i) = INT(y)
              y2(i) = INT(y) + 1
          ELSE
              p(i) = 0
              y1(i) = y
          END IF
      END DO

      DO i = 1, mplone
          tol(i) = 1.d-06
      END DO

      alpha(mplone) = -1.0          ! No initial estimate for sigma

      CALL REGRES(N, Y1, Y2, P, MPLONE, X, ROWX, COLX, W, LENW,
*          VCOV, WORK, LENWRK, ALPHA, TOL, MAXITS, IFAULT)

      IF (ifault .LT. 0) THEN
          WRITE(*, *)'IFAULT = ', ifault
          STOP
      ELSE
          WRITE(*, *)'No. of iterations = ', ifault
      END IF

```

```

WRITE(*, 900) (alpha(i), i=1,m)
900 FORMAT(1x, 'Regression coefficients: '/ 1x, 5f10.4)
DO i = 1, m
  se(i) = SQRT( vcov((i-1)*mplone + i) )
END DO
WRITE(*, 910) (se(i), i=1,m)
910 FORMAT(1x, 'Estimated standard errors: '/ 1x, 5f10.4)
WRITE(*, 920) alpha(mplone)
920 FORMAT(1x, 'Residual variance estimate = ', f10.4)
WRITE(*, *) 'Variance-covariance matrix:-'
i1 = 1
DO i = 1, m
  WRITE(*, '(1x, 7f10.4)') (vcov(j), j=i1,i1+m-1)
  i1 = i1 + mplone
END DO
end

```

```
REAL FUNCTION RAND()
```

```

C
C The Wichmann & Hill random number generator
C Algorithm AS183, Appl. Statist., 31, 188-190, 1982.
C The cycle length is 6.95E+12.
C This random number generator is very slow compared with most
C others, but it is dependable, and the results are reproducible.
C

```

```

INTEGER IX, IY, IZ
COMMON /RANDC/ IX, IY, IZ

```

```

C
C Initialize IX, IY & IZ if necessary
C

```

```

IF(IX .LE. 0) IX = 777
IF(IY .LE. 0) IY = 777
IF(IZ .LE. 0) IZ = 777

```

```

C
10 IX = MOD(171*IX, 30269)
IY = MOD(172*IY, 30307)
IZ = MOD(170*IZ, 30323)
RAND = MOD(FLOAT(IX)/30269. + FLOAT(IY)/30307. +
1      FLOAT(IZ)/30323. , 1.0)
RETURN
END

```

```
REAL FUNCTION RANDN()
```

```

C
C ALGORITHM 712, COLLECTED ALGORITHMS FROM ACM.
C THIS WORK PUBLISHED IN TRANSACTIONS ON MATHEMATICAL SOFTWARE,
C VOL. 18, NO. 4, DECEMBER, 1992, PP. 434-435.
C

```

```

C The function RANDN() returns a normally distributed pseudo-random
C number with zero mean and unit variance. Calls are made to a
C function subprogram RAND() which must return independent random
C numbers uniform in the interval (0,1).
C

```

```

C The algorithm uses the ratio of uniforms method of A.J. Kinderman
C and J.F. Monahan augmented with quadratic bounding curves.
C

```

```

DATA S,T,A,B / 0.449871, -0.386595, 0.19600, 0.25472/
DATA R1,R2/ 0.27597, 0.27846/

```

```
C
C Generate P = (u,v) uniform in rectangle enclosing acceptance region
50  U = RAND()
    V = RAND()
    V = 1.7156 * (V - 0.5)
C Evaluate the quadratic form
    X = U - S
    Y = ABS(V) - T
    Q = X**2 + Y*(A*Y - B*X)
C Accept P if inside inner ellipse
    IF (Q .LT. R1) GO TO 100
C Reject P if outside outer ellipse
    IF (Q .GT. R2) GO TO 50
C Reject P if outside acceptance region
    IF (V**2 .GT. -4.0*ALOG(U)*U**2) GO TO 50
C Return ratio of P's coordinates as the normal deviate
100 RANDN = V/U
    RETURN
    END
```

```
        SUBROUTINE REGRES(N, Y1, Y2, P, MPLONE, X, ROWX, COLX, W, LENW,
*        VCOV, WORK, LENWRK, ALPHA, TOL, MAXITS, IFAULT)
```

```
C***** NOTE: this routine uses the auxiliary routine
C***** AS7 with the modified argument lists suggested by Freeman
C***** Vol 31 No 3 p336--339.
```

```
C
C as r31 Vol 29 No 2 1980 p228 -- incorporated
C as r32 Vol 30 No 1 1981 p105 -- incorporated
C as r91 Vol 42 No 3 1993 p583 -- incorporated
```

```
C        ALGORITHM AS139 APPL. STATIST. (1979) VOL.28, NO.2
```

```
C        COMPUTE MAXIMUM LIKELIHOOD ESTIMATES
C        FROM A LINEAR MODEL WITH NORMAL HETEROGENOUS VARIANCE.
C        THE DESIGN MATRIX MUST BE NON-SINGULAR. THE DEPENDENT
C        VARIABLE MAY INCLUDE OBSERVATIONS CENSORED IN EITHER TAIL
C        AND/OR OBSERVATIONS CONFINED BETWEEN FINITE LIMITS.
```

```
C        Auxiliary routine required: RMILLS which is the last routine in
C        AS138.
```

```
C        IMPLICIT NONE
```

```
        INTEGER N, MPLONE, ROWX, COLX, P(N), LENW, LENWRK, MAXITS, IFAULT
        DOUBLE PRECISION X(ROWX,COLX), TOL(MPLONE), Y1(N), Y2(N),
*        ALPHA(MPLONE)
        DOUBLE PRECISION VCOV(LenWRK), WORK(LenWRK), W(LenW)
```

```
C        Local variables
```

```
C        INTEGER M, I, J, K, II, NDIMC, NUL, JJ, IIK, IJ, IPT, NJ, IIJ,
*        JJI, KK
        DOUBLE PRECISION QLIMIT, RLIMIT, C, ZERO, HALF, ONE
        PARAMETER (QLIMIT = 0.00001D0, RLIMIT=0.00001D0, C=0.39894228D0)
        PARAMETER (zero=0.d0, half=0.5D0, one=1.D0)
        DOUBLE PRECISION TEMP, SUM2, DEMP, R, R2, XSIG, TD, YMEAN, F, A,
*        FU, YN, YQ, TMPU, YNU, YQU, TINT, TEMP2, YS, YSU, B
```

```
C        INITIALIZATION
```

```
C
      M = MPLONE-1
C
C      CHECK ARRAY SIZES, ETC
C
      IFAULT = -7
      IF(ROWX.LT.N) RETURN
      IFAULT = -8
      IF(COLX.LT.M) RETURN
      IFAULT = -9
      IF(LENW.LT.(MPLONE+N)) RETURN
      IFAULT = -10
      IF(LENWRK.LT.(M*N)) RETURN
C
C      COMPUTE X'X IN LOWER TRIANGULAR FORM
C
      II = 0
      DO 53 I = 1, M
        DO 50 J = 1, I
          TEMP = ZERO
          DO 40 K = 1, N
40          TEMP = TEMP + X(K,I)*X(K,J)
          II = II + 1
          VCOV(II) = TEMP
50          CONTINUE
53          CONTINUE
      NDIMC = M*(M+1)/2
      CALL SYMINV(VCOV, M, NDIMC, WORK, W, NUL, IFAULT)
      IF(IFAULT.NE.0) GOTO 60
      IF(NUL.EQ.0) GOTO 70
60      VCOV(2) = IFAULT
      VCOV(1) = NUL
      IFAULT = -5
      RETURN
C
C      MATRIX NON-SINGULAR AND INVERSE OBTAINED
C      COMPUTE (X'X)INVERSE*X
C      FOLLOWING SCHEME USED TO REDUCE NUMBER OF STORAGE ARRAYS
C      NEEDED.   EXPAND FROM TRIANGULAR TO SQUARE MATRIX
C
70      CALL UNPACK(WORK, M, LENWRK)
C
C      DO MULTIPLICATION - ONE ROW AT A TIME - STARTING
C      WITH THE LAST ONE
C
      JJ = N*M
      II = M*M
      DO 220 I = 1, M
        II = II - M
        DO 200 J = 1, N
          TEMP = ZERO
          DO 170 K = 1, M
            IIK = II + K
            TEMP = TEMP + WORK(IIK)*X(J,K)
170          CONTINUE
          W(J) = TEMP
200          CONTINUE
        DO 210 J = 1, N
          IJ = N+1-J
          WORK(JJ) = W(IJ)
          JJ = JJ-1
```

```
210 CONTINUE
220 CONTINUE
C
  XSIG = ALPHA(MPLONE)
  IF(XSIG.GT.ZERO) GOTO 500
C
C      NO ACCEPTABLE INITIAL VALUE FOR SIGMA HAS BEEN INPUT,
C      OBTAIN INITIAL ESTIMATES FROM EXACTLY SPECIFIED
C      OBSERVATIONS ONLY (ALTHOUGH MATRIX BASED ON ALL
C      OBSERVATIONS) AND CONFINED OBSERVATIONS
C
  II = -N
  DO 300 I = 1, M
    II = II + N
    TEMP = ZERO
    DO 280 J = 1, N
      IIJ = II + J
      IPT = P(J)
      IF(IPT.EQ.0) GOTO 270
      IF(IPT.EQ.2) TEMP = TEMP + WORK(IIJ)*(Y1(J) + Y2(J))*HALF
      GOTO 280
270    TEMP = TEMP + WORK(IIJ)*Y1(J)
280    CONTINUE
    ALPHA(I) = TEMP
300 CONTINUE
C
C      CALCULATE INITIAL ESTIMATE OF SIGMA
C
  SUM2 = ZERO
  TEMP = ZERO
  DO 350 I = 1, N
    IPT = P(I)
    IF(IABS(IPT).EQ.1) GOTO 350
    DEMP = Y1(I)
    IF(IPT.EQ.2) DEMP = (DEMP + Y2(I))*HALF
    DO 320 J = 1, M
320    DEMP = DEMP - ALPHA(J)*X(I, J)
    SUM2 = SUM2 + DEMP**2
    TEMP = TEMP + ONE
350 CONTINUE
  XSIG = SQRT(SUM2/TEMP)
C
C      COMPUTE SOME CONSTANTS NEEDED THROUGHOUT
C
500 R = ZERO
  R2 = ZERO
  IFAULT = -2
  DO 600 I = 1, N
    IPT = P(I)
    IF(IPT.EQ.0) GOTO 550
    IF(IPT.EQ.2 .AND. ABS(Y1(I)-Y2(I)).LE. QLIMIT*ABS(Y1(I)))
      *          GOTO 540
    IF(IPT.NE.2) GOTO 600
    R2 = R2 + ONE
    IF(Y1(I).LT.Y2(I)) GOTO 600
    RETURN
540  P(I) = 0
550  R = R + ONE
    W(I) = Y1(I)
600 CONTINUE
  I = R + R2 + 0.01
```



```

        IFAULT = -4
        IF(I.LT.MPLONE) RETURN
        IFAULT = 0
C
C      START OF ITERATION PROCEDURE
C
620 TD = R
    SUM2 = ZERO
C
C      COMPLETE W-VECTOR
C
    DO 1000 I = 1, N
        IPT = P(I)
        YMEAN = ZERO
        DO 650 J = 1, M
650   YMEAN = YMEAN + ALPHA(J)*X(I,J)
        IF(IPT.EQ.0) GOTO 990
C
C      OBSERVATION NOT EXACTLY SPECIFIED
C
        TEMP = (Y1(I) - YMEAN)/XSIG
        IF(IPT-1)750, 700, 800
C
C      OBSERVATION CENSORED FROM ABOVE - LOWER BOUND KNOWN
C
700   CALL RMILLS(TEMP, F, RLIMIT)
        W(I) = YMEAN + XSIG*F
        TD = TD + F*(F-TEMP)
        GOTO 990
C
C      OBSERVATION CENSORED FROM BELOW - UPPER BOUND KNOWN
C
750   CALL RMILLS(-TEMP, F, RLIMIT)
        W(I) = YMEAN - XSIG*F
        TD = TD + F*(F+TEMP)
        GOTO 990
C
C      OBSERVATION CONFINED TO LIE BETWEEN TWO FINITE LIMITS
C
800   YN = EXP(-HALF*TEMP**2)*C
        CALL RMILLS(TEMP, F, RLIMIT)
        YQ = YN/F
        TMPU = (Y2(I) - YMEAN)/XSIG
        YNU = EXP(-HALF*TMPU**2)*C
        CALL RMILLS(TMPU, FU, RLIMIT)
        YQU = YNU/FU
        TINT = YQ - YQU
        IF(TINT.GE.QLIMIT) GOTO 820
C
C      AFTER STANDARDIZING, UPPER AND LOWER LIMITS RESULT IN
C      SAME PROBABILITY INTEGRAL
C
        IFAULT = -3
        RETURN
820   A = (YN - YNU)/TINT
        W(I) = YMEAN + XSIG*A
        TD = TD + (A**2 + (TMPU*YNU - TEMP*YN)/TINT)
C
C      CALCULATE RESIDUAL SUM OF SQUARES
C
990   SUM2 = SUM2 + (W(I) - YMEAN)**2

```

```
1000 CONTINUE
C
C      UPDATE PARAMETER ESTIMATES - STORE IN END OF W-VECTOR
C
      JJ = -N
      DO 1200 J = 1, M
        JJ = JJ + N
        TEMP = ZERO
        DO 1100 I = 1, N
          JJI = JJ + I
          TEMP = TEMP + WORK(JJI)*W(I)
1100    CONTINUE
        NJ = N + J
        W(NJ) = TEMP
1200 CONTINUE
      NJ = N + MPLONE
      W(NJ) = SQRT(SUM2/TD)
C
C      TEST FOR CONVERGENCE
C
      DO 1300 J = 1, MPLONE
        NJ = N + J
        IF(ABS(ALPHA(J)-W(NJ)).GE.TOL(J)) GOTO 1400
1300 CONTINUE
C
C      IF WE REACH HERE, CONVERGENCE OBTAINED
C
      IJ = IFAULT
      IFAULT = -1
C
C      UPDATE VALUES
C
1400 DO 1450 J = 1, MPLONE
      NJ = N + J
      ALPHA(J) = W(NJ)
1450 CONTINUE
      XSIG = ALPHA(MPLONE)
      IFAULT = IFAULT + 1
      IF(IFAULT.EQ.0) GOTO 1600
      IF(IFAULT.LE.MAXITS) GOTO 620
      IFAULT = -1
      RETURN
C
C      CONVERGENCE OBTAINED - COMPUTE VARIANCE-COVARIANCE
C      MATRIX. INITIALIZE WORK ARRAY
C
1600 II = MPLONE*(MPLONE + 1)/2
      DO 1650 I = 1, II
1650 WORK(I) = ZERO
      DO 2500 I = 1, N
        IPT = P(I)
        YS = Y1(I)
        DO 1680 J = 1, M
1680    YS = YS - ALPHA(J)*X(I,J)
        YS = YS/XSIG
        JJ = 0
        IF(IPT.NE.0) GOTO 1900
C
C      EXACTLY SPECIFIED OBSERVATION
C
      DO 1750 K = 1, M
```

```

      DO 1720 J = 1, K
        JJ = JJ + 1
        WORK(JJ) = WORK(JJ) + X(I,K)*X(I,J)
1720   CONTINUE
        KK = II - MPLONE + K
        WORK(KK) = WORK(KK) + YS*X(I,K)
1750   CONTINUE
        WORK(II) = WORK(II) + ONE + YS**2
        GOTO 2500
1900   IF(IPT-1) 2100, 2000, 2300
C
C     OBSERVATION CENSORED FROM ABOVE - LOWER BOUND KNOWN
C
2000   CALL RMILLS(YS, F, RLIMIT)
        TEMP = F*(F - YS)
        GOTO 2150
C
C     OBSERVATION CENSORED FROM BELOW - UPPER BOUND KNOWN
C
2100   CALL RMILLS(-YS, F, RLIMIT)
        TEMP = F*(F + YS)
C
C     ROUTINE FOR CENSORED OBSERVATIONS
C
2150   DO 2190 K = 1, M
        DO 2170 J = 1, K
          JJ = JJ + 1
          WORK(JJ) = WORK(JJ) + X(I,J)*X(I,K)*TEMP
2170   CONTINUE
          KK = II - MPLONE + K
          WORK(KK) = WORK(KK) + YS*X(I,K)*TEMP
2190   CONTINUE
          WORK(II) = WORK(II) + YS**2*TEMP
          GOTO 2500
C
C     OBSERVATION CONFINED BETWEEN TWO FINITE LIMITS
C
2300   YN = EXP(-HALF*YS**2)*C
        CALL RMILLS(YS, F, RLIMIT)
        YQ = YN/F
        YSU = YS + (Y2(I) - Y1(I))/XSIG
        CALL RMILLS(YSU, FU, RLIMIT)
        YNU = EXP(-HALF*YSU**2)*C
        YQU = YNU/FU
        TINT = YQ - YQU
        A = (YN - YNU)/TINT
        B = (YNU*YSU - YN*YS)/TINT
        TEMP = A**2 + B
        TEMP2 = A*B + (YS**2 * YN - YSU**2 * YNU) / TINT
        DO 2350 K = 1, M
          DO 2330 J = 1, K
            JJ = JJ + 1
            WORK(JJ) = WORK(JJ) + X(I,J)*X(I,K)*TEMP
2330   CONTINUE
            KK = II - MPLONE + K
            WORK(KK) = WORK(KK) - X(I,K) * TEMP2
2350   CONTINUE
            TEMP = (YS**3*YN - YSU**3*YNU)/TINT
            WORK(II) = WORK(II) - TEMP + B**2
2500   CONTINUE
C

```

```

C          INVERT THE MATRIX
C
CALL SYMINV(WORK, MPLONE, II, VCOV, W, NUL, IFAULT)
IF(IFAULT.EQ.0 .AND. NUL.EQ.0) GOTO 2550
VCOV(2) = IFAULT
VCOV(1) = NUL
IFAULT = -6
RETURN

C
C          RESTORE ITERATION COUNTER
C
2550 IFAULT = IJ
C
C          MULTIPLY BY SIGMA-SQUARED
C
TEMP = XSIG**2
DO 2580 I = 1, II
2580 VCOV(I) = VCOV(I)*TEMP
C
C          UNPACK THE MATRIX
C
CALL UNPACK(VCOV, MPLONE, LENWRK)
RETURN
END
*****
SUBROUTINE UNPACK(X, N, LENX)
C
C          ALGORITHM AS139.1 APPL. STATIST. (1979) VOL.28 NO.2
C
C          THIS SUBROUTINE EXPANDS A SYMMETRIC MATRIX STORED IN LOWER
C          TRIANGULAR FORM IN THE FIRST N*(N+1)/2 POSITIONS OF X
C          INTO A MATRIX USING THE FIRST N*N POSITIONS
C
C          LENX = LENGTH OF VECTOR X - MUST BE LESS THAN N*N
C
INTEGER N, LENX
DOUBLE PRECISION X(LENX)
C
C          Local variables
C
INTEGER NSQ, II, JJ, I, IJ, KK, J

NSQ = N*N
II = NSQ
JJ = N*(N+1)/2
C
C          STORE LAST ROW
C
DO 10 I = 1, N
X(II) = X(JJ)
II = II-1
JJ = JJ-1
10 CONTINUE
DO 80 I = 2, N
C
C          OBTAIN UPPER PART OF MATRIX FROM PART ALREADY SHIFTED
C
IJ = I - 1
KK = NSQ+1-I
DO 50 J = 1, IJ
X(II) = X(KK)

```

```
        II = II - 1
        KK = KK - N
50    CONTINUE
C
C        OBTAIN LOWER PART OF MATRIX FROM
C        ORIGINAL TRIANGULAR STORAGE
C
        IJ = N - IJ
        DO 70 J = 1, IJ
            X(II) = X(JJ)
            II = II - 1
            JJ = JJ - 1
70    CONTINUE
80    CONTINUE
        RETURN
        END

SUBROUTINE RMILLS(X, FUNC, TOL)
C
C        ALGORITHM AS 138.1 APPL. STATIST. (1979) VOL.28 NO.2
C
C        COMPUTE THE RECIPROCAL OF MILLS RATIO
C
        DOUBLE PRECISION X, FUNC, TOL
C
C        Local variables
C
        DOUBLE PRECISION Y, SGN, S, A, T, R, B, B1, A1, A2, B2, A0, B0
        DOUBLE PRECISION FPI, FPII, ZERO, HALF, ONE, TWO, TEN, SMALL
        DATA FPI /1.2533141D0/, FPII /0.7978846D0/, ZERO /0.D0/,
*        HALF /0.5D0/, ONE /1.D0/, TWO /2.D0/, TEN /10.D0/,
*        SMALL /0.000001D0/
C
        FUNC = ZERO
        IF (X .LT. -TEN) RETURN
        FUNC = FPII
        Y = ABS(X)
        IF (Y .LT. SMALL) RETURN
        SGN = ONE
        IF (X .LT. ZERO) SGN = -ONE
        IF (Y .GT. TWO) GOTO 100
        S = ZERO
        A = ONE
        T = Y
        R = Y
        B = Y ** 2
40    A = A + TWO
        S = T
        R = R * B / A
        T = T + R
        IF (R .GT. TOL) GOTO 40
        FUNC = ONE / (FPI * EXP(HALF * B) - SGN * T)
        RETURN
C
100   A = TWO
        B1 = Y
        S = Y
        A1 = Y ** 2 + ONE
        A2 = Y * (A1 + TWO)
        B2 = A1 + ONE
```

```

      T = A2 / B2
140  A = A + ONE
      A0 = A1
      A1 = A2
      A2 = Y * A1 + A * A0
      B0 = B1
      B1 = B2
      B2 = Y * B1 + A * B0
      R = S
      S = T
      T = A2 / B2
      IF (T - R .GT. TOL .OR. T - S .GT. TOL) GOTO 140
      FUNC = T
      IF (SGN .LT. ZERO) FUNC = T / (TWO*FPI*EXP(HALF * Y**2) * T - ONE)
      RETURN
      END

```

```

      subroutine syminv(a, n, nn, c, w, nullty, ifault)
c
c      Algorithm AS7, Applied Statistics, vol.17, 1968, p.198.
c
c      Forms in c( ) as lower triangle, a generalised inverse
c      of the positive semi-definite symmetric matrix a( )
c      order n, stored as lower triangle.
c
c      arguments:-
c      a( )      = input, the symmetric matrix to be inverted, stored in
c                  lower triangular form
c      n         = input, order of the matrix
c      nn        = input, the size of the a and c arrays      n*(n+1)/2
c      c( )      = output, the inverse of a (a generalized inverse if c is
c                  singular), also stored in lower triangular.
c                  c and a may occupy the same locations.
c      w( )      = workspace, dimension at least n.
c      nullty    = output, the rank deficiency of a.
c      ifault    = output, error indicator
c                  = 1 if n < 1
c                  = 2 if a is not +ve semi-definite
c                  = 3 if nn < n*(n+1)/2
c                  = 0 otherwise
c
c*****
c
c      double precision a(nn), c(nn), w(n), x, zero, one
c
c      data zero, one /0.0d0, 1.0d0/
c
c      cholesky factorization of a, result in c
c
c      call chol(a, n, nn, c, nullty, ifault)
c      if(ifault.ne.0) return
c
c      invert c & form the product (cinv)'*cinv, where cinv is the inverse
c      of c, row by row starting with the last row.
c      irow = the row number, ndiag = location of last element in the row.
c
c      irow=n
c      ndiag=nn
10    l=ndiag

```

```

        if (c(ndiag) .eq. zero) goto 60
        do 20 i=irow,n
            w(i)=c(l)
            l=l+i
20      continue
        icol=n
        jcol=nn
        mdiag=nn
30      l=jcol
        x=zero
        if(icol.eq.irow) x=one/w(irow)
        k=n
40      if(k.eq.irow) go to 50
        x=x-w(k)*c(l)
        k=k-1
        l=l-1
        if(l.gt.mdiag) l=l-k+1
        go to 40
50      c(l)=x/w(irow)
        if(icol.eq.irow) go to 80
        mdiag=mdiag-icol
        icol=icol-1
        jcol=jcol-1
        go to 30
60      do 70 j=irow,n
            c(l)=zero
            l=l+j
70      continue
80      ndiag=ndiag-irow
        irow=irow-1
        if(irow.ne.0) go to 10
        return
        end

```

SUBROUTINE CHOL (A, N, NN, U, NULLTY, IFAULT)

```

C
C   Algorithm AS6, Applied Statistics, vol.17, (1968)
C
C   Given a symmetric matrix order n as lower triangle in a( )
C   calculates an upper triangle, u( ), such that uprime * u = a.
C   a must be positive semi-definite. eta is set to multiplying
C   factor determining effective zero for pivot.
C
C   arguments:-
C   a( )      = input, a +ve definite matrix stored in lower-triangula
C               form.
C   n        = input, the order of a
C   nn       = input, the size of the a and u arrays      n*(n+1)/2
C   u( )     = output, a lower triangular matrix such that u*u' = a.
C               a & u may occupy the same locations.
C   nullty   = output, the rank deficiency of a.
C   ifault   = output, error indicator
C               = 1 if n < 1
C               = 2 if a is not +ve semi-definite
C               = 3 if nn < n*(n+1)/2
C               = 0 otherwise
C
C*****
C

```

```

      DOUBLE PRECISION A(NN), U(NN), ETA, ETA2, X, W, ZERO
C
C      The value of eta will depend on the word-length of the
C      computer being used.  See introductory text.
C
      DATA ETA, ZERO/1.D-9, 0.0D0/
C
      IFAULT = 1
      IF (N.LE.0) RETURN
      IFAULT = 3
      IF (NN.LT.N*(N+1)/2) RETURN
      IFAULT = 2
      NULLTY = 0
      J = 1
      K = 0
      ETA2 = ETA*ETA
      II = 0
C
C      Factorize column by column, icol = column no.
C
      DO 80 ICOL = 1,N
        II = II+ICOL
        X = ETA2*A(II)
        L = 0
        KK = 0
C
C      IROW = row number within column ICOL
C
        DO 40 IROW = 1,ICOL
          KK = KK+IROW
          K = K+1
          W = A(K)
          M = J
          DO 10 I = 1,IROW
            L = L+1
            IF (I.EQ.IROW) GO TO 20
            W = W-U(L)*U(M)
            M = M+1
10          CONTINUE
20          IF (IROW.EQ.ICOL) GO TO 50
            IF (U(L).EQ.ZERO) GO TO 30
            U(K) = W/U(L)
            GO TO 40
30          IF (W*W.GT.ABS(X*A(KK))) RETURN
            U(K) = ZERO
40          CONTINUE
50          IF (ABS(W).LE.ABS(ETA*A(K))) GO TO 60
            IF (W.LT.ZERO) RETURN
            U(K) = SQRT(W)
            GO TO 70
60          U(K) = ZERO
            NULLTY = NULLTY+1
70          J = J+ICOL
80          CONTINUE
      IFAULT = 0
      END

```



```

      SUBROUTINE INIT(X, N, XLEN, NCLUS, MXCLUS, MXSIZE, ITYPE,
*      CLUS, Y, SIZE, P, IOLD, INEW, IFAULT)
C
C      ALGORITHM AS 140.1 APPL. STATIST. (1979) VOL.28, NO.2
C
C      CONSTRUCT AN INITIAL PARTITION OF THE NODES
C
      INTEGER XLEN, FIRST, X(XLEN), Y(XLEN), CLUS(N), SIZE(MXCLUS),
*      INEW(N), IOLD(N)
      REAL P(MXCLUS, MXCLUS)
      LOGICAL FLAG
C
C      CHECK INPUTS
C
      IFAULT = 1
      IF (NCLUS .LE. 1 .OR. NCLUS .GE. N .OR. NCLUS .GT. MXCLUS) RETURN
      IFAULT = 2
      IF (NCLUS * MXSIZE .LE. N) RETURN
      IFAULT = 3
      DO 1 I = 2, N
      L = I - 1
      IF (X(I) .LE. X(L)) RETURN
1      CONTINUE
      M = N + 1
      IF (X(1) .NE. M .OR. X(N) .GT. XLEN) RETURN
      IFAULT = 4
      DO 2 I = M, XLEN
      IF (X(I) .LE. 0 .OR. X(I) .GT. N) RETURN
2      CONTINUE
      IFAULT = 5
      DO 5 I = 1, N
      FIRST = X(I)
      L = I + 1
      LAST = X(L) - 1
      IF (I .EQ. N) LAST = XLEN
      IF (FIRST .EQ. LAST) GOTO 5
      JLAST = LAST - 1
      DO 4 J = FIRST, JLAST
      JTEST = X(J)
      KFIRST = J + 1
      DO 3 K = KFIRST, LAST
      IF (JTEST .EQ. X(K)) RETURN
3      CONTINUE
4      CONTINUE
5      CONTINUE
C
C      CONSTRUCT Y VECTOR.  THE Y VECTOR HOLDS THE ASSOCIATION
C      MATRIX BY COLUMNS RATHER THAN BY ROWS AS X DOES.
C
      DO 6 I = 1, N
      INEW(I) = 0
      Y(I) = N + 1
6      CONTINUE
      Y(M) = 0
      DO 7 I = 1, N
      FIRST = X(I)
      LAST = X(I + 1) - 1
      IF (I .EQ. N) LAST = XLEN
      DO 7 J = FIRST, LAST
      KFIRST = X(J) + 1
      DO 7 K = KFIRST, N

```

```
7      Y(K) = Y(K) + 1
      CONTINUE
      DO 8 I = 1, N
      FIRST = X(I)
      LAST = X(I + 1) - 1
      IF (I .EQ. N) LAST = XLEN
      DO 8 J = FIRST, LAST
      ITEMP = X(J)
      L = Y(ITEMP) + INEW(ITEMP)
      Y(L) = I
      INEW(ITEMP) = INEW(ITEMP) + 1
8      CONTINUE
      IFAULT = 6
      DO 9 I = 2, N
      IF (Y(I) .LE. Y(I - 1)) RETURN
9      CONTINUE
      IF (Y(1) .NE. M .OR. Y(N) .GT. XLEN) RETURN
      IF (ITYPE .EQ. 1) GOTO 33
      IFAULT = 0
```

```
C
C      APPROXIMATE FIRST EIGENVECTOR
C
```

```
11     DO 11 I = 1, N
      IOLD(I) = 1
      DO 13 ITER = 1, 8
      DO 12 I = 1, N
      LAST = X(I + 1) - 1
      IF (I .EQ. N) LAST = XLEN
      DO 12 J = FIRST, LAST
      ITEMP = X(J)
      INEW(I) = INEW(I) + IOLD(ITEMP)
12     CONTINUE
      DO 13 I = 1, N
      IOLD(I) = INEW(I)
13     CONTINUE
```

```
C
C      SORT BY FIRST EIGENVECTOR
C
```

```
14     DO 14 I = 1, N
      INEW(I) = I
      DO 16 I = 1, N
      FLAG = .TRUE.
      DO 15 J = 2, N
      L = J - 1
      ITEMP = INEW(L)
      M = INEW(J)
      IF (IOLD(M) .GE. IOLD(ITEMP)) GOTO 15
      FLAG = .FALSE.
      INEW(J) = INEW(L)
      INEW(L) = M
15     CONTINUE
      IF (FLAG) GOTO 17
16     CONTINUE
```

```
C
C      PARTITION INTO INITIAL CLUSTERS
C
```

```
17     KSTART = N / NCLUS
      DO 21 I = 1, NCLUS
21     SIZE(I) = KSTART
      ILAST = MOD(N, NCLUS)
      IF (ILAST .EQ. 0) GOTO 31
```

```

DO 22 I = 1, ILAST
22  SIZE(I) = SIZE(I) + 1
31  J = 1
    DO 32 I = 1, NCLUS
    KLAST = SIZE(I)
    DO 32 K = 1, KLAST
    ITEMP = INEW(J)
    CLUS(ITEMP) = I
    J = J + 1
32  CONTINUE
    GOTO 40
33  DO 34 I = 1, NCLUS
34  SIZE(I) = 0
    IFAULT = 7
    DO 35 I = 1, N
    J = CLUS(I)
    IF (J .LE. 0 .OR. J .GT. NCLUS) RETURN
    SIZE(J) = SIZE(J) + 1
35  CONTINUE
    IFAULT = 8
    DO 36 I = 1, NCLUS
    IF (SIZE(I) .LE. 0 .OR. SIZE(I) .GT. MXSIZE) RETURN
36  CONTINUE
    IFAULT = 0

C
C      SET UP P MATRIX, SUCCESS COUNTS
C
40  DO 41 I = 1, NCLUS
    DO 41 J = 1, NCLUS
41  P(I, J) = 0.0
    DO 42 I = 1, N
    FIRST = X(I)
    LAST = X(I + 1) - 1
    IF (I .EQ. N) LAST = XLEN
    DO 42 J = FIRST, LAST
    IF (X(J) .EQ. I) GOTO 42
    ITEMP = X(J)
    ITEMP = CLUS(ITEMP)
    ITEMP2 = CLUS(I)
    P(ITEMP2, ITEMP) = P(ITEMP2, ITEMP) + 1.0
42  CONTINUE
    RETURN
    END

C
C      SUBROUTINE ALLOC(X, Y, N, XLEN, NCLUS, MXCLUS, MXSIZE,
* TH, MXS2, CLUS, SIZE, P, R1, R2, TLOG, IOLD, INEW)
C
C      ALGORITHM AS 140.2 APPL. STATIST. (1979) VOL.28, NO.2
C
C      FROM AN INITIAL PARTITION OF THE NODES OF A GRAPH,
C      REALLOCATE NODES TO CLUSTERS TO FIND A LOCALLY
C      MAXIMUM LIKELIHOOD PARTITION
C
C      INTEGER XLEN, FIRST, X(XLEN), Y(XLEN), CLUS(N),
* SIZE(MXCLUS), IOLD(N), INEW(N)
    REAL P(MXCLUS, MXCLUS), TLOG(MXS2), R1(MXCLUS), R2(MXCLUS)
    LOGICAL GLOBAL
C
C      INITIALIZE TLOG, INEW, IOLD, PASS.
C
DO 1 I = 1, MXS2

```

```

1      TLOG(I) = FLOAT(I) * ALOG(FLOAT(I))
2      DO 3 I = 1, NCLUS
      INEW(I) = 0
      IOLD(I) = 1
3      CONTINUE
      GLOBAL = .TRUE.

C
C      MOVE A NODE TO A NEW CLUSTER IF THE MOVE INCREASES
C      THE LIKELIHOOD.
C      ONLY CHECK MOVES IF ONE OF THE CLUSTERS HAS IOLD = 1.
C
4      DO 59 ITER = 1, N
      NBEST = CLUS(ITER)
      BTEST = TH

C
C      SET UP ARRAY OF ASSOCIATIONS (R) FOR THIS NODE
C
      DO 10 I = 1, NCLUS
      R1(I) = 0.0
      R2(I) = 0.0
10     CONTINUE
      FIRST = X(ITER)
      L = ITER + 1
      LAST = X(L) - 1
      IF (ITER .EQ. N) LAST = XLEN
      DO 11 I = FIRST, LAST
      IF (X(I) .EQ. ITER) GOTO 11
      ITEMP = X(I)
      ITEMP = CLUS(ITEMP)
      R1(ITEMP) = R1(ITEMP) + 1.0
11     CONTINUE
      FIRST = Y(ITER)
      LAST = Y(L) - 1
      IF (ITER .EQ. N) LAST = XLEN
      DO 12 I = FIRST, LAST
      IF (Y(I) .EQ. ITER) GOTO 12
      ITEMP = Y(I)
      ITEMP = CLUS(ITEMP)
      R2(ITEMP) = R2(ITEMP) + 1.0
12     CONTINUE

C
C      CHECK EACH CLUSTER FOR AN INCREASE IN LIKELIHOOD
C
      L = CLUS(ITER)
      DO 49 M = 1, NCLUS
      IF (L .EQ. M .OR. SIZE(M) .GE. MXSIZE .OR.
*      IOLD(L) + IOLD(M) .EQ. 0) GOTO 49
      TEST = 0.0
      DO 20 J = 1, NCLUS
      IF (J .EQ. L .OR. J .EQ. M) GOTO 20
      IF (P(L, J) .GT. 0.0) TEST = TEST + XLIKE(P(L, J), R1(J), SIZE(L),
*      SIZE(J), SIZE(L) - 1, SIZE(J), 1.0, TLOG, MXS2)
      IF (P(M, J) .GT. 0.0 .OR. R1(J) .GT. 0.0) TEST = TEST +
*      XLIKE(P(M, J), R1(J), SIZE(M), SIZE(J), SIZE(M) + 1, SIZE(J),
*      -1.0, TLOG, MXS2)
      IF (P(J, L) .GT. 0.0) TEST = TEST + XLIKE(P(J, L), R2(J), SIZE(L),
*      SIZE(J), SIZE(L) - 1, SIZE(J), 1.0, TLOG, MXS2)
      IF (P(J, M) .GT. 0.0 .OR. R2(J) .GT. 0.0) TEST = TEST +
*      XLIKE(P(J, M), R2(J), SIZE(M), SIZE(J), SIZE(M) + 1, SIZE(J),
*      -1.0, TLOG, MXS2)
20     CONTINUE

```

```

TEST = TEST + XLIKE(P(L, L), R1(L) + R2(L) , SIZE(L) - 1, SIZE(L),
* SIZE(L) - 1, SIZE(L) - 2, 1.0, TLOG, MXS2) +
* XLIKE(P(L, M), R1(M) - R2(L) , SIZE(L), SIZE(M), SIZE(L) - 1,
* SIZE(M) + 1, 1.0, TLOG, MXS2) +
* XLIKE(P(M, L), R2(M) - R1(L) , SIZE(L), SIZE(M), SIZE(L) - 1,
* SIZE(M) + 1, -1.0, TLOG, MXS2) +
* XLIKE(P(M, M), R1(M) + R2(M) , SIZE(M) - 1, SIZE(M),
* SIZE(M) + 1, SIZE(M), -1.0, TLOG, MXS2)
IF (TEST .LE. BTEST) GOTO 49
BTEST = TEST
NBEST = M
49 CONTINUE
C
C MOVE TO BEST CLUSTER
C
IF (NBEST .EQ. L) GOTO 59
M = NBEST
DO 50 II = 1, NCLUS
P(L, II) = P(L, II) - R1(II)
P(M, II) = P(M, II) + R1(II)
P(II, L) = P(II, L) - R2(II)
P(II, M) = P(II, M) + R2(II)
50 CONTINUE
SIZE(L) = SIZE(L) - 1
SIZE(M) = SIZE(M) + 1
CLUS(ITER) = NBEST
INEW(L) = 1
INEW(M) = 1
59 CONTINUE
C
C CHECK FOR OPTIMUM, WERE THERE ANY MOVES THIS PASS.
C
DO 60 I = 1, NCLUS
IF (INEW(I) .GT. 0) GOTO 62
60 CONTINUE
C
C NO MOVES, IF A GLOBAL CHECK, FINISH,
C IF A LOCAL CHECK, MAKE A GLOBAL CHECK.
C
IF (GLOBAL) GOTO 70
GOTO 2
C
C SOME MOVES, RESET IOLD, INEW, MAKE A LOCAL CHECK.
62 GLOBAL = .FALSE.
DO 63 I = 1, NCLUS
IOLD(I) = INEW(I)
INEW(I) = 0
63 CONTINUE
GOTO 4
C
C COMPUTE OVERALL LOG LIKELIHOOD
C
70 R1(I) = 0.0
DO 72 I = 1, NCLUS
R1(1) = R1(1) + XLIKE(0.0, P(I, I), I, I, SIZE(I) - 1,
* SIZE(I), -1.0, TLOG, MXS2)
DO 71 J = 1, NCLUS
IF (I .NE. J) R1(1) = R1(1) + XLIKE(0.0, P(I, J),
* I, I, SIZE(I), SIZE(J), -1.0, TLOG, MXS2)
71 CONTINUE
72 CONTINUE

```

```
RETURN  
END
```

```
C  
REAL FUNCTION XLIKE(P1, R1, S1, S2, S3, S4, Y1, TLOG, MXS2)
```

```
C  
C      ALGORITHM AS 140.3 APPL. STATIST. (1979) VOL.28, NO.2
```

```
C      EVALUATE THE CHANGE IN LOG LIKELIHOOD BETWEEN P SUCCESSES IN  
C      S1 * S2 TRIALS AND P1 - Y1 * R1 SUCCESSES IN S3 * S4 TRIALS.
```

```
C  
INTEGER S1, S2, S3, S4, P, R, X, Z  
REAL TLOG(MXS2)  
XLIKE = 0.0  
P = P1  
Z = S1 * S2  
R = Z - P  
IF (R .NE. 0 .AND. P .NE. 0) XLIKE = TLOG(Z) - TLOG(P) - TLOG(R)  
X = P1 - Y1 * R1  
Z = S3 * S4  
R = Z - X  
IF (R .NE. 0 .AND. X .NE. 0)  
* XLIKE = XLIKE + TLOG(X) + TLOG(R) - TLOG(Z)  
RETURN  
END
```

```
C UKC NETLIB DISTRIBUTION COPYRIGHT 1990 RSS
C
C     SUBROUTINE SINV(A, K, L, LO, PVT, IFAULT)
C
C     ALGORITHM AS 141 APPL. STATIST. (1979) VOL.28, NO.2
C
C     CALCULATE THE INVERSE OF A SYMMETRIC MATRIX
C     IGNORING A SPECIFIED ROW/COLUMN IF LO .NE. 0,
C     USING EITHER THE ORIGINAL MATRIX OR A COMPLETE INVERSE OF IT.
C
C Correction mentioned in vol 28 no 3 1979 p 336 applied
C
C     DIMENSION A(L, L)
C     REAL A, AA, AIP, BIG, EP, PVT, SMALL, T
C     INTEGER P, PM, PP
C
C     PARAMETER (BIG=1.0E38, SMALL=1.0E-7)
C
C     PARAMETER CHECKS
C
C     IFAULT = 3
C     IF (ABS(LO) .GT. K .OR. K .LT. 1 .OR. K .GT. L) RETURN
C
C     INITIAL VALUES
C
C     IFAULT = 0
C     IF (LO .GE. 0) GOTO 1
C     EP = 1.0
C     P = -LO
C     PVT = ABS(A(P, P))
C     T = PVT
C     GOTO 3
1     EP = -1.0
C     P = 1
C     PVT = BIG
C
C     PIVOT BY PIVOT INVERSION
C
C     IF (P .EQ. LO) GOTO 12
C     T = ABS(A(P, P))
C     IF (T .LT. PVT) PVT = T
3     IF (T .LT. SMALL) IFAULT = 1
C     IF (T .EQ. 0.0) GOTO 15
C     PM = P - 1
C     PP = P + 1
C     AA = 1.0 / A(P, P)
C     A(P, P) = -AA
C     IF (P .EQ. 1) GOTO 8
C     DO 7 I = 1, PM
C         AIP = A(I, P) * AA
C         DO 4 J = I, PM
4             A(I, J) = A(I, J) - AIP * A(J, P)
C         IF (P .EQ. K) GOTO 6
C         DO 5 J = PP, K
5             A(I, J) = A(I, J) - AIP * A(P, J)
6             A(I, P) = AIP * EP
7     CONTINUE
8     IF (P .EQ. K) GOTO 11
C     DO 10 I = PP, K
C         AIP = A(P, I) * AA
C         DO 9 J = I, K
```

```
9      A(I, J) = A(I, J) - AIP * A(P, J)
      A(P, I) = AIP * EP
10     CONTINUE
11     IF (EP .GT. 0.0) RETURN
12     P = P + 1
      IF (P .LE. K) GOTO 2
C
C      SIGN CORRECTION
C
      DO 14 I = 1, K
        DO 13 J = I, K
13      A(I, J) = -A(I, J)
14     CONTINUE
      RETURN
C
C      NIL PIVOT EXIT
C
15     IFAULT = 2
      RETURN
      END
```



```

SUBROUTINE EXACT(X, YOBS, ALPHA, N, K, P, XSIZE, PLT, PEQ, IFAULT)
C
C   ALGORITHM AS 142 APPL. STATIST. (1979) VOL.28, NO.3
C
C   CALCULATES THE EXACT PROBABILITIES
C   P(T(P) .LT. ALPHA) AND P(T(P) .EQ. ALPHA)
C   WHERE T(P) IS THE CONDITIONAL TEST STATISTIC FOR THE
C   REGRESSION PARAMETER BETA(P) IN A BINARY REGRESSION MODEL
C
C   INTEGER P, XSIZE, YOBS(N), Y(30), P1
C   INTEGER CLT, CEQ, CTOT
C   REAL ALPHA, PLT, PEQ, X(XSIZE, P)
C   REAL T(10), SUM
C
C   CHECK FOR INPUT PARAMETERS OUT OF RANGE
C
C   IFAULT = 1
C   IF (N .GT. 30) RETURN
C   IFAULT = 2
C   IF (P .GT. 10) RETURN
C   IFAULT = 3
C   IF (K .LT. 0 .OR. K .GT. N) RETURN
C   IFAULT = 0
C   PEQ = 1.0
C   PLT = 0.0
C   IF (K .EQ. 0 .OR. K .EQ. N) RETURN
C
C   INITIALIZATION
C   1.  CALCULATE OBSERVED VALUES OF CONDITIONING STATISTICS
C       T(2), ... ,T(P-1)
C   2.  CALCULATE INITIAL PERMUTATION OF K ONES AND
C       N-K ZEROES (1, ..., 1, 0, ..., 0)
C   3.  INITIALIZE NUMERATORS AND DENOMINATOR TO ZERO
C
C   DO 2 I = 1, P
C       T(I) = 0
C   DO 1 J = 1, N
C1      IF (YOBS(J) .EQ. 1) T(I) = T(I) + X(J, I)
C2      CONTINUE
C       P1 = P - 1
C   DO 3 I = 1, K
C3      Y(I) = 1
C       KK = K + 1
C   DO 4 I = KK, N
C4      Y(I) = 0
C       CLT = 0
C       CEQ = 0
C       CTOT = 0
C
C   CALCULATE VALUES OF CONDITIONING STATISTICS (T(2),...T(P-1))
C   FOR CURRENT PERMUTATION.
C   ADD ONE TO DENOMINATOR ONLY IF ALL MATCH OBSERVED VALUES
C
C5      IF (P1 .EQ. 0) GOTO 8
C       DO 7 I = 1, P1
C           SUM = 0.0
C           DO 6 J = 1, N
C6          IF (Y(J) .NE. 0) SUM = SUM + X(J, I)
C7          CONTINUE
C           IF (SUM .NE. T(I)) GOTO 10
C           CONTINUE

```

```
8      CTOT = CTOT + 1
C
C      CALCULATE VALUE OF T(P) FOR CURRENT PERMUTATION
C
      SUM = 0.0
      DO 9 I = 1, N
      IF (Y(I) .NE. 0) SUM = SUM + X(I, P)
9     CONTINUE
C
C      ADD ONE TO NUMERATOR(S) ONLY IF TEST IS PASSED
C
      IF (SUM .LT. ALPHA) CLT = CLT + 1
      IF (SUM .EQ. ALPHA) CEQ = CEQ + 1
C
C      GET ANOTHER PERMUTATION.
C      IF LAST IS ALREADY PROCESSED THEN CALCULATE
C      PROBABILITY AS NUMERATOR/DENOMINATOR
C
10    CALL GETONE(Y, N, IFLAG)
      IF (IFLAG .EQ. 0) GOTO 5
      PEQ = FLOAT(CEQ) / FLOAT(CTOT)
      PLT = FLOAT(CLT) / FLOAT(CTOT)
      RETURN
      END
C
      SUBROUTINE GETONE(RET, N, IFLAG)
C
C      ALGORITHM AS 142.1 APPL. STATIST. (1979) VOL.28, NO.3
C
C      SET DEFAULT RETURN FLAG
C      FLAG=1 - LAST PERMUTATION
C      (0, ..., 0, 1, ..., 1) GENERATED ON PREVIOUS CALL
C      FLAG=0 - RETURNED PERMUTATION SHOULD BE PROCESSED
C
      INTEGER RET(N)
      IFLAG = 0
C
C      INITIAL ACTION DEPENDS ON LEADING ONE OR ZERO
C
      IF (RET(1) .EQ. 0) GOTO 2
C
C      IF LEADING ONE, LOOK FOR FIRST ZERO, THEN
C      INTERCHANGE WITH LAST ONE
C
      DO 1 I = 2, N
      IF (RET(I) .EQ. 1) GOTO 1
      RET(I) = 1
      RET(I - 1) = 0
      RETURN
1     CONTINUE
      RETURN
C
C      INITIAL DIGIT IS ZERO
C      FIND FIRST ONE THEN NEXT ZERO (COORDINATE J)
C      CHECK FOR LAST PERMUTATION
C
2     N2 = N - 1
      DO 3 I = 2, N2
      IF (RET(I) .EQ. 1) GOTO 4
3     CONTINUE
      IFLAG = 1
```

```
      RETURN
4     I2 = I + 1
      DO 5 J = I2, N
      IF (RET(J) .EQ. 0) GOTO 6
5     CONTINUE
      IFLAG = 1
      RETURN
C
C     NOT ON LAST PERMUTATION THEREFORE
C     DEMOTE LAST ONE (INTERCHANGE LAST ONE - NEXT ZERO)
C     AND REVERSE PRECEDING ZEROES-ONES
C
6     RET(J) = 1
      RET(J - 1) = 0
      IF (J .EQ. 2) RETURN
      K = J - 2
      J = K / 2
      DO 7 I = 1, J
      SAVE = RET(K)
      RET(K) = RET(I)
      RET(I) = SAVE
      K = K - 1
7     CONTINUE
      RETURN
      END
```

```

subroutine median (m, n, x, norm, c, f, med, ifault,
*                maxm, maxn, md, g, q, l)
c
c   Algorithm AS 143  Appl. Statist. (1979) Vol. 28, No. 3
c
c   The Mediancentre
c   At least 10 times faster than AS 78.
c
c   Parameters:
c
c   m      integer      input: number of dimensions
c   n      integer      input: number of sample points
c   x      real array   input: data, n points, m dimensions
c   norm   real         output: norm of gradient
c   c      real         output: multiplicity of m in S ; 0 if m not in S
c   med    real array   output: coordinates of the mediancentre
c   ifault integer      output: -1 if m or n out of range
c                               0 if matrix of second derivatives
c                               is positive definite
c                               1 if matrix of second derivatives
c                               is not positive definite
c
c   implicit double precision (a-h, o-z)
c   dimension x(maxn,maxm), med(maxm), md(maxm), g(maxm),
*           q(maxm,maxm), l(maxn)
c   double precision norm, med, md
c
c   data zero, one /0.0d0, 1.0d0/
c   data eps /0.0001d0/
c
c   ifault = -1
c   if (m .lt. 1 .or. m .gt. maxm .or. n .lt. 1 .or. n .gt. maxn)
*     return
c   ifault = 0
c   do 1 i = 1, m
1 med(i) = zero
c   nn = n
c   do 2 i = 1, n
2 l(i) = i
c
c   computation of (residual) mean
c
c   3 f = one / float(nn)
c   do 5 i = 1, m
c     s = zero
c     g(i) = zero
c     do 4 j = 1, nn
c       k = l(j)
c       s = s + x(k, i)
4 continue
c     md(i) = s * f
c     med(i) = med(i) + md(i)
5 continue
c
c   Computation of function, gradient, and norm of gradient
c
c   c = zero
c   f = zero
c   s = zero
c   do 9 i = 1, n
c     t = zero

```

```
        do 6 j = 1, n
          x(i, j) = x(i, j) - md(j)
          t = t + x(i, j) * x(i, j)
6      continue
      if (t .gt. zero) goto 7
      c = c + one
      goto 9
7      t = sqrt(t)
      r = one / t
      s = s + r
      f = f + t
      do 8 j = 1, m
        g(j) = g(j) - r * x(i, j)
8      continue
9      continue
      norm = zero
      do 10 i = 1, m
        norm = norm + g(i) * g(i)
10     continue
      norm = sqrt(norm)
c
c      Check for extremal points
c
      if (norm .le. c + eps) return
      if (nn .eq. 1) goto 13
c
c      Simplex
c
      nt = nn
      nn = 0
      do 12 i = 1, nt
        k = l(i)
        ang = zero
        do 11 j = 1, m
          ang = ang + g(j) * x(k, j)
11     continue
        if (ang .gt. zero) goto 12
        nn = nn + 1
        l(nn) = k
12     continue
      if (nn .gt. 0) goto 3
c
c      Starting value
c
13     r = (c / norm - one) / s
        do 14 i = 1, m
          md(i) = r * g(i)
14     continue
c
c      Newton - Raphson procedure
c
15     c = zero
        f = zero
        s = zero
        do 16 i = 1, m
          g(i) = zero
          med(i) = med(i) + md(i)
          do 16 j = i, m
            q(i, j) = zero
16     continue
        do 19 i = 1, n
```

```

    t = zero
    do 17 j = 1, m
      x(i, j) = x(i, j) - md(j)
      t = t + x(i, j) * x(i, j)
17  continue
    if (t .eq. zero) goto 19
    t = sqrt(t)
    r = one / t
    s = s + r
    rr = r * r * r
    f = f + t
    do 18 j = 1, m
      g(j) = g(j) - r * x(i, j)
      do 18 k = j, m
        q(j, k) = q(k, j) - rr * x(i, j) * x(i, k)
18  continue
19  continue
    norm = zero
    do 20 j = 1, m
      norm = norm + g(j) * g(j)
20  continue
    norm = sqrt(norm)
    if (norm .le. eps) return
c
c      Cholesky and solution of equation
c
    ifault = 1
    if (q(1,1) + s .le. zero) return
    q(1,1) = sqrt(q(1,1) + s)
    do 21 i = 2, m
      q(i, 1) = q(1, i) / q(1, 1)
21  continue
    do 25 j = 2, m
      tmp = s + q(j, j)
      j1 = j - 1
      do 22 i = 1, j1
        tmp = tmp - q(j, i) * q(j, i)
22  continue
      if (tmp .le. zero) return
      q(j, j) = sqrt(tmp)
      j2 = j + 1
      if (j2 .gt. m) goto 25
      do 24 k = j2, m
        tmp = q(j, k)
        do 23 i = 1, j1
          tmp = tmp - q(j, i) * q(k, i)
23  continue
        q(k, j) = tmp / q(j, j)
24  continue
25  continue
    md(1) = -g(1) / q(1, 1)
    do 27 j = 2, m
      j1 = j - 1
      tmp = -g(j)
      do 26 i = 1, j1
        tmp = tmp - q(j, i) * md(i)
26  continue
      md(j) = tmp / q(j, j)
27  continue
    md(m) = md(m) / q(m, m)
    j1 = m - 1

```

```
do 29 j2 = 1, j1
  i = m - j2
  tmp = md(i)
  k = i + 1
  do 28 j = k, m
    tmp = tmp - q(j, i) * md(j)
28  continue
  md(i) = tmp / q(i, i)
29  continue
  ifault = 0
  goto 15
end
```

```
C UKC NETLIB DISTRIBUTION COPYRIGHT 1990 RSS
C
      SUBROUTINE MULMAX(N, K, NMIN, NN, NNK, PROB, A, FAC, IFAULT)
C
C      ALGORITHM AS 145 APPL. STATIST. (1979) VOL.28, NO.3
C
C      N IS THE NUMBER OF BALLS
C      K IS THE NUMBER OF BOXES
C      PROB(I) IS THE PROBABILITY THAT THE MAXIMUM
C      NUMBER OF BALLS IN A BOX IS I + NMIN - 1
C
      REAL PROB(NN), FAC(NNK), NUM, NUP
      INTEGER A(K), SUM
C
      PARAMETER (ZERO=0.0,TEN=10.0,EXPLIM=75.0)
C
      IFAULT = 1
      NUP = FLOAT(N) * ALOG10(FLOAT(K))
      IF (NUP .GT. EXPLIM) RETURN
      NUP = TEN ** NUP
      IFAULT = 2
      SUM = (N + K - 1) / K
      IF (NMIN .GT. N .OR. NMIN .LT. SUM) RETURN
      IFAULT = 3
      IF (N .LE. 1) RETURN
      IFAULT = 0
      DO 1 I = 1, NN
1      PROB(I) = ZERO
C
C      THIS GENERATES THE FIRST PARTITION
C
      M = 1
      A(1) = N
C
C      A NEW PARTITION IS STORED IN A(1) TO A(M)
C
2      NUM = FAC(N)
C
C      THIS COMPUTES THE LOGARITHM OF THE NUMBER
C      OF PARTITIONS OF BALLS
C
      DO 3 I = 1, M
          NA = A(I)
          NUM = NUM - FAC(NA)
3      CONTINUE
C
C      THIS COMPUTES THE LOGARITHM OF THE NUMBER
C      OF PERMUTATIONS OF BOXES
C
      NUM = NUM + FAC(K)
      KM = K - M
      IF (M .LT. K) NUM = NUM - FAC(KM)
      IF (M .EQ. 1) GOTO 6
      I = 1
      II = 2
4      IF (A(II) .EQ. A(I)) GOTO 5
      IJ = II - I
      NUM = NUM - FAC(IJ)
      I = II
5      II = II + 1
      IF (II .LE. M) GOTO 4
```



```
      IJ = II - I
      IF (IJ .GT. 1) NUM = NUM - FAC(IJ)
C
C      THE NUMBER OF ALLOCATIONS GIVING RISE TO THIS PARTITION
C      IS CUMULATED ACCORDING TO THE MAXIMUM FREQUENCY
C
6      KX = A(1) - NMIN + 1
      PROB(KX) = PROB(KX) + EXP(NUM)
C
C      THE MAIN ALGORITHM FOR GENERATING PARTITIONS STARTS HERE
C
7      IF (A(M) .EQ. 1) GOTO 11
      A(M) = A(M) -1
      IF (A(1) .LT. NMIN) GOTO 13
8      M = M + 1
      IF (M .GT. K) GOTO 12
      SUM = A(1)
      L = 2
9      IF (L .GE. M) GOTO 10
      SUM = SUM + A(L)
      L = L + 1
      GOTO 9
10     A(M) = N - SUM
      IF (A(M) .LE. A(M -1)) GOTO 2
      IF (M .GE. K) GOTO 12
      A(M) = A(M -1)
      GOTO 8
11     M = M -1
      GOTO 7
12     M = M -2
      GOTO 7
C
C      ALL PARTITIONS HAVE NOW BEEN GENERATED
C
13     DO 14 I = 1, NN
14     PROB(I) = PROB(I) / NUP
      RETURN
      END
```

```
double precision function gammds (y,p,ifault)
```

```
c
c      Algorithm AS 147  Appl. Statist. (1980) Vol. 29, No. 1
c
c      Computes the incomplete gamma integral for positive
c      parameters y,p using an infinite series
c
c      Auxiliary function required: ALNGAM = CACM algorithm 291
c
c      AS239 should be considered as an alternative to AS147
c
```

```
implicit double precision (a-h,o-z)
data e/1.0d-9/, zero/0.0d0/, one/1.0d0/, uflo/1.0d-37/
```

```
c
c      Checks admissibility of arguments and value of f
c
```

```
ifault = 1
gammds = zero
if(y.le.zero .or. p.le.zero) return
ifault = 2
```

```
c
c      alngam is natural log of gamma function
c
```

```
arg = p*log(y)-alngam(p+one)-y
if(arg.lt.log(uflo)) return
f = exp(arg)
if(f.eq.zero) return
ifault = 0
```

```
c
c      Series begins
c
```

```
c = one
gammds = one
a = p
1 a = a+one
c = c*y/a
gammds = gammds+c
if (c/gammds.gt.e) goto 1
gammds = gammds*f
return
end
```

```

SUBROUTINE JKKN(X, XX, K, N, TH, THJ, LTH, COV, PS, NGRP, IGSIZE,
* IFAULT)
C
C     REMARK ASR62 ON AS 148 APPL. STATIST. (1980) VOL. 29 NO. 1.
C
C     REMOVAL OF BIAS BY THE JACKKNIFE PROCEDURE
C
C     INTEGER K, N, LTH, NGRP, IGSIZE, IFAULT
C     REAL X(K, N), TH(LTH), THJ(LTH), COV(LTH, LTH), PS(LTH, NGRP),
* XX(K, N)
C
C     IFAULT = 1
C     IF (NGRP .LE. 1) RETURN
C     IFAULT = 0
C     NGRP1 = NGRP - 1
C     NN = NGRP1 * IGSIZE
C     ENGRP = NGRP
C     ENGRP1 = NGRP1
C     ENN = ENGRP * ENGRP1
C     IGSZ1 = IGSIZE + 1
C     KI = K * IGSIZE
C
C     KI = NUMBER OF X COMPONENTS IN A GROUP
C
C     LIN = NGRP1 * KI
C
C     FIRST CALCULATE NGRP*THETAHAT AND STORE IT IN TH
C
C     CALL THTHT(X, K, N, TH, LTH)
C     DO 10 I = 1, LTH
10 TH(I) = ENGRP * TH(I)
C
C     CALCULATE THE NGRP PSEUDOVALUES
C
C     IG1 = 0
C     DO 12 J = 1, K
C     DO 11 IN = I, NGRP
C 11 XX(J, IN) = X(J, IN)
C 12 CONTINUE
C     DO 50 I = 1, NGRP
C
C     MOVE THE I-TH GROUP OF OBSERVATIONS TO THE NGRP-TH GROUP
C     POSITION, THEN MOVE POSITION OF THE I+1-TH GROUP I-TH
C     POSITION, I+2-TH TO I+1-TH AND SO ON
C
C     DO 20 IG = 1, IGSIZE
C     DO 15 J = 1, K
C     TEMP = XX(J, I)
C     DO 14 IN = I, NN
C     NUM = IN + 1
14 XX(J, IN) = XX(J, NUM)
C     XX(J, NGRP) = TEMP
15 CONTINUE
20 CONTINUE
C     CALL THTHT(XX, K, NN, THJ, LTH)
C     DO 22 J = 1, K
C     DO 21 IN = I, NGRP
21 XX(J, IN) = X(J, IN)
22 CONTINUE
C     DO 35 II = 1, LTH
35 PS(II, I) = TH(II) - THJ(II) * ENGRP1

```

```
50 CONTINUE
C
C      INITIALIZE
C
      DO 75 I = 1, LTH
        THJ(I) = 0.0
        DO 75 J = 1, LTH
          COV(I, J) = 0.0
75 CONTINUE
C
C      CALCULATE JACKKNIFED VERSION OF THETAHAT AND STORE IN THJ
C
      DO 100 I = 1, NGRP
        DO 90 II = 1, LTH
          90 THJ(II) = THJ(II) + PS(II, I)
100 CONTINUE
        DO 110 II = 1, LTH
          110 THJ(II) = THJ(II) / ENGRP
C
C      CALCULATE THE APPROXIMATE COVARIANCE MATRIC OF THE JACKKNIFED
C      THETAHAT AND STORE IT IN COV
C
      DO 125 II = 1, LTH
        THJII = THJ(II)
        DO 125 JJ = II, LTH
          THJJJ = THJ(JJ)
          DO 115 I = 1, NGRP
            COV(II, JJ) = COV(II, JJ) + (PS(II, I) - THJII) * (PS(JJ, I)
            *
              - THJJJ)
115 CONTINUE
125 CONTINUE
C
C      IF LTH .GT. 1, COPY THE UPPER-TRIANGULAR SECTION OF COV INTO
C      THE LOWER TRIANGULAR SECTION
C
      IF (LTH .EQ. 1) GOTO 200
      DO 175 II = 2, LTH
        III = II - 1
        DO 175 JJ = 1, III
          COV(II, JJ) = COV(JJ, II)
175 CONTINUE
200 DO 210 II = 1, LTH
        DO 210 JJ = 1, LTH
          210 COV(II, JJ) = COV(II, JJ) / ENN
      RETURN
      END
```

```
SUBROUTINE AMALGM(K, XO, WO, X, W, XA, IFAULT)
```

```

C
C<<<<<  Acquired in machine-readable form from 'Applied Statistics'
C<<<<<  algorithms editor, January 1983.
C
C
C      ALGORITHM AS 149 APPL. STATIST. (1980) VOL.29, NO.2
C
C      AMALGAMATION OF MEANS BY THE UP-AND-DOWN BLOCKS ALGORITHM
C      OF KRUSKAL (BARLOW ET AL. ,1972, P.72 )
C
DIMENSION XO(K),WO(K),X(K),W(K),XA(K)
DATA TOL /1.0E-6/
IFAULT = 1
C
C      CHECK THAT K .GE. 2
C
IF (K .LT. 2) RETURN
IFAULT = 2
C
C      CHECK THAT THE WEIGHTS ARE POSITIVE
C
DO 1 I = 1,K
IF (WO(I) .LE. 0.0) RETURN
1 CONTINUE
IFAULT = 0
DO 2 I = 1,K
X(I) = XO(I)
W(I) = WO(I)
2 CONTINUE
M = K
I = 1
3 IF (I .EQ. M) GOTO 4
IF (X(I) .GT. X(I+1)) GOTO 9
IF (I .EQ. 1) GOTO 13
4 IF (X(I-1) .GT. X(I)) GOTO 6
IF (I .LT. M) GOTO 13
GOTO 14
C
C      POOL THE ACTIVE BLOCK WITH THE NEXT LOWER BLOCK
C
6 IM1 = I - 1
WW = W(IM1) + W(I)
X(IM1) = (W(IM1)*X(IM1) + W(I)*X(I))/WW
W(IM1) = WW
MM1 = M - 1
IF (I .EQ. M) GOTO 8
DO 7 J = I,MM1
J1 = J + 1
X(J) = X(J1)
W(J) = W(J1)
7 CONTINUE
8 I = IM1
M = MM1
IF (M .EQ. 1) GOTO 14
GOTO 3
C
C      POOL THE ACTIVE BLOCK WITH THE NEXT HIGHER BLOCK
C
9 I1 = I + 1
WW = W(I) + W(I1)

```

```
X(I) = (W(I)*X(I) + W(I1)*X(I1))/WW
W(I) = WW
MM1 = M - 1
IF (I1 .EQ. M) GOTO 11
DO 10 J = I1,MM1
J1 = J + 1
X(J) = X(J1)
W(J) = W(J1)
10 CONTINUE
11 M = MM1
IF (M .EQ. 1) GOTO 14
IF (I .EQ. 1) GOTO 12
IF (X(I-1) .GT. X(I)) GOTO 6
12 IF (I .EQ. M) GOTO 14
IF (X(I) .GT. X(I+1)) GOTO 9
13 I = I + 1
GO TO 12
```

```
C
C      OBTAIN THE AMALGAMATED MEANS XA(K) FROM THE WORKING ARRAY X(M)
C
```

```
14 I1 = 1
DO 17 I = 1,M
S = 0.0
DO 15 J = I1,K
S = S + WO(J)
XA(J) = X(I)
IF (ABS(S - W(I)) .LT. TOL) GOTO 16
15 CONTINUE
16 I1 = J + 1
17 CONTINUE
RETURN
END
```

```
      SUBROUTINE SCOUNT(NEVENT,TZERO,NF,NW,T,SPEC,FREQ,C,S,IFault)
C
C<<<<<  Acquired in machine-readable form from 'Applied Statistics'
C<<<<<  algorithms editor, January 1983.
C
C      ALGORITHM AS 150 APPL. STATIST. (1980) VOL.29, NO.2
C
C      COMPUTES ESTIMATES OF THE SPECTRUM OF A POINT PROCESS
C      BY TAKING A CENTRED MOVING AVERAGE OF THE NORMALISED
C      PERIODOGRAM OF THE COUNTING PROCESS
C
C
C      DIMENSION T(NEVENT),FREQ(NF),SPEC(NF),C(NF),S(NF)
C      REAL TWOPI
C      DATA TWOPI,NRECUR/6.283185307196E0,100/
C
C      TEST FOR ERRORS
C
C      IFAULT = 0
C      IF(NW.LE.0) GO TO 10
C      IF(NW.GT.NF) GO TO 11
C      IF(MOD(NW,2).EQ.0) GO TO 12
C      IF(NEVENT.LE.0) GO TO 13
C      IF(TZERO.LE.0.0) GO TO 14
C      IF(T(1).LT.0.0 .OR. T(NEVENT).GT.TZERO) GO TO 15
C      DO 1 I = 2,NEVENT
C      IF(T(I).LE.T(I-1)) GO TO 15
1 CONTINUE
C
C      END OF ERROR-TESTING SECTION
C
C      FW = NW
C      FN = NEVENT
C      RTZERO = 1.0/TZERO
C
C      INITIALISE ARRAYS FOR SUMS OF SINES AND COSINES
C      AND CALCULATE FREQUENCIES
C
C      DO 2 I = 1,NF
C      C(I) = 0.0
C      S(I) = 0.0
C      SPEC(I) = I
C      FREQ(I) = SPEC(I)*RTZERO
2 CONTINUE
C
C      CALCULATE SUMS OF SINES AND COSINES USING THE DOUBLE-
C      ANGLE SINE AND COSINE FORMULAS - EXCEPT COMPUTE EVERY
C      (NRECUR)TH. DIRECTLY
C
C      DO 6 I = 1,NEVENT
C      ANGLE = TWOPI*T(I)*RTZERO
C      COSINI = COS(ANGLE)
C      SININI = SIN(ANGLE)
C      COSREC = 1.0
C      SINREC = 0.0
C      DO 5 J = 1,NF
C
C      TEST WHETHER NEED TO COMPUTE SINE AND COSINE DIRECTLY
C
C      IF(MOD(J,NRECUR).NE.0) GO TO 3
C
```

```
C      RECALL THAT SPEC(J) = J
C
      FMULT = SPEC(J)*ANGLE
      COSREC = COS(FMULT)
      SINREC = SIN(FMULT)
      GOTO 4
3 TEMP = COSREC*COSINI - SINREC*SININI
  SINREC = COSREC*SININI + SINREC*COSINI
  COSREC = TEMP
4 C(J) = C(J) + COSREC
  S(J) = S(J) + SINREC
5 CONTINUE
6 CONTINUE

C
C      S(.) AND C(.) NOW CONTAIN THE SUMS OF SINES AND
C      COSINES,RESPECTIVELY
C
C
C      NOW USE SPEC(.) FOR THE NORMALISED PERIODOGRAM
C
      CNORM = 2.0/FN
      DO 7 I = 1,NF
7 SPEC(I) = CNORM*(C(I)*C(I) + S(I)*S(I))

C
C      NOW OBTAIN THE SMOOTHED SPECTRAL ESTIMATES -
C      RETURN IF WANT ONLY THE PERIODOGRAM
C
      IF(NW.EQ.1) RETURN
      KU = NF - NW + 1
      L = NW/2
      DO 9 I = 1,KU
      SUM = 0.0
      J = I + NW - 1
      DO 8 K = I,J
8 SUM = SUM + SPEC(K)

C
C      STORE THE SMOOTHED ESTIMATES AND THE CORRESPONDING
C      FREQUENCIES IN THE FIRST (NF - NW + 1) ELEMENTS OF
C      SPEC(.) AND FREQ(.)
C
      SPEC(I) = SUM/FW
      M = I + L
      FREQ(I) = FREQ(M)
9 CONTINUE
  RETURN
10 IFAULT = 1
  RETURN
11 IFAULT = 2
  RETURN
12 IFAULT = 3
  RETURN
13 IFAULT = 4
  RETURN
14 IFAULT = 5
  RETURN
15 IFAULT = 6
  RETURN
  END
```



```
      SUBROUTINE BIVCNT(N1,N2,TZERO,NSECT,T1,T2,NF,TTEMP,SPC1,SPC2,C1,
* S1,C2,S2,NT1,NT2,NN1,NN2,SPEC1,SPEC2,COHERE,PHASE,FREQ,IFAU
C
C<<<<< Acquired in machine-readable form from 'Applied Statistics'
C<<<<< algorithms editor, January 1983.
C
C      ALGORITHM AS 151 APPL. STATIST. (1980) VOL.29, NO.2
C
C      CALCULATES SMOOTHED SPECTRAL ESTIMATES FOR A BIVARIATE POINT
C      PROCESS BY SPLITTING THE PERIOD OF OBSERVATION INTO NONOVERLAPPING
C      SECTIONS OF EQUAL LENGTH
C
C      DIMENSION T1(N1),T2(N2),FREQ(NF),SPEC1(NF),SPEC2(NF),COHERE(NF),
1 PHASE(NF),C1(NF),S1(NF),C2(NF),S2(NF),TTEMP(NF),SPC1(NF),SPC2(NF)
      INTEGER NT1(NSECT),NT2(NSECT),NN1(NSECT),NN2(NSECT)
C
C      TEST FOR PARAMETER ERRORS
C
C      IF(TZERO.LE.0.0) GO TO 9
C      IF(N1.LE.0 .OR. N2.LE.0) GO TO 10
C      IF(T1(N1).GT.TZERO .OR. T2(N2).GT.TZERO) GO TO 11
C      IF(NSECT.LE.0) GO TO 12
C      IF(NF.LT.NSECT) GO TO 13
C      IFAULT = 0
C
C      INITIALISE ARRAYS FOR ACCUMULATING SPECTRAL ESTIMATES
C
C      DO 1 I = 1,NF
C      SPEC1(I) = 0.0
C      SPEC2(I) = 0.0
C      COHERE(I) = 0.0
C      PHASE(I) = 0.0
1 CONTINUE
C
C      UNLESS NSECT = 1,CALL SPLIT TO SECTION THE PERIOD OF OBSERVATION
C      AND CALCULATE THE EVENT TIMES RELATIVE TO THE SECTION ORIGINS
C
C      NT1(1) = N1
C      NT2(1) = N2
C      NN1(1) = N1
C      NN2(1) = N2
C      IF(NSECT.EQ.1) GO TO 3
C      CALL SPLIT(NSECT, N1, TZERO, T1, NT1, TTEMP, IFAULT)
C      IF (IFAU
C      CALL SPLIT(NSECT, N2, TZERO, T2, NT2, TTEMP, IFAULT)
C      IF(IFAU
C
C      CALCULATE NO. OF EVENTS IN EACH SECTION OF BOTH SERIES
C
C      NN1(1) = NT1(1)
C      NN2(1) = NT2(1)
C
C      TEST WHETHER THE WORKSPACE ARRAY TTEMP(.) IS LARGE ENOUGH
C      TO STORE THE EVENT TIMES IN SECTION 1 OF EACH SERIES
C
C      IF(NN1(1).GT.NF.OR.NN2(1).GT.NF) GO TO 14
C      DO 2 I = 2,NSECT
C      NN1(I) = NT1(I)-NT1(I-1)
C      NN2(I) = NT2(I)-NT2(I-1)
C
C      DO THE SAME FOR THE OTHER SECTIONS
```

```

C
  IF(NN1(I).GT.NF.OR.NN2(I).GT.NF) GO TO 14
2 CONTINUE

C
C  CALL SCOUNT SECTION BY SECTION,USING TTEMP(.) TO STORE
C  THE EVENT TIMES TEMPORARILY
C
3 FN = 1.0/FLOAT(NSECT)
  TS = TZERO*FN
  KU1 = 0
  KU2 = 0
  DO 7 J = 1,NSECT
  KL1 = KU1+1
  KU1 = NT1(J)
  KL2 = KU2+1
  KU2 = NT2(J)
  DO 4 I = KL1,KU1
  K = I-KL1+1
  TTEMP(K) = T1(I)
4 CONTINUE

C
C  CALL SCOUNT WITH NW-1 TO OBTAIN THE NORMALISED PERIODOGRAM AND
C  THE SUM OF SINES AND COSINES FOR SECTION J OF SERIES 1
C
  CALL SCOUNT(NN1(J), TS, NF, 1, TTEMP, SPC1, FREQ, C1, S1, IFAULT)
  IF(IFAULT.NE.0) RETURN
  DO 5 I = KL2, KU2
  K = I-KL2+1
  TTEMP(K) = T2(I)
5 CONTINUE

C
C  DO THE SAME FOR SERIES 2
C
  CALL SCOUNT(NN2(J), TS, NF, 1, TTEMP, SPC2, FREQ, C2, S2, IFAULT)
  IF(IFAULT.NE.0) RETURN
  SQNN = 1.0/SQRT(FLOAT(NN1(J)*NN2(J)))

C
C  ACCUMULATE(OVER THE NSECT SECTIONS) THE SPECTRAL ESTIMATES
C  AT EACH FREQUENCY
C
  DO 6 I = 1,NF
  SPEC1(I) = SPEC1(I) + SPC1(I)
  SPEC2(I) = SPEC2(I) + SPC2(I)
  COHERE(I) = COHERE(I) + (C1(I)*C2(I) + S1(I)*S2(I))*SQNN
  PHASE(I) = PHASE(I) + (C2(I)*S1(I) - C1(I)*S2(I))*SQNN
6 CONTINUE
7 CONTINUE

C
C  NOW FIND THE SMOOTHED ESTIMATES
C
  DO 8 I = 1,NF
  SPEC1(I) = SPEC1(I)*FN
  SPEC2(I) = SPEC2(I)*FN
  TEMP = COHERE(I)
  COHERE(I) = 4.0*FN*FN*(TEMP*TEMP + PHASE(I)*PHASE(I))/
1 (SPEC1(I)*SPEC2(I))
  PHASE(I) = ATAN2(PHASE(I),TEMP)
8 CONTINUE
  RETURN
9 IFAULT = 7
  RETURN

```

```
10 IFAULT = 8
    RETURN
11 IFAULT = 9
    RETURN
12 IFAULT = 10
    RETURN
13 IFAULT = 11
    RETURN
14 IFAULT = 12
    RETURN
    END
    SUBROUTINE SPLIT(NSECT,NEVENT,TZERO,T,NT,TSECT,IFAU)
C
C   ALGORITHM AS 151.1 APPL. STATIST. (1980) VOL.29, NO.2
C
C   SPLITS A PERIOD OF OBSERVATION ON A POINT PROCESS INTO
C   NONOVERLAPPING SECTIONS OF EQUAL LENGTH AND COMPUTES
C   THE EVENT TIMES RELATIVE TO THE SECTION ORIGINS
C
C
C   DIMENSION T(NEVENT),TSECT(NSECT)
C   INTEGER NT(NSECT)
C   IFAULT = 0
C
C   TEST FOR PARAMETER ERRORS
C
C   IF (NSECT.LE.1.OR.NSECT.GT.NEVENT) GO TO 7
C   IF(TZERO.LE.0.0) GO TO 8
C   IF(T(NEVENT).GT.TZERO) GO TO 9
C
C   INITIA = NEVENT/NSECT
C   JJ = NSECT-1
C   FN = TZERO/FLOAT(NSECT)
C   DO 4 I = 1,JJ
C
C   COMPUTE THE TIMES AT WHICH THE SECTIONS END
C
C   TSECT(I) = FLOAT(I)*FN
C
C   AS A STARTING POINT,ASSUME THAT ALL SECTIONS CONTAIN THE
C   SAME NUMBER OF EVENTS
C
C   NT(I) = I*INITIA
C   INDEX = NT(I)
C
C   TEST WHETHER THE FINISHING POINT FOR SECTION I IS TOO
C   SMALL,JUST RIGHT OR TOO HIGH
C
C   IF(T(INDEX)-TSECT(I))1,4,3
1  NT(I) = NT(I)+1
   INDEX = NT(I)
   IF(INDEX.GT.NEVENT) GO TO 2
   IF(T(INDEX)-TSECT(I))1,4,2
2  NT(I) = NT(I)-1
   GOTO 4
3  NT(I) = NT(I)-1
   INDEX = NT(I)
   IF(INDEX.LT.1) GO TO 4
   IF(T(INDEX).GT.TSECT(I)) GO TO 3
4  CONTINUE
   NT(NSECT) = NEVENT
```

```
C
C      NT(I) IS NOW EQUAL TO THE TOTAL NUMBER OF EVENTS IN
C      THE FIRST I SECTIONS
C
C      NOW COMPUTE THE EVENT TIMES RELATIVE TO THE SECTION ORIGINS -
C      FIRST TEST WHETHER SECTION 1 CONTAINS NO EVENTS
C
      IF(NT(1).EQ.0) GO TO 10
      DO 6 I = 2,NSECT
      KK = I-1
      LK = NT(KK)+1
      LU = NT(I)
C
C      TEST WHETHER THE SECTION CONTAINS NO EVENTS
C
      IF(LK.GT.LU) GO TO 10
      DO 5 J = LK,LU
5     T(J) = T(J)-TSECT(KK)
6     CONTINUE
      RETURN
7     IFAULT = 13
      RETURN
8     IFAULT = 14
      RETURN
9     IFAULT = 15
      RETURN
10    IFAULT = 16
      RETURN
      END
```

```

REAL FUNCTION CHYPER(POINT, KK, LL, MM, NN, IFAULT)
C
C ALGORITHM AS R77 APPL. STATIST. (1989), VOL.38, NO.1
C Replaces AS 59 and AS 152
C Incorporates AS R86 from vol.40(2)
C
C Auxiliary routines required: ALNFAC (AS 245), ALNORM (AS 66)
C
INTEGER          KK, LL, MM, NN, IFAULT, K, L, M, N, I, J, NL, KL,
*                MNKL, MVBIG, MBIG
REAL             ZERO, ONE, P, PT, HALF, ALNFAC, ELIMIT, MEAN,
*                SIG, ALNORM, SXTEEN, SCALE, ROOTPI, ARG, HUNDRD
LOGICAL          POINT, DIR
PARAMETER (ZERO = 0.0, HALF = 0.5, ONE = 1.0, MVBIG = 1000,
*          MBIG = 600, ELIMIT = -88.0, SXTEEN = 16.0,
*          SCALE = 1.0E35, ROOTPI = 2.50662 82746 31001,
*          HUNDRD = 100.0)
C
K = KK + 1
L = LL + 1
M = MM + 1
N = NN + 1
DIR = .TRUE.
C
C Check arguments are within permitted limits
C
IFAULT = 1
CHYPER = ZERO
IF (N .LT. 1 .OR. M .LT. N .OR. K .LT. 1 .OR. K .GT. M) RETURN
C
IFAULT = 2
IF (L .LT. 1 .OR. K-L .GT. M-N) RETURN
IF (.NOT. POINT) CHYPER = ONE
IF (L .GT. N .OR. L .GT. K) RETURN
IFAULT = 0
CHYPER = ONE
IF (K .EQ. 1 .OR. K .EQ. M .OR. N .EQ. 1 .OR. N .EQ. M) RETURN
IF (.NOT. POINT .AND. LL .EQ. MIN(KK, NN)) RETURN
C
P = REAL(NN) / REAL(MM - NN)
IF (REAL(MIN(KK, MM-KK)) .GT. SXTEEN * MAX(P, ONE/P) .AND.
*   MM .GT. MVBIG .AND. ELIMIT .GT. -HUNDRD) THEN
C
C Use a normal approximation
C
MEAN = REAL(KK) * REAL(NN) / REAL(MM)
SIG = SQRT(MEAN * (REAL(MM-NN) / REAL(MM)) * (REAL(MM-KK) /
*   (REAL(MM-1))))
IF (POINT) THEN
  ARG = -HALF * (((REAL(LL) - MEAN) / SIG)**2)
  CHYPER = ZERO
  IF (ARG .GE. ELIMIT) CHYPER = EXP(ARG) / (SIG * ROOTPI)
ELSE
  CHYPER = ALNORM((REAL(LL) + HALF - MEAN) / SIG, .FALSE.)
END IF
C
ELSE
C
C Calculate exact hypergeometric probabilities.
C Interchange K and N if this saves calculations.
C

```

```

        IF (MIN(K-1, M-K) .GT. MIN(N-1, M-N)) THEN
            I = K
            K = N
            N = I
        END IF
        IF (M-K .LT. K-1) THEN
            DIR = .NOT. DIR
            L = N - L + 1
            K = M - K + 1
        END IF
C
        IF (MM .GT. MBIG) THEN
C
C        Take logarithms of factorials.
C
            P = ALNFAC(NN) - ALNFAC(MM) + ALNFAC(MM-KK) + ALNFAC(KK) +
*           ALNFAC(MM-NN) - ALNFAC(LL) - ALNFAC(NN-LL) - ALNFAC(KK-LL)
*           - ALNFAC(MM-NN-KK+LL)
            CHYPER = ZERO
            IF (P .GE. ELIMIT) CHYPER = EXP(P)
            ELSE
C
C        Use Freeman/Lund algorithm
C
            DO 3 I = 1, L-1
                CHYPER = CHYPER * REAL(K-I) * REAL(N-I) / (REAL(L-I) *
*                 REAL(M-I))
            3   CONTINUE
            IF (L .NE. K) THEN
                J = M - N + L
                DO 5 I = L, K-1
                    CHYPER = CHYPER * REAL(J-I) / REAL(M-I)
                5   CONTINUE
            END IF
C
            END IF
C
            IF (POINT) RETURN
            IF (CHYPER .EQ. ZERO) THEN
C
C        We must recompute the point probability since it has underflowed.
C
                IF (MM .LE. MBIG) P = ALNFAC(NN) - ALNFAC(MM) + ALNFAC(KK) +
*                 ALNFAC(MM-NN) - ALNFAC(LL) - ALNFAC(NN-LL) - ALNFAC(KK-LL) -
*                 ALNFAC(MM-NN-KK+LL) + ALNFAC(MM-KK)
                P = P + LOG(SCALE)
                IF (P .LT. ELIMIT) THEN
                    IFAULT = 3
                    IF (LL .GT. REAL(NN*KK + NN + KK + 1)/(MM + 2)) CHYPER = ONE
                    RETURN
                ELSE
                    P = EXP(P)
                END IF
            ELSE
C
C        Scale up at this point.
C
                P = CHYPER * SCALE
            END IF
C
            PT = ZERO

```

```
      NL = N - L
      KL = K - L
      MNKL = M - N - KL + 1
      IF (L .LE. KL) THEN
      DO 7 I = 1, L-1
        P = P * REAL(L-I) * REAL(MNKL-I) /
*          (REAL(NL+I) * REAL(KL+I))
        PT = PT + P
7      CONTINUE
      IF (P .EQ. ZERO) IFAULT = 3
      ELSE
      DIR = .NOT. DIR
      DO 9 J = 0, KL-1
        P = P * REAL(NL-J) * REAL(KL-J) / (REAL(L+J) * REAL(MNKL+J))
        PT = PT + P
9      CONTINUE
      IF (P .EQ. ZERO) IFAULT = 3
      END IF
C
      IF (DIR) THEN
      CHYPER = CHYPER + (PT / SCALE)
      ELSE
      CHYPER = ONE - (PT / SCALE)
      END IF
C
      END IF
C
      END
```

```
DOUBLE PRECISION FUNCTION GRADSOL(A, M, C, N)
```

```
C
C TRANSLATION OF AMENDED VERSION OF APPLIED STATISTICS ALGORITHM
C AS 153 (AS R52), VOL. 33, 363-366, 1984.
C BY R.W. FAREBROTHER (ORIGINALLY NAMED GRADSOL OR PAN)
C
C GRADSOL EVALUATES THE PROBABILITY THAT A WEIGHTED SUM OF
C SQUARED STANDARD NORMAL VARIATES DIVIDED BY X TIMES THE UNWEIGHTED
C SUM IS LESS THAN A GIVEN CONSTANT, I.E. THAT
C  $A1.U1^{**2} + A2.U2^{**2} + \dots + AM.UM^{**2} <$ 
C  $X*(U1^{**2} + U2^{**2} + \dots + UM^{**2}) + C$ 
C WHERE THE U'S ARE STANDARD NORMAL VARIABLES.
C FOR THE DURBIN-WATSON STATISTIC, X = DW, C = 0, AND
C A ARE THE NON-ZERO EIGENVALUES OF THE "M*A" MATRIX.
```

```
C THE ELEMENTS A(I) MUST BE ORDERED. A(0) = X
C N = THE NUMBER OF TERMS IN THE SERIES. THIS DETERMINES THE
C ACCURACY AND ALSO THE SPEED. NORMALLY N SHOULD BE ABOUT 10-15.
```

```
C -----
C ORIGINALLY FROM STATLIB. REVISED 5/3/1996 BY CLINT CUMMINS:
```

- C 1. DIMENSION A STARTING FROM 0 (FORTRAN 77)
- C IF THE USER DOES NOT INITIALIZE A(0) = X,
- C THERE WOULD BE UNPREDICTABLE RESULTS, SINCE A(0) IS ACCESSED
- C WHEN J2=0 FOR THE FINAL DO 60 LOOP.
- C 2. USE X VARIABLE TO AGREE WITH PUBLISHED CODE
- C 3. FIX BUG 2 LINES BELOW DO 60 L2 = J2, NU, D
- C PROD = A(J2) --> PROD = A(L2)
- C (PRIOR TO THIS FIX, ONLY THE TESTS WITH M=3 WORKED CORRECTLY)
- C 4. TRANSLATE TO UPPERCASE AND REMOVE TABS

```
C TESTED SUCCESSFULLY ON THE FOLLOWING BENCHMARKS:
```

- C 1. FAREBROTHER 1984 TABLE (X=0):

A	C	PROBABILITY
1,3,6	1	.0542
1,3,6	7	.4936
1,3,6	20	.8760
1,3,5,7,9	5	.0544
1,3,5,7,9	20	.4853
1,3,5,7,9	50	.9069
3,4,5,6,7	5	.0405
3,4,5,6,7	20	.4603
3,4,5,6,7	50	.9200

- C 2. DURBIN-WATSON 1951/71 SPIRITS DATASET, FOR X=.2,.3,...,3.8, C=0
- C COMPARED WITH BETA APPROXIMATION (M=66), A SORTED IN REVERSE ORDER
- C 3. JUDGE, ET AL 2ND ED. P.399 DATASET, FOR X=.2,.3,...,3.8, C=0
- C COMPARED WITH BETA APPROXIMATION (M=8), A SORTED IN EITHER ORDER

```
C INTEGER M, N
```

```
C DOUBLE PRECISION A(0:M), C, X
```

```
C LOCAL VARIABLES
```

```
C INTEGER D, H, I, J1, J2, J3, J4, K, L1, L2, NU, N2
```

```
C DOUBLE PRECISION NUM, PIN, PROD, SGN, SUM, SUM1, U, V, Y
```

```
C DOUBLE PRECISION ZERO, ONE, HALF, TWO
```

```
C DATA ZERO/0.D0/, ONE/1.D0/, HALF/0.5D0/, TWO/2.D0/
```

```
C SET NU = INDEX OF 1ST A(I) >= X.
```

```
C ALLOW FOR THE A'S BEING IN REVERSE ORDER.
```

```
C IF (A(1) .GT. A(M)) THEN
```

```
    H = M
```



```

      K = -1
      I = 1
ELSE
      H = 1
      K = 1
      I = M
ENDIF
X = A(0)
DO 10 NU = H, I, K
      IF (A(NU) .GE. X) GO TO 20
10 CONTINUE
C
C      IF ALL A'S ARE -VE AND C >= 0, THEN PROBABILITY = 1.
C
      IF (C .GE. ZERO) THEN
          GRADSOL = ONE
          RETURN
      ENDIF
C
C      SIMILARLY IF ALL THE A'S ARE +VE AND C <= 0, THEN PROBABILITY = 0.
C
20 IF (NU .EQ. H .AND. C .LE. ZERO) THEN
      GRADSOL = ZERO
      RETURN
  ENDIF
C
      IF (K .EQ. 1) NU = NU - 1
      H = M - NU
      IF (C .EQ. ZERO) THEN
          Y = H - NU
      ELSE
          Y = C * (A(1) - A(M))
      ENDIF
C
      IF (Y .GE. ZERO) THEN
          D = 2
          H = NU
          K = -K
          J1 = 0
          J2 = 2
          J3 = 3
          J4 = 1
      ELSE
          D = -2
          NU = NU + 1
          J1 = M - 2
          J2 = M - 1
          J3 = M + 1
          J4 = M
      ENDIF
      PIN = TWO * DATAN(ONE) / N
      SUM = HALF * (K + 1)
      SGN = K / DBLE(N)
      N2 = N + N - 1
C
C      FIRST INTEGRALS
C
DO 70 L1 = H-2*(H/2), 0, -1
DO 60 L2 = J2, NU, D
      SUM1 = A(J4)
C      FIX BY CLINT CUMMINS 5/3/96
```

```
C      PROD = A(J2)
      PROD = A(L2)
      U = HALF * (SUM1 + PROD)
      V = HALF * (SUM1 - PROD)
      SUM1 = ZERO
      DO 50 I = 1, N2, 2
        Y = U - V * DCOS(DBLE(I)*PIN)
        NUM = Y - X
        PROD = DEXP(-C/NUM)
        DO 30 K = 1, J1
          PROD = PROD * NUM / (Y - A(K))
30      CONTINUE
        DO 40 K = J3, M
          PROD = PROD * NUM / (Y - A(K))
40      CONTINUE
        SUM1 = SUM1 + DSQRT(DABS(PROD))
50      CONTINUE
      SGN = -SGN
      SUM = SUM + SGN * SUM1
      J1 = J1 + D
      J3 = J3 + D
      J4 = J4 + D
60     CONTINUE
C
C     SECOND INTEGRAL.
C
      IF (D .EQ. 2) THEN
        J3 = J3 - 1
      ELSE
        J1 = J1 + 1
      ENDIF
      J2 = 0
      NU = 0
70     CONTINUE
C
      GRADSOL = SUM
      RETURN
      END
```

```

CSTART OF AS 154
      SUBROUTINE STARMA(IP, IQ, IR, NP, PHI, THETA, A, P, V, THETAB,
$ XNEXT, XROW, RBAR, NRBAR, IFAULT)
C
C      ALGORITHM AS 154  APPL. STATIST. (1980) VOL.29, P.311
C
C      INVOKING THIS SUBROUTINE SETS THE VALUES OF V AND PHI, AND
C      OBTAINS THE INITIAL VALUES OF A AND P.
C      THIS ROUTINE IS NOT SUITABLE FOR USE WITH AN AR(1) PROCESS.
C      IN THIS CASE THE FOLLOWING INSTRUCTIONS SHOULD BE USED FOR
C      INITIALISATION.
C      V(1) = 1.0
C      A(1) = 0.0
C      P(1) = 1.0 / (1.0 - PHI(1) * PHI(1))
C
      REAL PHI(IR), THETA(IR), A(IR), P(NP), V(NP), THETAB(NP),
$ XNEXT(NP), XROW(NP), RBAR(NRBAR), VJ, PHII, PHIJ, SSQERR,
$ RECRES, YNEXT, ZERO, ONE
C
      DATA ZERO, ONE /0.0, 1.0/
C
      CHECK FOR FAILURE INDICATION.
C
      IFAULT = 0
      IF (IP .LT. 0) IFAULT = 1
      IF (IQ .LT. 0) IFAULT = IFAULT + 2
      IF (IP .EQ. 0 .AND. IQ .EQ. 0) IFAULT = 4
      K = IQ + 1
      IF (K .LT. IP) K = IP
      IF (IR .NE. K) IFAULT = 5
      IF (NP .NE. IR * (IR + 1) / 2) IFAULT = 6
      IF (NRBAR .NE. NP * (NP - 1) / 2) IFAULT = 7
      IF (IR .EQ. 1) IFAULT = 8
      IF (IFAULT .NE. 0) RETURN
C
      NOW SET A(0), V AND PHI.
C
      DO 10 I = 2, IR
      A(I) = ZERO
      IF (I .GT. IP) PHI(I) = ZERO
      V(I) = ZERO
      IF (I .LE. IQ + 1) V(I) = THETA(I - 1)
10 CONTINUE
      A(1) = ZERO
      IF (IP .EQ. 0) PHI(1) = ZERO
      V(1) = ONE
      IND = IR
      DO 20 J = 2, IR
      VJ = V(J)
      DO 20 I = J, IR
      IND = IND + 1
      V(IND) = V(I) * VJ
20 CONTINUE
C
      NOW FIND P(0).
C
      IF (IP .EQ. 0) GOTO 300
C
      THE SET OF EQUATIONS  $S * \text{VEC}(P(0)) = \text{VEC}(V)$ 
C      IS SOLVED FOR  $\text{VEC}(P(0))$ .
C      S IS GENERATED ROW BY ROW IN THE ARRAY XNEXT.

```

```
C      THE ORDER OF ELEMENTS IN P IS CHANGED, SO AS TO
C      BRING MORE LEADING ZEROS INTO THE ROWS OF S,
C      HENCE ACHIEVING A REDUCTION OF COMPUTING TIME.
C
      IRANK = 0
      SSQERR = ZERO
      DO 40 I = 1, NRBAR
40  RBAR(I) = ZERO
      DO 50 I = 1, NP
      P(I) = ZERO
      THETAB(I) = ZERO
      XNEXT(I) = ZERO
50  CONTINUE
      IND = 0
      IND1 = 0
      NPR = NP - IR
      NPR1 = NPR + 1
      INDJ = NPR1
      IND2 = NPR
      DO 110 J = 1, IR
      PHIJ = PHI(J)
      XNEXT(INDJ) = ZERO
      INDJ = INDJ + 1
      INDI = NPR1 + J
      DO 110 I = J, IR
      IND = IND + 1
      YNEXT = V(IND)
      PHII = PHI(I)
      IF (J .EQ. IR) GOTO 100
      XNEXT(INDJ) = -PHII
      IF (I .EQ. IR) GOTO 100
      XNEXT(INDI) = XNEXT(INDI) - PHIJ
      IND1 = IND1 + 1
      XNEXT(IND1) = -ONE
100  XNEXT(NPR1) = -PHII * PHIJ
      IND2 = IND2 + 1
      IF (IND2 .GT. NP) IND2 = 1
      XNEXT(IND2) = XNEXT(IND2) + ONE
      CALL INCLU2(NP, NRBAR, ONE, XNEXT, XROW, YNEXT,
      $ P, RBAR, THETAB, SSQERR, RECRES, IRANK, IFAIL)
C
C      NO NEED TO CHECK IFAIL AS WEIGHT = 1.0
C
      XNEXT(IND2) = ZERO
      IF (I .EQ. IR) GOTO 110
      XNEXT(INDI) = ZERO
      INDI = INDI + 1
      XNEXT(IND1) = ZERO
110  CONTINUE
      CALL REGRES(NP, NRBAR, RBAR, THETAB, P)
C
C      NOW RE-ORDER P.
C
      IND = NPR
      DO 200 I = 1, IR
      IND = IND + 1
      XNEXT(I) = P(IND)
200  CONTINUE
      IND = NP
      IND1 = NPR
      DO 210 I = 1, NPR
```

```
      P(IND) = P(IND1)
      IND = IND - 1
      IND1 = IND1 - 1
210 CONTINUE
      DO 220 I = 1, IR
220 P(I) = XNEXT(I)
      RETURN
C
C      P(0) IS OBTAINED BY BACKSUBSTITUTION FOR
C      A MOVING AVERAGE PROCESS.
C
300 INDN = NP + 1
      IND = NP + 1
      DO 310 I = 1, IR
      DO 310 J = 1, I
      IND = IND - 1
      P(IND) = V(IND)
      IF (J .EQ. 1) GOTO 310
      INDN = INDN - 1
      P(IND) = P(IND) + P(INDN)
310 CONTINUE
      RETURN
      END
C
      SUBROUTINE KARMA(IP, IQ, IR, NP, PHI, THETA, A, P,
$ V, N, W, RESID, SUMLOG, SSQ, IUPD, DELTA, E, NIT)
C
C      ALGORITHM AS 154.1 APPL. STATIST. (1980) VOL.29, P.311
C
C      INVOKING THIS SUBROUTINE UPDATES A, P, SUMLOG AND SSQ BY
C      INCLUSION OF DATA VALUES W(1) TO W(N). THE CORRESPONDING
C      VALUES OF RESID ARE ALSO OBTAINED.
C      WHEN FT IS LESS THAN (1 + DELTA), QUICK RECURSIONS ARE USED.
C
      REAL PHI(IR), THETA(IR), A(IR), P(NP), V(NP), W(N), RESID(N),
$ E(IR), SUMLOG, SSQ, DELTA, WNEXT, A1, DT, ET, FT, UT, G,
$ ZERO, ZLOG, ZSQRT
C
      DATA ZERO /0.0/
C
      ZLOG(G) = ALOG(G)
      ZSQRT(G) = SQRT(G)
C
      IR1 = IR - 1
      DO 10 I = 1, IR
10 E(I) = ZERO
      INDE = 1
C
C      FOR NON-ZERO VALUES OF NIT, PERFORM QUICK RECURSIONS.
C
      IF (NIT .NE. 0) GOTO 600
      DO 500 I = 1, N
      WNEXT = W(I)
C
C      PREDICTION.
C
      IF (IUPD .EQ. 1 .AND. I .EQ. 1) GOTO 300
C
      HERE DT = FT - 1.0
C
      DT = ZERO
```

```

      IF (IR .NE. 1) DT = P(IR + 1)
      IF (DT .LT. DELTA) GOTO 610
      A1 = A(1)
      IF (IR .EQ. 1) GOTO 110
      DO 100 J = 1, IR1
100  A(J) = A(J + 1)
110  A(IR) = ZERO
      IF (IP .EQ. 0) GOTO 200
      DO 120 J = 1, IP
120  A(J) = A(J) + PHI(J) * A1
200  IND = 0
      INDN = IR
      DO 210 L = 1, IR
      DO 210 J = L, IR
      IND = IND + 1
      P(IND) = V(IND)
      IF (J .EQ. IR) GOTO 210
      INDN = INDN + 1
      P(IND) = P(IND) + P(INDN)
210  CONTINUE
C
C      UPDATING.
C
300  FT = P(1)
      UT = WNEXT - A(1)
      IF (IR .EQ. 1) GOTO 410
      IND = IR
      DO 400 J = 2, IR
      G = P(J) / FT
      A(J) = A(J) + G * UT
      DO 400 L = J, IR
      IND = IND + 1
      P(IND) = P(IND) - G * P(L)
400  CONTINUE
410  A(1) = WNEXT
      DO 420 L = 1, IR
420  P(L) = ZERO
      RESID(I) = UT / ZSQRT(FT)
      E(INDE) = RESID(I)
      INDE = INDE + 1
      IF (INDE .GT. IQ) INDE = 1
      SSQ = SSQ + UT * UT / FT
      SUMLOG = SUMLOG + ZLOG(FT)
500  CONTINUE
      NIT = N
      RETURN
C
C      QUICK RECURSIONS
C
600  I = 1
610  NIT = I - 1
      DO 650 II = I, N
      ET = W(II)
      INDW = II
      IF (IP .EQ. 0) GOTO 630
      DO 620 J = 1, IP
      INDW = INDW - 1
      IF (INDW .LT. 1) GOTO 630
      ET = ET - PHI(J) * W(INDW)
620  CONTINUE
630  IF (IQ .EQ. 0) GOTO 645

```

```
      DO 640 J = 1, IQ
      INDE = INDE - 1
      IF (INDE .EQ. 0) INDE = IQ
      ET = ET - THETA(J) * E(INDE)
640 CONTINUE
645 E(INDE) = ET
      RESID(II) = ET
      SSQ = SSQ + ET * ET
      INDE = INDE + 1
      IF (INDE .GT. IQ) INDE = 1
650 CONTINUE
      RETURN
      END

C
      SUBROUTINE KALFOR(M, IP, IR, NP, PHI, A, P, V, WORK)
C
C      ALGORITHM AS 154.2  APPL. STATIST. (1980) VOL.29, P.311
C
C      INVOKING THIS SUBROUTINE OBTAINS PREDICTIONS
C      OF A AND P, M STEPS AHEAD.
C
      REAL PHI(IR), A(IR), P(NP), V(NP), WORK(IR), DT,
      $  A1, PHII, PHIJ, PHIJDT, ZERO
C
      DATA ZERO /0.0/
C
      IR1 = IR - 1
      DO 300 L = 1, M
C
C      PREDICT A.
C
      A1 = A(1)
      IF (IR .EQ. 1) GOTO 110
      DO 100 I = 1, IR1
100 A(I) = A(I + 1)
110 A(IR) = ZERO
      IF (IP .EQ. 0) GOTO 200
      DO 120 J = 1, IP
120 A(J) = A(J) + PHI(J) * A1
C
C      PREDICT P.
C
200 DO 210 I = 1, IR
210 WORK(I) = P(I)
      IND = 0
      IND1 = IR
      DT = P(1)
      DO 220 J = 1, IR
      PHIJ = PHI(J)
      PHIJDT = PHIJ * DT
      DO 220 I = J, IR
      IND = IND + 1
      PHII = PHI(I)
      P(IND) = V(IND) + PHII * PHIJDT
      IF (J .LT. IR) P(IND) = P(IND) + WORK(J + 1) * PHII
      IF (I .EQ. IR) GOTO 220
      IND1 = IND1 + 1
      P(IND) = P(IND) + WORK(I + 1) * PHIJ + P(IND1)
220 CONTINUE
300 CONTINUE
      RETURN
```

END

```

C
SUBROUTINE INCLU2(NP, NRBAR, WEIGHT, XNEXT, XROW, YNEXT, D, RBAR,
$ THETAB, SSQERR, RECRES, IRANK, IFAULT)
C
C     ALGORITHM AS 154.3  APPL. STATIST. (1980) VOL.29, P.311
C
C     FORTRAN VERSION OF REVISED VERSION OF ALGORITHM AS 75.1
C     APPL. STATIST. (1974) VOL.23, P.448
C     SEE REMARK AS R17 APPL. STATIST. (1976) VOL.25, P.323
C
REAL XNEXT(NP), XROW(NP), D(NP), RBAR(NRBAR), THETAB(NP),
$ WEIGHT, YNEXT, SSQERR, RECRES, WT, Y, DI, DPI, XI, XK,
$ CBAR, SBAR, RBTHIS, ZERO, ZSQRT
C
DATA ZERO /0.0/
C
ZSQRT(Y) = SQRT(Y)
C
C     INVOKING THIS SUBROUTINE UPDATES D, RBAR, THETAB, SSQERR
C     AND IRANK BY THE INCLUSION OF XNEXT AND YNEXT WITH A
C     SPECIFIED WEIGHT. THE VALUES OF XNEXT, YNEXT AND WEIGHT WILL
C     BE CONSERVED. THE CORRESPONDING VALUE OF RECRES IS CALCULATED.
C
Y = YNEXT
WT = WEIGHT
DO 10 I = 1, NP
10 XROW(I) = XNEXT(I)
RECRES = ZERO
IFAULT = 1
IF (WT .LE. ZERO) RETURN
IFAULT = 0
C
ITHISR = 0
DO 50 I = 1, NP
IF (XROW(I) .NE. ZERO) GOTO 20
ITHISR = ITHISR + NP - I
GOTO 50
20 XI = XROW(I)
DI = D(I)
DPI = DI + WT * XI * XI
D(I) = DPI
CBAR = DI / DPI
SBAR = WT * XI / DPI
WT = CBAR * WT
IF (I .EQ. NP) GOTO 40
I1 = I + 1
DO 30 K = I1, NP
ITHISR = ITHISR + 1
XK = XROW(K)
RBTHIS = RBAR(ITHISR)
XROW(K) = XK - XI * RBTHIS
RBAR(ITHISR) = CBAR * RBTHIS + SBAR * XK
30 CONTINUE
40 XK = Y
Y = XK - XI * THETAB(I)
THETAB(I) = CBAR * THETAB(I) + SBAR * XK
IF (DI .EQ. ZERO) GOTO 100
50 CONTINUE
SSQERR = SSQERR + WT * Y * Y
RECRES = Y * ZSQRT(WT)

```



```
      RETURN
100  IRANK = IRANK + 1
      RETURN
      END
C
      SUBROUTINE REGRES(NP, NRBAR, RBAR, THETAB, BETA)
C
C      ALGORITHM AS 154.4  APPL. STATIST. (1980) VOL.29, P.311
C
C      REVISED VERSION OF ALGORITHM AS 75.4
C      APPL. STATIST. (1974) VOL.23, P.448
C      INVOKING THIS SUBROUTINE OBTAINS BETA BY BACKSUBSTITUTION
C      IN THE TRIANGULAR SYSTEM RBAR AND THETAB.
C
      REAL RBAR(NRBAR), THETAB(NP), BETA(NP), BI
      ITHISR = NRBAR
      IM = NP
      DO 50 I = 1, NP
      BI = THETAB(IM)
      IF (IM .EQ. NP) GOTO 30
      I1 = I - 1
      JM = NP
      DO 10 J = 1, I1
      BI = BI - RBAR(ITHISR) * BETA(JM)
      ITHISR = ITHISR - 1
      JM = JM - 1
10  CONTINUE
30  BETA(IM) = BI
      IM = IM - 1
50  CONTINUE
      RETURN
      END
CEND OF AS 154
```

```

REAL FUNCTION QF(ALB,ANC,N,IRR,SIGMA,CC,LIM1,ACC,ITH,TRACE,IFAUULT)
C
C ALGORITHM AS 155 APPL. STATIST. (1980) VOL.29, NO.3
C
C Distribution of a linear combination of non-central chi-squared
C random variables.
C
INTEGER IRR,LIM1,IFAUULT
REAL SIGMA,CC,ACC
REAL TRACE(7),ALB(IRR),ANC(IRR)
INTEGER N(IRR),ITH(IRR)
INTEGER J,NJ,NT,NTM
REAL ACC1,ALMX,XLIM,XNT,XNTM
REAL UTX,TAUSQ,SD,AINTV,AINTV1,X,UP,UN,D1,D2,ALJ,ANCL
DOUBLE PRECISION AINTL,ERSM
REAL PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,ZERO,HALF,ONE,TWO,FOUR,
1 SIXTN,FOURP5,PT07,PT2,QUART,TEN,PT33,PT67,PT75,ONEPT5,THREE,
2 ONEPT1
INTEGER ICOUNT,IR,LIM
LOGICAL NDTSTR,FAIL
COMMON /QFCOM/ AINTL,ERSM,PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,
1 ICOUNT,IR,NDTSTR,FAIL,LIM
DATA ZERO /0.0/,HALF/0.5/,ONE/1.0/,TWO/2.0/,FOUR/4.0/,SIXTN/16.0/,
1 FOURP5/4.5/,PT07/0.07/,PT2/0.2/,QUART/0.25/,TEN/10.0/,
2 PT33/0.33/,PT67/0.67/,PT75/0.75/,ONEPT5/1.5/,THREE/3.0/,
3 ONEPT1/1.1/
C
C IROUND(X) = INT(X + SIGN(HALF,X))
C
C Setting constants in COMMON. ALN28 = ln(2) / 8.
C
PI = 3.14159265358979
ALN28 = 0.0866
C
C = CC
IR = IRR
LIM = LIM1
DO 10 J = 1,7
TRACE(J) = ZERO
10 CONTINUE
IFAUULT = 0
ICOUNT = 0
AINTL = ZERO
ERSM = ZERO
QF = -ONE
ACC1 = ACC
NDTSTR = .TRUE.
FAIL = .FALSE.
C
C Find mean, sd, max & min of ALB.
C Check that parameter values are valid.
C
XLIM = LIM
SIGSQ = SIGMA**2
SD = SIGSQ
ALMAX = ZERO
ALMIN = ZERO
AMEAN = ZERO
J = 1
20 IF (.NOT.(J.LE.IR)) GO TO 60
NJ = N(J)

```

```
ALJ = ALB(J)
ANCJ = ANC(J)
IF (.NOT.(NJ.LT.0.OR.ANCJ.LT.ZERO)) GO TO 30
IF AULT = 3
GO TO 260
30 SD = SD + ALJ**2*(2*NJ + FOUR*ANCJ)
AMEAN = AMEAN + ALJ*(NJ + ANCJ)
IF (.NOT.(ALMAX.LT.ALJ)) GO TO 40
ALMAX = ALJ
GO TO 50
40 IF (.NOT.(ALMIN.GT.ALJ)) GO TO 50
ALMIN = ALJ
50 J = J + 1
GO TO 20
60 IF (.NOT.(SD.EQ.ZERO)) GO TO 80
IF (.NOT.(C.GT.ZERO)) GO TO 70
QF = ONE
GO TO 260
70 QF = ZERO
GO TO 260
80 IF (.NOT.(ALMIN.EQ.ZERO.AND.ALMAX.EQ.ZERO.AND.SIGMA.EQ.ZERO))
1 GO TO 90
IF AULT = 3
GO TO 260
90 SD = SQRT(SD)
IF (.NOT.(ALMAX.LT.-ALMIN)) GO TO 100
ALMX = -ALMIN
GO TO 110
100 ALMX = ALMAX
C
C Starting values for FINDU * CTFF.
C
110 UTX = SIXTN/SD
UP = FOURP5/SD
UN = -UP
C
C Truncation point with no convergence factor.
C
CALL FINDU (N,ALB,ANC,UTX,HALF*ACC1)
C
C Does convergence factor help ?
C
IF (.NOT.(C.NE.ZERO.AND.ALMX.GT.PT07*SD)) GO TO 130
TAUSQ = QUART*ACC1/CFE(N,ALB,ANC,ITH,C)
IF (.NOT.(FAIL)) GO TO 120
FAIL = .FALSE.
GO TO 130
120 IF (.NOT.(TRUNCN(N,ALB,ANC,UTX,TAUSQ).LT.PT2*ACC1)) GO TO 130
SIGSQ = SIGSQ + TAUSQ
CALL FINDU (N,ALB,ANC,UTX,QUART*ACC1)
TRACE(6) = SQRT(TAUSQ)
130 TRACE(5) = UTX
ACC1 = HALF*ACC1
C
C Find 'range' of distribution, quit if outside of this.
C
140 D1 = CTFF(N,ALB,ANC,ACC1,UP) - C
IF (.NOT.(D1.LT.ZERO)) GO TO 150
QF = ONE
GO TO 260
150 D2 = C - CTFF(N,ALB,ANC,ACC1,UN)
```

```
        IF (.NOT.(D2.LT.ZERO)) GO TO 160
        QF = ZERO
        GO TO 260
C
C   Find integration interval.
C
160   IF (.NOT.(D1.GT.D2)) GO TO 170
        AINTV = D1
        GO TO 180
170   AINTV = D2
180   AINTV = TWO*PI/AINTV
C
C   Calculate number of terms required for main & auxiliary
C   integrations.
C
        XNT = UTX/AINTV
        XNTM = THREE/SQRT(ACC1)
        IF (.NOT.(XNT.GT.XNTM*ONEPT5)) GO TO 220
        IF (.NOT.(XNTM.GT.XLIM)) GO TO 190
        IFAULT = 1
        GO TO 260
C
C   Parameters for auxiliary integration.
C
190   NTM = IROUND(XNTM)
        AINTV1 = UTX/XNTM
        X = TWO*PI/AINTV1
        IF (.NOT.(X.LE.ABS(C))) GO TO 200
        GO TO 220
C
C   Calculate convergence factor.
C
200   TAUSQ = CFE(N,ALB,ANC,ITH,C - X) + CFE(N,ALB,ANC,ITH,C + X)
        TAUSQ = PT33*ACC1/(ONEPT1*TAUSQ)
        IF (.NOT.(FAIL)) GO TO 210
        GO TO 220
210   ACC1 = PT67*ACC1
C
C   Auxiliary integration.
C
        CALL INTEGR (N,ALB,ANC,NTM,AINTV1,TAUSQ,.FALSE.)
        XLIM = XLIM - XNTM
        SIGSQ = SIGSQ + TAUSQ
        TRACE(3) = TRACE(3) + 1
        TRACE(2) = TRACE(2) + NTM + 1
C
C   Find truncation point with new convergence factor.
C
        CALL FINDU (N,ALB,ANC,UTX,QUART*ACC1)
        ACC1 = PT75*ACC1
        GO TO 140
C
C   Main integration.
C
220   TRACE(4) = AINTV
        IF (.NOT.(XNT.GT.XLIM)) GO TO 230
        IFAULT = 1
        GO TO 260
230   NT = IROUND(XNT)
        CALL INTEGR (N,ALB,ANC,NT,AINTV,ZERO,.TRUE.)
        TRACE(3) = TRACE(3) + 1
```

```

        TRACE(2) = TRACE(2) + NT + 1
        QF = HALF - AINTL
        TRACE(1) = ERSM
        UP = ERSM
C
C   Test whether round-off error could be significant.
C   Allow for radix 8 or 16 machines.
C
        X = UP + ACC/TEN
        J = 1
240   IF (.NOT.(J.LE.8)) GO TO 260
        IF (.NOT.(J*X.EQ.J*UP)) GO TO 250
        IFAULT = 2
250   J = J*2
        GO TO 240
260   TRACE(7) = ICOUNT
        RETURN
        END
C
        SUBROUTINE COUNTR
C
C   Count number of calls to ERRBD, TRUNCN & CFE.
C
        DOUBLE PRECISION AINTL,ERSM
        REAL PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C
        INTEGER ICOUNT,IR,LIM
        LOGICAL NDSRT,FAIL
        COMMON /QFCOM/ AINTL,ERSM,PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,
1     ICOUNT,IR,NDTSRT,FAIL,LIM
C
        ICOUNT = ICOUNT + 1
        IF (.NOT.(ICOUNT.GT.LIM)) GO TO 20
        WRITE (6,10)
10    FORMAT (' qf: cannot locate integration parameters'//)
        STOP
20    RETURN
        END
C
        REAL FUNCTION ALOG1(X,FIRST)
C
C   If FIRST then return ln(1 + x) else ln(1 + x) - x.
C
        REAL X
        LOGICAL FIRST
        REAL S,S1,TERM,Y,AK,PT1,ONE,TWO,THREE
        DATA PT1/0.1/,ONE/1.0/,TWO/2.0/,THREE/3.0/
C
        F1(I) = S + TERM/AK
C
        IF (.NOT.(ABS(X).GT.PT1)) GO TO 20
        IF (.NOT.(FIRST)) GO TO 10
        ALOG1 = LOG(ONE + X)
        GO TO 70
10    ALOG1 = LOG(ONE + X) - X
        GO TO 70
20    Y = X/(TWO + X)
        TERM = TWO*Y**3
        AK = THREE
        IF (.NOT.(FIRST)) GO TO 30
        S = TWO
        GO TO 40

```

```
30 S = -X
40 S = S*Y
   Y = Y**2
   S1 = F1(0)
50 IF (.NOT.(S1.NE.S)) GO TO 60
   AK = AK + TWO
   TERM = TERM*Y
   S = S1
   S1 = F1(0)
   GO TO 50
60 ALOG1 = S
70 RETURN
   END
```

```
C
   REAL FUNCTION EXP1(X)
   REAL X
   REAL ZERO,NEG50
   DATA ZERO/0.0/,NEG50/-50.0/

C
   IF (.NOT.(X.LT.NEG50)) GO TO 10
   EXP1 = ZERO
   GO TO 20
10 EXP1 = EXP(X)
20 RETURN
   END
```

```
C
   SUBROUTINE ORDER (ALB,ITH)

C
C   Find order of absolute values of ALB.
C
```

```
   REAL ALB(*)
   INTEGER ITH(*)
   INTEGER J,K,K1,ITHK
   REAL ALJ
   DOUBLE PRECISION AINTL,ERSM
   REAL PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C
   INTEGER ICOUNT,IR,LIM
   LOGICAL NDSRT,FAIL
   COMMON /QFCOM/ AINTL,ERSM,PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,
1  ICOUNT,IR,NDTSRT,FAIL,LIM
```

```
C
   J = 1
10 IF (.NOT.(J.LE.IR)) GO TO 60
   ALJ = ABS(ALB(J))
   K = J - 1
20 IF (.NOT.(K.GT.0)) GO TO 40
   ITHK = ITH(K)
   K1 = K + 1
   IF (.NOT.(ALJ.GT.ABS(ALB(ITHK)))) GO TO 50
   ITH(K1) = ITHK
   GO TO 30
30 K = K - 1
   GO TO 20
40 K = 0
   K1 = 1
50 ITH(K1) = J
   J = J + 1
   GO TO 10
60 NDTSRT = .FALSE.
   RETURN
   END
```

```

C
REAL FUNCTION ERRBD(N,ALB,ANC,UU,CX)
C
C Find bound on tail probability using mgf.
C Cut-off point returned to CX.
C
REAL U,UU,CX
INTEGER N(*)
REAL ALB(*),ANC(*)
REAL SUM1,ALJ,ANCJ,X,Y,CONST
INTEGER J,NJ
DOUBLE PRECISION AINTL,ERSM
REAL PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,HALF,ONE,TWO
INTEGER ICOUNT,IR,LIM
LOGICAL NDTSTRT,FAIL
COMMON /QFCOM/ AINTL,ERSM,PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,
1 ICOUNT,IR,NDTSTRT,FAIL,LIM
DATA HALF/0.5/,ONE/1.0/,TWO/2.0/
C
CALL COUNTR
U = UU
CONST = U*SIGSQ
SUM1 = U*CONST
U = TWO*U
J = IR
10 IF (.NOT.(J.GT.0)) GO TO 20
NJ = N(J)
ALJ = ALB(J)
ANCJ = ANC(J)
X = U*ALJ
Y = ONE - X
CONST = CONST + ALJ*(ANCJ/Y + NJ)/Y
SUM1 = SUM1 + ANCJ*(X/Y)**2
SUM1 = SUM1 + NJ*(X**2/Y + ALOG1(-X,.FALSE.))
J = J - 1
GO TO 10
20 ERRBD = EXP1(-HALF*SUM1)
CX = CONST
RETURN
END
C
REAL FUNCTION CTFF(N,ALB,ANC,ACCX,UPN)
C
C Find CTFF so that  $P(QF > CTFF) < ACCX$  if  $UPN > 0$ ;
C  $P(QF < CTFF) < ACCX$  otherwise.
C
REAL ACCX,UPN
INTEGER N(*)
REAL ALB(*),ANC(*)
REAL U1,U2,U,RB,CONST,C1,C2
DOUBLE PRECISION AINTL,ERSM
REAL PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,ZERO,ONE,TWO
INTEGER ICOUNT,IR,LIM
LOGICAL NDTSTRT,FAIL
COMMON /QFCOM/ AINTL,ERSM,PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,
1 ICOUNT,IR,NDTSTRT,FAIL,LIM
DATA ZERO/0.0/,ONE/1.0/,TWO/2.0/
C
F1(I) = U2/(ONE + U2*RB)
F2(I) = (C1 - AMEAN)/(C2 - AMEAN)
C

```

```

    U2 = UPN
    U1 = ZERO
    C1 = AMEAN
    IF (.NOT.(U2.GT.ZERO)) GO TO 10
    RB = ALMAX
    GO TO 20
10  RB = ALMIN
20  RB = TWO*RB
    U = F1(0)
30  IF (.NOT.(ERRBD(N,ALB,ANC,U,C2).GT.ACCX)) GO TO 40
    U1 = U2
    C1 = C2
    U2 = TWO*U2
    U = F1(0)
    GO TO 30
40  U = F2(0)
50  IF (.NOT.(U.LT.0.9)) GO TO 80
    U = (U1 + U2)/TWO
    IF (.NOT.(ERRBD(N,ALB,ANC,U/(ONE + U*RB),CONST).GT.ACCX)) GO TO 60
    U1 = U
    C1 = CONST
    GO TO 70
60  U2 = U
    C2 = CONST
70  U = F2(0)
    GO TO 50
80  CTFF = C2
    UPN = U2
    RETURN
    END

```

```

C
    REAL FUNCTION TRUNCN(N,ALB,ANC,UU,TAUSQ)
C
C   Bound integration error due to truncation at U.
C
    REAL U,UU,TAUSQ
    INTEGER N(*)
    REAL ALB(*),ANC(*)
    REAL SUM1,SUM2,PROD1,PROD2,PROD3,ALJ,ANCJ,X,Y,ERR1,ERR2
    INTEGER J,NJ,NS
    DOUBLE PRECISION AINTL,ERSM
    REAL PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,ZERO,QUART,HALF,ONE,TWO
    INTEGER ICOUNT,IR,LIM
    LOGICAL NDTSTR,FAIL
    COMMON /QFCOM/ AINTL,ERSM,PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,
1   ICOUNT,IR,NDTSTR,FAIL,LIM
    DATA ZERO/0.0/,QUART/0.25/,HALF/0.5/,ONE/1.0/,TWO/2.0/

```

```

C
    CALL COUNTR
    U = UU
    SUM1 = ZERO
    PROD2 = ZERO
    PROD3 = ZERO
    NS = 0
    SUM2 = (SIGSQ + TAUSQ)*U**2
    PROD1 = TWO*SUM2
    U = TWO*U
    J = 1
10  IF (.NOT.(J.LE.IR)) GO TO 40
    ALJ = ALB(J)
    ANCJ = ANC(J)

```



```

      NJ = N(J)
      X = (U*ALJ)**2
      SUM1 = SUM1 + ANCJ*X/(ONE + X)
      IF (.NOT.(X.GT.ONE)) GO TO 20
      PROD2 = PROD2 + NJ*LOG(X)
      PROD3 = PROD3 + NJ*ALOG1(X,.TRUE.)
      NS = NS + NJ
      GO TO 30
20    PROD1 = PROD1 + NJ*ALOG1(X,.TRUE.)
30    J = J + 1
      GO TO 10
40    SUM1 = HALF*SUM1
      PROD2 = PROD1 + PROD2
      PROD3 = PROD1 + PROD3
      X = EXP1(-SUM1 - QUART*PROD2)/PI
      Y = EXP1(-SUM1 - QUART*PROD3)/PI
      IF (.NOT.(NS.EQ.0)) GO TO 50
      ERR1 = ONE
      GO TO 60
50    ERR1 = X*TWO/NS
60    IF (.NOT.(PROD3.GT.ONE)) GO TO 70
      ERR2 = 2.5*Y
      GO TO 80
70    ERR2 = ONE
80    IF (.NOT.(ERR2.LT.ERR1)) GO TO 90
      ERR1 = ERR2
90    X = HALF*SUM2
      IF (.NOT.(X.LE.Y)) GO TO 100
      ERR2 = ONE
      GO TO 110
100   ERR2 = Y/X
110   IF (.NOT.(ERR1.LT.ERR2)) GO TO 120
      TRUNCN = ERR1
      GO TO 130
120   TRUNCN = ERR2
130   RETURN
      END
C
      SUBROUTINE FINDU (N,ALB,ANC,UTX,ACCX)
C
C   Find U such that TRUNCN(U) < ACCX & TRUNCN(U / 1.2) > ACCX.
C
      REAL UTX,ACCX
      INTEGER N(*)
      REAL ALB(*),ANC(*)
      REAL U,UT
      REAL DIVIS(4)
      INTEGER I
      DOUBLE PRECISION AINTL,ERSM
      REAL PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,FOUR
      INTEGER ICOUNT,IR,LIM
      LOGICAL NDSRT,FAIL
      COMMON /QFCOM/ AINTL,ERSM,PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,
1    ICOUNT,IR,NDSRT,FAIL,LIM
      DATA DIVIS/2.0,1.4,1.2,1.1/, FOUR/4.0/
C
      UT = UTX
      U = UT/FOUR
      IF (.NOT.(TRUNCN(N,ALB,ANC,U,ZERO).GT.ACCX)) GO TO 20
      U = UT
10    IF (.NOT.(TRUNCN(N,ALB,ANC,U,ZERO).GT.ACCX)) GO TO 40

```

```

      UT = UT*FOUR
      U = UT
      GO TO 10
20    UT = U
      U = U/FOUR
30    IF (.NOT.(TRUNCN(N,ALB,ANC,U,ZERO).LE.ACCX)) GO TO 40
      UT = U
      U = U/FOUR
      GO TO 30
40    DO 50 I = 1,4
      U = UT/DIVIS(I)
      IF (.NOT.(TRUNCN(N,ALB,ANC,U,ZERO).LE.ACCX)) GO TO 50
      UT = U
50    CONTINUE
      UTX = UT
      RETURN
      END

C
      SUBROUTINE INTEGR (N,ALB,ANC,NTERM,AINTRV,TAUSQ,MAIN)
C
C      Carry out integration with NTERM terms, at interval AINTRV.
C      If not MAIN then multiply integrand by 1 - exp(-0.5 * TAUSQ *
C      U**2).
C
      INTEGER NTERM
      REAL AINTRV,TAUSQ
      LOGICAL MAIN
      INTEGER N(*)
      REAL ALB(*),ANC(*)
      REAL AINPI,U,SUM1,SUM2,SUM3,X,Y,Z
      INTEGER K,J,NJ
      DOUBLE PRECISION AINTL,ERSM
      REAL PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,QUART,HALF,ONE,TWO
      INTEGER ICOUNT,IR,LIM
      LOGICAL NDTSRF,FAIL
      COMMON /QFCOM/ AINTL,ERSM,PI,ALN28,SIGSQ,ALMAX,ALMIN,AMEAN,C,
1    ICOUNT,IR,NDTSRT,FAIL,LIM
      DATA QUART/0.25/,HALF/0.5/,ONE/1.0/,TWO/2.0/

C
      AINPI = AINTRV/PI
      K = NTERM
10    IF (.NOT.(K.GE.0)) GO TO 50
      U = (K + HALF)*AINTRV
      SUM1 = -TWO*U*C
      SUM2 = ABS(SUM1)
      SUM3 = -HALF*SIGSQ*U**2
      J = IR
20    IF (.NOT.(J.GT.0)) GO TO 30
      NJ = N(J)
      X = TWO*ALB(J)*U
      Y = X**2
      SUM3 = SUM3 - QUART*NJ*ALOG1(Y,.TRUE.)
      Y = ANC(J)*X/(ONE + Y)
      Z = NJ*ATAN(X) + Y
      SUM1 = SUM1 + Z
      SUM2 = SUM2 + ABS(Z)
      SUM3 = SUM3 - HALF*X*Y
      J = J - 1
      GO TO 20
30    X = AINPI*EXP1(SUM3)/U
      IF (.NOT.(.NOT.MAIN)) GO TO 40

```

```

      X = X*(ONE - EXP1(-HALF*TAUSQ*U**2))
40    SUM1 = SIN(HALF*SUM1)*X
      SUM2 = HALF*SUM2*X
      AINTL = AINTL + SUM1
      ERSM = ERSM + SUM2
      K = K - 1
      GO TO 10
50    RETURN
      END
C
      REAL FUNCTION CFE(N,ALB,ANC,ITH,X)
C
C      Coefficient of TAUSQ in error when convergence factor of
C      exp(-0.5 * TAUSQ * U**2) is used when df is evaluated at X.
C
      REAL X
      INTEGER N(*), ITH(*)
      REAL ALB(*), ANC(*)
      REAL AXL, AXL1, AXL2, SXL, SUM1, ALJ
      INTEGER J, K, IT, ITK
      DOUBLE PRECISION AINTL, ERSM
      REAL PI, ALN28, SIGSQ, ALMAX, ALMIN, AMEAN, C, ZERO, ONE, FOUR, HUNDRD
      INTEGER ICOUNT, IR, LIM
      LOGICAL NDTSTR, FAIL
      COMMON /QFCOM/ AINTL, ERSM, PI, ALN28, SIGSQ, ALMAX, ALMIN, AMEAN, C,
1     ICOUNT, IR, NDTSTR, FAIL, LIM
      DATA ZERO/0.0/, ONE/1.0/, FOUR/4.0/, HUNDRD/100.0/
C
      CALL COUNTR
      IF (.NOT.(NDTSTR)) GO TO 10
      CALL ORDER (ALB, ITH)
10     AXL = ABS(X)
      SXL = SIGN(ONE, X)
      SUM1 = ZERO
      J = IR
20     IF (.NOT.(J.GT.0)) GO TO 70
      IT = ITH(J)
      IF (.NOT.(ALB(IT)*SXL.GT.ZERO)) GO TO 60
      ALJ = ABS(ALB(IT))
      AXL1 = AXL - ALJ*(N(IT) + ANC(IT))
      AXL2 = ALJ/ALN28
      IF (.NOT.(AXL1.GT.AXL2)) GO TO 30
      AXL = AXL1
      GO TO 60
30     IF (.NOT.(AXL.GT.AXL2)) GO TO 40
      AXL = AXL2
40     SUM1 = (AXL - AXL1)/ALJ
      K = J - 1
50     IF (.NOT.(K.GT.0)) GO TO 70
      ITK = ITH(K)
      SUM1 = SUM1 + (N(ITK) + ANC(ITK))
      K = K - 1
      GO TO 50
60     J = J - 1
      GO TO 20
70     IF (.NOT.(SUM1.GT.HUNDRD)) GO TO 80
      CFE = ONE
      FAIL = .TRUE.
      GO TO 90
80     CFE = 2**((SUM1/FOUR)/(PI*AXL**2))
90     RETURN

```

END

```

SUBROUTINE UDRUNS(X, N, UV, DV, IFAULT)
C
C     ALGORITHM AS 157 APPL. STATIST. (1981), VOL. 30, NO. 1
C
C     THE RUNS-UP AND FUNS-DOWN TEST
C
C     INTEGER UCOUNT, DCOUNT, RU, RD
C     DIMENSION X(N), A(6, 6), B(6), UCOUNT(6), DCOUNT(6)
C
C     SET-UP THE A AND B MATRICES
C
C     DATA
*   A(1, 1), A(1, 2), A(1, 3), A(1, 4), A(1, 5), A(1, 6), A(2, 2),
*   A(2, 3), A(2, 4), A(2, 5), A(2, 6), A(3, 3), A(3, 4), A(3, 5),
*   A(3, 6), A(4, 4), A(4, 5), A(4, 6), A(5, 5), A(5, 6), A(6, 6)
*   /4529.4, 9044.9, 13568.0, 18091.0, 22615.0, 27892.0, 18097.0,
*   27139.0, 36187.0, 45234.0, 55789.0, 40721.0, 54281.0, 67852.0,
*   83685.0, 72414.0, 90470.0, 111580.0, 113262.0, 139476.0,
*   172860.0/
IFAUULT = 0
IF (N .LT. 4000) GOTO 500
DO 1 J = 2, 6
  J1 = J - 1
  DO 1 I = 1, J1
    A(J, I) = A(I, J)
1 CONTINUE
B(1) = 1.0 / 6.0
B(2) = 5.0 / 24.0
B(3) = 11.0 / 120.0
B(4) = 19.0 / 720.0
B(5) = 29.0 / 5040.0
B(6) = 1.0 / 840.0
C
DO 100 I = 1, 6
  UCOUNT(I) = 0
  DCOUNT(I) = 0
100 CONTINUE
C
C     THE LOOP THAT ENDS AT LINE 300 DETERMINES THE NUMBER OF
C     RUNS-UP AND RUNS-DOWN OF LENGTH I FOR I=1(1)5 AND THE NUMBER
C     OF RUNS-UP AND RUNS-DOWN OF LENGTH GREATER OR EQUAL TO 6
C
C     RU = 1
C     RD = 1
C     DO 300 J = 2, N
C
C     THE FOLLOWING STATEMENT TESTS FOR BOTH RUNS-UP AND
C     RUNS-DOWN BREAK-POINTS.  IF A RUN-DOWN BREAK-POINT IS
C     DETECTED - GOTO 200, OTHERWISE - GOTO 150.
C     ( RU AND RD ACT AS LOCAL COUNTERS FOR THE NUMBER OF
C     RUNS-UP AND RUNS-DOWN RESPECTIVELY.)
C     A TEST IS ALSO MADE FOR DATA TIES BEWTEEN ADJACENT
C     ELEMENTS.  IF A TIE IS DETECTED - GOTO 600.
C
C     IF (X(J) - X(J - 1)) 150, 600, 200
150   UCOUNT(RU) = UCOUNT(RU) + 1
      RU = 1
      IF (RD .LT. 6) RD = RD + 1
      GOTO 300
200   DCOUNT(RD) = DCOUNT(RD) + 1
      RD = 1

```

```
      IF (RU .LT. 6) RU = RU + 1
300 CONTINUE
      UCOUNT(RU) = UCOUNT(RU) + 1
      DCOUNT(RD) = DCOUNT(RD) + 1
C
C      CALCULATE THE TEST STATISTICS UV AND DV.
C
      UV = 0.0
      DV = 0.0
      RN = FLOAT(N)
      DO 400 I = 1, 6
        DO 400 J = 1, 6
          UV = UV + (FLOAT(UCOUNT(I)) - RN * B(I)) *
*             (FLOAT(UCOUNT(J)) - RN * B(J)) * A(I, J)
          DV = DV + (FLOAT(DCOUNT(I)) - RN * B(I)) *
*             (FLOAT(DCOUNT(J)) - RN * B(J)) * A(I, J)
400 CONTINUE
      UV = UV / RN
      DV = DV / RN
      GOTO 700
500 IFAULT = N
      GOTO 700
600 IFAULT = 1
700 RETURN
      END
```

```

SUBROUTINE PROBS(K, W, P, IFAULT)

```

```

C
C     ALGORITHM AS 158 APPL. STATIST. (1981) VOL.30, NO.1
C
C     CALCULATION OF THE PROBABILITIES P(L,K) FOR
C     THE CASE OF SIMPLE ORDER,
C     FOR EQUAL WEIGHTS, K .GE. 3 AND .LE. 10 .
C     FOR UNEQUAL WEIGHTS, K .GE. 3 AND .LE. 6
C

```

```

DIMENSION W(10), P(10), Q(10, 10)
REAL ZERO, HALF, ONE, THREE, SIX
DATA ZERO/0.0/, HALF/0.5/, ONE/1.0/, THREE/3.0/,
*     SIX/6.0/, C1 /1.0E-6/

```

```

C
C     CHECK THAT WEIGHTS ARE POSITIVE
C

```

```

IFAULT = 0
DO 1 I = 1, K
  IF (W(I) .LE. ZERO) GOTO 101
1 CONTINUE

```

```

C
C     CHECK THAT K .GE. 3 AND .LE. 10
C

```

```

IF (K .LT. 2 .OR. K .GT. 10) GOTO 102
WW = W(1)
DO 2 I = 2, K
  IF (ABS(WW - W(I)) .GT. C1) GOTO 7
2 CONTINUE

```

```

C
C     EQUAL WEIGHTS
C

```

```

Q(1, 3) = ONE / THREE
Q(2, 3) = HALF
Q(3, 3) = ONE / SIX
IF (K .EQ. 3) GOTO 5
DO 4 J = 4, K
  AJ = J
  A1 = ONE /AJ
  A2 = (AJ - ONE) * A1
  Q(1, J) = A1
  J1 = J - 1
  DO 3 L = 2, J1
    L1 = L - 1
3   Q(L, J) = A1 * Q(L1, J1) + A2 * Q(L, J1)
  Q(J, J) = ONE / FACT(J, IFAULT)
  IF (IFAULT .NE. 0) RETURN
4 CONTINUE
5 CONTINUE
DO 6 J = 1, K
6 P(J) = Q(J, K)
RETURN

```

```

C
C     UNEQUAL WEIGHTS - CHECK THAT K .LE. 6
C

```

```

7 IF (K .GT. 6) GOTO 102
K2 = K - 2
GOTO (8, 9, 10, 11), K2
8 P(1) = PR1(1, 3, W)
P(2) = HALF
P(3) = HALF - P(1)
RETURN

```

```

    9 P(1) = PR1(1, 4, W)
      P(4) = PR1(4, 4, W)
      P(2) = HALF - P(4)
      P(3) = HALF - P(1)
      RETURN
    10 P(5) = PR1(5, 5, W)
      P(4) = PR1(4, 5, W)
      P(2) = HALF - P(4)
      P(1) = PR1(1, 5, W)
      P(3) = HALF - P(1) - P(5)
      RETURN
    11 SUM = ZERO
      DO 12 I = 2, 6
        PP = PR2(I, 2)
        P(I) = PP
        SUM = SUM + PP
    12 CONTINUE
      P(1) = ONE - SUM
      IF (P(1) .LT. ZERO) P(1) = ZERO
      RETURN
101 IFAULT = 1
      RETURN
102 IFAULT = 2
      RETURN
      END

C
      FUNCTION PR1(I, J, W)

C
C      ALGORITHM AS 158.1 APPL. STATIST. (1981) VOL.30, NO.1
C
C      EXPLICIT CALCULATION OF PROBABILITIES FOR K .LE. 5
C      ALSO CALLED BY FUNCTION F2
C
      DIMENSION W(10)
      REAL ZERO, HALF, QTR, EIGHTH, PT0625, PT375, PII
      DATA ZERO/0.0/, HALF/0.5/, QTR/0.25/, EIGHTH/0.125/,
*      PT0625/0.0625/, PT375/0.375/, PII/0.318309886/

C
      IF (J .NE. 3) GOTO 40
      C = HALF * PII * F1(W(1), W(2), W(3))
      IF (I .EQ. 3) GOTO 30
      PR1 = QTR - C
      RETURN
    30 PR1 = QTR + C
      RETURN
    40 W1 = W(1)
      W2 = W(2)
      W3 = W(3)
      W4 = W(4)
      W12 = W1 + W2
      W23 = W2 + W3
      W34 = W3 + W4
      S12 = F1(W1, W2, W3)
      S23 = F1(W2, W3, W4)
      IF (J .EQ. 5) GOTO 50
      IF (I .EQ. 4) GOTO 41
      C1 = QTR * PII *
*      (F1(W1, W2, W34) + F1(W1, W23, W4) + F1(W12, W3, W4))
      PR1 = EIGHTH - C1
      RETURN
    41 C2 = QTR *PII * (S12 + S23)
```



```
PR1 = EIGHTH + C2
RETURN
50 W5 = W(5)
W45 = W4 + W5
W123 = W12 + W3
W234 = W23 + W4
W345 = W34 + W5
S34 = F1(W3, W4, W5)
IF (I .EQ. 4) GOTO 52
C5 = PT0625 + EIGHTH * PII * (S12 + S23 + S34) +
* QTR * PII * PII * S12 * S34
IF (I .EQ. 1) GOTO 51
PR1 = C5
IF (PR1 .LT. ZERO) PR1 = ZERO
RETURN
51 S113 = F1(W1, W2, W345)
S131 = F1(W1, W234, W5)
S311 = F1(W123, W4, W5)
C3 = PT375 + EIGHTH * PII * (S113 + S131 + S311 + F1(W1, W23, W45)
* + F1(W12, W3, W45) + F1(W12, W34, W5) - S12 - S23 - S34)
* - QTR * PII * PII * (S12 * S311 + S23 * S131 + S34 * S113)
PR1 = HALF - C3 - C5
RETURN
52 C2 = EIGHTH * PII * (S12 + S34 + F1(W1, W2, W34) + F1(W12, W3, W4)
* + F1(W1, W23, W4) + F1(W2, W3, W45) + F1(W23, W4, W5) +
* F1(W2, W34, W5))
PR1 = QTR + C2
RETURN
END
```

```
C
C
FUNCTION F1(V1, V2, V3)
C
C   ALGORITHM AS 158.2 APPL. STATIST. (1981) VOL.30, NO.1
C
RHO = -SQRT(V1 * V3 / ((V1 + V2) * (V2 + V3)))
F1 = ASIN(RHO)
RETURN
END
```

```
C
FUNCTION PR2(I, W)
C
C   ALGORITHM AS 158.3 APPL. STATIST. (1981) VOL.30, NO.1
C
C   CALCULATION OF PROBABILITIES FOR K .EQ. 6 USING
C   RECURRENCE RELATION
```

```
C
DIMENSION W(10)
REAL ZERO, HALF, EIGHTH, PT0625, P03125, QTR, PII
DATA ZERO/0.0/, HALF/0.5/, EIGHTH/0.125/, PT0625/0.0625/,
* P03125/0.03125/, QTR/0.25/
DATA PII /0.318309886/
```

```
C
W1 = W(1)
W2 = W(2)
W3 = W(3)
W4 = W(4)
W5 = W(5)
W6 = W(6)
W12 = W1 + W2
W23 = W2 + W3
```

```

W34 = W3 + W4
W45 = W4 + W5
W56 = W5 + W6
W123 = W12 + W3
W234 = W23 + W4
W345 = W34 + W5
W456 = W45 + W6
W1234 = W123 + W4
W2345 = W234 + W5
W3456 = W345 + W6
D4 = ZERO
D5 = ZERO
I1 = I - 1
GOTO (2, 3, 4, 5, 6), I1
2 PR2 = HALF * (F2(1, 5, W2, W3, W4, W5, W6) +
* F2(1, 5, W1, W2, W3, W4, W5) + F2(1, 3, W1, W2, W3, D4, D5) *
* F2(1, 3, W4, W5, W6, D4, D5)) + QTR *
* (F2(1, 4, W3, W4, W5, W6, D5) + F2(1, 4, W1, W2, W3, W4, D5))
RETURN
3 PR2 = F2(3, 3, W1, W2, W3456, D4, D5) *
* F2(1, 4, W3, W4, W5, W6, D5) + F2(3, 3, W1, W2345, W6, D4, D5) *
* F2(1, 4, W2, W3, W4, W5, D5) + F2(3, 3, W1234, W5, W6, D4, D5) *
* F2(1, 4, W1, W2, W3, W4, D5) + HALF *
* (F2(3, 3, W1, W23, W456, D4, D5) * F2(1, 3, W4, W5, W6, D4, D5)
* + F2(3, 3, W1, W234, W56, D4, D5) * F2(1, 3, W2, W3, W4, D4, D5)
* + F2(3, 3, W12, W3, W456, D4, D5) * F2(1, 3, W4, W5, W6, D4, D5)
* + F2(3, 3, W12, W345, W6, D4, D5) * F2(1, 3, W3, W4, W5, D4, D5)
* + F2(3, 3, W123, W4, W56, D4, D5) * F2(1, 3, W1, W2, W3, D4, D5)
* + F2(3, 3, W123, W45, W6, D4, D5) * F2(1, 3, W1, W2, W3, D4, D5))
* + EIGHTH * F2(3, 3, W12, W34, W56, D4, D5)
RETURN
4 PR2 = F2(4, 4, W1, W2, W3, W456, D5) *
* F2(1, 3, W4, W5, W6, D4, D5) + F2(4, 4, W1, W2, W345, W6, D5) *
* F2(1, 3, W3, W4, W5, D4, D5) + F2(4, 4, W1, W234, W5, W6, D5) *
* F2(1, 3, W2, W3, W4, D4, D5) + F2(4, 4, W123, W4, W5, W6, D5) *
* F2(1, 3, W1, W2, W3, D4, D5) + QTR *
* (F2(4, 4, W1, W2, W34, W56, D5) + F2(4, 4, W1, W23, W4, W56, D5)
* + F2(4, 4, W1, W23, W45, W6, D5) +
* F2(4, 4, W12, W3, W4, W56, D5) + F2(4, 4, W12, W3, W45, W6, D5)
* + F2(4, 4, W12, W34, W5, W6, D5))
RETURN
5 PR2 = HALF * (F2(5, 5, W1, W2, W3, W4, W56) +
* F2(5, 5, W1, W2, W3, W45, W6) + F2(5, 5, W1, W2, W34, W5, W6) +
* F2(5, 5, W1, W23, W4, W5, W6) + F2(5, 5, W12, W3, W4, W5, W6))
RETURN
6 S12 = F1(W1, W2, W3)
S23 = F1(W2, W3, W4)
S34 = F1(W3, W4, W5)
S45 = F1(W4, W5, W6)
PR2 = P03125 + PT0625 * PII * (S12 + S23 + S34 + S45) +
* EIGHTH * PII * PII * (S12 * S34 + S12 * S45 + S23 * S45)
IF (PR2 .LT. ZERO) PR2 = ZERO
RETURN
END
C
FUNCTION F2(I, J, V1, V2, V3, V4, V5)
C
C     ALGORITHM AS 158.4 APPL. STATIST. (1981) VOL.30, NO.1
C
DIMENSION VV(10)
VV(1) = V1

```

```
VV(2) = V2  
VV(3) = V3  
VV(4) = V4  
VV(5) = V5  
F2 = PR1(I, J, VV)  
RETURN  
END
```

C

```
FUNCTION FACT(M, IFAULT)
```

C

C

```
ALGORITHM AS 158.5 APPL. STATIST. (1981) VOL.30, NO.1
```

C

C

```
CALCULATION OF M FACTORIAL
```

C

```
REAL ONE
```

```
DATA ONE/1.0/, MAXM /50/
```

C

```
IFault = 3
```

```
IF (M .LT. 0 .OR. M .GT. MAXM) RETURN
```

```
IFault = 0
```

```
FACT = ONE
```

```
IF (M .LE. 1) RETURN
```

```
A1 = ONE
```

```
DO 1 I = 2, M
```

```
AI = I
```

```
A1 = A1 * AI
```

```
1 CONTINUE
```

```
FACT = A1
```

```
RETURN
```

```
END
```

```
      SUBROUTINE RCONT2(NROW, NCOL, NROWT, NCOLT, JWORK, MATRIX,  
*      KEY, IFAULT)  
C  
C      ALGORITHM AS 159  APPL. STATIST. (1981) VOL.30, NO.1  
C  
C      Generate random two-way table with given marginal totals  
C  
C      N.B. The call to the NAG random number function G05AAF has been  
C      replaced by the use of the random number generator from AS 183.  
C  
C      N.B. See the journal article for the significance of the lines  
C      which start with C*  
C  
      INTEGER NROWT(NROW), NCOLT(NCOL), MATRIX(NROW, NCOL),  
*      JWORK(NCOL)  
      REAL FACT(5001), DUMMY, ZERO, ONE, HALF  
      LOGICAL KEY  
      LOGICAL LSP, LSM  
      COMMON /B/ NTOTAL, NROWM, NCOLM, FACT  
C  
C*      COMMON /TEMPRY/ HOP  
C  
      DATA MAXTOT /5000/, ZERO/0.0/, ONE/1.0/, HALF/0.5/  
C  
      IFAULT = 0  
      IF (KEY) GO TO 103  
C  
C      Set KEY for subsequent calls  
C  
      KEY = .TRUE.  
C  
C      Check for faults and prepare for future calls  
C  
      IF (NROW .LE. 1) GO TO 212  
      IF (NCOL .LE. 1) GO TO 213  
      NROWM = NROW - 1  
      NCOLM = NCOL - 1  
      DO 100 I = 1, NROW  
        IF (NROWT(I) .LE. 0) GO TO 214  
100 CONTINUE  
      NTOTAL = 0  
      DO 101 J = 1, NCOL  
        IF (NCOLT(J) .LE. 0) GO TO 215  
        NTOTAL = NTOTAL + NCOLT(J)  
101 CONTINUE  
      IF (NTOTAL .GT. MAXTOT) GO TO 216  
C  
C      Calculate log-factorials  
C  
      X = ZERO  
      FACT(1) = ZERO  
      DO 102 I = 1, NTOTAL  
        X = X + LOG(FLOAT(I))  
        FACT(I+1) = X  
102 CONTINUE  
C  
C      -----  
C      Construct random matrix  
C      -----  
C  
103 DO 105 J = 1, NCOLM
```

```
105 JWORK(J) = NCOLT(J)
      JC = NTOTAL
C
C*      HOP = ONE
C
      DO 190 L = 1, NROWM
          NROWTL = NROWT(L)
          IA = NROWTL
          IC = JC
          JC = JC - NROWTL
          DO 180 M = 1, NCOLM
              ID = JWORK(M)
              IE = IC
              IC = IC - ID
              IB = IE - IA
              II = IB - ID
C
C      Test for zero entries in MATRIX
C
          IF (IE .NE. 0) GO TO 130
          DO 121 J = M, NCOL
121      MATRIX(L,J) = 0
          GO TO 190
C
C      Generate pseudo-random number
C
130      DUMMY = RAND()
C
C      Compute conditional expected value of MATRIX(L, M)
C
131      NLM = IA * ID / FLOAT(IE) + HALF
          IAP = IA + 1
          IDP = ID + 1
          IGP = IDP - NLM
          IHP = IAP - NLM
          NLMP = NLM + 1
          IIP = II + NLMP
          X = EXP(FACT(IAP) + FACT(IB+1) + FACT(IC+1) + FACT(IDP) -
*          FACT(IE+1) - FACT(NLMP) - FACT(IGP) - FACT(IHP) - FACT(IIP))
          IF (X .GE. DUMMY) GO TO 160
          SUMPRB = X
          Y = X
          NLL = NLM
          LSP = .FALSE.
          LSM = .FALSE.
C
C      Increment entry in row L, column M
C
140      J = (ID - NLM) * (IA - NLM)
          IF (J .EQ. 0) GO TO 156
          NLM = NLM + 1
          X = X * J / FLOAT(NLM * (II + NLM))
          SUMPRB = SUMPRB + X
          IF (SUMPRB .GE. DUMMY) GO TO 160
150      IF (LSM) GO TO 155
C
C      Decrement entry in row L, column M
C
          J = NLL * (II + NLL)
          IF (J .EQ. 0) GO TO 154
          NLL = NLL - 1
```

```
      Y = Y * J / FLOAT((ID - NLL) * (IA - NLL))
      SUMPRB = SUMPRB + Y
      IF (SUMPRB .GE. DUMMY) GO TO 159
      IF (.NOT. LSP) GO TO 140
      GO TO 150
154    LSM = .TRUE.
155    IF (.NOT. LSP) GO TO 140
      DUMMY = SUMPRB * RAND()
      GO TO 131
156    LSP = .TRUE.
      GO TO 150
159    NLM = NLL
C
C*      HOP = HOP * Y
C*      GO TO 161
C*160    HOP = HOP * X
C*161    MATRIX(L,M) = NLM
C
160    MATRIX(L,M) = NLM
      IA = IA - NLM
      JWORK(M) = JWORK(M) - NLM
180    CONTINUE
      MATRIX(L,NCOL) = IA
190    CONTINUE
C
C      Compute entries in last row of MATRIX
C
      DO 192 M = 1, NCOLM
192    MATRIX(NROW,M) = JWORK(M)
      MATRIX(NROW,NCOL) = IB - MATRIX(NROW,NCOLM)
      RETURN
C
C      Set faults
C
212    IFAULT = 1
      RETURN
213    IFAULT = 2
      RETURN
214    IFAULT = 3
      RETURN
215    IFAULT = 4
      RETURN
216    IFAULT = 5
      RETURN
      END
```

```
      SUBROUTINE SCREEN(NVAR, MP, MM, NTAB, TABLE, DIM, GSQ, DGFR,  
*   PART, MARG, DFS, IP, IM, ISET, JSET, CONFIG, FIT, SIZE,  
*   COORD, X, Y, IFAULT)  
C  
C   ALGORITHM AS 160 APPL. STATIST. (1981) VOL.30, NO.1  
C  
C   Screen all effects for partial and marginal association.  
C  
      INTEGER NVAR, MP, MM, NTAB, IP(NVAR,MP), IM(NVAR,MM), DGFR(NVAR),  
*   DFS(NVAR,MP), ISET(NVAR), JSET(NVAR), CONFIG(NVAR,MP),  
*   DIM(NVAR), DF, SIZE(NVAR), COORD(NVAR)  
      REAL GSQ(NVAR), PART(NVAR,MP), MARG(NVAR,MP), TABLE(NTAB),  
*   FIT(NTAB), X(NTAB), Y(NTAB), ZERO  
      DATA ZERO /0.0/  
C  
C   Check for input errors  
C  
      IFAULT = 1  
      IF (NVAR .LE. 1) RETURN  
      ISZ = 1  
      DO 100 I = 1, NVAR  
         IF (DIM(I) .LE. 1) IFAULT = 2  
         ISZ = ISZ * DIM(I)  
100 CONTINUE  
      IF (ISZ .NE. NTAB) IFAULT = 2  
      MAX = 1  
      LIM = NVAR / 2  
      DO 110 I = 1, LIM  
110 MAX = MAX * (NVAR - I + 1) / I  
      IF (MP .LT. MAX) IFAULT = 3  
      MAX = 1  
      LIM = (NVAR - 1) / 2  
      DO 120 I = 1, LIM  
120 MAX = MAX * (NVAR - I) / I  
      MAX = MAX * NVAR  
      IF (MM .LT. MAX) IFAULT = 4  
      IF (IFAULT .GT. 1) RETURN  
C  
C   Fit the no effect model  
C  
      DGFR(NVAR) = NTAB - 1  
      AVG = ZERO  
      IFAULT = 5  
      DO 130 I = 1, NTAB  
         IF (TABLE(I) .LT. ZERO) RETURN  
         AVG = AVG + TABLE(I)  
130 CONTINUE  
      IFAULT = 0  
      AVG = AVG / NTAB  
      CALL RESET(FIT, NTAB, AVG)  
      CALL LIKE(GSQ, FIT, TABLE, NTAB)  
C  
C   Begin fitting effects  
C  
      NV1 = NVAR - 1  
      DO 200 M = 1, NV1  
C  
C   Set up the arrays IP and IM  
C  
         CALL CONF(NVAR, M, MP, MM, ISET, JSET, IP, IM, NP)  
C
```

```
C      Fit the saturated model
C
      CALL RESET(FIT, NTAB, AVG)
      CALL EVAL(IP, NP, M, 1, NVAR, MP, CONFIG, DIM, DGFR(M))
      CALL LOGFIT(NVAR, NTAB, NP, DIM, CONFIG, TABLE, FIT, SIZE,
*        COORD, X, Y)
      CALL LIKE(GSQ(M+1), FIT, TABLE, NTAB)
C
C      Move the first column of IP to the last
C
      DO 150 I = 1, M
        ITP = IP(I,1)
        NP1 = NP - 1
        DO 140 J = 1, NP1
140      IP(I,J) = IP(I,J+1)
        IP(I,NP) = ITP
150      CONTINUE
        L3 = -M + 1
        DO 190 J = 1, NP
C
C      Fit the effects in IP ignoring the last column
C
      CALL RESET(FIT, NTAB, AVG)
      CALL EVAL(IP, NP-1, M, 1, NVAR, MP, CONFIG, DIM, DF)
      CALL LOGFIT(NVAR, NTAB, NP-1, DIM, CONFIG, TABLE, FIT, SIZE,
*        COORD, X, Y)
      CALL LIKE(G21, GIT, TABLE, NTAB)
      DFS(M,J) = DGFR(M) - DF
      PART(M,J) = G21 - GSQ(M+1)
C
C      For M = 1, partials and marginals are equal
C
      IF (M .GT. 1) GO TO 160
      MARG(1,J) = PART(1,J)
      GO TO 170
C
C      Fit the last column alone
C
160      CALL RESET(FIT, NTAB, AVG)
      CALL EVAL(IP, 1, M, NP, NVAR, MP, CONFIG, DIM, DF)
      CALL LOGFIT(NVAR, NTAB, 1, DIM, CONFIG, TABLE, FIT, SIZE,
*        COORD, X, Y)
      CALL LIKE(G22, FIT, TABLE, NTAB)
C
C      Locate the appropriate columns of IM and fit them
C
      L3 = L3 + M
      CALL RESET(FIT, NTAB, AVG)
      CALL EVAL(IM, M, M-1, L3, NVAR, MM, CONFIG, DIM, DF)
      CALL LOGFIT(NVAR, NTAB, M, DIM, CONFIG, TABLE, FIT, SIZE,
*        COORD, X, Y)
      CALL LIKE(G23, FIT, TABLE, NTAB)
      MARG(M,J) = G23 - G22
C
C      Move the next effect to be ignored to the last in IP
C
170      DO 180 I = 1, M
        ITP = IP(I,NP)
        IP(I,NP) = IP(I,J)
        IP(I,J) = ITP
180      CONTINUE
```



```
190 CONTINUE
C
      DGFR(NVAR) = DGFR(NVAR) - DGFR(M)
      GSQ(M) = GSQ(M) - GSQ(M+1)
200 CONTINUE
C
      RETURN
      END
C
C
      SUBROUTINE CONF(N, M, MP, MM, ISET, JSET, IP, IM, NP)
C
C      ALGORITHM AS 160.1 APPL. STATIST. (1981) VOL.30, NO.1
C
C      Set up the arrays IP and IM for a given N and M.  Essentially
C      IP contains all possible combinations of (N choose M).  For each
C      combination found IM contains all combinations of degree M-1.
C
      INTEGER ISET(N), JSET(N), IP(N,MP), IM(N,MM)
      LOGICAL ILAST, JLAST
C
      ILAST = .TRUE.
      NP = 0
      NM = 0
C
C      Get IP
C
100 CALL COMBO(ISET, N, M, ILAST)
      IF (ILAST) RETURN
      NP = NP + 1
      DO 110 I = 1, M
110 IP(I,NP) = ISET(I)
      IF (M .EQ. 1) GO TO 100
C
C      Get IM
C
      JLAST = .TRUE.
      L = M - 1
120 CALL COMBO(JSET, M, L, JLAST)
      IF (JLAST) GO TO 100
      NM = NM + 1
      DO 130 I = 1, L
          JS = JSET(I)
          IM(I,NM) = ISET(JS)
130 CONTINUE
      GO TO 120
C
      END
C
C
      SUBROUTINE COMBO(ISET, N, M, LAST)
C
C      ALGORITHM AS 160.2 APPL. STATIST. (1981) VOL.30, NO.1
C
C      Subroutine to generate all possible combinations of M of the
C      integers from 1 to N in a stepwise fashion.  Prior to the first
C      call, LAST should be set to .FALSE.  Thereafter, as long as LAST
C      is returned .FALSE., a new valid combination has been generated.
C      When LAST goes .TRUE., there are no more combinations.
C
      LOGICAL LAST
```

```
      INTEGER N, M, ISET(M)
C
      IF (LAST) GO TO 110
C
C      Get next element to increment
C
      K = M
100   L = ISET(K) + 1
      IF (L + M - K .LE. N) GO TO 150
      K = K - 1
C
C      See if we are done
C
      IF (K .LE. 0) GO TO 130
      GO TO 100
C
C      Initialize first combination
C
110   DO 120 I = 1, M
120   ISET(I) = I
130   LAST = .NOT. LAST
      RETURN
C
C      Fill in remainder of combination.
C
150   DO 160 I = K, M
      ISET(I) = L
      L = L + 1
160   CONTINUE
C
      RETURN
      END
C
C
      SUBROUTINE EVAL(IAR, NC, NV, IBEG, NVAR, MAX, CONFIG, DIM, DF)
C
C      ALGORITHM AS 160.3 APPL. STATIST. (1981) VOL.30, NO.1
C
C      IAR = array containing the effects to be fitted
C      NC  = number of columns of IAR to be used
C      NV  = number of variables in each effect
C      IBEG = beginning column
C      DF  = degrees of freedom
C
C      CONFIG is in a format compatible with algorithm AS 51
C
      INTEGER IAR(NVAR,MAX), CONFIG(NVAR,NC), DIM(NVAR), DF
C
      DF = 0
      DO 110 J = 1, NC
      KK = 1
      DO 100 I = 1, NV
      L = IBEG + J - 1
      K = IAR(I,L)
      KK = KK * (DIM(K) - 1)
      CONFIG(I,J) = K
100   CONTINUE
      CONFIG(NV+1,J) = 0
      DF = DF + KK
110  CONTINUE
C
```

```
      RETURN
      END
C
C
      SUBROUTINE RESET(FIT, NTAB, AVG)
C
C   ALGORITHM AS 160.4 APPL. STATIST. (1981) VOL.30, NO.1
C
C   Initialize the fitted values to the average entry
C
      REAL FIT(NTAB)
C
      DO 100 I = 1, NTAB
         FIT(I) = AVG
100 CONTINUE
      RETURN
      END
C
C
      SUBROUTINE LIKE(GSQ, FIT, TABLE, NTAB)
C
C   ALGORITHM AS 160.5 APPL. STATIST. (1981) VOL.30, NO.1
C
C   Compute the likelihood-ratio chi-square
C
      REAL FIT(NTAB), TABLE(NTAB), ZERO, TWO
      DATA ZERO /0.0/, TWO /2.0/
C
      GSQ = ZERO
      DO 100 I = 1, NTAB
         IF (FIT(I) .EQ. ZERO .OR. TABLE(I) .EQ. ZERO) GO TO 100
         GSQ = GSQ + TABLE(I) * LOG(TABLE(I) / FIT(I))
100 CONTINUE
      GSQ = TWO * GSQ
      RETURN
      END
C
C
      SUBROUTINE LOGFIT(NVAR, NTAB, NCON, DIM, CONFIG, TABLE, FIT, SIZE,
*      COORD, X, Y)
C
C   ALGORITHM AS 160.6 APPL. STATIST. (1981) VOL.30, NO.1
C
C   Iterative proportional fitting of the marginals of a contingency
C   table. Relevant code from AS 51 is used.
C
      REAL TABLE(NTAB), FIT(NTAB), MAXDEV, X(NTAB), Y(NTAB), ZERO
      INTEGER CONFIG(NVAR,NCON), DIM(NVAR), SIZE(NVAR), COORD(NVAR)
      LOGICAL OPTION
      DATA MAXDEV /0.25/, MAXIT /25/, ZERO /0.0/
C
      DO 230 KK = 1, MAXIT
C
C   XMAX is the maximum deviation between fitted and true marginal
C
         XMAX = ZERO
         DO 220 II = 1, NCON
            OPTION = .TRUE.
C
C   Initialize arrays
C
C
```

```
        SIZE(1) = 1
        NV1 = NVAR - 1
        DO 100 K = 1, NV1
            L = CONFIG(K,II)
            IF (L .EQ. 0) GO TO 110
            SIZE(K+1) = SIZE(K) * DIM(L)
100     CONTINUE
        K = NVAR
110     N = K - 1
        ISZ = SIZE(K)
        DO 120 J = 1, ISZ
            X(J) = ZERO
            Y(J) = ZERO
120     CONTINUE
C
C     Initialize co-ordinates
C
130     DO 140 K = 1, NVAR
140     COORD(K) = 0
C
C     Find locations in tables
C
        I = 1
150     J = 1
        DO 160 K = 1, N
            L = CONFIG(K,II)
            J = J + COORD(L) * SIZE(K)
160     CONTINUE
        IF (.NOT. OPTION) GO TO 170
C
C     Compute marginals
C
        X(J) = X(J) + TABLE(I)
        Y(J) = Y(J) + FIT(I)
        GO TO 180
C
C     Make adjustments
C
170     IF (Y(J) .LE. ZERO) FIT(I) = ZERO
        IF (Y(J) .GT. ZERO) FIT(I) = FIT(I) * X(J) / Y(J)
C
C     Update co-ordinates
C
180     I = I + 1
        DO 190 K = 1, NVAR
            COORD(K) = COORD(K) + 1
            IF (COORD(K) .LT. DIM(K)) GO TO 150
            COORD(K) = 0
190     CONTINUE
        IF (.NOT. OPTION) GO TO 200
        OPTION = .FALSE.
        GO TO 130
C
C     Find the largest deviation
C
200     DO 210 I = 1, ISZ
        E = ABS(X(I) - Y(I))
        IF (E .GT. XMAX) XMAX = E
210     CONTINUE
220     CONTINUE
C
```

```
C      Test convergence
C
      IF (XMAX .LT. MAXDEV) RETURN
230 CONTINUE
C
      RETURN
      END
```

```

SUBROUTINE TABLE(N1, N2, ALPHA, MM, A1, PMAX, FSUM, A2, PMAX2,
* FSUM2, IFAULT)
C
C     ALGORITHM AS 161 APPL. STATIST. (1981) VOL.30, NO.2
C
DIMENSION MM(101, 2), FSUM(201), X(101, 101), COM(101),
* FSUM2(201), COMB(101), COMBO(201)
C
IFAULT = 0
IF (N2 .GT. 100) IFAULT = IFAULT + 1
IF (N1 .GT. N2) IFAULT = IFAULT + 2
IF (ALPHA .LE. 0.0 .OR. ALPHA .GE. 0.3) IFAULT = IFAULT + 4
IF (IFAULT .NE. 0) RETURN
N11 = N1 + 1
N21 = N2 + 1
CALL COMBIN(N11, COM)
CALL COMBIN(N21, COMB)
CALL COMBIN(N1 + N2 + 1, COMBO)
DO 10 I = 1, N11
    MM(I, 1) = 999
    MM(I, 2) = -999
10 CONTINUE
DO 15 I = 1, N11
    DO 15 J = 1, N21
        X(I, J) = -1.0
15 CONTINUE
C
C     INCREASE CHECK UNTIL SIG, THE LEAST UPPER BOUND ON
C     THE SIZE OF CRITICAL REGION, IS .GE. ALPHA + 0.0005
C
DEL = 0.1
CHECK = 3.0 * ALPHA
20 IF (CHECK .GT. 1.0) GOTO 30
CALL UMPUAL(N1, N2, CHECK, MM, X, SIG, FSUM, PMAX,
* COM, COMB, COMBO)
IF (SIG .GE. ALPHA) GOTO 40
CHECK = CHECK + DEL
GOTO 20
30 CHECK = 1.0
CALL UMPUAL(N1, N2, CHECK, MM, X, SIG, FSUM, PMAX,
* COM, COMB, COMBO)
40 IF (SIG .LE. ALPHA + 0.0005) GOTO 50
C
C     BACKUP SIG UNTIL LESS THAN ALPHA BY REPEATEDLY
C     ELIMINATING THE POINT WITH LARGEST PROBABILITY
C     FROM THE CRITICAL REGION
C
J = 1
IF (MM(J, 1) .EQ. 999) GOTO 50
JOLD = MM(J, 1)
DO 45 I = 1, N11
    IF (MM(I, 1) .EQ. 999) GOTO 47
    INEW = MM(I, 1)
    IF (X(I, INEW) .LE. X(J, JOLD)) GOTO 45
    J = I
    JOLD = MM(J, 1)
45 CONTINUE
C
C     REMOVE ALL X VALUES CLOSE TO THE MAXIMUM VALUE
C
47 XVAL = X(J, JOLD)

```

```
DO 49 I = 1, N11
  IF (MM(I, 1) .EQ. 999) GOTO 49
  INEW = MM(I, 1)
  IF (ABS(X(I, INEW) - XVAL) .GT. 0.00005) GOTO 49
  MM(I, 1) = MM(I, 1) + 1
  IF (MM(I, 1) .GT. N21) MM(I, 1) = 999
49 CONTINUE
CALL TMAX(MM, N1, N2, SIG, PMAX, FSUM, COM, COMB)
GOTO 40
50 A1 = SIG
DO 60 I = 1, N11
  IF (MM(I, 1) .EQ. 999) GOTO 60
  IREV = N11 - I + 1
  MM(IREV, 2) = N21 + 1 - MM(I, 1)
60 CONTINUE
CALL TMAX(MM, N1, N2, A2, PMAX2, FSUM2, COM, COMB)
DO 70 J = 1, N11
  IF (MM(J, 1) .NE. 999) MM(J, 1) = MM(J, 1) - 1
  IF (MM(J, 2) .NE. -999) MM(J, 2) = MM(J, 2) - 1
70 CONTINUE
RETURN
END
```

C  
C

```
SUBROUTINE COMBIN(NP1, C)
```

C  
C  
C  
C  
C  
C  
C  
C

```
ALGORITHM AS 161.1 APPL. STATIST. (1981) VOL.30, NO.2
```

```
COMPUTE THE COMBINATIONS OF N = NP1 - 1 ITEMS  
TAKING J AT A TIME AND STORE THEM IN THE ARRAY  
C(J + 1), J = 0, 1, 2, ..., N
```

```
DIMENSION C(NP1)
N = NP1 - 1
C(1) = 1.0
C(2) = FLOAT(N)
C(N) = FLOAT(N)
C(N + 1) = 1.0
IF (N .LE. 3) RETURN
M = N / 2 + 1
DO 10 J = 3, M
  NMJP2 = N - J + 2
  C(J) = C(J - 1) * (FLOAT(NMJP2) / FLOAT(J - 1))
  C(NMJP2) = C(J)
```

```
10 CONTINUE
RETURN
END
```

C  
C

```
SUBROUTINE UMPUAL(N1, N2, CHECK, MM, X, SIG, FSUM, PMAX, COM,  
* COMB, COMBO)
```

C  
C  
C

```
ALGORITHM AS 161.2 APPL. STATIST. (1981) VOL.30, NO.2
```

```
DIMENSION MM(101, 2), COMBO(201), COMB(101), COM(101), FSUM(201)
DIMENSION X(101, 101)
N11 = N1 + 1
N21 = N2 + 1
BETA0 = CHECK
```

C  
C

```
ADD POINTS TO CRITICAL REGION WITH X1 + X2 CONSTANT, UNTIL
```

```
C      THE SUM OF THE PROBABILITIES (BY THE HYPERGEOMETRIC) IS AS
C      LARGE AS POSSIBLE WITHOUT EXCEEDING CHECK
C
C      THE CRITICAL REGION IS REPRESENTED BY MM AND HAS BEEN
C      INITIALIZED IN SUBROUTINE TABLE.
C
C      ADJUST THE CURRENT MM VALUES ROW BY ROW (J1 = 1, N11).
C
DO 100 J1 = 1, N11
C
C      IF NO ENTRY IN ROW IS CURRENTLY IN THE CRITICAL REGION,
C      ASSUME THE LAST ENTRY (N21) IS.
C
      IF (MM(J1, 1) .EQ. 999) MM(J1, 1) = N2
C
C      INITIALIZE BETAU AND START J2 INCREASED BY 1 FOR THE LOOP
C
      J2 = MM(J1, 1) + 1
      BETAU = -1.0
C
C      WHILE WE ARE STILL IN THE ROW AND THE POSITION IS IN THE
C      CRITICAL REGION, CALCULATE BETAU BY THE HYPERGEOMETRIC
C      ON THE DIAGONAL. THE SUM OF THE PROBABILITIES IS STORED
C      IN X, AN N11 * N21 ARRAY. THE COMPUTATION IS BYPASSED
C      IF DONE EARLIER.
C
10 IF (J2 .LE. 1 .OR. BETAU .GT. BETA0) GOTO 40
      J2 = J2 - 1
      IF (X(J1, J2) .NE. -1.0) GOTO 30
      J1J2M1 = J1 + J2 - 1
      BETAU = COM(J1) * COMB(J2) / COMBO(J1J2M1)
      IF (J1 .NE. 1 .AND. J2 .NE. N21) BETAU = BETAU + X(J1 - 1, J2 + 1)
      X(J1, J2) = BETAU
      GOTO 10
C
C      RETRIEVE BETAU FROM X ARRAY
C
30 BETAU = X(J1, J2)
      GOTO 10
C
C      IF WE STOPPED BECAUSE J2 = 1, CONTINUE WITH J1 LOOP
C      OTHERWISE, BACKUP J2 FIRST.
C
40 IF (BETAU .GT. BETA0) J2 = J2 + 1
C
C      CHECK TO SEE IF ANY POINT IN ROW IS IN THE CRITICAL REGION
C
      IF (J2 .GT. N21) J2 = 999
      MM(J1, 1) = J2
100 CONTINUE
C
C      FOR THE CRITICAL REGION WITH SIZE LESS THAN OR
C      EQUAL TO CHECK UNDER THE NONRANDOMIZED UMPU TEST,
C      FIND SIG THE LEAST UPPER BOUND ON ITS SIZE UNDER
C      THE UNCONDITIONAL NON-RANDOMIZED TEST
C
      CALL TMAX(MM, N1, N2, FMAX, PMAX, FSUM, COM, COMB)
      SIG = FMAX
      RETURN
      END
```



```
C
C
SUBROUTINE TMAX(MM, N1, N2, FMAX, PMAX, FSUM, COM, COMB)
C
C     ALGORITHM AS 161.3 APPL. STATIST. (1981) VOL.30, NO.2
C
C     DIMENSION FSUM(201), MM(101, 2), P(201), DFSUM(201), COM(101),
*     COMB(101)
C     DATA EPS /0.00001/
C
C     EVALUATE THE PROBABILITY, FSUM(P), OF THE CRITICAL REGION
C     UNDER THE HYPOTHESIS  $P_1 = P_2 = P$  FOR  $P = 0.0, \dots, 1.0$ 
C
C     F = 0.0
C     KSTEP = N1 + N2 + 1
C     DEL = 1.0 / FLOAT(N1 + N2)
C     DO 10 K = 1, KSTEP
C         P(K) = F
C         CALL SRCH(MM, F, N1, N2, FSUM(K), DFSUM(K), COM, COMB)
C         F = F + DEL
10 CONTINUE
C     FMAX = 0.0
C     PMAX = 0.0
C     IF (MM(1, 1) .EQ. 999 .AND. MM(N1 + 1, 2) .EQ. -999) RETURN
C
C     APPROXIMATE THE LEAST UPPER BOUND, FMAX, FOR THE PROBABILITY
C     OF THE CRITICAL REGION ON THE INTERVAL 0.0 TO 1.0
C
C     J = 1
C     DO 20 I = 2, KSTEP
C         IF (FSUM(I) .GT. FSUM(J)) J = I
20 CONTINUE
C     FMAX = FSUM(J)
C     PMAX = P(J)
C
C     IF FMAX OCCURS AT EITHER ENDPOINT OF (0, 1) BRANCH OUT
C
C     PJMID = P(J)
C     SUMID = FSUM(J)
C     DSUMID = DFSUM(J)
C     IF (J .EQ. 1) GOTO 60
C     IF (J .EQ. KSTEP) GOTO 70
C
C     BRANCH OUT IF THE FUNCTION FSUM(P) IS FLAT ENOUGH IN THE
C     NEIGHBORHOOD OF FMAX
C
25 IF (DFSUM(J - 1) * DFSUM(J + 1) .GT. 0.0) GOTO 40
C     SUMLO = FSUM(J - 1)
C     PJLO = P(J - 1)
C     SUMHI = FSUM(J + 1)
C     PJHI = P(J + 1)
30 IF (ABS(SUMID - SUMLO) .LE. EPS .AND.
*     ABS(SUMID - SUMHI) .LE. EPS) GOTO 40
C     IF (DSUMID) 34, 40, 32
32 PJLO = PJMID
C     SUMLO = SUMID
C     GOTO 38
34 PJHI = PJMID
C     SUMHI = SUMID
38 PJMID = (PJLO + PJHI) * 0.5
C     CALL SRCH(MM, PJMID, N1, N2, SUMID, DSUMID, COM, COMB)
```

```
GOTO 30
40 FMAX = SUMID
   PMAX = PJMID
   RETURN
60 IF (FMAX .GE. 0.9999) RETURN
   G = 0.0001
   CALL SRCH(MM, G, N1, N2, RUM, DRUM, COM, COMB)
C
C   IF FMAX OCCURS AT 0, RETURN.
C
   IF (RUM .LT. FMAX) RETURN
   J = 2
   GOTO 25
70 IF (FMAX .GE. 0.9999) RETURN
   G = 0.9999
   CALL SRCH(MM, G, N1, N2, RUM, DRUM, COM, COMB)
C
C   IF FMAX OCCURS AT 1, RETURN.
C
   IF (RUM .LT. FMAX) RETURN
   J = KSTEP - 1
   GOTO 25
END
C
C
SUBROUTINE SRCH(MM, PP, N1, N2, SUMS, DSUMS, COM, COMB)
C
C   ALGORITHM AS 161.4 APPL. STATIST. (1981) VOL.30, NO.2
C
C   FIND THE SIZE OF THE CRITICAL REGION UNDER THE UNCONDITIONAL
C   NONRANDOMIZED TEST WITH PROBABILITY P1 = P2 = PP
C
DIMENSION MM(101, 2), COM(101), COMB(101)
C
N11 = N1 + 1
N21 = N2 + 1
SUM = 0.0
SUMM = 0.0
DSUM = 0.0
DSUMM = 0.0
IF (PP .GE. 0.99999) GOTO 30
IF (PP .LE. 0.00001) GOTO 40
C
C   SEARCH THE ONE-SIDED CRITICAL REGION
C
PP1 = 1.0 - PP
DO 20 I = 1, N11
IF (MM(I, 1) .EQ. 999) GOTO 50
NE = N21
DP1EXP = PP1 ** (I + N2)
PPEXP = PP ** (I + N2)
DPPEXP = PP ** (N1 - I)
PP1EXP = PP1 ** (N1 - I)
DO 10 J = 1, N21
IF (MM(I, 1) .GT. NE) GOTO 20
PPEXP = PPEXP / PP
PP1EXP = PP1EXP * PP1
C
C   EVALUATE THE PROBABILITY OF A POINT IN THE CRITICAL REGION
C   BY THE PRODUCT OF INDEPENDENT BINOMIAL TERMS AND ACCUMULATE
C   IN SUM. ALSO EVALUATE THE DERIVATIVE OF SUM AT P1 = P2 = PP.
```

```
C
  IF (MM(1, 1) .EQ. 999) GOTO 4
  SUM = SUM + COM(I) * COMB(NE) * PPEXP * PP1EXP
  DSUM = DSUM + COM(I) * COMB(NE) * (FLOAT(I + N2 - J) * PPEXP /
* PP * PP1EXP - FLOAT(N1 + J - I) * PPEXP * PP1EXP / PP1)
4 IF (MM(N11, 2) .EQ. -999) GOTO 5
  DPPEXP = DPPEXP * PP
  DP1EXP = DP1EXP / PP1
  SUMM = SUMM + COM(I) * COMB(NE) * DPPEXP * DP1EXP
  DSUMM = DSUMM + COM(I) * COMB(NE) * (FLOAT(N1 + J - I) * DPPEXP /
* PP * DP1EXP - FLOAT(N2 + I - J) * DPPEXP * DP1EXP / PP1)
5 NE = NE - 1
10 CONTINUE
20 CONTINUE
  GOTO 50
30 IF (MM(N11, 1) .NE. 999) SUM = 1.0
  SUMS = SUM + SUMM
  RETURN

C
40 IF (MM(1, 1) .EQ. 1) SUM = 1.0
  SUMS = SUM
  RETURN

C
50 SUMS = SUM + SUMM
  DSUMS = DSUM + DSUMM
  RETURN
  END
```

```
      subroutine logccs(ns, nca, nct, nimax, nmax2, nvmax, nv, nv1, z,
+         ivar, covi, w, ww, dl, iw, is, b, cov, chi2, st, ifault)
c
c   ALGORITHM AS 162  APPL. STATIST. (1981) VOL. 30, NO. 2
c
c   Logistic analysis of case-control studies
c
c   Auxiliary routine required: SYMINV from AS 7.
c   N.B. The description in the journal states that AS 6 is also
c       needed, but where ?
c
c   integer    nca(ns), nct(ns), ivar(nv), iw(nmax2), is(ns)
c   real       z(nvmax, nimax), covi(nv1), w(nv), ww(nv), dl(nv),
+         b(nv), cov(nv1)
c   real       one, zero, two
c   logical    ifg, id
c   data maxit /20/, eps /1.e-6/, one/1.0/, zero/0.0/, two/2.0/
c
c   Initial settings
c
c   rlikp = one
c   ifault = 0
c   if (nvmax .lt. nv) go to 27
c   do 1 i = 1, ns
c     if (nmax2 .lt. nca(i) + nct(i) + 2) go to 27
1  continue
c   is(1) = 0
c   IF(NS .EQ. 1) GOTO 28
c   do 2 j = 2, ns
c     j1 = j - 1
c     is(j) = is(j1) + nca(j1) + nct(j1)
2  continue
28  if (nimax .lt. is(ns) + nca(ns) + nct(ns)) go to 27
c   its = 0
c
c   Start of iteration
c
c   3  its = its + 1
c     if (its .gt. maxit) go to 24
c     rlik = zero
c     k = 0
c     do 4 j = 1, nv
c       dl(j) = zero
c       do 4 jj = 1, j
c         k = k + 1
c         covi(k) = zero
4  continue
c
c   Loop through strata
c
c   do 17 i = 1, ns
c     if (nca(i) * nct(i) .eq. 0) go to 17
c     ifg = .false.
c     sx = zero
c     k = 0
c     do 5 j = 1, nv
c       w(j) = zero
c       ww(j) = zero
c       do 5 jj = 1, j
c         k = k + 1
c         cov(k) = zero
```

```
5  continue
   m = nca(i)
   n = m + nct(i)
   xx = one
   x = zero
   iw(1) = n + 1
   iw(n + 2) = -2
   kk = nct(i) + 1
   do 6 j = 2, kk
6  iw(j) = 0
   do 7 j = 1, m
     jj = kk + j
     iw(jj) = j
7  continue
c
c  Calculator numerator of terms of likelihood
c
   do 9 k = 1, nv
     l = ivar(k)
     bk = b(k)
     wk = zero
     do 8 j = 1, m
       ji = is(i) + j
       wk = wk + z(l, ji)
       x = x + bk * z(l, ji)
8     continue
     w(k) = wk
9   continue
c
c  Go through all possible combinations to calculate denominator
c  terms of likelihood
c
10  xx = exp(x)
    sx = sx + xx
    if (ifg) go to 12
    rlik = rlik + log(sx)
    do 11 k = 1, nv
11  dl(k) = dl(k) + w(k)
    ifg = .true.
12  l = 0
    do 13 k = 1, nv
      ww(k) = ww(k) + xx * w(k)
      do 13 kk = 1, k
        l = l + 1
        cov(l) = cov(l) + xx * w(k) * w(kk)
13  continue
    call twidl(ips, im, iz, id, iw, nmax2)
    if (id) go to 15
c
c  Use the special features of TWIDL that only one element is altered
c  at a time, to calculate contribution of succeeding combinations
c  with minimal arithmetic.
c
    ipsli = is(i) + n - ips + 1
    imli = is(i) + n - im + 1
    do 14 k = 1, nv
      l = ivar(k)
      zc = z(l, ipsli) - z(l, imli)
      w(k) = w(k) + zc
      x = x + b(k) * zc
14  continue
```

```
        go to 10
c
15  rlik = rlik - log(sx)
    l = 0
    do 16 j = 1, nv
        dl(j) = dl(j) - ww(j) / sx
        do 16 k = 1, j
            l = l + 1
            covi(l) = covi(l) + (sx * cov(l) - ww(j) * ww(k)) / sx**2
16  continue
17  continue
c
    if (its .eq. 1) rliks = rlik
    call syminv(covi, nv, cov, w, nullty, ifault, nv1)
    if (ifault .ne. 0) go to 25
c
c  Calculate new parameter estimates.
c
    do 20 i = 1, nv
        w(i) = zero
        i2 = i * (i - 1) / 2
        do 18 j = 1, i
            k = i2 + j
            w(i) = w(i) + dl(j) * cov(k)
18  continue
        i1 = i + 1
        if (i1 .gt. nv) go to 20
        do 19 k = i1, nv
            j = k * (k - 1) / 2 + i
            w(i) = w(i) + dl(k) * cov(j)
19  continue
20  continue
        do 21 i = 1, nv
21  b(i) = b(i) + w(i)
        if (its .ne. 1) go to 23
c
c  Calculate score test
c
    st = zero
    do 22 i = 1, nv
22  st = st + w(i) * dl(i)
c
c  Test for convergence
c
23  rlik = rlik - rliks
    if (abs(rlikp - rlik) .le. eps) go to 26
    rlikp = rlik
    go to 3
24  ifault = 1
    return
25  ifault = 2
    return
26  chi2 = two * rlik
    return
27  ifault = 3
    return
end
c
c
c
    subroutine twidl(x, y, z, done, p, n2)
```

```
integer x, y, z, n2, p(n2)
logical done
```

```
c
c      Algorithm AS 162.1  Appl. Statist. (1981) Vol.30, No. 2
```

```
c      This subroutine is a fortran version of
c      CACM Algorithm 382 for generating all combinations
c      of M out of N objects.  All subscripts in the array P have
c      been increased by unity to avoid reference to P(0).
```

```
c      Ref:- P.J. Chase (1970), Comm. ACM, Vol.13, No.6, p368.
```

```
c      Parameters:-
```

```
c      done          logical      input: Initially set to .false.
c                                   output: If all combinations have been
c                                           found then done is set to .true.
c                                           Otherwise done=.false.
```

```
c      p             integer array input: Initially, p(1)=N+1, p(N+2)=-2
c                   of length      p(2,...,N-M+1)=0,
c                   N+2            p(N-M+2,...,N+1)=1,...,M
c                                   If M=0, set p(2)=1.
```

```
c      n2            integer       input: n2=n+2
```

```
c      x, y, z       integers      output: See below.
```

```
c      Initially, let A(1,...,N)=1,...,N
c                   let C(1,...,M)=A(N-M+1),...,A(N) = N-M+1,...,N
c                   be the initial combination.
```

```
c      Then the next combination is given by setting C(Z)=A(X)
```

```
c      Alternatively, initially let B(1,...,N-M)=0 and B(N-M+1,...,N)=1
c                                   be the initial sequence of zeros and ones.
```

```
c      Then the next sequence of zeros and ones is obtained by setting
c      B(X)=1 and B(Y)=0.
```

```
c
```

```
      j = 0
1  j = j + 1
   if (p(j + 1) .le. 0) goto 1
   if (p(j) .ne. 0) goto 4
   if (j .lt. 3) goto 3
   do 2 i = 3, j
2  p(i) = -1
3  p(j + 1) = 0
   p(2) = 1
   x = 1
   z = 1
   y = j
   goto 10
4  if (j .gt. 1) p(j) = 0
5  j = j + 1
   j1 = j + 1
   if (p(j1) .gt. 0) goto 5
   i = j - 1
   k = i
6  i = i + 1
   i1 = i + 1
   if (p(i1) .ne.0) goto 7
```

```
    p(i1) = -1
    goto 6
7  if (p(i1) .ne. -1) goto 8
    z = p(k + 1)
    p(i1) = z
    x = i
    y = k
    p(k + 1) = -1
    goto 10
8  if (i .ne. p(1)) goto 9
    done = .true.
    goto 10
9  z = p(i1)
    p(j1) = z
    p(i1) = 0
    x = j
    y = i
10 return
    end
```

```
c
c
c*****
```

```
c The routine below initializes TWIDL. It is NOT part of AS 162.
c It enables TWIDL to be used for other applications.
```

```
c
c      subroutine initp(n, m, p, n2, done)
c      integer p(n2)
c      logical done
```

```
c
c      done = .false.
c      n1 = n + 1
c      nm1 = n - m + 1
c      p(1) = n1
c      p(n+2) = -2
c      do 1 i = 2, nm1
1  p(i) = 0
c      do 2 i = 1,m
c      i1 = nm1 + i
2  p(i1) = i
c      return
c      end
```



```
      subroutine gtrans(r, nr, m, n, ifault)
c
c      Algorithm AS163 Applied Statistics (1981) vol.30, no. 2
c
c      Transposes rows m and m+1 in the standardized lower-triangular
c      working matrix r and restores the triangular structure by plane
c      rotations.  r is of length nr = n(n+1)/2 and is stored row by
c      row, shortest row first.
c
c      double precision r(nr), a, b, c, d, zero, one
c
c      data zero, one/0.d0, 1.d0/
c
c      ifault = 1
c      if (n .lt. 2 .or. m .lt. 1 .or. m .ge. n) return
c      ifault = 0
c      ma = m * (m + 1) / 2
c      mb = ma + m
c
c      Exchange columns
c
c      i = mb
20    i = i - 1
c      if (i .eq. ma) go to 30
c      j = i - m
c      a = r(i)
c      r(i) = r(j)
c      r(j) = a
c      go to 20
30    mc = mb + 1
c
c      a will now be set equal to element (m,m)
c      b = element (m,m+1), and c = element (m+1,m+1).
c      If a and c are zero, there is nothing to do.
c
c      a = r(ma)
c      c = r(mc)
c      if (a .le. zero .and. c .le. zero) return
c
c      Other special cases where one or more of a, b or c is zero.
c
c      b = r(mb)
c      j = m + 2
c      mi = mb + j
c      if (b .ne. zero) go to 50
c      r(mc) = a
c      r(ma) = c
c      if (j .gt. n) return
c      do 40 i = j, n
c          b = r(mi-1)
c          r(mi-1) = r(mi)
c          r(mi) = b
c          mi = mi + i
40    continue
c      return
c
50    if (c .gt. zero) go to 70
c      r(ma) = a * b * b
c      r(mb) = one / b
c      if (j .gt. n) return
c      do 60 i = j, n
```

```

        r(mi-1) = r(mi-1) / b
        mi = mi + i
60    continue
    return
c
c    General case - a, b, c all non-zero
c
70    d = a * b * b + c
    r(ma) = d
    c = c / d
    r(mc) = a * c
    a = a * b / d
    r(mb) = a
    if (j .gt. n) return
    do 80 i = j, n
        d = r(mi-1)
        r(mi-1) = a * d + c * r(mi)
        r(mi) = d - b * r(mi)
        mi = mi + i
80    continue
    return
end

c
c
c    subroutine update(r, x, w, n, nr)
c
c    Algorithm AS163.1 Applied Statistics (1981) vol.30, no.2
c
c    Uses plane rotations to update the standardized square root
c    (Cholesky factor) of a matrix of sums of squares and products
c    when another data vector x is to be included.  r is of length
c    nr = n(n+1)/2 and is stored row by row, shortest row first.
c
c    double precision x(n), r(nr), w, y, d, c, s, eps
c
c    data eps/0.d0/
c
c    l = 0
    do 20 i = 1, n
        if (w .le. eps) return
        l = l + i
        y = x(i)
        if (abs(y) .le. eps) go to 20
        d = r(l) + w * y * y
        if (abs(d) .le. eps) go to 20
        c = r(l) / d
        r(l) = d
        if (i .eq. n) return
        s = w * y / d
        w = c * w
        k = l
        m = i + 1
        do 10 j = m, n
            k = k + j - 1
            d = x(j)
            r(k) = c * r(k) + s * d
10        continue
20    continue
    return
end

```

SUBROUTINE GIVENC(R, IR, NVAR, X, V, IFAULT)

```
C
C<<<<< Acquired in machine-readable form from 'Applied Statistics'
C<<<<< algorithms editor, January 1983.
C
C      ALGORITHM AS 164  APPL. STATIST. (1981) VOL.30, NO.2
C
C      APPLIES GIVENS TRANSFORMS TO INCLUDE A NEW ROW OF DATA
C      OR CONSTRAINT
C
C      The corrections detailed on p.357 of 'Applied Statistics', Vol.30,
C      have been incorporated.
C
REAL R(IR), X(NVAR)
DATA ZERO/0.0/
C
C      SMALL CONSTANTS THAT THE USER CAN MODIFY
C
DATA EPS0/0.0/, EPS1/0.0/
C
C      CHECK FOR VALID PARAMETERS
C
IFAILT = 0
IRUSED = NVAR*(NVAR+1)/2
IF (IR.LT.IRUSED) GO TO 1003
IF (V.LT.ZERO) GO TO 1002
VLOCAL = V
C
C      FOR EACH ROW OF UPPER TRIANGULAR R
C
II = 0
DO 60 I = 1, NVAR
  II = II + I
  XI = X(I)
  XI2 = XI*XI
  IF (XI2.LE.ABS(VLOCAL)*EPS0) GO TO 60
  CTEMP = R(II)
  IJ = II
  IPLUS = I + 1
C
C      IF ZERO WEIGHT ON ROW OF R, SIMPLE PIVOT
C
IF (CTEMP.GE.ZERO) GO TO 20
R(II) = VLOCAL/XI2
IF (I.EQ.NVAR) GO TO 70
DO 10 J = IPLUS, NVAR
  IJ = IJ + J - 1
  R(IJ) = X(J)/XI
10 CONTINUE
RETURN
C
C      IF INFINITE WEIGHT ON ROW OF R, SIMPLE PIVOT
C
20 IF (CTEMP.GT.EPS1) GO TO 40
DO 30 J = IPLUS, NVAR
  IJ = IJ + J - 1
  X(J) = X(J) - XI*R(IJ)
30 CONTINUE
GO TO 60
C
C      OTHERWISE ORDINARY GIVENS ROTATION
```

```
C
  40  VNEW = VLOCAL + CTEMP*XI2
      C = VLOCAL/VNEW
      S = CTEMP*XI/VNEW
      VLOCAL = VNEW
      R(II) = CTEMP*C
      IF (I.EQ.NVARS) GO TO 70
      DO 50 J = IPLUS, NVARS
        IJ = IJ + J - 1
        RTEMP = C*R(IJ) + S*X(J)
        X(J) = X(J) - XI*R(IJ)
        R(IJ) = RTEMP
  50  CONTINUE
C
  60  CONTINUE
C
      CHECK FOR INCONSISTENT OR DUPLICATED CONSTRAINTS
C
  70  IF (ABS(R(IRUSED)).LE.EPS1) GO TO 1001
      IF (VLOCAL.LE.EPS1) IFAULT = -1
      RETURN
C
      ERROR FLAG SET
C
  1001 IFAULT = IFAULT + 1
  1002 IFAULT = IFAULT + 1
  1003 IFAULT = IFAULT + 1
      RETURN
      END
C
      SUBROUTINE BSUB(R, IR, IDEP, COEFF, IC, IFAULT)
C
      ALGORITHM AS 164.1  APPL. STATIST. (1981) VOL.30, NO.2
C
      PERFORM BACK SUBSTITUTION TO GET PARAMETER ESTIMATES
C
      REAL R(IR), COEFF(IC)
      DATA ZERO/0.0/
C
      CHECK FOR VALID PARAMETERS
C
      IFAULT = 0
      II = IDEP*(IDEP+1)/2
      NXVARS = IDEP - 1
      IF (IR.LT.II.OR.IC.LT.NXVARS) GO TO 1001
      IF (NXVARS.LT.1) RETURN
C
      BACK SUBSTITUTION
C
      K = II
      NX = IDEP
      DO 30 I = 1, NXVARS
        II = II - NX
        K = K - 1
        TEMP = R(K)
        IF (R(II).LT.ZERO) IFAULT = IFAULT - 1
        IF (I.EQ.1) GO TO 20
        IJ = II
        DO 10 J = NX, NXVARS
          IJ = IJ + J - 1
          TEMP = TEMP - R(IJ)*COEFF(J)
```

```
10 CONTINUE
20 NX = NX - 1
   COEFF(NX) = TEMP
30 CONTINUE
   RETURN
C
1001 IFAULT = 1
   RETURN
   END
C
SUBROUTINE SSCOMP(R, IR, IDEP, NOBS, ICOMP, SSQ, IDF, IFAULT)
C
C   ALGORITHM AS 164.2 APPL. STATIST. (1981) VOL.30, NO.2
C
C   FINDS (ICOMP)TH COMPONENT OF TOTAL SUM OF SQRS
C   ZERO-TH COMPONENT IS RESIDUAL SSQ
C
DIMENSION R(IR)
DATA ZERO/0.0/, ONE/1.0/
C
C   SMALL CONSTANT THAT THE USER CAN MODIFY
C
DATA EPS1/0.0/
C
C   CHECK FOR VALID PARAMETERS
C
IFAULT = 0
IRUSED = IDEP*(IDEP + 1)/2
IF (IR.LT.IRUSED) IFAULT = IFAULT + 1
IF (ICOMP.LT.0.OR.ICOMP.GE.IDEP) IFAULT = IFAULT + 2
IF (IFAULT.GT.0) RETURN
C
C   TEST IF RESIDUAL SSQ REQUIRED
C
IF (ICOMP.GE.1) GO TO 20
NXVARS = IDEP - 1
IDF = NOBS - NXVARS
II = 0
DO 10 I = 1, NXVARS
  II = II + I
  IF (R(II).LE.EPS1) IDF = IDF + 1
10 CONTINUE
SSQ = ZERO
IF (R(IRUSED).GT.EPS1) SSQ = ONE/R(IRUSED)
RETURN
C
C   ORDINARY COMPONENT
C
20 IDF = 0
SSQ = ZERO
II = ICOMP*(ICOMP+1)/2
IF (R(II).LE.EPS1) RETURN
IDF = 1
IJ = IRUSED - IDEP + ICOMP
SSQ = R(IJ)*R(IJ)/R(II)
RETURN
END
C
SUBROUTINE VAR(R, IR, S, IS, IDEP, NOBS, IFAULT)
C
C   ALGORITHM AS 164.3 APPL. STATIST. (1981) VOL.30, NO.2
```

```
C
C      FINDS ESTIMATE OF VAR/COVAR MATRIX OF ESTIMATES
C
REAL R(IR), S(IS)
DATA ZERO/0.0/, ONE/1.0/

C
C      SMALL CONSTANT THAT THE USER CAN MODIFY
C
DATA EPS1/0.0/

C
C      CHECK FOR VALID PARAMETERS
C
IFAUULT = 0
IRUSED = IDEP*(IDEP+1)/2
IF (IR.LT.IRUSED.OR.IS.LT.(IRUSED-IDEP)) GO TO 1002
NXVARS = IDEP - 1

C
C      INVERT UNIT UPPER TRIANGULAR MATRIX
C
NCONS = 0
IJ = 0
DO 50 I = 1, NXVARS
  JJ = 0
  J = 0
10  J = J + 1
  IJ = IJ + 1
  JJ = JJ + J
  IF (J.LT.I) GO TO 20
  IF (R(IJ).LE.EPS1) NCONS = NCONS + 1
  GO TO 50
20  STEMP = -R(IJ)
  IK = IJ
  KJ = JJ
  KMAX = I - 1
  KMIN = J + 1
  IF (KMAX.LT.KMIN) GO TO 40
  DO 30 K = KMIN, KMAX
    IK = IK + 1
    KJ = KJ + K - 1
    STEMP = STEMP - R(IK)*S(KJ)
30  CONTINUE
40  S(IJ) = STEMP
  GO TO 10
50 CONTINUE

C
C      ESTIMATE VARIANCE AND APPLY IDENTIFIABILITY CONSTRAINTS
C
IDF = NOBS - NXVARS + NCONS
IF (IDF.LE.0) GO TO 1001
SIGMA = ZERO
IF (R(IRUSED).GT.ZERO) SIGMA = ONE/(R(IRUSED)*FLOAT(IDF))
II = 0
DO 60 I = 1, NXVARS
  II = II + I
  S(II) = SIGMA*R(II)
  IF (R(II).LT.ZERO) S(II) = ZERO
60 CONTINUE

C
C      MULTIPLY MATRICES TOGETHER TO FORM EST OF VAR
C
II = 0
```

```
      IJ = 0
      DO 90 I = 1, NXVARS
        II = II + I
        DO 90 J = 1, I
          KK = II
          IJ = IJ + 1
          KI = IJ
          KJ = II
          STEMP = S(KK)
          IF (I.NE.J) STEMP = STEMP*S(IJ)
          K = I
70      K = K + 1
          IF (K.GT.NXVARS) GO TO 80
          KK = KK + K
          KI = KI + K - 1
          KJ = KJ + K - 1
          STEMP = STEMP + S(KI)*S(KJ)*S(KK)
          GO TO 70
C
      80      S(IJ) = STEMP
      90 CONTINUE
      RETURN
C
      1001 IFAULT = IFAULT + 1
      1002 IFAULT = IFAULT + 1
      RETURN
      END
C
      SUBROUTINE ALIAS(R, IR, NVAR, EPS, WORKSP, IFAULT)
C
C      ALGORITHM AS 164.4  APPL. STATIST. (1981) VOL.30, NO.2
C
C      ASSUMES ANY DIAGONAL ELEMENTS OF D LESS THAN EPS ARE
C      ROUNDING ERRORS AND REDUCES THEM TO ZERO
C
      REAL R(IR), WORKSP(NVAR)
      DATA ZERO/0.0/, ONE/1.0/, ONENEG/-1.0/
C
C      CHECK FOR VALID PARAMETERS
C
      IFAULT = 0
      IRUSED = NVAR*(NVAR+1)/2
      IF (IR.LT.IRUSED) GO TO 1001
      NXVARS = NVAR - 1
C
C      FOR EACH ROW OF TRIANGULAR R
C
      II = 0
      DO 20 I = 1, NXVARS
        II = II + I
        WORKSP(I) = ZERO
C
C      CHECK FOR WEIGHT OF ROW NEAR ZERO
C
      IF (ABS(R(II))*EPS.LE.ONE) GO TO 20
      IFAULT = IFAULT - 1
      V = R(II)
      R(II) = ONENEG
      IJ = II
      IPLUS = I + 1
C
```

```
C          ROTATE MODIFIED ROW WITH GIVENS
C
      DO 10 J = IPLUS, NVAR5
        IJ = IJ + J - 1
        WORKSP(J) = R(IJ)
        R(IJ) = ZERO
10     CONTINUE
      CALL GIVENC(R, IR, NVAR5, WORKSP, V, IFAIL)
20    CONTINUE
      RETURN
C
C          SET FAULT INDICATOR
C
1001  IFAULT = 1
      RETURN
      END
```



```
      SUBROUTINE KKEY(IDATA,ICLSS,ILCSE,ILSYM,ISMSB,NCASE,NCLAS,NSCOR,
1         NSYM,ISIG,NUM,NKEY,MAXLEV,NPRINT,NPUNCH,IFAU)
C
C<<<<<  Acquired in machine-readable form from 'Applied Statistics'
C<<<<<  algorithms editor, January 1983.
C
C         ALGORITHM AS 165  APPL. STATIST. (1981) VOL.30, NO.3
C
C         Constructs a discriminant function in Fortran for categorical data.
C
      DIMENSION IDATA(NSYM,NCASE),ICLSS(NCASE),ILCSE(NCASE),
1         ILSYM(3,NKEY),ISMSB(NSYM)
      DIMENSION ITABL(10,10),MTAB(10,10),IFST(10),IT(10),ITERM(10),
1         ITMIN(10),MEST(10),MINC(10),MSC(10),NOC(10)
      DATA ITWO/1/
C
C         CHECK INPUT VALUES
C
      IF(NCASE.LT.3) GO TO 52
      IF(NSYM.LT.3) GO TO 53
      IF(NSCOR.LT.2 .OR. NSCOR.GT.10) GO TO 54
      IF(NCLAS.LT.2 .OR. NCLAS.GT.10) GO TO 55
      DO 1 J = 1,NCASE
      IF(ICLSS(J).LT.1 .OR. ICLSS(J).GT.NCLAS) GO TO 56
      DO 1 I = 1,NSYM
      IF(IDATA(I,J).LT.0 .OR. IDATA(I,J).GE.NSCOR) GO TO 57
1     CONTINUE
      IF(ISIG.LT.0 .OR. ISIG.GT.2) GO TO 58
      IF(NPRINT.LT.1 .OR. NPUNCH.LT.1) GO TO 59
C
C         CONSTRUCT KEY AND WRITE FORTRAN FUNCTION
C
C         INDIVIDUAL LABELS STORED IN ILCSE - INITIALISE TO ONES
C
      IFAULT = 0
      IFLAG = 2
      LEVEL = 1
      LEV10 = 10
      ILSYM(3,1) = 0
      ILSYM(3,2) = 1
      DO 2 I = 1,NCASE
2     ILCSE(I) = 1
      DO 3 I = 1,NCLAS
3     ITERM(I) = 1
      WRITE(NPUNCH,80)NSYM
C
C         VARIABLE LABELS STORED IN ILSYM - NSYMU GIVES NUMBER STORED
C
      NSYMU = 0
C
C         NEW LEVEL
C         LABEL IS CURRENT INDIVIDUAL LABEL - LABNO GIVES FIRST
C         INDIVIDUAL FOR INSPECTION
C
4     LABEL = -1
      LABNO = 1
C
C         TAKE NEXT INDIVIDUAL LABEL - SAME LEVEL
C
5     DO 6 I = LABNO,NCASE
C
```

```
C          IF INDIVIDUAL LABEL NEGATIVE MOVE ON
C
          IF(ILCSE(I).GT.0) GO TO 7
6        CONTINUE
C
          NO POSITIVE INDIVIDUAL LABELS - END OF KEY
C
          GO TO 50
C
          FIND NEXT INDIVIDUAL LABEL IGNORING INDIVIDUALS ALREADY
C          PROCESSED AT THIS LEVEL
C
7        DO 8 J = I,NCASE
          IF(ILCSE(J).LT.LEV10.AND.ILCSE(J).GE.0) GO TO 9
8        CONTINUE
C
          ALL INDIVIDUALS DONE - GO ON TO NEXT LEVEL IF ANY VARIABLES
C          LEFT - OTHERWISE END KEY
C
          LEVEL = LEVEL+1
          LEV10 = LEV10*10
          IF(LEVEL.GT.NSYM ) GO TO 49
          GO TO 4
C
          TEST WHETHER VARIABLE HAS BEEN USED ON THESE INDIVIDUALS
C          PICK OUT VARIABLES THAT MATCH THE INDIVIDUAL LABEL OR THE
C          FIRST N DIGITS OF IT
C          THESE VARIABLES HAVE 1 PLACED IN ISMSB - OTHERS HAVE ZERO.
C
9        LABEL = ILCSE(J)
          LABNO = J
          DO 10 I = 1,NSYM
10       ISMSB(I) = 0
          IF(NSYMU.EQ.0) GO TO 13
          LAB = LABEL
          DO12 I = 1,LEVEL
          DO 11 J = 1,NSYMU
          ISM = ILSYM(1,J)
          IF(ILSYM(2,J).EQ.LAB)ISMSB(ISM) = 1
11       CONTINUE
          IF(LEVEL.NE.I)LAB = LABEL/10
12       CONTINUE
C
          FIND THE VARIABLE OF THE SUBSET THAT IS MOST DISCRIMINATING
C          FOR THESE INDIVIDUALS
C
13      MAXP = 0
          DO 16 I = 1,NSYM
          IF(ISMSB(I).EQ.1) GO TO 16
          CALL IPOWR(I,LABEL,IP,IT,MSC,NOC,ITABL,IDATA,ICLSS,ILCSE,NCASE,
1         NCLAS,NSCOR,NSYM,IFAUULT)
          IF(IFAUULT.NE.0) RETURN
          IF(IP.LE.MAXP) GO TO 16
          MAXP = IP
          IPN = I
          DO 15 J = 1,10
          MEST(J) = MSC(J)
          MINC(J) = NOC(J)
          ITMIN(J) = IT(J)
          DO 15 J1 = 1,10
          MTAB(J1,J) = ITABL(J1,J)
```

```
15 CONTINUE
16 CONTINUE
C
C     APPLY ERROR-RATE STOP RULE
C
MAXV = 0
DO 20 L = 1,NCLAS
IT(L) = 0
DO 17 M = 1,NSCOR
17 IT(L) = IT(L)+MTAB(L,M)
IF(IT(L)-MAXV)20,18,19
18 ITWO = 3-ITWO
IF(ITWO.EQ.2) GO TO 20
19 MAXV = IT(L)
MCLAS = L
20 CONTINUE
NMIN = 0
DO 21 L = 1,NSCOR
21 NMIN = NMIN+MINC(L)
IIP = IT(MCLAS)
IF(MAXP - IIP.GE.NUM) GO TO 27
WRITE(NPRINT,91)
GO TO 28
C
C     TEST FOR SIGNIFICANCE FOR ADDITION OF VARIABLE TO KEY
C
27 IF(LEVEL-1.GE.MAXLEV) GO TO 35
CALL TRUNC(MTAB,NO,IFFAULT)
IF(IFFAULT.EQ.1)RETURN
IF(NO + ISIG.LT.3) GO TO 36
IFFAULT = 0
WRITE(NPRINT,92)
C
C     STOP THAT BRANCH
C
28 IIP = NMIN-IIP
WRITE(NPRINT,95)LABEL,MCLAS,NMIN,IIP
DO 30 II = 1,IFLAG
IF(ILSYM(3,II).EQ.LABEL) GO TO 31
30 CONTINUE
31 IF(ITERM(MCLAS).EQ.1) GO TO 32
WRITE(NPUNCH,85)II,ITERM(MCLAS)
GO TO 33
32 ITERM(MCLAS) = II
WRITE(NPUNCH,81)II,MCLAS
33 DO 34 II = LABNO,NCASE
34 IF(ILCSE(II).EQ.LABEL) ILCSE(II) = -MCLAS
GO TO 48
C
C     MAXIMUM LEVELS REACHED
C
35 WRITE(NPRINT,93)
GO TO 28
C
C     WRITE BRANCH STATEMENT
C
36 WRITE(NPRINT,96)LABEL,IPN,NMIN
DO 37 II = 1,IFLAG
IF(ILSYM(3,II).EQ.LABEL) GO TO 38
37 CONTINUE
38 DO 41 J = 1,10
```

```
41  IFST(J) = 1
    WRITE(NPUNCH,82)II,IPN
    DO 43 J = 1,NSCOR
    J1 = J-1
    IF(MINC(J).EQ.0) GO TO 43
    WRITE(NPRINT,97)J1,LABEL,J1,ITMIN(J)
    IFLAG = IFLAG+1
    IF(IFLAG.GT.NKEY) GO TO 60
    ILSYM(3,IFLAG) = LABEL*10+J1
    IFST(J) = IFLAG
43  CONTINUE
    WRITE(NPUNCH,83)IFST
C
C      WRITE BRANCH TERMINAL IE. CLASS =
C
    DO 46 J = 1,NSCOR
    IF(MINC(J).EQ.0 .OR. ITMIN(J).GT.0) GO TO 46
    LAB = LABEL*10+J-1
    WRITE(NPRINT,95)LAB,MEST(J),MINC(J),ITMIN(J)
    MEJ = MEST(J)
    IMJ = ITERM(MEJ)
    IF(IMJ.EQ.1) GO TO 44
    WRITE(NPUNCH,85)IFST(J),IMJ
    GO TO 46
44  ITERM(MEJ) = IFST(J)
    WRITE(NPUNCH,81)IFST(J),MEST(J)
46  CONTINUE
C
C      LABEL THE VARIABLE, CREATING NEW ROW IN ILSYM
C
    NSYMU = NSYMU+1
    IF(NSYMU.GT.NKEY) GO TO 61
    ILSYM(1,NSYMU) = IPN
    ILSYM(2,NSYMU) = LABEL
C
C      ADD A DIGIT TO INDIVIDUAL LABEL
C
    DO 47 I = LABNO,NCASE
    IF(ILCSE(I).NE.LABEL) GO TO 47
    IDA = IDATA(IPN,I) +1
    LAB = ILCSE(I)*10+IDA-1
    IF(ITMIN(IDA).EQ.0) LAB = -MEST(IDA)
    ILCSE(I) = LAB
47  CONTINUE
48  LABNO = LABNO+1
    IF(LABNO.LE.NCASE) GO TO 5
    LEVEL = LEVEL+1
    LEV10 = LEV10*10
    IF(LEVEL.LE.NSYM ) GO TO 4
C
C      TERMINATE PROCEDURE - SUCCESSFUL RETURN
C
49  WRITE(NPRINT,94)
50  LREJ = NCLAS+1
    DO 51 I = 1,NCASE
    ILCSE(I) = -ILCSE(I)
51  CONTINUE
    WRITE(NPUNCH,84)LREJ
    RETURN
C
C      FAULT RETURNS
```

```
C
52  IFAULT = 6
    RETURN
53  IFAULT = 7
    RETURN
54  IFAULT = 8
    RETURN
55  IFAULT = 9
    RETURN
56  IFAULT = 10
    RETURN
57  IFAULT = 11
    RETURN
58  IFAULT = 12
    RETURN
59  IFAULT = 13
    RETURN
60  IFAULT = 14
    RETURN
61  IFAULT = 15
    RETURN
```

```
C
C      FORMATS FOR PUNCHED CARD OUTPUT
C
80  FORMAT(6X,21H FUNCTION ICLAS(ISYM)/6X,16H DIMENSION ISYM(,I5,2H ))
81  FORMAT(1X,I4,1X,7H ICLAS = ,I2/6X,7H RETURN)
82  FORMAT(1X,I4,1X,8H I = ISYM(,I3,3H)+1)
83  FORMAT(6X,8H GO TO (,9(I3,1H, ),I3,3H),I)
84  FORMAT(3X,2H 1,2X,6HICLAS = ,I2/6X,7H RETURN/6X,4H END)
85  FORMAT(1X,I4,1X,7H GO TO ,I3)
```

```
C
C      FORMATS FOR PRINTED OUTPUT
C
91  FORMAT(1H0,47X,61H * REMAINING VARIABLES DO NOT SUFFICIENTLY IMPRO
1VE ERROR RATE)
92  FORMAT(1H0,47X,38H * REMAINING VARIABLES NOT SIGNIFICANT)
93  FORMAT(1H0,47X,34H * SPECIFIED MAXIMUM LEVEL REACHED)
94  FORMAT(1H0,47X,31H * ALL VARIABLES HAVE BEEN USED)
95  FORMAT(1H ,I8,7H CLASS = ,I2,30X,26H * THIS RULE DERIVED USING,I4,
113H INDIVIDUALS.,I6)
96  FORMAT(1H0,I8,13H IF VARIABLE ,I3,9H SCORES -,14X,26H * THIS RULE
1DERIVED USING,I4,20H INDIVIDUALS. ERRORS)
97  FORMAT(32X,I1,6H GO TO,I7,I1,2X,1H*,43X,I4)
    END
```

```
C
    SUBROUTINE IPOWR(I,J,IP,IT,MAXSC,NOC,ITABL,IDATA,ICLSS,ILCSE,NCASE
1,NCLAS,NSCOR,NSYM,IFAU)LT)
```

```
C
C      ALGORITHM AS 165.1  APPL. STATIST. (1981) VOL.30, NO.3
C
C      COMPUTE DISCRIMINATING POWER, IP, OF VARIABLE I FOR A SUBSET OF THE
C      DATA DEFINED BY INDIVIDUAL LABEL J.
C
    DIMENSION IDATA(NSYM,NCASE),ICLSS(NCASE),ILCSE(NCASE)
    DIMENSION ITABL(10,10),IT(10),MAXSC(10),NOC(10)
    DATA ITWO/1/
```

```
C
C      CHECK INPUT VALUES
C
    IF(I.GT.NSYM .OR. I.LT.1) GO TO 9
    IF(NCASE.LT.3) GO TO 10
```

```
      IF(NSYM.LT.3) GO TO 11
      IF(NSCOR.LT.2 .OR. NSCOR.GT.10) GO TO 12
      IF(NCLAS.LT.2 .OR. NCLAS.GT.10) GO TO 13
      DO 1 L = 1,NCASE
      IF(ICLSS(L).LT.1 .OR. ICLSS(L).GT.NCLAS) GO TO 14
      IF(IDATA(I,L).LT.0 .OR. IDATA(I,L).GE.NSCOR) GO TO 15
1     CONTINUE
C
C       TABULATE CLASS BY VARIABLE SCORE FOR THE APPROPRIATE
C       SUBSET OF THE DATA
C
      DO 2 L = 1,10
      DO 2 M = 1,10
2     ITABL(L,M) = 0
      DO 3 L = 1,NCASE
      IF(ILCSE(L).NE.J) GO TO 3
      IND = IDATA(I,L)+1
      ICS = ICLSS(L)
      ITABL(ICS,IND) = ITABL(ICS,IND)+1
3     CONTINUE
      IP = 0
      DO 8 L = 1,NSCOR
      MAX = 1
      NOC(L) = ITABL(1,L)
      DO 7 M = 2,NCLAS
      NOC(L) = NOC(L)+ITABL(M,L)
      IF(ITABL(MAX,L)-ITABL(M,L))5,4,7
4     ITWO = 3-ITWO
      IF(ITWO.EQ.2) GO TO 7
5     MAX = M
7     CONTINUE
      IT(L) = NOC(L) - ITABL(MAX,L)
      MAXSC(L) = MAX
      IP = IP+ITABL(MAX,L)
8     CONTINUE
      IFAULT = 0
      RETURN
C
C       FAULT RETURNS
C
9     IFAULT = 5
      RETURN
10    IFAULT = 6
      RETURN
11    IFAULT = 7
      RETURN
12    IFAULT = 8
      RETURN
13    IFAULT = 9
      RETURN
14    IFAULT = 10
      RETURN
15    IFAULT = 11
      RETURN
      END
C
      SUBROUTINE TRUNC(ITABL,NO,IFAU)
C
C       ALGORITHM AS 165.2 APPL. STATIST. (1981) VOL.30, NO.3
C
      DIMENSION CRIT(36,2),ITABL(10,10),IRT(10),ICT(10)
```

```

DATA CRIT(1,1),CRIT(2,1),CRIT(3,1),CRIT(4,1),CRIT(5,1),CRIT(6,1),
1CRIT( 7,1),CRIT( 8,1),CRIT( 9,1),CRIT(10,1),CRIT(11,1),CRIT(12,1),
1CRIT(13,1),CRIT(14,1),CRIT(15,1),CRIT(16,1),CRIT(17,1),CRIT(18,1),
1CRIT(19,1),CRIT(20,1),CRIT(21,1),CRIT(22,1),CRIT(23,1),CRIT(24,1),
1CRIT(25,1),CRIT(26,1),CRIT(27,1),CRIT(28,1),CRIT(29,1),CRIT(30,1),
1CRIT(31,1),CRIT(32,1),CRIT(33,1),CRIT(34,1),CRIT(35,1),CRIT(36,1)/
1      3.84,      5.99,      7.81,      9.49,      11.07,      12.59,
1      14.07,     15.51,     16.92,     18.31,     19.68,     21.03,
1      22.36,     23.68,     25.00,     26.30,     27.59,     28.87,
1      30.14,     31.41,     32.67,     33.92,     35.17,     36.42,
1      37.65,     38.89,     40.11,     41.34,     42.56,     43.77,
1      55.76,     67.50,     79.08,     90.53,    101.9 ,    113.1/

```

```

DATA CRIT(1,2),
1CRIT( 2,2),CRIT( 3,2),CRIT( 4,2),CRIT( 5,2),CRIT( 6,2),CRIT( 7,2),
1CRIT( 8,2),CRIT( 9,2),CRIT(10,2),CRIT(11,2),CRIT(12,2),CRIT(13,2),
1CRIT(14,2),CRIT(15,2),CRIT(16,2),CRIT(17,2),CRIT(18,2),CRIT(19,2),
1CRIT(20,2),CRIT(21,2),CRIT(22,2),CRIT(23,2),CRIT(24,2),CRIT(25,2),
1CRIT(26,2),CRIT(27,2),CRIT(28,2),CRIT(29,2),CRIT(30,2),CRIT(31,2),
1CRIT(32,2),CRIT(33,2),CRIT(34,2),CRIT(35,2),CRIT(36,2)/
16.63, 9.21,     11.34,     13.28,     15.09,     16.81,     18.48,
1      20.09,     21.67,     23.21,     24.73,     26.22,     27.69,
1      29.14,     30.58,     32.00,     33.41,     34.81,     36.19,
1      37.57,     38.93,     40.29,     41.64,     42.98,     44.31,
1      45.64,     46.96,     48.28,     49.59,     50.89,     63.69,
1      76.15,     88.38,    100.4 ,    112.3 ,    124.1/

```

```

NO = 0
IFFAULT = 0

```

```

C
C      COMPUTE ROW AND COLUMN TOTALS, NOTING EMPTY ROWS AND COLUMNS
C

```

```

NROWS = 0
DO 2 I = 1,10
  IR = 0
  DO 1 J = 1,10
    IF(ITABL(I,J).LT.0) GO TO 13
    IR = IR+ITABL(I,J)
1  CONTINUE
  IF(IR.GT.0)NROWS = NROWS+1
  IRT(I) = IR
2  CONTINUE
  IF(NROWS.LT.2) GO TO 15
  NCOLS = 0
  DO 4 I = 1,10
    IC = 0
    DO 3 J = 1,10
      IC = IC+ITABL(J,I)
3  CONTINUE
  IF(IC.GT.0)NCOLS = NCOLS+1
  ICT(I) = IC
4  CONTINUE
  IF(NCOLS.LT.2) GO TO 16
  IGT = 0
  DO 5 I = 1,10
    IGT = IGT+IRT(I)
5  IF(IGT.EQ.0) GO TO 14

```

```

C
C      COMPUTE G STATISTIC (LIKELIHOOD RATIO TEST)
C
G = 0.0
DO 8 J = 1,10
  IF(ICT(J).EQ.0) GO TO 8

```

```
FAC = FLOAT(IGT)/FLOAT(ICT(J))
DO 7 I = 1,10
IF(IRT(I).EQ.0) GO TO 7
IJOBS = ITABL(I,J)
IF(IJOBS.EQ.0) GO TO 7
OBSIJ = FLOAT(IJOBS)
AL = OBSIJ*FAC/FLOAT(IRT(I))
G = G + OBSIJ*ALOG(AL)
7 CONTINUE
8 CONTINUE
G = 2.0*G
NDF = (NROWS - 1)*(NCOLS - 1)
C
C     COMPARE G WITH TABLE OF CRITICAL VALUES OF CHI-SQUARE,
C     OR INTERPOLATE
C
IF(NDF.LE.30) GO TO 11
NC = NDF/10
NCRITL = NC*10
IF(NCRITL.EQ.NDF) GO TO 10
CL1 = CRIT(NC+27,1)
CL2 = CRIT(NC+27,2)
CH1 = CRIT(NC+28,1)
CH2 = CRIT(NC+28,2)
F = FLOAT(NDF - NCRITL)/10.0
CRIT1 = CL1 + (CH1 - CL1)*F
CRIT2 = CL2 + (CH2 - CL2)*F
GO TO 12
10 NDF = NC+27
11 CRIT1 = CRIT(NDF,1)
CRIT2 = CRIT(NDF,2)
12 IF(G.LT.CRIT2)NO = 1
IF(G.LT.CRIT1)NO = 2
RETURN
C
C     FAULT RETURNS
C
13 IFAULT = 1
RETURN
14 IFAULT = 2
RETURN
15 IFAULT = 3
RETURN
16 IFAULT = 4
RETURN
END
```



```

SUBROUTINE ENTNGL(IP, L, M, NPTS, IDES, NP, NINTER, ITERMS, NTP,
*   A, NA, X, NX, W, NW, IFAULT)
C
C   ALGORITHM AS 166  APPL. STATIST. (1981) VOL.30, NO.3
C
C   CALCULATES THE ENTANGLEMENT MATRIX FOR A SPECIFIED DESIGN
C
C   *** Warning ***
C   A scanner was used to enter this text - it may contain errors!
C
C   INTEGER L(IP), M(IP), IDES(NP), ITERMS(NTP)
C   REAL W(NW), A(NA), X(NX)
C   LOGICAL XXONLY
C   DATA ZERO, POINT4, ONE /0.0, 0.4, 1.0/
C
C   CHECK PARAMETERS FOR ERRORS
C
C   IFAULT = 0
C   ID = 0
C   XXONLY = NINTER .EQ. 0
C   IF (IP .LE. 0 .OR. NPTS .LE. 0 .OR. NINTER .LT. 0 .OR.
*   NTP .LT. IP * NINTER) IFAULT = 5
C   IF (NP .LT. NPTS * IP) IFAULT = 6
C   LSUM = 0
C   MSUM = 0
C   LMSUM = 0
C   MAXL = 0
C   DO 10 JA = 1, IP
C     LJA = IABS(L(JA))
C     MJA = M(JA)
C     IF (MJA .LE. 0 .OR. MJA .GE. LJA .OR. LJA .EQ. 0 .OR.
*     LJA .GT. NPTS) IFAULT = 7
C     IF (XXONLY) GOTO 3
C     IT = JA
C     DO 2 JB = 1, NINTER
C       J = ITERMS(IT)
C       IF (J .LT. 0 .OR. J .GT. MJA) IFAULT = 13
C       IT = IT + IP
2    CONTINUE
3    IF (LJA .GT. MAXL) MAXL = LJA
C     LSUM = LSUM + LJA
C     MSUM = MSUM + MJA
C     LMSUM = LMSUM + LJA * MJA
C     DO 5 I = 1, NPTS
C       ID = ID + 1
C       LIJ = IDES(ID)
C       IF (LIJ .LT. 0 .OR. LIJ .GE. LJA) IFAULT = 1
5    CONTINUE
10   CONTINUE
C   MSIZE = MSUM + NINTER
C   LASTA = MSIZE * (MSIZE + 1) / 2
C   IF (NA .LT. LASTA) IFAULT = 8
C   XXONLY = NX .EQ. 1
C   IF (NX .LT. MSIZE * NPTS .AND. .NOT. XXONLY) IFAULT = 9
C   LASTW = LSUM + MAXL + MAXL + 2 + LMSUM + MSUM + NINTER + NINTER
C   IF (NW .LT. LASTW) IFAULT = 10
C   IF (IFAULT .NE. 0) RETURN
C
C   INITIALIZE LAST PART OF W TO ZERO
C
C   IWG = LASTW - NINTER + 1

```

```
      DO 15 IW = IWG, LASTW
15  W(IW) = ZERO
C
C      CALCULATE ORTHOGONAL POLYNOMIAL COEFFICIENTS FOR EACH FACTOR
C
      LIMWD = LSUM + MAXL + MAXL + 2
      IWD = LIMWD
      ID = 0
      LIMWB = LSUM + 1
      LIMWC = LIMWB + MAXL
      DO 100 JA = 1, IP
        KR = 0
        LJA = IABS(L(JA))
        MJA = M(JA)
        IF (LJA .EQ. 2) GOTO 52
C
C      (1)  FACTORS WITH THREE OR MORE LEVELS
C
      DO 16 J = 1, LJA
        IW = LSUM + J
        W(IW) = ZERO
16  CONTINUE
      DO 18 I = 1, NPTS
        ID = ID + 1
        IW = IDES(ID) + LIMWB
        W(IW) = W(IW) + ONE
18  CONTINUE
      CONST = FLOAT(NPTS / LJA)
      IFAULT = 12
      DO 19 J = 1, LJA
        IW = LSUM + J
        IF (ABS(W(IW) - CONST) .GT. POINT4) RETURN
19  CONTINUE
      CONST = ONE / SQRT(CONST)
      IFAULT = 0
      IF (L(JA) .LT. 0) GOTO 40
      DO 20 J = 1, LJA
        IW = IWA + J
        W(IW) = FLOAT(J)
20  CONTINUE
40  IW = IWA + 1
      CALL ORTHON(0, W(IW), W(LIMWB), W(LIMWC), LJA, LJA+2, IFAULT)
      IF (IFAILT .NE. 0 .AND. IFAULT .NE. 2) RETURN
      IF (IFAILT .EQ. 2) IFAIL = 2
50  KR = KR + 1
      IF (KR .GT. MJA) GOTO 80
      CALL ORTHON(KR, W(IW), W(LIMWB), W(LIMWC), LJA, LJA+2, IFAULT)
      IF (IFAILT .NE. 0 .AND. IFAULT .NE. 2) RETURN
      GOTO 58
C
C      (2)  FACTORS WITH TWO LEVELS ONLY (POSSIBLY OCCURRING UNEQUALLY)
C
52  ISUM = 0
      DO 54 I = 1, NPTS
        ID = ID + 1
        ISUM = ISUM + IDES(ID)
54  CONTINUE
      CONST = FLOAT(ISUM) / FLOAT(NPTS)
      W(LIMWB) = -CONST
      W(LIMWB + 1) = ONE - CONST
      CONST = 1.0 / SQRT(CONST * FLOAT(NPTS - ISUM))
```

```
C
C          COPY COEFFICIENTS FROM WORKSPACE AREA TO STORAGE AREA
C
58 DO 60 J = 1, LJA
    IWD = IWD + 1
    IWB = LSUM + J
    W(IWD) = W(IWB) + CONST
60 CONTINUE
    IF (LJA .NE. 2) GOTO 50
80 IWA = IWA + LJA
100 CONTINUE
C
C          PREPARE TO SET UP A
C
    LIMWE = IWD
    DO 120 IA = 1, LASTA
120 A(IA) = ZERO
C
C          ADD EACH DESIGN POINT INTO A
C
    LIMWD = LIMWD + 1
    DO 240 I = 1, NPTS
    ID = 0
C
C          (1) MAIN EFFECTS
C
    IWD = LIMWD
    IWE = LIMWE
    DO 140 JA = 1, IP
    LJA = IABS(L(JA))
    MJA = M(JA)
    LIJ = ID + I
    LIJ = IDES(LIJ)
    DO 130 J = 1, MJA
    IWE = IWE + 1
    IW = IWD + LIJ
    W(IWE) = W(IW)
    IWD = IWD + LJA
130 CONTINUE
    ID = ID + NPTS
140 CONTINUE
C
C          (2) INTERACTIONS
C
    IF (NINTER .EQ. 0) GOTO 200
    IT = 0
    IWF = IWE
    IWG = IWF + NINTER
    DO 180 JB = 1, NINTER
    IWF = IWF + 1
    IWG = IWG + 1
    WW = ONE
    IWE = LIMWE
    DO 160 JA = 1, IP
    IT = IT + 1
    IF (ITERMS(IT) .EQ. 0) GOTO 150
    IW = IWE + ITERMS(IT)
    WW = WW * W(IW)
150 IWE = IWE + M(JA)
160 CONTINUE
    W(IWF) = WW
```

```

      W(IWG) = W(IWG) + WW
180 CONTINUE
C
C      CALCULATE THE TERMS IN THE SSP MATRIX
C
200 IA = 1
   DO 220 JA = 1, MSIZE
      IW = LIMWE + JA
      DO 210 JB = 1, JA
         IW2 = LIMWE + JB
         A(IA) = A(IA) + W(IW) * W(IW2)
         IA = IA + 1
210 CONTINUE
220 CONTINUE
C
C      STORE CONTRASTS IN X
C
   IF (XXONLY) GOTO 240
   I X = I
   DO 230 JA = 1, MSIZE
      IW = LIMWE + JA
      X(IX) = W(IW)
      IX = IX + NPTS
230 CONTINUE
240 CONTINUE
C
C      ADJUST INT X INT TERMS IN A ABOUT THEIR MEANS
C      (TERMS INVOLVING MAIN EFFECTS ARE ALREADY CENTRED)
C
   IF (NINTER .EQ. 0) RETURN
   J = MSUM + 1
   IA = J * MSUM / 2
   IA2 = IA
   IWG = IWG - MSIZE
   CONST = ONE / FLOAT(NPTS)
   DO 260 JA = J, MSIZE
      IA = IA + J - 1
      IW = IWG + JA
      DO 250 JB = J, JA
         IA = IA + 1
         IW2 = IWG + JB
         A(IA) = A(IA) - W(IW) * W(IW2) * CONST
250 CONTINUE
260 CONTINUE
C
C      CALCULATE 1 / SQRT(DIAG(A)) AND STORE
C
   IWE = LIMWE
   IA = 0
   DO 320 JA = 1, MSIZE
      IA = IA + JA
      IWE = IWE + 1
      W(IWE) = 1.0 / SQRT(LA(IA))
320 CONTINUE
C
C      CONVERT A FROM A SSP-TYPE MATRIX TO A CO
C
   DO 360 JA = J, MSIZE
      IW = LIMWE + JA
      WW = W(IW)
```

```
      DO 350 JB = 1, JA
        IW2 = LIMWE + JB
        IA2 = IA2 + 1
        A(IA2) = A(IA2) * WW * W(IW2)
350    CONTINUE
360    CONTINUE
C
C      STANDARDIZE INTERACTION CONTRASTS
C
      IF (XXONLY) RETURN
      IWG = IWE
      IWE = IWE - NINTER
      IX = (J - 1) * NPTS
      DO 400 JA = 1, NINTER
        IWE = IWE + 1
        IWG = IWG + 1
        XBAR = W(IWG) + 1
        WW = W(IWE)
        DO 380 I = 1, NPTS
          IX = IX + 1
          X(IX) = WW * (X(IX) - XBAR)
380    CONTINUE
400    CONTINUE
      RETURN
      END
```

```

SUBROUTINE FIT(A, NA, NTERMS, MSIZE, IE, INC, NINC, NADD,
*   GVAR, KEY, EFF, EPS, IFAULT)

```

```

C
C   ALGORITHM AS 167  APPL. STATIST. (1981)  VOL.30, NO.3
C
C   CALCULATES EFFICIENCIES OF ESTIMATION OF TERMS IN
C   THE CURRENT MODEL AND ITS GENERALIZED VARIANCE
C
C   *** Warning: This text has been read using a scanner and may
C               contain errors
C

```

```

REAL A(NA), EFF(NTERMS)
INTEGER INC(NINC), IE(NTERMS), KEY(NTERMS)
DATA ONE /1.0/
IFault = 0
IA = NTERMS * (NTERMS + 1) / 2
IF (NA .LT. IA) IFAULT = 2
IF (MSIZE .LT. 0 .OR. NADD .LE. 0 .OR. NADD .GT. NINC)
+   IFAULT = 3
IF (MSIZE .NE. 0 .OR. IFAULT .NE. 0) GOTO 5
ONEPLS = ONE + EPS
ONEMIN = ONE - EPS
IA = 0
DO 3 J1 = 1, NTERMS
DO 1 J2 = 1, J1
IA = IA + 1
R = A(IA)
IF (R .LT. -ONEPLS .OR. R .GT. ONEPLS) IFAULT = 1
1 CONTINUE
IF (R .LT. ONEMIN) IFAULT = 1
IE(J1) = -1
3 CONTINUE
GVAR = ONE
5 IF (IFault .NE. 0) RETURN
DO 20 J = 1, NADD
JP = INC(J)
IF (JP .LE. 0 .OR. JP .GT. NTERMS) GOTO 50
IF (IABS(IE(JP)) .NE. 1) GOTO 50
IA = JP * (JP + 1) / 2
IF (ABS(A(IA)) .LE. EPS) GOTO 19
IF (IE(JP) .LT. 0) GOTO 16

```

```

C
C   DROP TERM FROM MODEL
C
K = MSIZE - 1
DO 12 J1 = 1, K
IF (JP .NE. KEY(J1)) GOTO 12
DO 8 J2 = J1, K
8 KEY(J2) = KEY(J2 + 1)
GOTO 13
12 CONTINUE
13 MSIZE = K
GVAR = -GVAR / A(IA)
CALL PIVOT(A, NA, NTERMS, JP, IE)
GOTO 20

```

```

C
C   ADD TERM TO MODEL
C
16 MSIZE = MSIZE + 1
KEY(MSIZE) = JP
CALL PIVOT(A, NA, NTERMS, JP, IE)

```

```
      GVAR = -GVAR * A(IA)
      GOTO 20
C
C      LEAVE TERM IN OR OUT OF MODEL AS PIVOT TOO SMALL
C
19 IFAULT = -JP
20 CONTINUE
C
C      CALCULATE EFFICIENCIES OF EACH TERM IN MODEL
C
      DO 40 J = 1, MSIZE
      IA = IA * (IA + 1) / 2
      EFF(J) = -ONE / A(IA)
40 CONTINUE
      RETURN
50 IFAULT = 4
      RETURN
      END
C
      SUBROUTINE PIVOT(A, NA, K, IP, IE)
C
C      ALGORITHM AS 167.1  APPL. STATIST. (1981) VOL.30, NO.3
C
C      ROW BY ROW INVERSION IN SITU OF A SYMMETRIC MATRIX STORED AS
C      LOWER TRIANGLE. A FORTRAN TRANSLATION OF ALGORITHM AS 37
C      (GARSIDE, 1971)
      REAL A(NA)
      INTEGER IE(K)
C
      DATA ONE /1.0/
      JP = IABS(IP)
      JPP = JP * (JP + 1) / 2
      JOP = JPP - JP
      AA = ONE / A(JPP)
      A(JPP) = -AA
      NIJ = 0
      IF (JP .EQ. 1) GOTO 100
      JP1 = JP - 1
      DO 80 I = 1, JP1
      NIP = JOP + I
      AIP = -A(NIP) * FLOAT(IE(JP))
      A(NIP) = AIP * AA
      DO 60 J = 1, I
      NIJ = NIJ + 1
      NJP = JOP + J
      A(NIJ) = A(NIJ) - AIP * A(NJP)
60 CONTINUE
80 CONTINUE
100 IF (JP .EQ. K) GOTO 190
      NIJ = NIJ + JP
      JP2 = JP + 1
      NIP = JPP
      DO 150 I = JP2, K
      NIP = NIP + I - 1
      AIP = -A(NIP) * FLOAT(IE(JP))
      A(NIP) = AIP * AA
      IF (JP .EQ. 1) GOTO 130
      DO 110 J = 1, JP1
      NIJ = NIJ + 1
      NJP = JOP + J
      A(NIJ) = A(NIJ) - AIP * A(NJP)
```

```
110 CONTINUE
130 NIJ = NIJ + 1
    NJP = JPP + JP
    DO 140 J = JP2, I
    NIJ = NIJ + 1
    A(NIJ) = A(NIJ) - AIP * A(NJP)
    NJP = NJP + J
140 CONTINUE
150 CONTINUE
190 IE(JP) = -IE(JP)
    RETURN
    END
```



```

      subroutine scale(fmn, fmx, n, mpv, valmin, step, nvals,
*   ir, ifault)
c
c   algorithm as 168  appl. statist. (1981) vol.30, no.3
c
c   calculates neat values for lowest print position and
c   step between printed values on a scale to include fmn
c   and fmx
c
      real unit(12)
      real tol, bias
      data nunit /12/
      data unit(1), unit(2), unit(3), unit(4), unit(5), unit(6),
*   unit(7), unit(8), unit(9), unit(10), unit(11), unit(12)
*   /12.0, 15.0, 20.0, 25.0, 30.0, 40.0,
*   50.0, 60.0, 80.0, 100.0, 120.0, 150.0/
      data tol /5.0e-6/, bias /1.0e-5/
      data minn /2/, maxn /10000/, cover /0.7/
c
      fmax = fmx
      fmin = fmn
c
      test for valid parameters
c
      ifault = 0
      if (fmax .lt. fmin) ifault = ifault + 1
      if (n .lt. minn .or. n .gt. maxn) ifault = ifault + 2
      if (mpv .le. 0 .or. mpv .ge. n) ifault = ifault + 4
      if (ifault .ne. 0) return
      nvals = (n - 1) / mpv + 1
c
      test for values effectively equal
c
      if (fmax - fmin .gt. tol * amax1(abs(fmax), abs(fmin))) goto 20
      ifault = -1
      if (fmax) 5, 10, 15
5 fmax = 0.0
      goto 20
10 fmax = 1.0
      goto 20
15 fmin = 0.0
c
      find neat trial step size
c
20 finter = float(n) / float(mpv)
      s = (fmax - fmin) * (1.0 + 2.0 * bias) / finter
      ir = 0
25 if (s .gt. 10.0) goto 30
      s = s * 10.0
      ir = ir + 1
      goto 25
30 if (s .le. 100.0) goto 35
      s = s / 10.0
      ir = ir - 1
      goto 30
35 do 40 i = 1, nunit
      if (s .le. unit(i)) goto 45
40 continue
45 step = 10.0 ** (-ir) * unit(i)
c
c   find neat trial start value
c

```

```
    aj = 0.0
50  aj = aj + 1.0
    if (unit(i) - 0.1 .gt. aint((unit(i) + 0.1) / aj) * aj) goto 50
    tstep = step / aj
    temp = fmin / tstep + aj * (0.5 / float(mpv) - finter * bias)
    valmin = aint(temp) * tstep
    if (temp .lt. 0.0 .and. temp .ne. aint(temp))
*   valmin = valmin - tstep
c
c     test whether fmax is in scale
c
c     if (fmax .lt. valmin + step *
*   (finter * (1.0 - bias) - 0.5 / float(mpv))) goto 55
c
c     try new step or start value
c
c     if (unit(i) / unit(i + 1) * (1.0 - 1.0 / (aj * finter)) .lt.
*   cover) goto 50
    i = i + 1
    goto 45
c
c     get position of least significant figure on scale
c
55 do 60 j = 1, 2
    aj = aj * 10.0
    if (unit(i) - 0.1 .lt. aint((unit(i) + 0.1) / aj) * aj)
*       ir = ir - 1
60 continue
    return
end
c
c   subroutine axis(valmin, step, nvals, maxpr, ir, irprin, offset,
*   ifact, vals, iv, ifault)
c
c     algorithm as 168.1 appl. statist. (1981) vol.30, no.3
c
c     sets up values and formats for printing on an axis
c
c   real vals(iv)
c   data irmax /20/, mprmax /20/
c
c     check for valid parameters
c
c   ifault = 0
c   if (nvals .lt. 2) ifault = ifault + 1
c   fmax = valmin + step * float(nvals - 1)
c   if (nvals .ge. 2 .and. fmax .le. valmin) ifault = ifault + 2
c   if (maxpr .lt. 2 .or. maxpr .gt. mprmax) ifault = ifault + 4
c   if (nvals .gt. iv) ifault = ifault + 8
c   if (ir .gt. irmax) ifault = ifault + 16
c   if (ifault .gt. 0) return
c
c     find position of most significant digit(il) and number of
c     significant digits overall(is) and varying(it)
c
c   tmax = 10.0 ** maxpr
c   fl = abs(fmax)
c   fs = abs(valmin)
c   il = 0
10  if (fl .lt. 1.0 .and. fs .lt. 1.0) goto 20
    fl = fl / 10.0
    fs = fs / 10.0
```

```
    il = il + 1
    goto 10
c
20 if (fl .ge. 0.1 .or. fs .ge. 0.1) goto 30
    fl = fl * 10.0
    fs = fs * 10.0
    il = il - 1
    goto 20
c
30 is = il + ir
    it = is
    if (valmin .le. 0.0 .and. fmax .ge. 0.0) goto 50
40 fl = mod(fl, 1.0) * 10.0
    fs = mod(fs, 1.0) * 10.0
    if (it .le. 0) goto 1016
    if (int(fl) .ne. int(fs)) goto 50
    it = it - 1
    goto 40
c
c    decide on printing format
c
50 ifact = 0
    offset = 0.0
    irprin = max(ir, 0)
    ilprin = max(il, 0)
c
    if (irprin + ilprin .le. maxpr) goto 70
    if (is .le. maxpr) goto 60
    irprin = maxpr - 1
    ifact = max(it, maxpr) - 1 - ir
    goto 70
60 ifact = il - 1
    irprin = is - 1
70 fs = 10.0 ** (-ifact)
    vstep = step * fs
    vmin = valmin * fs
    if (is .le. maxpr) goto 80
    offset = aint(vmin / 10.0) * 10.0
    vmin = vmin - offset
c
c    write values for axis
c
80 do 90 i = 1, nvals
    vals(i) = vmin
    vmin = vmin + vstep
90 continue
c
c    check that all values can be printed
c
    fs = 0.1 ** irprin
    if (abs(vals(1)) * fs + 0.5 .lt. tmax .and.
* abs(vals(nvals)) * fs + 0.5 .lt. tmax) return
    il = il + 1
    is = is + 1
    it = it + 1
    goto 50
c
c    error indicator
c
1016 ifault = 16
    return
```

end

```

      subroutine scatpl(a, n, m, icy, ncy, icx, ny, nx, scaley,
*   scalex, istand, ifault, iwrite)
c
c   algorithm as 169  appl. statist. (1981) vol.30, no.3
c
c   produces a scatter plot of one variable against several
c
character*1 iout,intch,markch,iblack,idot,icolon
character*1 icomma,iapost,isemi,itwo,idash,form21*14,form22*6
character iform1*20,iform2*21,form11*8,form12*11
dimension iout(161), vals(20), a(n, m), icy(ncy), scalex(2),
*   scaley(2), intch(11), markch(5)
data maxwid /132/, maxht /50/, maxy /5/
data mpvx /10/, mpvy /5/
data intch(1), intch(2), intch(3), intch(4), intch(5), intch(6),
*   intch(7), intch(8), intch(9), intch(10), intch(11)
*   /'0', '1', '2', '3', '4', '5', '6', '7', '8', '9', '9'/
data markch(1), markch(2), markch(3), markch(4), markch(5)
*   /'*', '0', '+', 'x', '='/
data iblack /' '/, idot /'.'/, icolon /':'/, icomma /','/,
*   iapost /'''/, isemi /';'/, itwo /'2'/, idash /'-'/
c
c   formats for printing
c
data iform1 /'(1h ,f8.0,1x,152a1) '/
data iform2 /'(1h ,5x,16(f8.0,2x)) '/
c
1 format(' ', 10x, ':', 151a1)
2 format(' times 10**', i3)
3 format(' offset', f10.0)
4 format(' ', 14x, 'times 10**', i3)
5 format(' ', 14x, 'offset', f10.0)
6 format(' ', 2x, 16(9x, a1))
c
c   test for valid parameters
c
ifault = 0
if (n .lt. 1) ifault = ifault + 1
if (m .lt. 2) ifault = ifault + 2
if (icx .lt. 1 .or. icx .gt. m) ifault = ifault + 4
if (ncy .le. 0 .or. ncy .gt. maxy) ifault = ifault + 8
if (ifault .gt. 0) return
do 10 i = 1, ncy
  if (icy(i) .lt. 1 .or. icy(i) .gt. m) goto 1016
10 continue
c
c   set plot size
c
nly = maxht - 5
if (nly .gt. ny) nly = ny
if (nly .le. mpvy) nly = mpvy + 1
nlx = maxwid - 11
if (nlx .gt. nx) nlx = nx
if (nlx .le. mpvx) nlx = mpvx + 1
c
c   calculate horizontal scale
c
xmin = scalex(1)
xmax = scalex(2)
if (xmax .gt. xmin) goto 30
xmin = a(1, icx)

```

```

    xmax = xmin
    if (n .eq. 1) goto 30
    do 20 i = 2, n
        ai = a(i, icx)
        if (ai .lt. xmin) xmin = ai
        if (ai .gt. xmax) xmax = ai
20 continue
c
30 call scale(xmin, xmax, nlx, mpvx, temp, xvstep,
* nxvals, irx, ifail)
    if (ifail .gt. 0) goto 1032
    xmin = temp
    xstep = xvstep / float(mpvx)
c
c     calculate vertical scale
c
    ymin = scaley(1)
    ymax = scaley(2)
    if (ymax .gt. ymin) goto 50
    k = icy(1)
    ymin = a(1, k)
    ymax = ymin
    do 40 j = 1, ncy
        k = icy(j)
        do 40 i = 1, n
            ai = a(i, k)
            if (ai .lt. ymin) ymin = ai
            if (ai .gt. ymax) ymax = ai
40 continue
c
50 call scale(ymin, ymax, nly, mpvy, temp, yvstep,
* nyvals, iry, ifail)
    if (ifail .gt. 0) goto 1064
    ymin = temp
    ystep = yvstep / float(mpvy)
c
c     calculate printed values and set mark for 2 points
c
    call axis(ymin, yvstep, nyvals, 6, iry, irpr, offset,
* ifact, vals, 20, ifail)
    if (ifail .gt. 0) goto 1064
    read(iform1, '(a8,lx,a11)')form11,form12
    write(iform1, '(a8,a1,a11)')form11,intch(irpr + 1),form12
    if (ifact .ne. 0) write (iwrite, 2) ifact
    if (offset .ne. 0.0) write (iwrite, 3) offset
    if (istand .eq. 0) intch(3) = isemi
c
c     for each line of output
c
    iplted = 0
    do 140 i = 1, nly
        iy = nly - i
        do 60 ix = 1, nlx
60    iout(ix) = iblank
c
c     scan data for points on current line
c
    do 120 l = 1, n
        indx = (a(1, icx) - xmin) / xstep + 1.5
        if (indx .lt. 1 .or. indx .gt. nlx) goto 120
        do 110 j = 1, ncy
```

```

        k = icy(j)
        y = (a(l, k) - ymin) / ystep
        indy = y + 0.5
        if (indy .ne. iy) goto 110
        iplted = iplted + 1
        if (iout(indx) .ne. iblank) goto 80
c
c      single point
c
        if (istand .eq. 0) goto 70
        iout(indx) = markch(j)
        goto 110
70      iout(indx) = icomma
        if (int(y) .eq. iy) iout(indx) = iapost
        goto 110
c
c      multiple points
c
80      do 90 ic = 3, 10
        if (iout(indx) .eq. intch(ic)) goto 100
90      continue
        ic = 2
100     iout(indx) = intch(ic + 1)
110     continue
120     continue
c
c      print line
c
        if (mod(iy, mpvy) .eq. 0) goto 130
        write (iwrite, 1) (iout(ix), ix = 1, nlx)
        goto 140
130    write (iwrite, iform1) vals(nyvals), idash, icolon,
*      (iout(ix), ix = 1, nlx)
        nyvals = nyvals - 1
140    continue
c
c      print horizontal axis using variable formats
c
        write (iwrite, 1) (idot, i = 1, nlx)
        call axis(xmin, xvstep, nxvals, 6, irx, irpr, offset,
* ifact, vals, 20, ifail)
        intch(3) = itwo
        read(iform2, '(a14,1x,a6)')form21,form22
        write(iform2, '(a14,a1,a6)')form21,intch(irpr + 1),form22
        if (ifail .gt. 0) goto 1032
        write (iwrite, 6) (icolon, i = 1, nxvals)
        write (iwrite, iform2) (vals(i), i = 1, nxvals)
        if (ifact .ne. 0) write (iwrite, 4) ifact
        if (offset .ne. 0.0) write (iwrite, 5) offset
        ifault = iplted - n * ncy
        return
c
c      set error indicator
c
1064   ifault = ifault + 32
1032   ifault = ifault + 16
1016   ifault = ifault + 16
        return
        end

```

```
C UKC NETLIB DISTRIBUTION COPYRIGHT 1990 RSS
C
C     FUNCTION CHISQN(X, DF, FL, IFAULT)
C
C<<<<<  Acquired in machine-readable form from 'Applied Statistics'
C<<<<<  algorithms editor, January 1983.
C
C
C     ALGORITHM AS 170  APPL. STATIST. (1981) VOL.30, NO.3
C
C     The non-central chi-squared distribution.
C
C     Auxiliary routines required: GAMMDS = AS147, ALOGAM = CACM 291.
C     See AS245 for an alternative to ALOGAM.
C
C     CHISQN = 0.0
C     IFAULT = 0
C
C     TEST FOR ADMISSIBILITY OF ARGUMENTS
C
C     IF (DF.LE.0.0) IFAULT = 1
C     IF (X.LT.0.0) IFAULT = 2
C     IF (FL.LT.0.0) IFAULT = 3
C     IF (IFAUULT.GT.0.OR.X.EQ.0.0) RETURN
C
C     DF2 = 0.5*DF
C     X2 = 0.5*X
C     FXP = GAMMDS(X2,DF2,IFAUULT)
C     CHISQN = CHI(X2,DF2,FL,FXP)
C     RETURN
C     END
C
C     SUBROUTINE CHISQL(X, DF, FX, FL, IFAULT)
C
C     ALGORITHM AS 170.1  APPL.STATIST. (1981) VOL.30, NO.3
C
C     DEFINE ACCURACY AND INITIALIZE
C
C     N SHOULD BE SPECIFIED SUCH THAT ACC IS GREATER THAN
C     OR EQUAL TO (AU-AL)/2**N
C
C     PARAMETER (ACC = 1.0E-6, N = 30)
C
C     AL = 0.0
C     AINC = 80.0
C     AU = 80.0
C
C     IFAULT = 0
C
C     TEST FOR ADMISSIBILITY OF ARGUMENTS
C
C     IF (DF.LE.0.0) IFAULT = 1
C     IF (X.LT.0.0) IFAULT = 2
C     IF (FX.LE.0.0) IFAULT = 3
C     IF (IFAUULT.GT.0) GO TO 4
C
C     DF2 = 0.5*DF
C     X2 = 0.5*X
C     FX1 = GAMMDS(X2,DF2,IFAUULT)
C 1 APROX = CHI(X2,DF2,AU,FX1)
C     IF (FX.GT.APROX) GOTO 2
```



```
      IF (FX.LT.APROX) AL = AU
      AU = AU+AINC
      GO TO 1
2 DO 3 J = 1,N
      FL = 0.5*(AL+AU)
      APROX = CHI(X2, DF2, FL, FX1)
      IF (ABS(FX-APROX).LT.ACC) GO TO 4
      IF (FX.LT.APROX) AL = FL
      IF (FX.GE.APROX) AU = FL
3 CONTINUE
4 RETURN
END
```

```
C
      FUNCTION CHI(X, DF, FL, FXC)
C
C      ALGORITHM AS 170.2  APPL. STATIST. (1981) VOL.30, NO.3
C
      PARAMETER (ACC2 = 1.0E-8)
C
      CHI = FXC
      DF1 = DF
      FL2 = 0.5*FL
      C = 1.0
      T = 0.0
1 T = T+1.0
      C = C*FL2/T
      DF1 = DF1+1.0
      TERM = C*GAMMDS(X, DF1, IFAULT)
      CHI = CHI+TERM
      IF (TERM.GE.ACC2) GO TO 1
      CHI = CHI*EXP(-FL2)
      RETURN
END
```

```

SUBROUTINE TPSHV(N, T, NTMAX, SY2, PROB, KGP, KPR, A, KF, DLF,
*      IFAULT)
C
C      ALGORITHM AS 171 APPL. STATIST. (1982) VOL.31, NO.3
C
C      Fisher's exact variance test for the Poisson distribution
C
      INTEGER T, SY2, TS, A(T), KF(T)
      REAL DD, DC, DM, DMIN, DP, D1, DZ, DPRB, DLF(NTMAX)
      DATA MAXP /1000000/, MAXT /80/
C
      IFAULT = 0
      DPRB = DZ
      DM = D1 - DMIN
      IF (N .LT. 2 .OR. N .GT. NTMAX) IFAULT = 2
      IF (T .LT. 2 .OR. T .GT. NTMAX .OR. T .GT. MAXT) IFAULT = 3
      IF (IFAULT .NE. 0) GO TO 200
      KGP = 0
      KPR = 0
C
C      Generate log factorials and constant
C
      DLF(1) = DZ
      DO 10 I = 2, NTMAX
10  DLF(I) = DLF(I-1) + LOG(FLOAT(I))
      DC = - T * LOG(FLOAT(N)) + DLF(N) + DLF(T)
C
C      Generate partitions of sample total (T) starting with M the
C      number of non-zero values in the sample.
C
      M = MIN(T, N)
      DO 15 J = 1, M
15  KF(J) = 0
      DO 20 J = 1, M
20  DO 25 J = 1, M
25  A(J) = 1
      TS = M - 1
30  A(M) = T
      DO 35 J = 2, M
35  A(M) = A(M) - A(J-1)
      TS = TS + A(M)**2
      KGP = KGP + 1
C
C      The current M-part partition of T:
C      A(1) + A(2) + ... + A(M) = T
C      with sums of squares TS = SUM A(J)**2
C      is admissible if TS < SY2
C
      IF (TS .GE. SY2) GO TO 80
C
C      Convert sample into frequency distribution.
C      KZ is the number of zero values in the sample.
C      KF(J) is the number of A()'s = J.
C
      KZ = N - M
      MX = A(M)
      DO 60 J = 1, M
      IAK = A(J)
      KF(IAK) = KF(IAK) + 1
60 CONTINUE
C
C      Compute DP = probability for this sample

```

```
C
  KPR = KPR + 1
  DD = DZ
  IF (KZ .GT. 0) DD = DLF(KZ)
  IAK = KF(1)
  IF (KF(1) .GT. 0) DD = DD + DLF(IAK)
  KF(1) = 0
  IF (MX .LT. 2) GO TO 70
  DO 65 J = 2, MX
    IF (KF(J) .EQ. 0) GO TO 65
    IAK = KF(J)
    DD = DD + DLF(IAK) + KF(J) * DLF(J)
    KF(J) = 0
65 CONTINUE
70 DP = EXP(DC - DD)
  DPRB = DPRB + DP
  IF (DPRB .LT. DM) GO TO 80
  IFAULT = 1
  DPRB = DM
  GO TO 200
80 CONTINUE
  IT = M - 1
90 IF (IT .EQ. 0) GO TO 120
C
C   Determine next M-partition & update sum of squares.
C
  IF ((A(M) - A(IT)) .GT. 1) GO TO 100
  IT = IT - 1
  GO TO 90
100 IAT = A(IT) + 1
  M1 = M - 1
  DO 110 J = IT, M1
    TS = TS - A(J)**2 + IAT**2
    A(J) = IAT
110 CONTINUE
  TS = TS - A(M)**2
C
C   New values for A(1), ..., A(M-1) are determined.
C
  IF (KGP .LT. MAXP) GO TO 30
  IFAULT = 1
  GO TO 200
120 M = M - 1
C
C   End evaluation of M-part partitions.
C   Decrease M by 1 and continue if SY2 > sum of squares for
C   the last partition.
C
  IF (TS .GE. SY2) GO TO 200
  IF (M .GT. 1) GO TO 20
C
200 PROB = D1 - DPRB
  RETURN
  END
```

```
      SUBROUTINE SIMDO(QIND, QFOR, IPROD, KDIM, JSUB, IVEC, IFAULT)
C
C   ALGORITHM AS 172  APPL. STATIST. (1982) VOL.31, NO.1
C
C   Generates the subscript vector (index subscript) given the index
C   subscript (subscript vector) for a sequence of Fortran DO-loops
C   nested to depth KDIM
C
C   LOGICAL QIND, QFOR
C   INTEGER IPROD(KDIM), IVEC(KDIM)
C
C   IFAULT = 0
C   IF (.NOT. QIND) GO TO 12
C
C   Index subscript to subscript vector conversion
C
C   IF (JSUB .LE. IPROD(KDIM)) GO TO 5
C   IFAULT = 1
C   RETURN
5  ITEMPV = JSUB - 1
C   IJ = KDIM - 1
C   DO 10 I = 1, IJ
C     IK = KDIM - I
C     IVEC(I) = ITEMPV / IPROD(IK)
C     ITEMPV = ITEMPV - IPROD(IK) * IVEC(I)
C     IVEC(I) = IVEC(I) + 1
10  CONTINUE
C   IVEC(KDIM) = ITEMPV + 1
C   IF (QFOR) CALL REVERS(IVEC, KDIM)
C   RETURN
C
C   Subscript vector to index subscript conversion
C
C   12 IF (IVEC(1) .LE. IPROD(1)) GO TO 14
C   IFAULT = 2
C   RETURN
14  DO 15 I = 2, KDIM
C     IF (IVEC(I) .LE. IPROD(I)/IPROD(I-1)) GO TO 15
C     IFAULT = 2
C     RETURN
15  CONTINUE
C   IF (.NOT. QFOR) CALL REVERS(IVEC, KDIM)
C   JSUB = IVEC(1)
C   DO 20 I = 2, KDIM
C     JSUB = JSUB + (IVEC(I) - 1) * IPROD(I-1)
20  CONTINUE
C   RETURN
C   END
C
C
C   SUBROUTINE REVERS(ITAB, IDIM)
C   INTEGER ITAB(IDIM)
C
C   ALGORITHM AS 172.1  APPL. STATIST. (1982) VOL.31, NO. 1
C
C   Reorders subscript vector, if required
C
C   ITER = IDIM / 2
C   K = IDIM + 1
C   DO 10 I = 1, ITER
C     ITEMP = ITAB(I)
```

IK = K - I

ITAB(I) = ITAB(IK)

ITAB(IK) = ITEMP

10 CONTINUE

C

RETURN

END

```
      SUBROUTINE DESMAT(MAXROW,MAXCOL,NDIM,NSUB,MXDINT,MSUB,  
      1LSUB,ISUB,IBEG,MATDES,IFAUULT)
```

```
C  
C<<<<<  Acquired in machine-readable form from 'Applied Statistics'  
C<<<<<  algorithms editor, January 1983.
```

```
C  
C      ALGORITHM AS 173  APPL. STATIST. (1982) VOL.31, NO.1
```

```
C  
C      GENERATES A DESIGN MATRIX FOR BALANCED FACTORIAL  
C      EXPERIMENTS
```

```
C  
C      DIMENSION MATDES(MAXROW,MAXCOL),NSUB(NDIM),MSUB(NDIM),  
1      LSUB(NDIM),ISUB(NDIM),IBEG(NDIM)
```

```
C  
C      PRIMARY INPUT PARAMETER CHECK
```

```
C  
C      IFAULT = 0  
C      DO 5 I = 1,NDIM  
C      IF(NSUB(I) .GE.2) GO TO 5  
C      IFAULT = 1  
C      RETURN
```

```
5 CONTINUE  
C      IF(MXDINT .LE.NDIM) GO TO 8  
C      IFAULT = 2  
C      RETURN
```

```
C  
C      CALCULATE PRODUCT VECTOR MSUB FOR M.E. GENERATION  
C      CALCULATE PRODUCT VECTOR LSUB FOR INTRT. GENERATION
```

```
C  
8 IBEG(1) = 1  
C      MSUB(1) = NSUB(1)  
C      LSUB(1) = NSUB(1)-1  
C      DO 40 I = 2,NDIM  
C      IK = I-1  
C      IBEG(I) = IBEG(IK)+NSUB(IK)-1  
C      MSUB(I) = MSUB(IK) * NSUB(I)  
C      LSUB(I) = LSUB(IK) *(NSUB(I)-1)
```

```
40 CONTINUE  
C  
C      RESERVE THE TOTAL NUMBER OF OBSERVATIONS
```

```
C  
C      NOBS = MSUB(NDIM)  
C  
C      SECONDARY INPUT PARAMETER CHECK  
C  
C      IF(NOBS .LE. MAXROW) GO TO 50  
C      IFAULT = 3  
C      RETURN
```

```
C  
C      GENERATE THE MAIN EFFECTS  
C  
50 CALL MANEFF(MAXROW,MAXCOL,NDIM,NSUB,MSUB,ISUB,MATDES,JCOL)
```

```
C  
C      GENERATE ALL POSSIBLE INTERACTIONS  
C  
C      IF(MXDINT.GE.2)CALL INTER(MAXROW,MAXCOL,NDIM,NOBS,NSUB,MXDINT,IBEG  
1,MSUB,LSUB,ISUB,MATDES,JCOL,IFAUULT)
```

```
C  
C      PASS BACK NOBS AND JCOL IRRESPECTIVE OF VALUE OF IFAULT  
C  
C      IBEG(1) = NOBS
```

```
      IBEG(2) = JCOL
      RETURN
      END
      SUBROUTINE MANEFF(MAXROW,MAXCOL,NDIM,NSUB,MSUB,ISUB,MATDES,
1JCOL)
C
C      ALGORITHM AS 173.1  APPL. STATIST. (1982) VOL.31, NO.1
C
C      COMPUTES THOSE COLUMNS OF THE DESIGN MATRIX (MATDES) ASSOCIATED
C      WITH THE MEAN AND THE MAIN EFFECTS
C
      DIMENSION MATDES(MAXROW,MAXCOL),NSUB(NDIM),MSUB(NDIM),ISUB(NDIM)
C
      SET THE TOTAL NUMBER OF OBSERVATIONS
C
      NOBS = MSUB(NDIM)
C
      SET UP MUU
C
      DO 10 I = 1,NOBS
      MATDES(I,1) = 1
10 CONTINUE
C
      SET UP OTHER MAIN EFFECTS
C
      DO 40 I = 1,NOBS
      CALL SIMDO(.TRUE.,.TRUE.,MSUB,NDIM,I,ISUB,JFALT)
C
      ROUTINE PROTECTED FROM FAILURE SO FAULT PARAMETER UNTESTED
C
      JCOL = 1
      DO 30 J = 1,NDIM
      IK = NSUB(J)-1
      DO 20 K = 1,IK
      JCOL = JCOL+1
      IF (ISUB(J) .EQ. K) GO TO 15
      IF (ISUB(J) .EQ. NSUB(J))GO TO 18
      MATDES(I,JCOL) = 0
      GO TO 20
15 MATDES(I,JCOL) = 1
      GO TO 20
18 MATDES(I,JCOL) = -1
20 CONTINUE
30 CONTINUE
40 CONTINUE
      RETURN
      END
      SUBROUTINE INTER(MAXROW,MAXCOL,NDIM,NOBS,NSUB,MXDINT,IBEG,
1ICOMB,LSUB,IREF,MATDES,JCOL,IFALT)
C
C      ALGORITHM AS 173.2  APPL. STATIST. (1982) VOL.31, NO.1
C
C      GENERATES THE SPECIFIED INTERACTION TERMS
C
      DIMENSION MATDES(MAXROW,MAXCOL),NSUB(NDIM),IBEG(NDIM),ICOMB(NDIM)
1,LSUB(NDIM),IREF(NDIM)
      LOGICAL QNXT
C
      GENERATE ALL POSSIBLE COMBINATIONS OF DIMENSION .LE. MXDINT
C
      QNXT = .FALSE.
```

```

        DO 50 ICMB = 2, MXDINT
    5 CALL COMB(NDIM, ICMB, ICOMB, QNXT)
C
C     HERE TO PROCESS CURRENT COMBINATION OF DIMENSION ICMB
C
C     CALCULATE THE ADDITIONAL COLUMNS REQUIRED TO STORE THIS
C     INTERACTION
C
        NPROD = 1
        DO 10 I = 1, ICMB
            IK = ICOMB(I)
            NPROD = NPROD*(NSUB(IK)-1)
    10 CONTINUE
C
C     CHECK IF SUFFICIENT COLUMNS ARE AVAILABLE IN MATDES
C
C     IF (JCOL+NPROD .LE. MAXCOL) GO TO 15
        IFAULT = 4
        RETURN
C
C     PROCESS THE CURRENT INTERACTION FOR WHICH THERE IS SPACE
C
    15 DO 40 J = 1, NPROD
        CALL SIMDO(.TRUE., .TRUE., LSUB, NDIM, J, IREF, JFALT)
C
C         ROUTINE PROTECTED FROM FAILURE SO FAULT PARAMETER UNTESTED
C
        JCOL = JCOL+1
        DO 30 I = 1, NOBS
            MATDES(I, JCOL) = 1
            DO 20 L = 1, ICMB
                IK = ICOMB(L)
                JREF = IBEG(IK) + IREF(L)
                MATDES(I, JCOL) = MATDES(I, JCOL)*MATDES(I, JREF)
    20 CONTINUE
    30 CONTINUE
    40 CONTINUE
C
C     FINISHED ADDING IN THIS INTERACTION - PROCESS NEXT ONE
C
C     IF(QNXT)GO TO 5
    50 CONTINUE
        RETURN
        END
        SUBROUTINE COMB(N, K, A, MTC)
C
C         ALGORITHM AS 173.3  APPL. STATIST. (1982) VOL.31, NO.1
C
C         GENERATES ALL POSSIBLE COMBINATIONS OF DIMENSION K
C         FROM N INTEGERS
C
        INTEGER A(K), H
        LOGICAL MTC
C
        IF(.NOT.MTC) GO TO 20
        DO 10 H = 1, K
            M = K + 1 - H
            M2 = A(M)
            IF(M2.NE.N+1-H)GO TO 30
    10 CONTINUE
    20 M2 = 0

```



```
H = K
30 DO 40 J = 1,H
    M = K + J - H
    A(M) = M2 + J
40 CONTINUE
    MTC = A(1).NE.N-K+1
    RETURN
    END
```

```

SUBROUTINE NONPAR(ISTAT, IT, NPOP, IN, IP, Y, NAR, ST, IDF,
*   VM, AR, W, VP, VR, VY, VV, IFAULT)

```

```

C
C   ALGORITHM AS 174  APPL. STATIST. (1982) VOL.31, NO.1
C
C   Computes the distribution-free test statistics for either the
C   multivariate multi-sample rank sum test (MMRST) or the multi-
C   variate multi-sample median test (MMMT)
C
C   INTEGER IN(NPOP)
C   REAL Y(IT,IP), VM(IP,IP), AR(NAR), W(IP), VP(NPOP,IP), VR(IP),
*   VY(IT), VV(NAR)
C   DATA ZERO/0.0/, HALF/0.5/, ONE/1.0/

```

```

C
C   IFAULT = 3
C   IF (ISTAT .NE. 0 .AND. ISTAT .NE. 1) GO TO 22
C   IFAULT = 4
C   IF (NPOP .LT. 2) GO TO 22
C   IFAULT = 5
C   IF (IP .LT. 1) GO TO 22
C   IFAULT = 6
C   ISUM = 0
C   DO 1 I = 1, NPOP
1  ISUM = ISUM + IN(I)
C   IF (ISUM .NE. IT) GO TO 22
C   IFAULT = 7
C   JP = IP * (IP+1) / 2
C   IF (NAR .NE. JP) GO TO 22
C   IFAULT = 0

```

```

C
C   DO 6 J = 1, IP
C     DO 5 I = 1, IT
C       R = HALF
C       DO 4 II = 1, IT
C         IF (Y(I,J) - Y(II,J)) 4, 2, 3
2       R = R + HALF
C         GO TO 4
3       R = R + ONE
4       CONTINUE
C       VY(I) = R
5       CONTINUE
C     DO 6 I = 1, IT
C       Y(I,J) = VY(I)
6 CONTINUE

```

```

C
C   Matrix Y now has the ranks replacing the observed values
C

```

```

C   B = IT
C   IF (ISTAT .EQ. 1) GO TO 9
C   A = HALF * B
C   DO 8 J = 1, IP
C     DO 8 IJ = 1, IT
C       IF (Y(IJ,J) .LE. A) GO TO 7
C       Y(IJ,J) = ZERO
C       GO TO 8
7     Y(IJ,J) = ONE
8 CONTINUE

```

```

C
C   If MMTT test is selected (ISTAT = 0), the Y-matrix will now
C   contain 1's and 0's.  1 indicates an observation <= the median;
C   0 if greater than the median.

```

C

```
9 DO 13 I = 1, IP
  IA = 0
  DO 11 IB = 1, NPOP
    IST = IN(IB)
    CST = ZERO
    DO 10 IC = 1, IST
      IA = IA + 1
      CST = CST + Y(IA,I)
10 CONTINUE
  VP(IB,I) = CST
11 CONTINUE
  DO 13 IR = 1, IP
    V = ZERO
    DO 12 JR = 1, IT
      V = V + Y(JR,I) * Y(JR,IR)
      VM(I,IR) = V
12 CONTINUE
13 CONTINUE
```

C  
C  
C  
C  
C  
C  
C

Matrix VP contains the sum of the Y-matrix elements for each population and each multivariate response.

Matrix VM contains the sum of squares and cross-products of the columns of Y, that is  $VM = Y'Y$ .

```
DO 14 I = 1, IP
14 VR(I) = ZERO
DO 15 I = 1, IP
  DO 15 IPR = 1, NPOP
    VR(I) = VR(I) + VP(IPR,I)
15 CONTINUE
```

C  
C  
C

Vector VR contains the sum of elements in each column of Y.

```
KPR = 0
DO 16 J = 1, IP
  DO 16 I = 1, J
    KPR = KPR + 1
    AR(KPR) = VM(I,J)/B - VR(I)*VR(J)/B**2
16 CONTINUE
```

C  
C  
C  
C  
C

Vector AR contains the upper triangular portion of VM adjusted for the overall means read in columnwise. This is the upper triangle of the dispersion matrix required for subroutine SYMINV.

```
DO 17 I = 1, NPOP
  AA = IN(I)
  DO 17 J = 1, IP
    VP(I,J) = VP(I,J)/AA - VR(J)/B
17 CONTINUE
```

C  
C  
C  
C  
C

Matrix VP now contains the sum of the Y-matrix elements for each population and multivariate response adjusted for the overall population response mean.

```
CALL SYMINV(AR, IP, VV, W, NULLTY, IFAULT)
IF (IFAULT .NE. 0) GO TO 22
K = 0
DO 18 J = 1, IP
  DO 18 I = 1, J
    K = K + 1
```

VM(I,J) = VV(K)

VM(J,I) = VV(K)

18 CONTINUE

C

C Matrix VM now is the inverse of the dispersion matrix.

C

ST = ZERO

DO 21 IPR = 1, NPOP

TSTAT = ZERO

DO 20 JPR = 1, IP

ACC = ZERO

DO 19 KPR = 1, IP

19 ACC = ACC + VM(KPR,JPR) \* VP(IPR,KPR)

TSTAT = TSTAT + ACC \* VP(IPR,JPR) \* IN(IPR)

20 CONTINUE

ST = ST + TSTAT

21 CONTINUE

IDF = IP \* (NPOP - 1)

C

22 RETURN

END

```

SUBROUTINE FACSVM(A, B, W, N1, ITER0, ITER1, ITER2, EPS, IFAULT)
C
C   ALGORITHM AS 175  APPL. STATIST. (1982) VOL.31, NO.1
C
C   Cramer-Wold factorization; 3-stage algorithm.
C   Factorizes:  $A(x) = a_0 + a_1(x + 1/x) + a_2(x^2 + 1/x^2) + \dots$ 
C                $= B(x).B(1/x)$ 
C   where       $B(x) = b_0 + b_1.x + b_2.x^2 + \dots + b_n.x^n$ 
C
C   Auxiliary routine required: SDSDOT from IMSL; an equivalent function
C   has been added to this file.
C
REAL A(N1), B(N1), W(N1,2), HALF
DATA HALF /0.5E0/
C
C   Generate initial values for B using Bauer algorithm
C
IFAULT = 0
DO 10 I = 1, N1
10 W(I,1) = A(I)
CALL BAUER(W, B, N1, ITER0, IER)
IF (IER .NE. 0) GO TO 130
C
C   Iterate to convergence using Wilson algorithm
C
IF (ITER1 .LE. 0) GO TO 50
DO 40 ITER = 1, ITER1
DO 20 I = 1, N1
W(I,1) = A(I)
W(I,2) = B(I)
20 CONTINUE
CALL RECURS(B, W, N1, IER)
IF (IER .NE. 0) GO TO 120
DO 30 I = 1, N1
30 B(I) = B(I) + HALF * W(I,2)
IF (B(1) .LE. ABS(B(N1))) GO TO 120
IF (W(1,2) - B(1) .LE. EOS * W(1,2) .AND. ITER .GT. 1) GO TO 50
40 CONTINUE
GO TO 110
C
C   Iterative improvement using incremental form
C
50 IF (ITER2 .EQ. 0) GO TO 140
DO 80 ITER = 1, ITER2
DO 60 I = 1, N1
W(I,1) = - A(I)
W(I,2) = B(I)
60 CONTINUE
CALL RESIDU(W, B, N1)
CALL RECURS(B, W, N1, IER)
IF (IER .NE. 0) GO TO 120
DO 70 I = 1, N1
70 B(I) = W(I,2) - B(I)
IF (B(1) .LE. ABS(B(N1))) GO TO 120
IF (B(1) .GE. W(1,2) .AND. ITER .GT. 1) GO TO 140
80 CONTINUE
GO TO 140
C
C   Exits from subroutine
C
110 IFAULT = 1

```

```
      GO TO 140
120  IFAULT = 2
      GO TO 140
130  IFAULT = 3
140  RETURN
      END
C
      SUBROUTINE BAUER(A, B, N1, MAXIT, IFAULT)
C
C   ALGORITHM AS 175.1  APPL. STATIST. (1982) VOL.31, NO.1
C
C   Bauer-Rissanen algorithm.
C
      REAL A(N1), B(N1), C, ONE, ZERO
      DATA ONE /1.0E0/, ZERO /0.0E0/
C
      N = N1 - 1
      IFAULT = 0
      DO 10 I = 1, N
10   B(I) = A(I+1)
      B(N1) = ZERO
      IF (MAXIT .EQ. 0) GO TO 30
      DO 20 ITER = 1, MAXIT
          IF (A(1) .LE. ABS(A(N1))) GO TO 100
          C = - B(1) / A(1)
          IF (ABS(C) .GT. ONE) GO TO 100
          DO 20 I = 1, N
              A(I) = A(I) + C * B(I)
              B(I) = B(I+1) + C * A(I+1)
20   CONTINUE
30   IF (A(1) .LE. ZERO) GO TO 100
      C = SQRT(A(1))
      DO 40 I = 1, N1
40   B(I) = A(I) / C
      RETURN
C
100  IFAULT = 1
      RETURN
      END
C
      SUBROUTINE RECURS(B, W, N1, IFAULT)
C
C   ALGORITHM AS 175.2  APPL. STATIST. (1982) VOL.31, NO.1
C
C   Recursive solution for polynomial coefficients
C
      REAL B(N1), W(N1), S, HALF, ZERO
      DATA HALF /0.5E0/, ZERO /0.0E0/
C
      N = N1 - 1
      M = N1
      W(1) = HALF * W(1)
      DO 20 I = 1, N
          IF (B(1) .LE. ZERO) GO TO 40
          S = W(M) / B(1)
          K = M
          DO 10 J = 1, M
              W(J) = W(J) - S * B(K)
              K = K - 1
10   CONTINUE
      W(M) = S
```

```
      S = B(M) / B(1)
      CALL LINCOM(B, S, M)
      B(M) = S
      M = M - 1
20 CONTINUE
C
      IF (B(1) .LE. ZERO) GO TO 40
      B(1) = W(1) / B(1)
      DO 30 I = 2, N1
        S = B(I)
        B(I) = ZERO
        CALL LINCOM(B, S, I)
        B(I) = B(I) + W(I)
30 CONTINUE
      IFAULT = 0
      RETURN
C
40 IFAULT = 1
      RETURN
      END
C
      SUBROUTINE LINCOM(X, P, M)
C
C      ALGORITHM AS 175.3 APPL. STATIST. (1982) VOL.31, NO.1
C
C      Replaces X with X - P * XSTAR
C
      REAL X(M), P, S
C
      I = 1
      J = M
10 S = X(I)
      X(I) = X(I) - P * X(J)
      IF (I .NE. J) X(J) = X(J) - P * S
      I = I + 1
      J = J - 1
      IF (I .LE. J) GO TO 10
C
      RETURN
      END
C
      SUBROUTINE RESIDU(A, B, N1)
C
C      ALGORITHM AS 175.4 APPL. STATIST. (1982) VOL.31, NO.1
C
C      Replaces A with A + B * BSTAR
C
      REAL A(N1), B(N1), SDSDOT
C
      DO 10 I = 1, N1
10 A(I) = SDSDOT(N1-I+1, A(I), B(1), 1, B(I), 1)
C
      RETURN
      END
C
C
      REAL FUNCTION SDSDOT(N, SB, SX, INCX, SY, INCY)
C
C      Evaluate the single-precision dot-product B + X'Y using double
C      precision internally.
C      Modified from the BLAS function SDOT by Alan Miller, CSIRO
```

```
C      Division of Mathematics & Statistics, Melbourne, Australia
C
      INTEGER N, INCX, INCY
      REAL SB, SX(*), SY(*)
C
C      Local variables
C
      DOUBLE PRECISION DDOT
      INTEGER I, IX, IY, M, MP1, NS
C***FIRST EXECUTABLE STATEMENT  SDSDOT
      DDOT = SB
      IF(N.LE.0) RETURN
      IF(INCX.EQ.INCY) IF(INCX-1)5, 20, 60
5 CONTINUE
C
C      CODE FOR UNEQUAL INCREMENTS OR NONPOSITIVE INCREMENTS.
C
      IX = 1
      IY = 1
      IF(INCX.LT.0) IX = (-N+1)*INCX + 1
      IF(INCY.LT.0) IY = (-N+1)*INCY + 1
      DO 10 I = 1, N
          DDOT = DDOT + DBLE(SX(IX)) * DBLE(SY(IY))
          IX = IX + INCX
          IY = IY + INCY
10 CONTINUE
      SDSDOT = DDOT
      RETURN
C
C      CODE FOR BOTH INCREMENTS EQUAL TO 1
C
C      CLEAN-UP LOOP SO REMAINING VECTOR LENGTH IS A MULTIPLE OF 5.
C
20 M = MOD(N, 5)
      IF( M .EQ. 0 ) GO TO 40
      DO 30 I = 1, M
          DDOT = DDOT + DBLE(SX(I)) * DBLE(SY(I))
30 CONTINUE
      IF( N .LT. 5 ) THEN
          SDSDOT = DDOT
          RETURN
      END IF
40 MP1 = M + 1
      DO 50 I = MP1, N, 5
          DDOT = DDOT + DBLE(SX(I)) * SY(I) + DBLE(SX(I+1)) * SY(I+1) +
1      DBLE(SX(I+2)) * SY(I+2) + DBLE(SX(I+3)) * SY(I+3) +
2      DBLE(SX(I+4)) * SY(I+4)
50 CONTINUE
      SDSDOT = DDOT
      RETURN
C
C      CODE FOR POSITIVE EQUAL INCREMENTS .NE.1.
C
60 CONTINUE
      NS = N*INCX
      DO 70 I = 1, NS, INCX
          DDOT = DDOT + DBLE(SX(I)) * DBLE(SY(I))
70 CONTINUE
      SDSDOT = DDOT
      RETURN
```



END

```
      SUBROUTINE DENEST(DT, NDT, DLO, DHI, WINDOW, FT, SMOOTH,  
*   NFT, ICAL, IFAULT)  
      REAL DT(NDT), FT(NFT), SMOOTH(NFT)  
C  
C   ALGORITHM AS 176 APPL. STATIST. (1982) VOL.31, NO.1  
C   Modified using AS R50 (Appl. Statist. (1984))  
C  
C   Find density estimate by kernel method using Gaussian kernel.  
C   The interval on which the estimate is evaluated has end points  
C   DLO and DHI.  If ICAL is not zero then it is assumed that the  
C   routine has been called before with the same data and end points  
C   and that the array FT has not been altered.  
C  
C   Auxiliary routines called: FORRT & REVRT from AS 97  
C  
C   DATA ZERO/0.0/, HALF/0.5/, ONE/1.0/, SIX/6.0/, THIR2/32.0/  
C   DATA BIG/30.0/, KFTLO/5/, KFTHI/11/  
C  
C   The constant BIG is set so that exp(-BIG) can be calculated  
C   without causing underflow problems and can be considered = 0.  
C  
C   Initialize and check for valid parameter values.  
C  
      IF (WINDOW .LE. ZERO) GO TO 92  
      IF (DLO .GE. DHI) GO TO 93  
      II = 2**KFTLO  
      DO 1 K = KFTLO, KFTHI  
        IF (II .EQ. NFT) GO TO 2  
        II = II + II  
1 CONTINUE  
      IFAULT = 1  
      RETURN  
2 STEP = (DHI - DLO) / FLOAT(NFT)  
  AINC = ONE / (NDT * STEP)  
  NFT2 = NFT / 2  
  HW = WINDOW / STEP  
  FAC1 = THIR2 * (ATAN(ONE) * HW / NFT) ** 2  
  IF (ICAL .NE. 0) GO TO 10  
C  
C   Discretize the data  
C  
      DLO1 = DLO - STEP * HALF  
      DO 3 J = 1, NFT  
3 FT(J) = ZERO  
      DO 4 I = 1, NDT  
        WT = (DT(I) - DLO1) / STEP  
        JJ = INT(WT)  
        IF (JJ .LT. 1 .OR. JJ .GT. NFT) GO TO 4  
        WT = WT - JJ  
        WINC = WT * AINC  
        KK = JJ + 1  
        IF (JJ .EQ. NFT) KK = 1  
        FT(JJ) = FT(JJ) + AINC - WINC  
        FT(KK) = FT(KK) + WINC  
4 CONTINUE  
C  
C   Transform to find FT.  
C  
      CALL FORRT(FT, NFT)  
C  
C   Find transform of density estimate.
```

```
C
10 JHI = SQRT(BIG / FAC1)
    JMAX = MIN(NFT2 - 1, JHI)
    SMOOTH(1) = FT(1)
    RJ = ZERO
    DO 11 J = 1, JMAX
        RJ = RJ + ONE
        RJFAC = RJ * RJ * FAC1
        BC = ONE - RJFAC / (HW * HW * SIX)
        FAC = EXP(-RJFAC) / BC
        J1 = J + 1
        J2 = J1 + NFT2
        SMOOTH(J1) = FAC * FT(J1)
        SMOOTH(J2) = FAC * FT(J2)
11 CONTINUE
C
C   Cope with underflow by setting tail of transform to zero.
C
    IF (JHI + 1 - NFT2) 21, 23, 20
20 SMOOTH(NFT2 + 1) = EXP(-FAC1 * FLOAT(NFT2)**2) * FT(NFT2 + 1)
    GO TO 24
21 J2LO = JHI + 2
    DO 22 J1 = J2LO, NFT2
        J2 = J1 + NFT2
        SMOOTH(J1) = ZERO
        SMOOTH(J2) = ZERO
22 CONTINUE
23 SMOOTH(NFT2 + 1) = ZERO
C
C   Invert Fourier transform of SMOOTH to get estimate and eliminate
C   negative density values.
C
24 CALL REVRT(SMOOTH, NFT)
    DO 25 J = 1, NFT
25 IF (SMOOTH(J) .LT. ZERO) SMOOTH(J) = ZERO
    IFAULT = 0
    RETURN
C
92 IFAULT = 2
    RETURN
93 IFAULT = 3
    RETURN
    END
```

```
      subroutine nscor1 (s, n, n2, work, ifault)
c
c      Algorithm AS 177  Appl. Statist. (1982) Vol. 31, No. 2
c
c      Exact calculation of Normal Scores
c
      double precision s(n2), work(4,721)
      double precision zero, one, c, scor, ail, ani, an, h
      data one/1.0d0/, zero/0.0d0/, h/0.025d0/, nstep/721/
c
      ifault=3
      if (n2 .ne. n/2) return
      ifault=1
      if (n .le. 1) return
      ifault=0
      if (n .gt. 2000) ifault=2
c
      an=n
      c=log(an)
c
c      Accumulate ordinates for calculation of integral for rankits
c
      do 20 i=1, n2
         il=i-1
         ni=n-i
         ail=il
         ani=ni
         scor=zero
         do 10 j=1,nstep
10      scor=scor+exp(work(2,j) + ail * work(3,j) + ani * work(4,j)
*          + c) * work(1,j)
         s(i)=scor * h
         c=c+log(ani/dble(i))
20 continue
      return
      end
c
c
      subroutine init(work)
c
c      Algorithm AS 177.1  Appl. Statist. (1982) Vol. 31, No. 2
c
c
      double precision work(4,721)
      double precision xstart, h, pi2, half, xx, alnorm
      data xstart/-9.0d0/, h/0.025d0/, pi2/-0.918938533d0/,
*      half/0.5d0/, nstep/721/
      xx=xstart
c
c      Set up arrays for calculation of integral
c
      do 10 i=1,nstep
         work(1,i)=xx
         work(2,i)=pi2 - xx * xx * half
         work(3,i)=log(alnorm(xx, .true.))
         work(4,i)=log(alnorm(xx, .false.))
         xx=xstart + dble(i) * h
10 continue
      return
      end
c
c
```

```

double precision function alnorm(x,upper)
c
c      Algorithm AS66 Applied Statistics (1973) vol22 no.3
c
c      Evaluates the tail area of the standardised normal curve
c      from x to infinity if upper is .true. or
c      from minus infinity to x if upper is .false.
c
double precision zero,one,half
double precision con,z,y,x
double precision p,q,r,a1,a2,a3,b1,b2,c1,c2,c3,c4,c5,c6
double precision d1,d2,d3,d4,d5
logical upper,up
c*** machine dependent constants
double precision ltone,utzero
data zero/0.0d0/, one/1.0d0/, half/0.5d0/
data ltone/7.0d0/, utzero/18.66d0/
data con/1.28d0/
data p/0.398942280444d0/, q/0.39990348504d0/, r/0.398942280385d0/
data a1/5.75885480458d0/, a2/2.62433121679d0/, a3/5.92885724438d0/
data b1/-29.8213557807d0/, b2/48.6959930692d0/
data c1/-3.8052d-8/, c2/3.98064794d-4/, c3/-0.151679116635d0/
data c4/4.8385912808d0/, c5/0.742380924027d0/, c6/3.99019417011d0/
data d1/1.00000615302d0/, d2/1.98615381364d0/, d3/5.29330324926d0/
data d4/-15.1508972451d0/, d5/30.789933034d0/
c
up=upper
z=x
if(z.ge.zero)goto 10
up=.not.up
z=-z
10 if(z.le.ltone.or.up.and.z.le.utzero)goto 20
alnorm=zero
goto 40
20 y=half*z*z
if(z.gt.con) goto 30
c
alnorm=half-z*(p-q*y/(y+a1+b1/(y+a2+b2/(y+a3))))
goto 40
30 alnorm=r*exp(-y)/(z+c1+d1/(z+c2+d2/(z+c3+d3/(z+c4+d4/(z+c5+d5/
2 (z+c6))))))
40 if(.not.up)alnorm=one-alnorm
return
end
c
c
c      subroutine nscor2(s,n,n2,ier)
c
c      algorithm as 177.3, applied statistics, v.31, 161-165, 1982.
c
c      calculates approximate expected values of normal order statistics.
c      claimed accuracy is 0.0001, though usually accurate to 5-6 dec.
c
c*** N.B. This routine is NOT in double precision ***
c
c      arguments:
c      s(n2) = output, the first n2 expected values.
c      n = input, the sample size.
c      n2 = input, the number of order statistics required; must
c          be <= n/2.
c      ier = output, error indicator

```

```

c          = 0 if no error detected
c          = 1 if n <= 1.
c          = 2 if n > 2000, in which case the order statistics
c          are still calculated, but may be inaccurate.
c          = 3 if n2 > n/2 (n.b. this differs from the
c          published algorithm which returns an error
c          if n2 is not equal to n/2.)
c
c  calls ppnd = applied statistics algorithm 111.
c  An alternative is ppnd7 in algorithm AS 241.
c
c  real s(n2), eps(4), dl1(4), dl2(4), gam(4), lam(4),
*  bb, d, b1, an, ai, e1, e2, l1, correc, ppnd
c  data eps/0.419885e0, 0.450536e0, 0.456936e0, 0.468488e0/,
1  dl1/0.112063e0, 0.121770e0, 0.239299e0, 0.215159e0/,
2  dl2/0.080122e0, 0.111348e0, -0.211867e0, -0.115049e0/,
3  gam/0.474798e0, 0.469051e0, 0.208597e0, 0.259784e0/,
4  lam/0.282765e0, 0.304856e0, 0.407708e0, 0.414093e0/,
5  bb/-0.283833/, d/-0.106136/, b1/0.5641896/
c
c  input parameter checks.
c
c  ier = 3
c  if(n2.gt.n/2) return
c  ier = 1
c  if(n.le.1) return
c  ier = 0
c  if(n.gt.2000) ier = 2
c  s(1) = b1
c  if(n.eq.2) return
c
c  calculate normal tail areas for first 3 order statistics.
c
c  an = n
c  k = 3
c  if(n2.lt.k) k = n2
c  do 5 i = 1,k
c    ai = i
c    e1 = (ai - eps(i))/(an + gam(i))
c    e2 = e1**lam(i)
c    s(i) = e1 + e2*(dl1(i) + e2*dl2(i))/an - correc(i,n)
5  continue
c  if(n2.eq.k) go to 20
c
c  calculate normal areas for other cases.
c
c  do 10 i = 4,n2
c    ai = i
c    l1 = lam(4) + bb/(ai + d)
c    e1 = (ai - eps(4))/(an + gam(4))
c    e2 = e1**l1
c    s(i) = e1 + e2*(dl1(4) + e2*dl2(4))/an - correc(i,n)
10 continue
c
c  convert tail areas to normal deviates.
c
c  20 do 30 i = 1,n2
c  30 s(i) = -ppnd(s(i),ier)
c    return
c  end
c

```

```

c
  real function correc(i,n)
c
c  calculates correction for tail area of the i-th largest of n
c  order statistics.
c
  dimension c1(7),c2(7),c3(7)
  real mic
  data c1/9.5, 28.7, 1.9, 0., -7.0, -6.2, -1.6/,
1 c2/-6195., -9569., -6728., -17614., -8278., -3570., 1075./,
2 c3/9.338e4, 1.7516e5, 4.1040e5, 2.1576e6, 2.376e6, 2.065e6,
3 2.065e6/, mic/1.e-6/, c14/1.9e-5/
c
  correc = c14
  if(i*n.eq.4) return
  correc = 0.0
  if(i.lt.1.or.i.gt.7) return
  if(i.ne.4.and.n.gt.20) return
  if(i.eq.4.and.n.gt.40) return
  an = n
  an = 1.0/(an*an)
  correc = (c1(i) + an*(c2(i) + an*c3(i)))*mic
  return
end

c
c
  function ppnd(p,ier)
c
c  algorithm as 111, appl.statist., vol.26, 118-121, 1977.
c
c  produces normal deviate corresponding to lower tail area = p.
c
  data split/0.42/
  data a0,a1,a2,a3/2.506628, -18.61500, 41.39120, -25.44106/,
1 b1,b2,b3,b4/-8.473511, 23.08337, -21.06224, 3.130829/,
2 c0,c1,c2,c3/-2.787189, -2.297965, 4.850141, 2.321213/,
3 d1,d2/3.543889, 1.637068/
  ier=0
  q=p-0.5
  if(abs(q).gt.split) go to 10
c
c  0.08 < p < 0.92
c
  r=q*q
  ppnd=q*(((a3*r+a2)*r+a1)*r+a0)/((((b4*r+b3)*r+b2)*r+b1)*r+1.)
  return
c
c  p < 0.08 or p > 0.92, set r = min(p,1-p)
c
10 r=p
  if(q.gt.0.) r=1.-p
  if(r.le.0.) go to 20
  r=sqrt(-log(r))
  ppnd=(((c3*r+c2)*r+c1)*r+c0)/((d2*r+d1)*r+1.)
  if(q.lt.0.) ppnd=-ppnd
  return
20 ier=1
  ppnd=0.
  return
end

```

```
double precision function alnfac(j)
c
c      algorithm as 177.2  appl. statist. (1982) vol.31, no.2
c
c      natural logarithm of factorial for non-negative agrument
c
implicit logical (a-z)
integer j
double precision r(7), one, half, a0, three, four, fourtn, fortty,
*  fivfty, w, z
data r(1), r(2), r(3), r(4), r(5), r(6), r(7) /0.0d0, 0.0d0,
*  0.69314718056d0, 1.79175946923d0, 3.17805383035d0,
*  4.78749174278d0, 6.57925121101d0/
data one, half, a0, three, four, fourtn, fortty, fivfty /
*  1.0d0, 0.5d0, 0.918938533205d0, 3.0d0, 4.0d0, 14.0d0, 420.0d0,
*  5040.0d0/
if (j .ge. 0) goto 10
alnfac = one
return
10 if (j .ge. 7) goto 20
alnfac = r(j + 1)
return
20 w = j + 1
z = one / (w * w)
alnfac = (w - half) * log(w) - w + a0 + (((four - three * z)
* * z - fourtn) * z + fortty) / (fivfty * w)
return
end
```



```
      subroutine gsweep (s, t, k, l, m, n, e, ifault)
c
c      Algorithm AS 178   Appl. Statist.   (1982)   Vol. 31, No. 2
c
c      Performs Gauss-Jordan pivot for row/col K in N by N working
c      array stored lower triangle only row by row, shortest row
c      first, in locations 1 to (N*N+N)/2 of T
c
      double precision a, b, e, s(n), t(m), zero, one
      data zero/0.0d0/, one/1.0d0/
c
      ifault=1
      if(n.lt.1 .or. m.lt.(n*n+n)/2) return
      if(k.lt.1 .or. k.gt.n) return
      if(e.lt.zero) return
      ifault=0
c
      Parameters in range so test for collinearity
c
      l=k
      kk=(k*k+k)/2
      if(t(kk).lt.zero) goto 20
      if(t(kk).lt.e*s(k)) return
      ii=0
      ik=kk-k
      do 10 l=1,n
         ii=ii+1
         ik=ik+1
         if (l.gt.k) ik=ik+1-2
         if (t(ii).ge.zero) goto 10
         if(one/(t(ik)*t(ik)/t(kk)-t(ii)).lt.e*s(l)) return
10      continue
c
      No collinearity so update triangle
c
20      l=0
      t(kK)=-one/t(kk)
      a=abs(t(kk))
      ik=kk-k
      ij=0
      do 90 i=1,n
         ik=ik+1
         if(i-k) 50,30,40
30      ij=ij+k
         goto 90
40      ik=ik+i-2
50      b=t(ik)
         if(t(kk).lt.zero) b=-b
         t(ik)=a*t(ik)
         jk=kk-k
         do 80 j=1,i
            ij=ij+1
            jk=jk+1
            if(j-k) 70,80,60
60      jk=jk+j-2
70      t(ij)=t(ij)+b*t(jk)
80      continue
90      continue
      return
      end
```

##### User Supplied Comment and Possible Correction #####

I think I've found a bug in routine 193 permut. There is an array overflow caused statement label "7", which currently reads

```
7 do 8 j = 1,t
```

t is equal to n at the end of the algorithm, therefore j equals n. However, the a(k,n) array is referenced in the following lines as a(i,j+1) which is outside the array bounds.

The correct line should read:

```
7 do 8 j = 1,t-1
```

I've tested the change and the program appears to behave the same. The program appeared to work previously but this relied on IFAULT being zero and immediately after A in memory.

cheers,

Mark

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#####

```
      subroutine permut(n,k,r,a,ifault)
c
c   Algorithm AS 179   Appl. Statist. (1982) Vol.31, No.2
c
c   A single call generates all possible permutations of N
c   objects, partitioned into K non-empty subsets, and passed
c   as array R.
c
c   integer a(k,n),r(k),t,t2,tj1
c
c   check for fault conditions
c
c   ifault = 1
c   do 1 i = 1,k
c     if (r(i).eq.0) return
1  continue
c   ifault = 2
c   isum = 0
c   do 2 i = 1,k
2  isum = isum + r(i)
c   if (isum.ne.n) return
c   ifault = 0
c
c   step 1.  To initialise array A, fill rows, 1 to k-1, with
c           paired marks.
c
c   kount = 1
c   l = n
c   k1 = k-1
c   do 5 i = 1,k1
c     ir = r(i)
c     do 3 j = 1,ir
3    a(i,j) = i
c     ir1 = r(i) + 1
c     do 4 j = ir1,1
4    a(i,j) = i+1
c     l = l - r(i)
5  continue
```

```
c
c   step 2.  Begin generation of permutations by setting looping
c           indices i and t.  i indicates a row in array a, j
c           indicates a column in array a, and t indicates the
c           number of marks in row i.
c           If this is the first permutation, go to step 5.
c
6  i = k - 1
   t = r(k) + r(i)
   if (kount.eq.1) goto 14
c
c   step 3.  Search for an i mark followed by an i+1 mark in
c           row i and interchange the two marks.  If an
c           interchange is made, left-shift any marks out of
c           sequence, otherwise go to step 4.
c
7  do 8 j = 1,t
   j1 = j + 1
   if (a(i,j).ne.i.or.a(i,j1).ne.i+1) goto 8
   limit = j - 2
   a(i,j) = a(i,j1)
   a(i,j1)= a(i,j) - 1
   if (limit) 14, 14, 12
8  continue
c
c   step 4.  Interchange not made, so return row i to its initial
c           configuration in step 1 and go to step 1.
c
   if (t.eq.1) goto 10
   t2 = t/2
   do 9 j = 1,t2
   tj1 = t - j + 1
   itemp = a(i,j)
   a(i,j) = a(i,tj1)
   a(i,tj1) = itemp
9  continue
c
c   Reset looping indices i and t.  Return if i = 0, otherwise
c   go to step 3.
c
10 i = i - 1
   if (i.gt.0) goto 11
   return
11 t = t + r(i)
   goto 7
c
c   Interchange made, so left-shift any marks out of sequence
c   and go to step 5.
c
12 iflag = 0
   do 13 j = 1,limit
   j1 = j + 1
   if (a(i,j).ne.i + 1.or.a(i,j1).ne.i) goto 13
   a(i,j) = a(i,j1)
   a(i,j1)= a(i,j) + 1
   iflag = 1
13 continue
   if (iflag.eq.1) goto 12
c
c   step 5.  Fill last row (k) of array a with marks from row 1
c           and generate current permutation in last row (k)
```

```
c          of array a.
c
c 14 do 15 j = 1,n
c 15 a(k,j) = a(1,j)
c
c     if (k.eq.2) goto 18
c     do 17 l = 2,k1
c       m = 1
c       do 16 j = 1,n
c         if (a(k,j).ne.1) goto 16
c         a(k,j) = a(1,m)
c         m = m + 1
c 16   continue
c 17   continue
c
c     step 6.  At this point, call subroutine job to process the
c             current permutation, or execute equivalent
c             statements, and go to step 2.
c
c 18 call job(n,k,a,kount)
c
c     kount = kount + 1
c     goto 6
c     end
```

```
REAL FUNCTION TRIMSD(X, N, K, IW, IFAULT)
C
C ALGORITHM AS 180 APPL. STATIST. (1982) VOL.31, NO.2
C
C The value returned is a linear estimate of the standard deviation
C from a sample of N values of X symmetrically trimmed to retain K
C values.
C
C INTEGER IW(N)
C REAL X(N), QTR, HALF, P74, P98, AMID, B, P, SUM, C(6)
C DATA C/1.06683, 1.72534, 0.403049, 1.32458, -3.91154, 17.5265/,
* QTR/0.25/, HALF/0.5/, P74/0.74/, P98/0.98/
C
C IFAULT = 1
C TRIMSD = -1.0
C IF (N .LT. 4) RETURN
C IFAULT = 2
C P = K / FLOAT(N)
C IF (P .LT. HALF .OR. P .GT. P98) RETURN
C IFAULT = 3
C IF (MOD(N-K, 2) .NE. 0) RETURN
C IFAULT = 0
C
C ILO = (N-K)/2 + 1
C IHI = N - ILO + 1
C AMID = N + 1
C
C Get ranks of X in IW
C
C IW(1) = 1
C DO 10 I = 2, N
C   IW(I) = 1
C   DO 10 J = 1, I-1
C     IF (X(I) .GE. X(J)) GO TO 9
C     IW(J) = IW(J) + 1
C     GO TO 10
C 9   IW(I) = IW(I) + 1
C 10 CONTINUE
C
C SUM = 0.0
C DO 12 I = 1, N
C 12 IF (IW(I) .GE. ILO .AND. IW(I) .LE. IHI) SUM =
*   SUM + (2.0 * IW(I) - AMID) * X(I)
C
C Calculate the unbiassing factor
C
C P = P74 - P
C B = (((C(6)*P + C(5))*P + C(4))*P + C(3))*P + C(2))*P + C(1)
C
C TRIMSD = EXP(B) * SUM / (QTR * (2*K*(2*K - 1)))
C RETURN
C END
```

```

      SUBROUTINE FORKAL(IP, IQ, IR, NP, IRD, IRZ, ID, IL, N, NRBAR,
*     PHI, THETA, DELTA, W, Y, AMSE, A, P, V, RESID, E, XNEXT, XROW,
*     RBAR, THETAB, STORE, IFAULT)
C
C     ALGORITHM AS 182  APPL. STATIST. (1982) VOL.31, NO.2
C
C     Finite sample prediction from ARIMA processes.
C
C     Auxiliary routines required: KARMA & STARMA from AS 154 and
C     routines called by them: INCLU2 from ASR 17 (a slight variant on
C     AS 75, and REGRES from AS 75.
C
      REAL PHI(IR), THETA(IR), DELTA(ID), W(N), Y(IL), AMSE(IL),
*     A(IRD), P(IRZ), V(NP), RESID(N), E(IR), XNEXT(NP), XROW(NP),
*     RBAR(NRBAR), THETAB(NP), STORE(IRD)
      REAL ZERO, ONE, TWO
      DATA ZERO/0.0/, ONE/1.0/, TWO/2.0/
C
C     Invoking this routine will calculate the finite sample predictions
C     and their conditional mean square errors for any ARIMA process.
C
C     Check for input faults.
C
      IFAULT = 0
      IF (IP .LT. 0) IFAULT = 1
      IF (IQ .LT. 0) IFAULT = IFAULT + 2
      IF (IP * IP + IQ * IQ .EQ. 0) IFAULT = 4
      K = IQ + 1
      IF (K .LT. IP) K = IP
      IF (IR .NE. K) IFAULT = 5
      IF (NP .NE. IR * (IR + 1) / 2) IFAULT = 6
      IF (NRBAR .NE. NP * (NP - 1) / 2) IFAULT = 7
      IF (ID .LT. 0) IFAULT = 8
      IF (IRD .NE. IR + ID) IFAULT = 9
      IF (IRZ .NE. IRD * (IRD + 1) / 2) IFAULT = 10
      IF (IL .LT. 1) IFAULT = 11
      IF (IFAULT .NE. 0) RETURN
C
C     Calculate initial conditions for Kalman filter
C
      A(1) = ZERO
      V(1) = ONE
      IF (NP .EQ. 1) GO TO 130
      DO 100 I = 2, NP
100  V(I) = ZERO
      IF (IQ .EQ. 0) GO TO 130
      IQ1 = IQ + 1
      DO 110 I = 2, IQ1
110  V(I) = THETA(I-1)
      DO 120 J = 1, IQ
          LL = J * (2*IR + 1 - J) / 2
          DO 120 I = J, IQ
              LLI = LL + I
              V(LLI) = THETA(I) * THETA(J)
120  CONTINUE
C
C     Find initial likelihood conditions.
C     IFAULT not tested on exit from STARMA as all possible errors
C     have been checked above.
C
130  IF (IR .EQ. 1) P(1) = ONE / (ONE - PHI(1) * PHI(1))

```

```

      IF (IR .NE. 1) CALL STARMA(IP, IQ, IR, NP, PHI, THETA, A, P, V,
*   THETAB, XNEXT, XROW, RBAR, NRBAR, IFAULT)
C
C   Calculate data transformations
C
      NT = N - ID
      IF (ID .EQ. 0) GO TO 170
      DO 140 J = 1, ID
        NJ = N - J
        STORE(J) = W(NJ)
140  CONTINUE
      DO 160 I = 1, NT
        AA = ZERO
        DO 150 K = 1, ID
          IDK = ID + I - K
          AA = AA - DELTA(K) * W(IDK)
150  CONTINUE
        IID = I + ID
        W(I) = W(IID) + AA
160  CONTINUE
C
C   Evaluate likelihood to obtain final KF conditions
C
170  SUMLOG = ZERO
      SSQ = ZERO
      IUPD = 1
      DEL = - ONE
      NIT = 0
      CALL KARMA(IP, IQ, IR, NP, PHI, THETA, A, P, V, NT, W, RESID,
*   SUMLOG, SSQ, IUPD, DEL, E, NIT)
C
C   Calculate M.L.E. of sigma squared
C
      SIGMA = ZERO
      DO 200 J = 1, NT
200  SIGMA = SIGMA + RESID(J)**2
      SIGMA = SIGMA / NT
C
C   Reset the initial A and P when differencing occurs
C
      IF (ID .EQ. 0) GO TO 250
      DO 210 I = 1, NP
210  XROW(I) = P(I)
      DO 220 I = 1, IRZ
220  P(I) = ZERO
      IND = 0
      DO 230 J = 1, IR
        K = (J-1) * (ID + IR + 1) - (J-1) * J / 2
        DO 230 I = J, IR
          IND = IND + 1
          K = K + 1
          P(K) = XROW(IND)
230  CONTINUE
      DO 240 J = 1, ID
        IRJ = IR + J
        A(IRJ) = STORE(J)
240  CONTINUE
C
C   Set up constants
C
250  IR2 = IR + 1

```

```

IR1 = IR - 1
ID1 = ID - 1
ID2R = 2 * IRD
ID2R1 = ID2R - 1
IDD1 = 2 * ID + 1
IDD2 = IDD1 + 1
I45 = ID2R + 1
IDRR1 = IRD + 1
IDDR = 2 * ID + IR
JKL = IR * (IDDR + 1) / 2
JKL1 = JKL + 1
ID2R2 = ID2R + 2
IBC = IR * (I45 - IR) / 2
DO 560 L = 1, IL

```

C  
C  
C

Predict A

```

A1 = A(1)
IF (IR .EQ. 1) GO TO 310
DO 300 I = 1, IR1
300 A(I) = A(I+1)
310 A(IR) = ZERO
IF (IP .EQ. 0) GO TO 330
DO 320 J = 1, IP
320 A(J) = A(J) + PHI(J) * A1
330 IF (ID .EQ. 0) GO TO 360
DO 340 J = 1, ID
IRJ = IR + J
A1 = A1 + DELTA(J) * A(IRJ)
340 CONTINUE
IF (ID .LT. 2) GO TO 360
DO 350 I = 1, ID1
IRI1 = IRD - I
A(IRI1 + 1) = A(IRI1)
350 CONTINUE
360 A(IR2) = A1

```

C  
C  
C

Predict P

```

IF (ID .EQ. 0) GO TO 480
DO 370 I = 1, ID
STORE(I) = ZERO
DO 370 J = 1, ID
LL = MAX(I,J)
K = MIN(I,J)
JJ = JKL + (LL - K) + 1 + (K-1) * (IDD2 - K) / 2
STORE(I) = STORE(I) + DELTA(J) * P(JJ)
370 CONTINUE
IF (ID .EQ. 1) GO TO 400
DO 380 J = 1, ID1
JJ = ID - J
LK = (JJ-1) * (IDD2 - JJ) / 2 + JKL
LK1 = JJ * (IDD1 - JJ) / 2 + JKL
DO 380 I = 1, J
LK = LK + 1
LK1 = LK1 + 1
P(LK1) = P(LK)
380 CONTINUE
DO 390 J = 1, ID1
JKLJ = JKL1 + J
IRJ = IR + J

```



```

      P(JKLJ) = STORE(J) + P(IRJ)
390  CONTINUE
400  P(JKL1) = P(1)
      DO 410 I = 1, ID
          IRI = IR + I
          P(JKL1) = P(JKL1) + DELTA(I) * (STORE(I) + TWO * P(IRI))
410  CONTINUE
      DO 420 I = 1, ID
          IRI = IR + I
          STORE(I) = P(IRI)
420  CONTINUE
      DO 430 J = 1, IR
          KK1 = J * (ID2R1 - J) / 2 + IR
          K1 = (J-1) * (ID2R - J) / 2 + IR
          DO 430 I = 1, ID
              KK = KK1 + I
              K = K1 + I
              P(K) = PHI(J) * STORE(I)
              IF (J .NE. IR) P(K) = P(K) + P(KK)
430  CONTINUE
C
      DO 440 J = 1, IR
          STORE(J) = ZERO
          KKK = J * (I45 - J) / 2 - ID
          DO 440 I = 1, ID
              KKK = KKK + 1
              STORE(J) = STORE(J) + DELTA(I) * P(KKK)
440  CONTINUE
      IF (ID .EQ. 1) GO TO 460
      DO 450 J = 1, IR
          K = J * IDRR1 - J * (J+1) / 2 + 1
          DO 450 I = 1, ID1
              K = K - 1
              P(K) = P(K-1)
450  CONTINUE
460  DO 470 J = 1, IR
          K = (J-1) * (ID2R - J) / 2 + IR + 1
          P(K) = STORE(J) + PHI(J) * P(1)
          IF (J .LT. IR) P(K) = P(K) + P(J+1)
470  CONTINUE
480  DO 490 I = 1, IR
490  STORE(I) = P(I)
C
      IND = 0
      DT = P(1)
      DO 500 J = 1, IR
          PHIJ = PHI(J)
          PHIJDT = PHIJ * DT
          IND2 = (J-1) * (ID2R2 - J) / 2
          IND1 = J * (I45 - J) / 2
          DO 500 I = J, IR
              IND = IND + 1
              IND2 = IND2 + 1
              PHII = PHI(I)
              P(IND2) = V(IND) + PHII * PHIJDT
              IF (J .LT. IR) P(IND2) = P(IND2) + STORE(J+1) * PHII
              IF (I .EQ. IR) GO TO 500
              IND1 = IND1 + 1
              P(IND2) = P(IND2) + STORE(I+1) * PHIJ + P(IND1)
500  CONTINUE
C

```

```
C      Predict Y
C
      Y(L) = A(1)
      IF (ID .EQ. 0) GO TO 520
      DO 510 J = 1, ID
          IRJ = IR + J
          Y(L) = Y(L) + A(IRJ) * DELTA(J)
510    CONTINUE
C
C      Calculate M.S.E. of Y
C
520    AMS = P(1)
      IF (ID .EQ. 0) GO TO 550
      DO 530 J = 1, ID
          JRJ = IBC + (J-1) * (IDD2 - J) / 2
          IRJ = IR + J
          AMS = AMS + TWO * DELTA(J) * P(IRJ) + P(JRJ+1) * DELTA(J)**2
530    CONTINUE
      IF (ID .EQ. 1) GO TO 550
      DO 540 J = 1, ID1
          J1 = J + 1
          JRK = IBC + 1 + (J-1) * (IDD2 - J) / 2
          DO 540 I = J1, ID
              JRK = JRK + 1
              AMS = AMS + TWO * DELTA(I) * DELTA(J) * P(JRK)
540    CONTINUE
550    AMSE(L) = AMS * SIGMA
560    CONTINUE
C
      RETURN
      END
```

```
real function random()
```

```
c  
c Algorithm AS 183 Appl. Statist. (1982) vol.31, no.2  
c  
c Returns a pseudo-random number rectangularly distributed  
c between 0 and 1. The cycle length is 6.95E+12 (See page 123  
c of Applied Statistics (1984) vol.33), not as claimed in the  
c original article.
```

```
c  
c IX, IY and IZ should be set to integer values between 1 and  
c 30000 before the first entry.
```

```
c  
c Integer arithmetic up to 30323 is required.
```

```
c  
integer ix, iy, iz  
common /randc/ ix, iy, iz
```

```
c  
ix = 171 * mod(ix, 177) - 2 * (ix / 177)  
iy = 172 * mod(iy, 176) - 35 * (iy / 176)  
iz = 170 * mod(iz, 178) - 63 * (iz / 178)
```

```
c  
if (ix .lt. 0) ix = ix + 30269  
if (iy .lt. 0) iy = iy + 30307  
if (iz .lt. 0) iz = iz + 30323
```

```
c  
c If integer arithmetic up to 5212632 is available, the preceding  
c 6 statements may be replaced by:
```

```
c  
ix = mod(171 * ix, 30269)  
iy = mod(172 * iy, 30307)  
iz = mod(170 * iz, 30323)
```

```
c  
random = mod(float(ix) / 30269. + float(iy) / 30307. +  
+ float(iz) / 30323., 1.0)
```

```
return  
end
```

```
c  
c  
c  
c  
real function uniform()
```

```
c  
c Generate uniformly distributed random numbers using the 32-bit  
c generator from figure 3 of:  
c L'Ecuyer, P. Efficient and portable combined random number  
c generators, C.A.C.M., vol. 31, 742-749 & 774-?, June 1988.
```

```
c  
c The cycle length is claimed to be 2.30584E+18
```

```
c  
c Seeds can be set by calling the routine set_uniform
```

```
c  
c It is assumed that the Fortran compiler supports long variable  
c names, and integer*4.
```

```
c  
integer*4 z, k, s1, s2  
common /unif_seeds/ s1, s2  
save /unif_seeds/
```

```
c  
k = s1 / 53668  
s1 = 40014 * (s1 - k * 53668) - k * 12211  
if (s1 .lt. 0) s1 = s1 + 2147483563
```

```
c
      k = s2 / 52774
      s2 = 40692 * (s2 - k * 52774) - k * 3791
      if (s2 .lt. 0) s2 = s2 + 2147483399

c
      z = s1 - s2
      if (z .lt. 1) z = z + 2147483562

c
      uniform = z / 2147483563.
      return
      end

      subroutine set_uniform(seed1, seed2)

c
c      Set seeds for the uniform random number generator.
c
      integer*4 s1, s2, seed1, seed2
      common /unif_seeds/ s1, s2
      save /unif_seeds/

      s1 = seed1
      s2 = seed2
      return
      end
```

```

SUBROUTINE PROB(EPSI, N, NU, C, M, VM, ANS, BOUND, RND, IFAULT)

```

```

C
C<<<<< Acquired in machine-readable form from 'Applied Statistics'
C<<<<< algorithms editor, January 1983.

```

```

C
C      ALGORITHM AS 184  APPL. STATIST. (1982) VOL.31, NO.3

```

```

C
C      CALCULATES EXPRESSION (1) OF THE PURPOSE SECTION.
C      USEFUL FOR NON-CENTRAL STUDENTIZED MAXIMUM, MAXIMUM MODULUS,
C      AND MULTIPLE T-TEST PROBABILITIES.

```

```

C
C      DIMENSION PROD(2), EK(3), PHI(2, 10), C(2, N), AC(2), AM(2), M(N),
*      PH(200, 10), S(5), G2(3), G1(3), GMX(4), G2S(200, 3), AD(2, 10),
*      ER(4), PHM(10), RS(10), VM(N), R(200), PR(200)

```

```

C
C      ALR2PI=ALOG(2.0*PI), AL2=ALOG(2.0),
C      ER CONTAINS ROUNDING ERROR BOUNDS

```

```

C
C      DATA ALR2PI /0.91893853320467274178/,AL2 /0.69314718055994530942/,
*      ER(1), ER(2), ER(3), ER(4) /5.0E-07, 5.0E-07, 5.0E-07, 5.0E-07/,
*      ZERO, HALF, ONE, TWO, SEVEN, EIGHT /0.0, 0.5, 1.0, 2.0, 7.0,
*      8.0/, EITH, SEVEIG, FOUR, TWEL, XNIN6 /0.125, 0.875, 4.0, 12.0,
*      96.0/, MAXN /10/

```

```

C
C      FUNCTION STATEMENTS

```

```

C
C      BDD1(X, Y, Z) = ABS((X - Z) / Y - X * Y)
C      BDD2(W, X, Y, Z) = ABS((W - Y) * (W - Z) + (X * X) * ((-Z * W + Y)
*      * W + W * W * X * X))
C      GABS(X) = ABS(X)
C      GEXP(X) = EXP(X)
C      GMAX1(X, Y) = AMAX1(X, Y)
C      TMAX1(X, Y, Z) = AMAX1(X, Y, Z)
C      GMIN1(X, Y) = AMIN1(X, Y)
C      GSQRT(X) = SQRT(X)
C      GFLOAT(IJ) = FLOAT(IJ)
C      GLOG(X) = ALOG(X)

```

```

C
C      CHECKING FOR FAULTY INPUT DATA

```

```

C
C      IFAULT = 0
C      IF (NU .LE. 0) IFAULT = 1
C      IF (EPSI .LE. ER(3)) IFAULT = 2
C      IF (N .LE. 0 .OR. N .GT. MAXN) IFAULT = 3
C      IF (IFAUULT .NE. 0) RETURN
C      IZERO = 0
C      DO 2 J = 1, N
C      IF (C(1, J) .EQ. C(2, J) .AND. M(J) .EQ. 0) IZERO = 1
C      IF (C(1, J) .GT. C(2, J) .AND. M(J) .EQ. 0) IFAULT = 100 + J
C      IF (M(J) .EQ. 1 .AND. C(1, J) .NE. ZERO) IFAULT = 200 + J
C      IF (M(J) .EQ. 2 .AND. C(2, J) .NE. ZERO) IFAULT = 300 + J
C      IF (M(J) .EQ. 3 .AND. (C(1, J) .NE. ZERO .OR. C(2, J) .NE. ZERO))
*      IFAULT = 400 + J
C      IF (M(J) .LT. 0 .OR. M(J) .GT. 3) IFAULT = 500 + J
2 CONTINUE
C      IF (IFAUULT .NE. 0) RETURN

```

```

C
C      IZERO=1 IF ONE OF THE RANGES (C1,C2) IS DEGENERATE

```

```

C
C      ANS = ZERO
C      BOUND = ZERO

```

```

RND = ZERO
IF (IZERO .EQ. 1) RETURN
C
C      INITIALIZING VALUES TO BE USED IN PROGRAM
C
NK = N - 1
ITCH = 2
INDXL = 3
DF = GFLOAT(NU)
HD = HALF * DF
COEFF = HD * GLOG(HD) - ALGAMA(HD) + AL2
COFF = GEXP(COEFF)
EG = ONE
FE = ZERO
K = 1
TD = HALF / DF
SDFT = GSQRT(EIGHT * DF - SEVEN) * TD
S(1) = ZERO
S(2) = GSQRT(ONE - TD - SDFT)
S(3) = GSQRT((DF - ONE) / DF)
S(4) = GSQRT(ONE - TD + SDFT)
S(5) = GMAX1(TWO, GSQRT(ONE + GSQRT(GSQRT(XNIN6 * (FOUR + DF)
* / (EPSI * DF ** 3))))))
EPSL = EPSI * SEVEIG / S(5)
ES = S(5) - (S(4) - S(2)) * GMIN1(ONE, GFLOAT(NU / 3))
EK(2) = ZERO
EK(3) = ZERO
PROD(1) = ONE
C
C      THE FIRST 4 LINES OF THE DO 6 LOOP DETERMINE WHERE THE FACTORS,
C      PHI( ,JK), OF PROD ARE MONOTONE.
C      THE LOOP COMPUTES PHI AND PROD FOR S=0.0
C
DO 6 JK = 1, N
RS(JK) = -ONE
SUMC = C(1, JK) + C(2, JK)
IF (C(1, JK) * C(2, JK) .GT. ZERO) RS(JK) = VM(JK) / SUMC +
* GSQRT(VM(JK) * VM(JK) + TWO * SUMC * GLOG(C(2, JK) / C(1, JK))
* / (C(2, JK) - C(1, JK))) / GABS(SUMC)
IF (M(JK) .EQ. 0) PHI(1, JK) = ZERO
IF (M(JK) .EQ. 1) PHI(1, JK) = ALNORM(-VM(JK), .FALSE.)
IF (M(JK) .EQ. 2) PHI(1, JK) = ONE - ALNORM(-VM(JK), .FALSE.)
IF (M(JK) .EQ. 3) PHI(1, JK) = ONE
PROD(1) = PROD(1) * PHI(1, JK)
6 CONTINUE
C
C      THESE 5 LINES AND THE FIRST 4 LINES OF THE DO 60 LOOP ARE
C      SPECIAL HANDLING FOR NU.LE.2
C
IXG = MIN0(2, NU - 1)
XH = GFLOAT((2 - IXG) / 2)
G1(1) = XH * COFF
G1(2) = GFLOAT(IXG - 2 * (IXG / 2)) * COFF
G1(3) = BDD2(DF, ZERO, ONE, TWO) + GFLOAT(1 - (1 + IXG) / 2)
C
C      INTEGRATION BEGINS. (FE,R(K)) IS CURRENT SUBINTERVAL
C
DO 60 L = 2, 5
IF ((NU .LE. 2 .AND. L .EQ. 2) .OR. (NU .EQ. 1 .AND. L .LE. 3))
* GOTO 60
R(1) = S(L)

```

```

      ITCH = 2
      IF (NU .LE. 2 .OR. L .EQ. 2 .OR. L .EQ. 5) GOTO 13
      INDXL = 2
      ITCH = 1
      GOTO 13
C
C      SETTING UP THE MESH.      STATEMENTS 9-12 MAKE THE MESH FINER
C
      9 IF (K .GE. 200) GOTO 62
      R(K + 1) = (R(K) + FE) * HALF
      PR(K) = PROD(2)
      DO 11 J = 1, N
11 PH(K, J) = PHI(2, J)
      DO 12 J = 1, INDXL
12 G2S(K, J) = G2(J)
      K = K + 1
      ITCH = INDXL - 1
C
C      COMPUTING PHI, PROD, DENSITY OF S, AND ITS DERIVATIVE AT S=R(K)
C
13 G2(1) = GEXP(COEFF + (DF - ONE) * GLOG(R(K)) - DF * R(K) * R(K)
* * HALF)
      G2(2) = G2(1) * BDD1(DF, R(K), ONE)
      PROD(2) = ONE
      DO 14 J = 1, N
      IF (M(J) .EQ. 0) PHI(2, J) = ALNORM(C(2, J) * R(K) - VM(J),
* .FALSE.) - ALNORM(C(1, J) * R(K) - VM(J), .FALSE.)
      IF (M(J) .EQ. 1) PHI(2, J) = ALNORM(C(2, J) * R(K) - VM(J),
* .FALSE.)
      IF (M(J) .EQ. 2) PHI(2, J) = ONE - ALNORM(C(1, J) * R(K) - VM(J),
* .FALSE.)
      IF (M(J) .EQ. 3) PHI(2, J) = ONE
      PROD(2) = PROD(2) * PHI(2, J)
14 CONTINUE
C
C      STATEMENTS 18-22 DECIDE WHETHER TO USE FORM A (INDXL=3)
C      OR FORM B (INDXL=2).
C      ITCH DETERMINES WHETHER OR NOT G2(3) NEEDS TO BE COMPUTED
C
18 EPS = R(K) * EPSL
      GMIN = GMIN1(G1(1), G2(1))
      IF (NU .LE. 2) GOTO 22
      IF (GMIN .LT. ONE) GOTO 20
      INDXL = 2
      GOTO 26
20 IF (((INDXL .EQ. 3) .OR. (L .EQ. 3)) .OR. (L .EQ. 4)) GOTO 22
      G1(3) = BDD2(DF, FE, ONE, TWO) / (FE * FE)
      INDXL = 3
      ITCH = 2
22 IF (ITCH .EQ. 2) G2(3) = BDD2(DF, R(K), ONE, TWO) / (R(K) * R(K))
C
C      THE DO 32 LOOP COMPUTES BOUNDS FOR FIRST (AD(1,J)) AND
C      SECOND (AD(2,J)) DERIVATIVES OF PHI( ,J)
C
26 PRM = ONE
      DO 32 J = 1, N
      PHM(J) = GMAX1(PHI(1, J), PHI(2, J))
      IF (FE .LT. RS(J) .AND. R(K) .GT. RS(J)) PHM(J) = ALNORM(C(2, J)
* * RS(J) - VM(J), .FALSE.) - ALNORM(C(1, J) * RS(J) - VM(J),
* .FALSE.)
      PRM = PRM * PHM(J)

```

```

DO 30 I = 1, 2
AC1 = GABS(GABS(C(I, J) * FE) - GABS(VM(J)))
AC2 = GABS(GABS(C(I, J) * R(K)) - GABS(VM(J)))
AC(I) = GMIN1(AC1, AC2)
IF (C(I, J) .EQ. ZERO) GOTO 28
RATC = VM(J) / C(I, J)
IF (FE .LT. RATC .AND. R(K) .GT. RATC) AC(I) = ZERO
28 AM(I) = GMAX1(AC1, AC2)
AC(I) = GABS(C(I, J)) * GEXP(-HALF * AC(I) * AC(I) - ALR2PI)
30 CONTINUE
AD(1, J) = AC(1) + AC(2)
AD(2, J) = GABS(C(2, J)) * AM(2) * AC(2) + GABS(C(1, J)) * AM(1)
* * AC(1)
32 CONTINUE
C
C     THE DO 33 AND DO 34 LOOPS BOUND FIRST (BOU1) AND
C     SECOND (BOU2) DERIVATIVES OF PROD
C
BOU1 = ZERO
BOU2 = ZERO
DO 33 J = 1, N
BOU2 = BOU2 + PRM / PHM(J) * AD(2, J)
33 BOU1 = BOU1 + PRM / PHM(J) * AD(1, J)
IF (N .EQ. 1) GOTO 36
DO 34 J = 1, NK
JJ = J + 1
DO 34 KM = JJ, N
BOU2 = BOU2 + TWO * PRM / (PHM(J) * PHM(KM)) * AD(1, J) *
* AD(1, KM)
34 CONTINUE
36 IF (INDXL .EQ. 2) GOTO 40
C
C     CHECKING THE BOUND FOR THE FORM A CASES
C
DEL = R(K) - FE
DO 38 J = 1, 3
38 GMX(J) = GMAX1(G1(J), G2(J))
GMX(4) = GMX(1) * GMX(3)
IF (NU .EQ. 3 .AND. FE .EQ. ZERO) GMX(4) = GMAX1(GMX(4), TWO *
* COFF)
CHECK = (DEL ** 3) * (PRM * GMX(4) + BOU2 * GMX(1) + BOU1 * TWO *
* GMX(2)) / TWEL
GA = G1(1)
GB = G2(1)
GOTO 43
C
C     CHECKING THE BOUND FOR THE FORM B CASES
C
40 DEL = GAMAIN(DF, R(K) * R(K) * DF) - GAMAIN(DF, FE * FE * DF)
BOU3 = GMAX1(BDD1(DF, FE, ONE), BDD1(DF, R(K), ONE))
CHECK = (DEL ** 3) * (BOU2 + BOU1 * BOU3) / (GMIN * GMIN * TWEL)
GA = ONE
GB = ONE
43 BOU4 = BOUND + CHECK
IF (BOU4 .GT. EPS) GOTO 9
ANS = ANS + HALF * (PROD(1) * GA + PROD(2) * GB) * DEL
EK(INDXL) = EK(INDXL) + ONE
C
C     ADVANCING THE INTEGRATION IF THE BOUND IS SMALL ENOUGH
C
BOUND = BOU4

```



```
      IF (INDXL .EQ. 3) EG = TMAX1(EG, G1(1), G2(1))
      FE = R(K)
      PROD(1) = PROD(2)
      DO 46 J = 1, INDXL
46    G1(J) = G2(J)
      DO 50 J = 1, N
50    PHI(1, J) = PHI(2, J)
      IF (K .LE. 1) GOTO 60
      K = K - 1
      ITCH = 1
      DO 54 J = 1, N
54    PHI(2, J) = PH(K, J)
      PROD(2) = PR(K)
      DO 56 J = 1, INDXL
56    G2(J) = G2S(K, J)
      GOTO 18
60    CONTINUE
      BOUND = BOUND + EPSI * EITH
```

C  
C  
C

COMPUTING THE BOUND ON ROUNDING ERROR

```
      AN = GFLOAT(N)
      EA = GABS(GEXP(ER(4)) - ONE)
      RND = (EG * TWO * AN * ER(1) + EG * EA / (ONE + EA) + ER(3))
* * (ES + EK(3) * ER(3)) + ER(3) * EK(3) * EG + TWO * AN * ER(1)
* + (ONE + TWO * AN * ER(1)) * EK(2) * ER(2)
      RETURN
62  IFAULT = 4
      RETURN
      END
```

```

SUBROUTINE ASRCH(NVAR, DIM, TABLE, NTAB, FIT, TFIT, INIT, CONFIG,
*   NCON, MCON, CONFIG1, CONFIG2, CONFIG3, MARG, NMAR, U, NU, MAXDEV,
*   MAXIT, DEV, L1, L2, IA, MA, IB, MB, NI, NA, IFAULT)

```

```

C
C   ALGORITHM AS 185  APPL. STATIST. (1982) VOL.31, NO.3
C
C   This algorithm searches for a best log-linear model in contingency
C   tables using backward elimination procedure.

```

```

C   This version permits up to 7 variables.  If this limit is too
C   small, change the value of MAXVAR to its new limit, and the value
C   of the dimension of LOCMAR, MASK, & DELEF to the values of MCON,
C   MAXVAR + 1, and MAXVAR respectively.  See also changes needed in
C   subroutines LOGLIN (AS 51, Haberman 1972), LOWEFF, and DEGREF.

```

```

C   AS R87 has been incorporated from AS vol.40(2)

```

```

C   Auxiliary routines required: AS 51 and AS 66

```

```

C   INTEGER DIM(NVAR), LOCMAR(35), CONFIG(NVAR, MCON), CONFIG1(NVAR,
*   MCON), CONFIG2(NVAR, MCON), CONFIG3(NVAR, MCON), DELEF(7),
*   MASK(8), IB(NVAR, MB), SIZE
C   REAL TABLE(NTAB), FIT(NTAB), TFIT(NTAB), MARG(NMAR), U(NU),
*   MAXDEV, DEV(MAXIT), IA(4, MA), L1, L2, LR, LR1, LR3, ZERO
C   DATA MAXVAR /7/, ZERO /0.0/

```

```

C
C   IFAULT = 0
C   NA = 0
C   NB = 0
C   IF (NVAR .GT. 0 .AND. NVAR .LE. MAXVAR) GO TO 10
5  IFAULT = 4
C   RETURN

```

```

C
10  SIZE = 1
C   DO 12 I = 1, NVAR
C     IF (DIM(I) .LE. 0) GO TO 5
C     SIZE = SIZE * DIM(I)
12  CONTINUE
C   IF (SIZE .NE. NTAB) GO TO 5
C   DO 15 I = 1, NTAB
C     IF (TABLE(I) .LT. ZERO .OR. FIT(I) .LT. ZERO) GO TO 5
C     TFIT(I) = FIT(I)
15  CONTINUE

```

```

C   Select a best initial fit.  Skip step if given initial fit by user.

```

```

C
C   DO 70 NWAY = 1, NVAR
C     IF (INIT .EQ. 1) GO TO 50

```

```

C   Construct CONFIG for model with full I-order effects

```

```

C
C   NCON = 1
C   DO 20 I = 1, NWAY
20  NCON = NCON * (NVAR - I + 1) / I
C   IF (MCON .LT. NCON) GO TO 400
C   DO 25 J = 1, NVAR
C     MASK(J) = J - 1
C     DO 25 I = 1, NCON
C       CONFIG(J,I) = 0
25  CONTINUE
C   MASK(NWAY+1) = NVAR

```

```

      DO 45 L = 1, NCON
      DO 35 J = 1, NWAY
35     CONFIG(J,L) = MASK(J) + 1
      DO 40 J = 1, NWAY
      MASK(J) = MASK(J) + 1
      IF (MASK(J) .LT. MASK(J+1)) GO TO 45
      MASK(J) = J - 1
40     CONTINUE
45     CONTINUE
C
C     LOGLIN performs an iterative proportional fit of the marginal
C     totals (described in CONFIG) for a contingency table.
C
50     CALL LOGLIN(NVAR, DIM, NCON, CONFIG, NTAB, TABLE, FIT, LOCMAR,
*       NMAR, MARG, NU, U, MAXDEV, MAXIT, DEV, NLAST, IFAULT)
      IF (IFAULT .GT. 0) RETURN
      NA = NA + 1
      NI = NA
      CALL LRCHSQ(TABLE, FIT, NTAB, LR)
      CALL DEGREF(NVAR, DIM, NCON, NTAB, CONFIG, DF)
      P = XTAIL(LR, DF)
      CALL CPYLR(LR, DF, P, IA(1,NA), IA(2,NA), IA(3,NA))
      IF (NA .GT. MA .OR. (NB + NCON) .GT. MB) GO TO 400
      IA(4,NA) = NCON
      DO 55 K = 1, NCON
      NB = NB + 1
      DO 55 I = 1, NVAR
      IB(I,NB) = CONFIG(I,K)
55     CONTINUE
      IF (INIT .EQ. 1) GO TO 90
      IF (NWAY .EQ. NVAR) RETURN
      IF (P .LE. L1) GO TO 70
      IF (NA .EQ. 1) GO TO 65
      LA = NA - 1
      IF (IA(3,LA) .LE. L1) GO TO 60
C
C     If the previous model is a good fit and the current fit does not
C     improve significantly over it, use the previous fit as the best
C     initial fit.
C
      DLR = IA(1,LA) - IA(1,NA)
      DDF = IA(2,LA) - IA(2,NA)
      DP = XTAIL(DLR,DDF)
      IF (DP .LE. L2) GO TO 60
      CALL CPYCON(CONFIG1, CONFIG, NVAR, NCON1, NCON)
      CALL CPYLR(IA(1,LA), IA(2,LA), IA(3,LA), LR, DF, P)
      GO TO 90
60     IF (NWAY .EQ. NVAR - 1) GO TO 90
65     CALL CPYCON(CONFIG, CONFIG1, NVAR, NCON, NCON1)
70     CONTINUE
C
C     Backward elimination of effects from the best initial fit.
C
90     PP = ZERO
      N = 0
      NA = NA + 1
      IF (NA .GT. MA .OR. NB + NCON .GT. MB) GO TO 400
      CALL CPYLR(LR, DF, P, IA(1,NA), IA(2,NA), IA(3,NA))
      IA(4,NA) = NCON
      DO 100 K = 1, NCON
      NB = NB + 1

```

```

        DO 100 I = 1, NVAR
            IB(I,NB) = CONFIG(I,K)
100 CONTINUE
        LCON = NCON - 1
        DO 300 J = 1, NCON
C
C     Re-initialize FIT when fitting a simpler model
C
        DO 150 I = 1, NTAB
150     FIT(I) = TFIT(I)
        CALL CPYCON(CONFIG, CONFIG1, NVAR, NCON, NCON1)
C
C     Store effect to be deleted in DELEF and compress CONFIG1.
C     Obtain lower order effects of DELEF not implied in CONFIG1 and
C     store them in CONFIG2.
C
        NCON2 = NCON1 - J + 1
        DO 200 I = 1, NVAR
            DELEF(I) = CONFIG1(I,NCON2)
            CONFIG1(I,NCON2) = CONFIG1(I,NCON1)
200 CONTINUE
        CALL LOWEFF(NVAR, LCON, MCON, CONFIG1, CONFIG2, DELEF, JJ)
        NCON1 = LCON + JJ
        IF (JJ .EQ. 0) GO TO 225
        DO 220 L = 1, JJ
            LL = LCON + L
            DO 220 I = 1, NVAR
                CONFIG1(I,LL) = CONFIG2(I,L)
220 CONTINUE
225     NA = NA + 1
        IF (NA .GT. MA .OR. NB + NCON1 .GT. MB) GO TO 400
        CALL LOGLIN(NVAR, DIM, NCON1, CONFIG1, NTAB, TABLE, FIT, LOCMAR,
*         NMAR, MARG, NU, U, MAXDEV, MAXIT, DEV, NLAST, IFAULT)
        IF (IFAULT .GT. 0) RETURN
        CALL LRCHSQ(TABLE, FIT, NTAB, LR1)
        CALL DEGREF(NVAR, DIM, NCON1, NTAB, CONFIG1, DF1)
        P1 = XTAIL(LR1, DF1)
        CALL CPYLR(LR1, DF1, P1, IA(1,NA), IA(2,NA), IA(3,NA))
        IA(4,NA) = NCON1
        DO 250 K = 1, NCON1
            NB = NB + 1
            DO 250 I = 1, NVAR
                IB(I,NB) = CONFIG1(I,K)
250 CONTINUE
        DLR = LR1 - LR
        DDF = DF1 - DF
        DP = XTAIL(DLR, DDF)
C
C     Select the best fitted model that does not result in a significant
C     increase in LR chi-squared value for further simplification.
C
        IF (P1 .LT. L1 .OR. DP .LT. L2) GO TO 300
        IF (P1 .LT. PP) GO TO 300
        PP = P1
        N = N + 1
        CALL CPYCON(CONFIG1, CONFIG3, NVAR, NCON1, NCON3)
        CALL CPYLR(LR1, DF1, P1, LR3, DF3, P3)
300 CONTINUE
        IF (N .EQ. 0) GO TO 500
C
C     Copy the best simplified fit of each iteration to CONFIG.

```

```

C
  CALL CPYCON(CONFIG3, CONFIG, NVAR, NCON3, NCON)
  CALL CPYLR(LR3, DF3, P3, LR, DF, P)
  IF (NCON .EQ. 1 .AND. CONFIG(2,1) .EQ. 0) GO TO 500
  GO TO 90
C
400 IFAULT = 5
  RETURN
C
  Obtain fitted table of the best final / intermediate fit.
C
500 CALL LOGLIN(NVAR, DIM, NCON, CONFIG, NTAB, TABLE, FIT, LOCMAR,
*   NMAR, MARG, NU, U, MAXDEV, MAXIT, DEV, NLAST, IFAULT)
  RETURN
  END
C
  SUBROUTINE LOWEFF(NVAR, NCON, MCON, CONFIG1, CONFIG2, DELEF, JJ)
C
  ALGORITHM AS 185.1  APPL. STATIST. (1982) VOL.31, NO.3
C
  Find lower order effects of DELEF not implied in CONFIG1 and store
  them in CONFIG2.  If NVAR is to be greater than 7, the dimensions
  of MASK, MASK1 and MASK2 must all be increased to the value NVAR.
C
  INTEGER CONFIG1(NVAR,NCON), CONFIG2(NVAR,MCON), DELEF(NVAR),
*   MASK(7), MASK1(7), MASK2(7)
C
  Determine the order of the deleted effect.
C
  NWAY = 0
  DO 100 I = 1, NVAR
100 IF (DELEF(I) .NE. 0) NWAY = NWAY + 1
  JJ = 0
  IF (NWAY .EQ. 1) RETURN
C
  Find all possible lower order effects of the deleted effect.
C
  DO 300 J = 1, NWAY
    MASK(J) = J - 1
    DO 300 I = 1, NVAR
      CONFIG2(I,J) = 0
300 CONTINUE
  N = NWAY - 1
  MASK(N+1) = NWAY
350 CONTINUE
  DO 360 I = 1, NVAR
360 MASK1(I) = 0
  JJ = JJ + 1
  DO 400 J = 1, N
    L = MASK(J) + 1
    K = DELEF(L)
    MASK1(K) = 1
    CONFIG2(J,JJ) = K
400 CONTINUE
  IF (NCON .EQ. 0) GO TO 810
  NN = 0
C
  Check if each lower order effect is implied in CONFIG1.
C
  DO 700 J = 1, NCON
  DO 450 I = 1, NVAR

```

```
450  MASK2(I) = 0
      DO 500 I = 1, NVAR
          K = CONFG1(I,J)
          IF (K .NE. 0) MASK2(K) = 1
500  CONTINUE
      DO 550 K = 1, NVAR
          IF (MASK1(K) .EQ. 1 .AND. MASK2(K) .NE. 1) GO TO 650
550  CONTINUE
      GO TO 800
650  NN = NN + 1
700  CONTINUE
      IF (NN .EQ. NCON) GO TO 810
800  JJ = JJ - 1
810  DO 850 J = 1, N
          MASK(J) = MASK(J) + 1
          IF (MASK(J) .LT. MASK(J+1)) GO TO 350
          MASK(J) = J - 1
850  CONTINUE
C
      RETURN
      END
C
      SUBROUTINE LRCHSQ(TABLE, FIT, NTAB, RATIO)
C
C  ALGORITHM AS 185.2  APPL. STATIST. (1982) VOL.31, NO.3
C
C  LRCHSQ calculates twice the likelihood ratio.
C
      REAL TABLE(NTAB), FIT(NTAB), ZERO
      DATA ZERO /0.0/
C
      SUM = ZERO
      DO 10 I = 1, NTAB
C
C  Note that FIT(I) = 0 implies TABLE(I) = 0.
C
10  IF (TABLE(I) .NE. ZERO) SUM = SUM + TABLE(I) * LOG(TABLE(I) /
*    FIT(I))
      RATIO = SUM + SUM
      RETURN
      END
C
      SUBROUTINE DEGREF(NVAR, DIM, NCON, NTAB, CONFIG, DF)
C
C  ALGORITHM AS 185.3  APPL. STATIST. (1982) VOL.31, NO.3
C
C  DEGREF computes the degrees of freedom of a model described in
C  CONFIG.  If NVAR is to be greater than 7, the dimensions of MASK
C  and HASH must be increased to the values (NVAR + 1) and
C  (2.NVAR - 1) respectively).
C
      INTEGER DIM(NVAR), CONFIG(NVAR,NCON), MASK(8), HASH(127)
C
      NP = 0
      N = 2 ** NVAR - 1
      DO 5 I = 1, N
5  HASH(I) = 0
      DO 100 I = 1, NCON
C
C  Find the order of each effect in CONFIG.
C
C
```

```

        DO 10 J = 1, NVAR
        IF (CONFIG(J,I) .EQ. 0) GO TO 20
10    CONTINUE
        J = NVAR + 1
20    N = J - 1
C
C    Set up MASK.
C
        DO 30 J = 1, N
30    MASK(J) = 0
C
C    Use MASK to find all possible lower order effects.
C
40    DO 50 J = 1, N
        MASK(J) = MASK(J) + 1
        IF (MASK(J) .EQ. 1) GO TO 60
        MASK(J) = 0
50    CONTINUE
        GO TO 100
60    K = 0
        L = 1
        DO 80 J = 1, N
            IF (MASK(J) .NE. 1) GO TO 80
C
C    Get the lower order effect degrees of freedom.
C
            IJ = CONFIG(J,I)
            L = L * (DIM(IJ) - 1)
            K = K + 2 ** (CONFIG(J,I) - 1)
80    CONTINUE
C
C    Check if the lower order effect already existed.
C
            IF (HASH(K) .EQ. 1) GO TO 40
            HASH(K) = 1
            NP = NP + L
            GO TO 40
100   CONTINUE
        DF = NTAB - NP - 1
C
        RETURN
        END
C
        REAL FUNCTION XTAIL(RATIO, DF)
C
C    ALGORITHM AS 185.4 APPL. STATIST. (1982) VOL.31, NO.3
C
C    Computes probability of a chi-squared variable > RATIO using an
C    approximation from JASA (1968) vol.68, p.1420.
C
        REAL RATIO, DF, ZERO, ONE, TWO, SIX, PT04
        DATA ZERO /0.0/, ONE /1.0/, TWO /2.0/, SIX /6.0/, PT04 /0.04/
C
        IF (RATIO .EQ. ZERO) GO TO 50
        IF (DF .EQ. ONE) GO TO 100
        S = (DF - ONE) / TWO
        T = RATIO / TWO
        D = T - S - ONE / SIX - PT04 / DF
        Z = (D * SQRT(TWO * S * LOG(S / T) + TWO * (T - S))) / ABS(S - T)
C
C    ALNORM (AS 66, Hill 1973) evaluates the tail prob. of Z = N(0,1)

```

```
C
    XTAIL = ALNORM(Z, .TRUE.)
    RETURN
C
    50 XTAIL = ONE
    RETURN
100 Z = SQRT(RATIO)
    XTAIL = TWO * ALNORM(Z, .TRUE.)
    RETURN
    END
C
    SUBROUTINE CPYCON(CONFG1, CONFG2, NVAR, NCON1, NCON2)
C
C    ALGORITHM AS 185.5  APPL. STATIST. (1982) VOL.31, NO.3
C
    INTEGER CONFG1(NVAR,NCON1), CONFG2(NVAR,NCON1)
C
    DO 10 J = 1, NCON1
        DO 10 I = 1, NVAR
            CONFG2(I,J) = CONFG1(I,J)
10 CONTINUE
    NCON2 = NCON1
    RETURN
    END
C
    SUBROUTINE CPYLR(LR1, DF1, P1, LR2, DF2, P2)
C
C    ALGORITHM AS 185.6  APPL. STATIST. (1982) VOL.31, NO.3
C
    REAL LR1, DF1, P1, LR2, DF2, P2
C
    LR2 = LR1
    DF2 = DF1
    P2 = P1
    RETURN
    END
```



```
C UKC NETLIB DISTRIBUTION COPYRIGHT 1990 RSS
C
C SUBROUTINE RBO(N, A, M, IFAULT)
C COMPLEX A(N), T
C
C<<<<< Acquired in machine-readable form from 'Applied Statistics'
C<<<<< algorithms editor, January 1983.
C
C
C ALGORITHM AS 186 APPL. STATIST. (1982) VOL.31, NO.3
C
C SUBROUTINE RBO (WITH AN AUXILIARY SUBROUTINE FFT)
C PERFORMS THE N-POINT DISCRETE FAST FOURIER TRANSFORM OF
C THE SAMPLED FUNCTION STORED IN A(N), WHERE N=2**M,
C M AN INTEGER
C
C CHECK IF VALUES OF N AND M ARE PROPERLY CHOSEN
C
C IFAULT = 1
C IF (N .LE. 0 .OR. 2 ** M .NE. N) RETURN
C IFAULT = 0
C
C PART 1: PROCEDURE OF REVERSE BINARY ORDER PERMUTATION.
C CONTENTS OF CELLS ARE INTERCHANGED WHEN J.GT.I
C
C NW = N / 2
C NV = N + 1
C IMAX = NW - 1
C J = 1
C DO 6 I = 1, IMAX, 2
C
C IN THIS LOOP THE MINIMAL SET Z10 OF PAIRS OF ADDRESSES (I,J)
C IS GENERATED. THE Z10 GENERATION INSTEAD OF ALL POSSIBLE
C PAIRS (I,J) GENERATION REDUCES TOTAL TIME OF RBO PERMUTATION.
C
C IF (J - I) 1, 3, 2
C
C THE PAIR OF ADDRESSES (I,J) AVAILABLE AT THIS POINT IS USED
C (DUE TO SYMMETRY PRINCIPLE (1)) FOR (IP,JP) ADDRESS
C GENERATION (IP.GT.N/2)
C
1 IP = NV - I
JP = NV - J
C
C CONTENTS OF IP AND JP CELLS ARE INTERCHANGED
C
C T = A(JP)
C A(JP) = A(IP)
C A(IP) = T
C
C THE NEXT PAIR OF ADDRESSES IS GENERATED USING EVEN ELEMENT
C PROPERTY AND APPROPRIATE PERMUTATION IS PERFORMED.
C
C GOTO 3
2 T = A(J)
A(J) = A(I)
A(I) = T
3 IP = I + 1
JP = J + NW
T = A(JP)
A(JP) = A(IP)
```

```
      A(IP) = T
C
C      THE NEXT PAIR OF ADDRESSES (I,J) IS GENERATED. THIS PART OF
C      THE PROCEDURE DOES NOT DIFFER FROM THE APPROPRIATE PART OF
C      THE RADER ALGORITHM IN RABINER AND GOLD (1975).
C
      K = NV
4     IF (K .GE. J) GOTO 5
      J = J - K
      K = K / 2
      GOTO 4
5     J = J + K
6     CONTINUE
C
C      PART 2: NOW THE FFT SUBROUTINE IS CALLED. ONE CAN USE ANY OF
C      THE KNOWN PROCEDURES TO PERFORM THE COOLEY-TUKEY ALGORITHM.
C
      CALL FFT(M, N, A)
      RETURN
      END
C
      SUBROUTINE FFT(M, N, A)
C
C      ALGORITHM AS 186.1  APPL. STATIST. (1982) VOL.31, NO.3
C
C      SUBROUTINE FFT USES (WITH A SLIGHT MODIFICATION) PART OF FFT
C      ALGORITHM PUBLISHED IN RABINER AND GOLD (1975).
C
      COMPLEX A(N), U, W, T
      PI = 3.141592653589793
      LE = 1
      DO 20 L = 1, M
        LE1 = LE
        LE = LE + LE
        U = (1.0, 1.0)
        W = CMPLX(COS(PI / FLOAT(LE1)), -SIN(PI / FLOAT(LE1)))
        DO 20 J = 1, LE1
          DO 10 I = J, N, LE
            IP = I + LE1
            T = A(IP) * U
            A(IP) = A(I) - T
            A(I) = A(I) + T
10         CONTINUE
          U = U * W
20      CONTINUE
      RETURN
      END
```

```

SUBROUTINE DIGAMI(D, X, P, GPLOG, GP1LOG, PSIP, PSIP1, PSIDP,
*      PSIDP1, IFAULT)

```

```

C
C      ALGORITHM AS 187  APPL. STATIST. (1982) VOL.31, NO.3
C
C      Computes derivatives of the incomplete gamma integral for positive
C      parameters, X, P, using a series expansion if P > X or X <= 1, and
C      a continued fraction expansion otherwise.
C
C      Calculation of D(4) in line 60 corrected 5 October 1993.
C
C      N.B. The user must input values of the incomplete gamma, digamma
C      and trigamma functions.  These can be obtained using AS 239
C      (or 32), AS 103 and AS 121 respectively.
C
      REAL PN(6), D(6), DP(6), DPP(6), ZERO, ONE, TWO
      DATA E, OFLO, TMAX, VSMALL/1.E-6, 1.E30, 100.0, 1.E-30/
      DATA ZERO/0.0/, ONE/1.0/, TWO/2.0/
C
      IFAULT = 0
C
C      Derivatives with respect to X
C
      PM1 = P - ONE
      XLOG = LOG(X)
      D(1) = EXP(-GPLOG + PM1*XLOG - X)
      D(2) = D(1) * (PM1/X - ONE)
      D(5) = D(1) * (XLOG - PSIP)
C
C      Derivatives with respect to P
C
      IF (X .GT. ONE .AND. X .GE. P) GO TO 30
C
C      Series expansion
C
      F = EXP(P*XLOG - GP1LOG - X)
      DFP = F * (XLOG - PSIP1)
      DFPP = DFP*DFP/F - F*PSIDP1
C
      TMAXP = TMAX + P
      C = ONE
      S = ONE
      CP = ZERO
      CPP = ZERO
      DSP = ZERO
      DSPP = ZERO
      A = P
1  A = A + ONE
      CPC = CP / C
      CP = CPC - ONE/A
      CPP = CPP/C - CPC*CPC + ONE/A**2
      C = C*X/A
      CP = CP*C
      CPP = CPP*C + CP*CP/C
      S = S + C
      DSP = DSP + CP
      DSPP = DSPP + CPP
      IF (A .GT. TMAXP) GO TO 1001
      IF (C .GT. E*S) GO TO 1
      D(6) = S*F
      D(3) = S*DFP + F*DSP

```

```

D(4) = S*DFPP + TWO*DFP*DSP + F*DSPP
RETURN

```

C  
C  
C

```
Continued fraction expansion
```

```

30 F = EXP(P*XLOG - GPLOG - X)
    DFP = F * (XLOG - PSIP)
    DFPP = DFP*DFP/F - F*PSIDP

```

C

```

A = PM1
B = X + ONE - A
TERM = ZERO
PN(1) = ONE
PN(2) = X
PN(3) = X + ONE
PN(4) = X * B
S0 = PN(3) / PN(4)
DO 31 I = 1, 4
    DP(I) = ZERO
    DPP(I) = ZERO

```

```

31 CONTINUE
    DP(4) = -X

```

C

```

32 A = A - ONE
    B = B + TWO
    TERM = TERM + ONE
    AN = A*TERM
    PN(5) = B*PN(3) + AN*PN(1)
    PN(6) = B*PN(4) + AN*PN(2)
    DP(5) = B*DP(3) - PN(3) + AN*DP(1) + PN(1)*TERM
    DP(6) = B*DP(4) - PN(4) + AN*DP(2) + PN(2)*TERM
    DPP(5) = B*DPP(3) + AN*DPP(1) + TWO*(TERM*DP(1) - DP(3))
    DPP(6) = B*DPP(4) + AN*DPP(2) + TWO*(TERM*DP(2) - DP(4))

```

C

```

IF (ABS(PN(6)) .LT. VSMALL) GO TO 35
S = PN(5) / PN(6)
C = ABS(S - S0)
IF (C*P .GT. E) GO TO 34
IF (C .LE. E*S) GO TO 42

```

C

```

34 S0 = S
35 DO 36 I = 1, 4
    I2 = I + 2
    DP(I) = DP(I2)
    DPP(I) = DPP(I2)
    PN(I) = PN(I2)

```

```
36 CONTINUE
```

C

```

IF (TERM .GT. TMAX) GO TO 1001
IF (ABS(PN(5)) .LT. OFLO) GO TO 32
DO 41 I = 1, 4
    DP(I) = DP(I) / OFLO
    DPP(I) = DPP(I) / OFLO
    PN(I) = PN(I) / OFLO

```

```

41 CONTINUE
GO TO 32

```

C

```

42 D(6) = ONE - F*S
    DSP = (DP(5) - S*DP(6)) / PN(6)
    DSPP = (DPP(5) - S*DPP(6) - TWO*DSP*DP(6)) / PN(6)
    D(3) = -F*DSP - S*DFP

```

```
D(4) = -F*DSPP - TWO*DSP*DFP - S*DFPP  
RETURN
```

C

C Set fault indicator

C

```
1001 IFAULT = 1  
RETURN  
END
```

```
C UKC NETLIB DISTRIBUTION COPYRIGHT 1990 RSS
C
  SUBROUTINE EODSEQ(KA, IKA, LENGTH, NSTATE, MAXDEP, MAXINT, REP,
* PERC, AU, CU, CU0, NPOINT, IFAULT)
C
C ALGORITHM AS 188 APPL. STATIST. (1983) VOL.32, NO.2 (pp185-196)
C
C Estimation of the order of dependence in sequences
C
  INTEGER MAXKA, MAXJF
  PARAMETER (MAXKA=10, MAXJF=20)
  INTEGER IKA, LENGTH, NSTATE, MAXDEP, MAXINT, NPOINT, IFAULT
  INTEGER KA(IKA,LENGTH)
  REAL AU(MAXDEP), CU(MAXDEP), CU0, PERC(MAXDEP)
  LOGICAL REP
C
C Local variables
C
  INTEGER NWORD, JFIX, NGP, KTEMP, KK
  INTEGER JRANGE, MURANG, IGF, NEOS, LAST, I, NGPSIZ
  INTEGER K, LIMIT, IPASSI, NCOUNT, JFIX2, JCTEMP, IW
  REAL SUM, ALN2, ACCX
C
C..NC AND JFROG ARE ARRAYS USED FOR TEMPORARY STORAGE
C..NC(MAXKA) NEEDS TO BE CHANGED TO NC(IKA) IF IKA .GT. MAXKA
C..JFROG(MAXJF) NEEDS TO BE CHANGED TO JFROG(MAXDEP)
C..
  IF MAXDEP .GT. MAXJF
C
  INTEGER NC(MAXKA), JFROG(MAXJF)
C
C..NEOS (END OF SECTION) IS A NEGATIVE INTEGER USED TO
C..SIGNIFY A BREAK IN THE INPUT SEQUENCE
C
  NEOS = -1
C
C..INITIALIZATION PROCEDURE
C..CHECK INPUT PARAMETERS AND INITIALISE LOCAL VARIABLES
C..USED IN PACKING THE CODED OBSERVATIONS
C..INTWRD = NO. OF OBSERVATIONS STORABLE IN AN INTEGER
C..NWORD = NO. OF INTEGERS REQUIRED TO STORE LARGEST GROUP
C
  IF (IKA.LE.0 .OR. LENGTH.LE.0) GO TO 300
  IF (IKA.GT.MAXKA .OR. MAXDEP.GT.MAXJF) GO TO 300
  IF (NSTATE.LE.0 .OR. MAXDEP.LE.0 .OR. MAXINT.LE.0) GO TO 300
  ALN2 = ALOG(2.0)
  JRANGE = 0
  MURANG = 1
10 JRANGE = JRANGE + 1
  IF (JRANGE.GT.MAXINT) GO TO 300
  MURANG = MURANG*2
  IF (NSTATE.GT.MURANG) GO TO 10
  INTWRD = MAXINT/JRANGE
  NWORD = MAXDEP/INTWRD
  JFIX = MURANG**(INTWRD-1)
  JFIX2 = JFIX
  IW3 = MAXDEP - NWORD*INTWRD
  IF (IW3.EQ.0) GO TO 20
  NWORD = NWORD + 1
  JFIX2 = MURANG**(IW3-1)
  GO TO 30
20 IW3 = INTWRD
```

```
C
C..SECTION FOR CODING DATA
C
C..CODE UP FIRST GROUP
C
  30 IF (NWORD.GT.IKA) GO TO 300
      NGPS = 0
      NPOINT = 0
  40 JCTEMP = 0
      IW = 0
      NW = 1
      LAST = -1
C
C..CONSTRUCT FIRST MAXDEP-TUPLE IN ARRAY NC
C
  DO 60 I=1,MAXDEP
  50  NPOINT = NPOINT + 1
      IF (NPOINT.GT.LENGTH) GO TO 320
      INNON = KA(1,NPOINT)
      IF (INNON.EQ.NEOS) GO TO 320
      IF (INNON.LT.0 .OR. INNON.GT.NSTATE-1) GO TO 310
      IF (.NOT.REP .AND. (INNON.EQ.LAST)) GO TO 50
C
C..CODE MAXDEP-TUPLES INTO SUCCESSIVE COLUMNS OF THE ARRAY KA
C
      JCTEMP = JCTEMP/MURANG + INNON*JFIX
      LAST = INNON
      IW = IW + 1
      IF (IW.LT.INTWRD) GO TO 60
C
C..NEED ANOTHER INTEGER TO STORE PACKED CODES
C
      IW = 0
      NC(NW) = JCTEMP
      JCTEMP = 0
      NW = NW + 1
  60 CONTINUE
      IF (IW.NE.0) NC(NW) = JCTEMP/(MURANG**(INTWRD - IW))
C
C..END OF CONSTRUCTION OF FIRST MAXDEP-TUPLE
C..STORE IT IN THE FIRST COLUMN OF KA
C
  70 NGPS = NGPS + 1
      DO 80 I=1,NWORD
          KA(I,NGPS) = NC(I)
  80 CONTINUE
C
C..CONSTRUCT NEW MAXDEP-TUPLE IN C
C
  90 NPOINT = NPOINT + 1
      IF (NPOINT.GT.LENGTH) GO TO 120
      INNON = KA(1,NPOINT)
C
C..NEW SEQUENCE TEST
C
      IF (INNON.EQ.NEOS) GO TO 40
      IF (INNON.LT.0 .OR. INNON.GT.NSTATE-1) GO TO 310
C
C..TEST REPEAT FLAG
C
      IF (.NOT.REP .AND. (INNON.EQ.LAST)) GO TO 90
```

```
C
C..SHIFT OUT MOST ANCIENT ELEMENT AND SHIFT OTHER ELEMENTS ALONG
C
      NC(1) = NC(1)/MURANG
      IF (NWORD.LT.2) GO TO 110
      DO 100 I=2,NWORD
        JCTEMP = NC(I)/MURANG
        NC(I-1) = NC(I-1) + (NC(I)-JCTEMP*MURANG)*JFIX
        NC(I) = JCTEMP
100 CONTINUE
110 NC(NWORD) = NC(NWORD) + JFIX2*INNON
    LAST = INNON
    GO TO 70

C
C..ALL MAXDEP-TUPLES CONSTRUCTED NOW SORT ARRAY KA BY COLUMNS
C
      120 CALL EODSRT(KA, IKA, NGPS, NWORD)
C
C..COUNT GROUPS - DECREASING GROUP SIZE AT THE SAME TIME
C..IF A GROUP IS FOUND TO BE REPEATED M TIMES THIS MEANS
C..THAT EACH SUBGROUP WILL ALSO BE REPEATED M TIMES. TO
C..SAVE HAVING TO RECOUNT THESE SUBGROUPS THE FIRST ELEMENT
C..OF THE COLUMN FOLLOWING THE REPEATED GROUP IS USED TO
C..STORE THE REPEAT COUNT AS -(M-1). THIS COUNT NEEDS TO
C..BE NEGATIVE TO DISTINGUISH IT FROM THE POSITIVE CODED GROUPS
C
      NW = 1
      IW = INTWRD + 1
      LAST = MAXDEP + 1
      DO 280 K=1,MAXDEP
        IW = IW - 1
        IF (IW.NE.0) GO TO 130
        IW = INTWRD
        NW = NW + 1
        IF (NW.EQ.NWORD) IW = IW3
130  NGPSIZ = LAST - K

C
C..SET USER DEFINED TRIPWIRES
C
      LIMIT = INT(FLOAT(NGPS)*PERC(NGPSIZ)/100.0)
      SUM = 0.0
      IPASSI = 1

C
C..START TO PROCESS NEW GROUP
C..FIRST - SAVE IT IN ARRAY NC
C
      140 DO 150 I=NW,NWORD
        NC(I) = KA(I,IPASSI)
      150 CONTINUE

C
C..REMOVE LEAST SIGNIFICANT GROUP ELEMENT
C
      KA(NW,IPASSI) = KA(NW,IPASSI)/MURANG

C
C..UNSET IGF (IDENTICAL GROUP FOUND) FLAG
C
      IGF = 0
      NCOUNT = 1

C
C..LOOK AT INFORMATION ON NEXT GROUP (IF ANY)
C
```



```
160  IPASSI = IPASSI + 1
      IF (IPASSI.GT.NGPS) GO TO 190
      KTEMP = KA(1,IPASSI)
      IF (KTEMP.GE.0) GO TO 170
C
C..A NEGATIVE ELEMENT MEANS THE CONTENTS ARE A REPEAT COUNT
C..SUBTRACT IT FROM BOTH THE POINTER AND THE COUNT
C
      NCOUNT = NCOUNT - KTEMP
      IPASSI = IPASSI - KTEMP
      IF (IPASSI.GT.NGPS) GO TO 190
C
C..REAL GROUP ENCOUNTERED - TEST IF SAME AS LAST ONE
C
170  DO 180 I=NW,NWORD
      IF (KA(I,IPASSI).NE.NC(I)) GO TO 190
180  CONTINUE
C
C..IDENTICAL GROUP FOUND  SET IGF FLAG
C
      IGF = 1
      NCOUNT = NCOUNT + 1
      GO TO 160
C
C..NEW GROUP FOUND OR NO MORE GROUPS
C..UPDATE AVERAGE UNCERTAINTY SUM
C
190  ACCX = FLOAT(NCOUNT)
      SUM = SUM + ACCX*ALOG(ACCX)
      IF (NCOUNT.LE.LIMIT) GO TO 260
C
C..LAST GROUP OCCURS SUFFICIENTLY FREQUENTLY - UNPACK GROUP AND
C..PASS GROUP, SIZE AND FREQUENCY TO USER SUPPLIED ROUTINE
C..OUTFRG
C..FIRST WORD - MAY NOT BE FULL
C
      NGP = NC(NW)
      J = 0
      DO 200 I=1,IW
        J = J + 1
        KTEMP = NGP/MURANG
        JFROG(J) = NGP - KTEMP*MURANG
        NGP = KTEMP
200  CONTINUE
C
C..MIDDLE WORDS - ALL FULL
C
      IF (NGPSIZ.EQ.IW) GO TO 250
      JCTEMP = NWORD - 1
      IF (NW.EQ.JCTEMP) GO TO 230
      NW2 = NW + 1
      KK = NW
      DO 220 I=NW2,JCTEMP
        KK = KK + 1
        NGP = NC(KK)
        DO 210 L=1,INTWRD
          J = J + 1
          KTEMP = NGP/MURANG
          JFROG(J) = NGP - KTEMP*MURANG
          NGP = KTEMP
210  CONTINUE
```

```
220 CONTINUE
C
C..LAST WORD - MAY NOT BE FULL
C
230 NGP = NC(NWORD)
DO 240 I=1,IW3
    J = J + 1
    KTEMP = NGP/MURANG
    JFROG(J) = NGP - KTEMP*MURANG
    NGP = KTEMP
240 CONTINUE
250 CONTINUE
    CALL OUTFRG(JFROG, NGPSIZ, NCOUNT)
260 IF (IGF.EQ.0) GO TO 270
C
C..IGF FLAG SET - STORE REPEAT COUNT
C
    KTEMP = IPASSI + 1 - NCOUNT
    KA(1,KTEMP) = 1 - NCOUNT
C
C..ESTIMATE AVERAGE UNCERTAINTY AND CONDITIONAL UNCERTAINTY
C
270 IF (IPASSI.LE.NGPS) GO TO 140
    ACCX = FLOAT(NGPS)
    AU(NGPSIZ) = -(SUM/ACCX - ALOG(ACCX))/ALN2
280 CONTINUE
    DO 290 K=2,MAXDEP
        CU(K) = AU(K) - AU(K-1)
290 CONTINUE
    CU(1) = AU(1)
    CU0 = ALOG(FLOAT(NSTATE))/ALN2
    IFAULT = 0
    RETURN
C
C..ERROR EXITS
C
C..IFAUULT=1 - NSTATE-1 NOT STORABLE IN AN INTEGER
C..
C.. OR NUMBER OF INTEGERS REQUIRED TO STORE TO
C.. GIVEN MAXDEP .GT. IKA
C..
C.. OR ONE OF IKA, LENGTH, NSTATE, MAXDEP OR
C.. MAXINT .LE. 0
C
300 IFAULT = 1
    RETURN
C
C..IFAUULT=2 - ILLEGAL ACTIVITY NUMBER AT POSITION NPOINT IN
C.. THE PREPARED DATA STRING. NUMBER EITHER GREATER
C.. THAN NSTATE-1 OR LESS THAN ZERO AND NOT EQUAL TO EOS
C
310 IFAULT = 2
    RETURN
C
C..IFAUULT=3 - DATA STRING IS TOO SHORT ENDING AT POSITION NPOINT
C.. IN THE PREPARED DATA STRING
C
320 IFAULT = 3
    RETURN
    END
    SUBROUTINE EODSRT(KA, IKA, NGPS, NWORD)
```

```
C
C..ROUTINE TO SORT ARRAY A BY COLUMNS FROM IKA TO 1
C..I.E. FIRST SORT KA(IKA,1).LT.KA(IKA,2).LT.KA(IKA,3).....
C..THEN          KA(IKA-1,1).LT.KA(IKA-1,2).LT.KA(IKA-1,3).....
C..E.T.C
C..THIS ROUTINE IS BASED ON M01AQF FROM THE NAG MK8
C..FORTRAN LIBRARY AND SINGLETON (1969)
C
```

```
    PARAMETER (MAXKA=10)
    INTEGER IKA, NWORD
    INTEGER KA(IKA,NGPS), IL(22), IU(22)
```

```
C
C..NOTE  IF MORE THAN 10 WORDS ARE REQUIRED FOR STORING
C..THE MAXIMUM SIZE GROUP THE FOLLOWING ARRAY
C..DECLARATIONS MUST BE INCREASED.
C
```

```
    INTEGER IT(MAXKA), ITT(MAXKA)
    NWORD1 = NWORD + 1
    M = 1
    I = 1
    J = NGPS
    II = I
10  IF (I-J.GE.0) GO TO 240
20  K = I
    IJ = (J+I)/2
    DO 30 MM=1,NWORD
        IT(MM) = KA(MM,IJ)
30  CONTINUE
    MM = NWORD1
    DO 40 NN=1,NWORD
        MM = MM - 1
        IF (KA(MM,I)-IT(MM)) 70, 40, 50
40  CONTINUE
    GO TO 70
50  DO 60 MM=1,NWORD
        KA(MM,IJ) = KA(MM,I)
        KA(MM,I) = IT(MM)
        IT(MM) = KA(MM,IJ)
60  CONTINUE
70  L = J
    MM = NWORD1
    DO 80 NN=1,NWORD
        MM = MM - 1
        IF (KA(MM,J)-IT(MM)) 90, 80, 160
80  CONTINUE
    GO TO 160
90  DO 100 MM=1,NWORD
        KA(MM,IJ) = KA(MM,J)
        KA(MM,J) = IT(MM)
        IT(MM) = KA(MM,IJ)
100 CONTINUE
    MM = NWORD1
    DO 110 NN=1,NWORD
        MM = MM - 1
        IF (KA(MM,I)-IT(MM)) 160, 110, 120
110 CONTINUE
    GO TO 160
120 DO 130 MM=1,NWORD
        KA(MM,IJ) = KA(MM,I)
        KA(MM,I) = IT(MM)
        IT(MM) = KA(MM,IJ)
```

```
130 CONTINUE
    GO TO 160
140 DO 150 MM=1,NWORD
    KA(MM,L) = KA(MM,K)
    KA(MM,K) = ITT(MM)
150 CONTINUE
160 L = L - 1
    MM = NWORD1
    DO 170 NN=1,NWORD
    MM = MM - 1
    IF (KA(MM,L)-IT(MM)) 180, 170, 160
170 CONTINUE
180 DO 190 MM=1,NWORD
    ITT(MM) = KA(MM,L)
190 CONTINUE
200 K = K + 1
    MM = NWORD1
    DO 210 NN=1,NWORD
    MM = MM - 1
    IF (KA(MM,K)-IT(MM)) 200, 210, 220
210 CONTINUE
220 IF (K-L.LE.0) GO TO 140
    IF (L-I-J+K.LE.0) GO TO 230
    IL(M) = I
    IU(M) = L
    I = K
    M = M + 1
    GO TO 250
230 IL(M) = K
    IU(M) = J
    J = L
    M = M + 1
    GO TO 250
240 M = M - 1
    IF (M.EQ.0) GO TO 360
    I = IL(M)
    J = IU(M)
250 IF (J-I-11.GE.0) GO TO 20
    IF (I-II) 270, 10, 270
260 I = I + 1
270 IF (I-J.EQ.0) GO TO 240
    I1 = I + 1
    DO 280 MM=1,NWORD
    IT(MM) = KA(MM,I1)
280 CONTINUE
    MM = NWORD1
    DO 290 NN=1,NWORD
    MM = MM - 1
    IF (KA(MM,I)-IT(MM)) 260, 290, 300
290 CONTINUE
    GO TO 260
300 K = I
310 K1 = K + 1
    DO 320 MM=1,NWORD
    KA(MM,K1) = KA(MM,K)
320 CONTINUE
    MM = NWORD1
    K = K - 1
    DO 330 NN=1,NWORD
    MM = MM - 1
    IF (IT(MM)-KA(MM,K)) 310, 330, 340
```

```
330 CONTINUE
340 K1 = K + 1
      DO 350 MM=1,NWORD
          KA(MM,K1) = IT(MM)
350 CONTINUE
      GO TO 260
360 RETURN
      END
```

```
C UKC NETLIB DISTRIBUTION COPYRIGHT 1990 RSS
C
C     SUBROUTINE BBML(N, IX, IN, W, P, RL, MRL, ITER, CCRIT, MEW, THETA,
*     SEM, SETH, RNL, IFAULT)
C
C     ALGORITHM AS189 APPL. STATIST. (1983) VOL.32, NO.2
C
C     SUBROUTINE FOR CALCULATING THE MAXIMUM LIKELIHOOD ESTIMATES
C     OF THE PARAMETERS OF THE BETA BINOMIAL DISTRIBUTION
C
C     REAL W(N), P(N), CCRIT, MEW, THETA, SEM, SETH, RNL, INF, DUM,
*     FD(2), SD(3), TD(4), UB(2), DEL, EPS, A, B, C, D, E, F
C     INTEGER IX(N), IN(N), RL(MRL,3), LM(3), RD1(2,2), RD2(2,3),
*     RD3(2,4)
C     LOGICAL MC
C     PARAMETER (INF = 1.0E6)
C     DATA
*     RD1(1,1), RD1(2,1), RD1(1,2), RD1(2,2)/1,-1,1,1/,
*     RD2(1,1), RD2(2,1), RD2(1,2), RD2(2,2),
*     RD2(1,3), RD2(2,3)/-1,-1,-1,1,-1,-1/,
*     RD3(1,1), RD3(2,1), RD3(1,2), RD3(2,2), RD3(1,3),
*     RD3(2,3), RD3(1,4), RD3(2,4)/2,-2,2,2,2,-2,2,2/
C
C     I = ITER
C     ITER = 0
C     MC = .TRUE.
C     UB(1) = 0.01
C     UB(2) = 0.01
C
C     SET THE ARRAYS RL AND LM
C
C     CALL SET(N, IX, IN, RL, MRL, LM, IFAULT)
C     IF(IFAULT.NE.0) RETURN
C     SEM = -1.0
C     SETH = -1.0
C     NND = 0
C
C     CALCULATION OF INITIAL ESTIMATES (BY MOMENTS)
C
C     CALL BBME(N, IX, IN, W, P, INF, MEW, THETA)
C     IF(THETA.EQ.INF) GOTO 50
C
C     NEWTON-RAPHSON ITERATION ON FIRST DERIVATIVES
C
C     5 IF(ITER.LE.I) GOTO 10
C     IFAULT = 7
C     GOTO 60
C
C     CALCULATE FIRST DERIVATIVES OF LOG LIKELIHOOD
C
C     10 CALL GDER(MEW, THETA, RL, MRL, LM, 2, RD1, FD)
C
C     CALCULATE SECOND DERIVATIVES OF LOG LIKELIHOOD
C
C     CALL GDER(MEW, THETA, RL, MRL, LM, 3, RD2, SD)
C
C     CALCULATE THIRD DERIVATIVES OF LOG LIKELIHOOD
C
C     CALL GDER(MEW, THETA, RL, MRL, LM, 4, RD3, TD)
C
C     CALCULATE INCREMENTS
```

```

C
DUM = SD(1)*SD(3) - SD(2)*SD(2)
IF(SD(1).LT.0.0.AND.DUM.GT.0.0) GOTO 15
C
C      NON NEGATIVE DEFINITE MATRIX
C
NND = NND+1
C
C      SD(1) IS ALWAYS NEGATIVE SO A GRADIENT STEP IS MADE ON MEW
C
A = MEW - FD(1)/SD(1)
B = THETA
IF(FD(2).NE.0.0) B = B + SIGN(UB(2),FD(2))
IF(A.LE.0.0) A = 0.0001
IF(A.GE.1.0) A = 0.9999
IF(B.LT.0.0) B = 0.0
IF(B.GT.INF) B = INF
CALL BBL(MEW, THETA, RL, MRL, LM, C)
CALL BBL(A, B, RL, MRL, LM, D)
IF(NND.GT.10.OR.C.GE.D) GOTO 40
ITER = ITER+1
MEW = A
THETA = B
GOTO 5
15 DEL = (FD(2)*SD(2) - FD(1)*SD(3))/DUM
EPS = (FD(1)*SD(2) - FD(2)*SD(1))/DUM
C
C      CHECK LIPSCHITZ CONDITION SATISFIED
C
A = SD(2)*TD(2) - TD(1)*SD(3)
B = SD(2)*TD(3) - TD(2)*SD(3)
C = TD(1)*SD(2) - TD(2)*SD(1)
D = SD(2)*TD(2) - SD(1)*TD(3)
E = SD(2)*TD(4) - TD(3)*SD(3)
F = TD(3)*SD(2) - TD(4)*SD(1)
A = DEL*A + EPS*B
C = DEL*C + EPS*D
E = DEL*B + EPS*E
F = DEL*D + EPS*F
DUM = (A*A + C*C + E*E + F*F)/(DUM*DUM)
IF(DUM.GE.1.0) GOTO 20
IF(ABS(DEL).LE.CCRIT.AND.ABS(EPS).LE.CCRIT) MC = .FALSE.
GOTO 45
C
C      FAILURE OF LIPSCHITZ CONDITION. A STEP IN THE DIRECTION OF THE
C      GRADIENT IS MADE.
C
20 A = FD(1)*FD(1)
B = FD(2)*FD(2)
C = A*SD(1) + 2.0*SD(2)*FD(1)*FD(2) + B*SD(3)
IF(C.NE.0.0) GOTO 25
DEL = 0.0
IF(FD(1).NE.0.0) DEL = SIGN(UB(1),FD(1))
EPS = 0.0
IF(FD(2).NE.0.0) EPS = SIGN(UB(2),FD(2))
GOTO 30
25 C = -(A+B)/C
DEL = C*FD(1)
EPS = C*FD(2)
IF(ABS(DEL).GT.UB(1)) DEL = SIGN(UB(1),DEL)
UB(1) = 2.0*ABS(DEL)

```

```

        IF(ABS(EPS).GT.UB(2)) EPS = SIGN(UB(2),EPS)
        UB(2) = 2.0*ABS(EPS)
30 CALL BBL(MEW, THETA, RL, MRL, LM, C)
35 A = MEW + DEL
    B = THETA + EPS
    IF(A.LE.0.0) A = 0.0001
    IF(A.GE.1.0) A = 0.9999
    DEL = A - MEW
    IF(B.LT.0.0) B = 0.0
    IF(B.GT.INF) B = INF
    EPS = B - THETA
    CALL BBL(A, B, RL, MRL, LM, D)
C
C     CHECK TO SEE IF GRADIENT STEP HAS INCREASED LOG LIKELIHOOD
C
    IF(D.GT.C) GOTO 45
    DEL = DEL/2.0
    EPS = EPS/2.0
    IF(ABS(DEL).GT.CCRIT.OR.ABS(EPS).GT.CCRIT) GOTO 35
40 IFAULT = 8
    GOTO 60
45 ITER = ITER + 1
    A = MEW + DEL
    B = THETA + EPS
    IF(A.GT.0.0.AND.A.LT.1.0.AND.B.GE.0.0.AND.B.LE.INF) GOTO 55
    IF(A.LE.0.0) MEW = 0.0
    IF(A.GE.1.0) MEW = 1.0
    IF(B.LT.0.0) THETA = 0.0
    IF(B.GT.INF) THETA = INF
50 IFAULT = 6
    GOTO 60
55 MEW = A
    THETA = B
    IF(MC) GOTO 5
C
C     CALCULATE LOG LIKELIHOOD AND S.E.S
C
    IF(SD(1).LT.0.0) SEM = SQRT(-1.0/SD(1))
    IF(SD(3).LT.0.0) SETH = SQRT(-1.0/SD(3))
60 CALL BBL(MEW, THETA, RL, MRL, LM, RNL)
    RETURN
    END
C
SUBROUTINE BBME(N, IX, IN, W, P, INF, MEW, THETA)
C
C     ALGORITHM AS 189.1 APPL. STATIST. (1983) VOL.32, NO.2
C
C     SUBROUTINE TO ESTIMATE MEW AND THETA OF THE BETA BINOMIAL
C     DISTRIBUTION BY THE METHOD OF MOMENTS
C
    REAL W(N), P(N), INF, MEW, THETA, D1, D2, R, S, TP, WT
    INTEGER IX(N), IN(N)
    LOGICAL J
C
    J = .FALSE.
    DO 5 I = 1,N
        W(I) = FLOAT(IN(I))
        P(I) = FLOAT(IX(I))/W(I)
    5 CONTINUE
10 WT = 0.0
    TP = 0.0

```



```
      DO 15 I = 1,N
        WT = WT+W(I)
        TP = TP+W(I)*P(I)
15  CONTINUE
      TP = TP/WT
      S = 0.0
      D1 = 0.0
      D2 = 0.0
      DO 20 I = 1,N
        R = P(I)-TP
        S = S+W(I)*R*R
        R = W(I)*(1.0-W(I)/WT)
        D1 = D1+R/FLOAT(IN(I))
        D2 = D2+R
20  CONTINUE
      S = FLOAT(N-1)*S/FLOAT(N)
      R = TP*(1.0-TP)
      IF(R.EQ.0.0) GOTO 30
      R = (S-R*D1)/(R*(D2-D1))
      IF(R.LT.0.0) R = 0.0
      IF(J) GOTO 30
      DO 25 I = 1,N
25  W(I) = W(I)/(1.0+R*(W(I)-1.0))
      J = .TRUE.
      GOTO 10
30  MEW = TP
      IF(R.GE.1.0) GOTO 35
      THETA = R/(1.0-R)
      IF(THETA.LE.INF) RETURN
35  THETA = INF
      RETURN
      END
```

```
C
      SUBROUTINE SET(N, IX, IN, RL, MRL, LM, IFAULT)
C
C      ALGORITHM AS 189.2 APPL. STATIST. (1983) VOL.32, NO.2
C
C      SUBROUTINE FOR SETTING UP ARRAY FOR CALCULATION OF
C      THE BETA BINOMIAL LOG LIKELIHOOD AND ITS DERIVATIVES
C
      INTEGER IX(N), IN(N), RL(MRL,3), LM(3)
C
C      TEST ADMISSIBILITY OF DATA
C
      IF(N.GT.1) GOTO 5
      IFAULT = 1
      RETURN
5  DO 10 I = 1,N
      IF(IX(I).GT.0) GOTO 15
10  CONTINUE
      IFAULT = 2
      RETURN
15  DO 20 I = 1,N
      IF(IX(I).LT.IN(I)) GOTO 25
20  CONTINUE
      IFAULT = 3
      RETURN
C
C      FORM MATRIX OF COUNTS
C
25  IFAULT = 4
```

```
DO 30 I = 1,3
  LM(I) = 0
  DO 30 J = 1,MRL
    RL(J,I) = 0
30 CONTINUE
DO 65 I = 1,N
  JJ = IX(I)
  MAR = 1
  GOTO 45
35  JJ = IN(I)-IX(I)
  MAR = 2
  GOTO 45
40  JJ = IN(I)
  MAR = 3
45  IF(JJ) 50,60,55
50  IFAULT = 5
  RETURN
55  IF(JJ.GT.MRL) RETURN
  IF(JJ.GT.LM(MAR)) LM(MAR) = JJ
  RL(JJ,MAR) = RL(JJ,MAR)+1
60  GOTO(35,40,65) MAR
65 CONTINUE
  IFAULT = 0
```

```
C
C      EVALUATE NUMBER OF CALLS TO DIFFERENT TERMS OF LIKELIHOOD
C      FUNCTION
C
```

```
DO 75 I = 1,3
  JJ = LM(I)-1
  IF(JJ.LE.0) GOTO 75
  K = JJ
  DO 70 J = 1,JJ
    RL(K,I) = RL(K,I)+RL(K+1,I)
    K = K-1
70  CONTINUE
75 CONTINUE
  RETURN
  END
```

```
C
C      SUBROUTINE BBL(MEW, THETA, RL, MRL, LM, RNL)
C
C      ALGORITHM AS 189.3 APPL. STATIST. (1983) VOL.32, NO.2
C
C      SUBROUTINE FOR CALCULATION OF THE BETA BINOMIAL LOG
C      LIKELIHOOD
C
```

```
REAL MEW, THETA, RNL, A
INTEGER RL(MRL,3), LM(3)
```

```
C
C      RNL = 0.0
C      MLM = LM(3)
C      DO 5 I = 1,MLM
C        A = FLOAT(I-1)*THETA
C        IF(I.LE.LM(1))RNL = RNL + FLOAT(RL(I,1))*ALOG(MEW+A)
C        IF(I.LE.LM(2))RNL = RNL + FLOAT(RL(I,2))*ALOG(1.0-MEW+A)
C        RNL = RNL - FLOAT(RL(I,3))*ALOG(1.0+A)
5 CONTINUE
  RETURN
  END
```

```
C
C      SUBROUTINE GDER(MEW, THETA, RL, MRL, LM, IDER, RD, PD)
```

```
C
C      ALGORITHM AS 189.4 APPL. STATIST. (1983) VOL.32, NO.2
C
C      GENERAL DERIVATIVE SUBROUTINE
C
REAL MEW, THETA, PD(IDER), A, B, C, D
INTEGER RL(MRL,3), LM(3), RD(2,IDER)
C
MLM = LM(3)
KK = IDER-1
DO 5 I = 1, IDER
5 PD(I) = 0.0
DO 45 I = 1, MLM
  C = FLOAT(I-1)
  A = C*THETA
  DO 40 J = 1, 3
    IF(I.GT.LM(J)) GOTO 40
    GOTO (10,15,20) J
10  D = MEW+A
    GOTO 25
15  D = 1.0-MEW+A
    GOTO 25
20  D = 1.0+A
25  B = FLOAT(RL(I,J))/D**KK
    IF(J.EQ.3) GOTO 35
    DO 30 K = 1, IDER
      PD(K) = PD(K)+FLOAT(RD(J,K))*B
      B = B*C
30  CONTINUE
    GOTO 40
35  D = -FLOAT(RD(1,1))*B*C**KK
    PD(IDER) = PD(IDER)+D
40  CONTINUE
45 CONTINUE
RETURN
END
```

```
double precision function prtrng(q, v, r, ifault)
implicit double precision (a-h, o-z)
```

```
c
c      Algorithm AS 190  Appl. Statist. (1983) Vol.32, No. 2
c      Incorporates corrections from Appl. Statist. (1985) Vol.34 (1)
c
c      Evaluates the probability from 0 to q for a studentized
c      range having v degrees of freedom and r samples.
c
c      Uses subroutine ALNORM = algorithm AS66.
c
c      Arrays vw and qw store transient values used in the
c      quadrature summation.  Node spacing is controlled by
c      step.  pcutj and pcutk control truncation.
c      Minimum and maximum number of steps are controlled by
c      jmin, jmax, kmin and kmax.  Accuracy can be increased
c      by use of a finer grid - Increase sizes of arrays vw
c      and qw, and jmin, jmax, kmin, kmax and 1/step proportionally.
c
```

```
double precision q,v,r,vw(30), qw(30), pcutj, pcutk, step,
#   vmax,zero,fifth,half,one,two,cv1,cv2,cvmax,cv(4)
double precision g, gmid, r1, c, h, v2, gstep, pk1, pk2, gk, pk
double precision w0, pz, x, hj, ehj, pj
data pcutj, pcutk, step, vmax /0.00003d0, 0.0001d0, 0.45d0,
#   120.0d0/, zero, fifth, half, one, two /0.0d0, 0.2d0, 0.5d0,
#   1.0d0, 2.0d0/, cv1, cv2, cvmax /0.193064705d0, 0.293525326d0,
#   0.39894228d0/, cv(1), cv(2), cv(3), cv(4) /0.318309886d0,
#   -0.268132716d-2, 0.347222222d-2, 0.833333333d-1/
data jmin, jmax, kmin, kmax/3, 15, 7, 15/
```

```
c
c      Check initial values
c
```

```
prtrng = zero
ifault = 0
if (v .lt. one .or. r .lt. two) ifault = 1
if (q .le. zero .or. ifault .eq. 1) goto 99
```

```
c
c      Computing constants, local midpoint, adjusting steps.
c
```

```
g = step * r ** (-fifth)
gmid = half * log(r)
r1 = r - one
c = log(r * g * cvmax)
if(v.gt.vmax) goto 20
```

```
c
c      h = step * v ** (-half)
c      v2 = v * half
c      if (v .eq. one) c = cv1
c      if (v .eq. two) c = cv2
c      if (.not. (v .eq. one .or. v .eq. two)) c = sqrt(v2)
#   * cv(1) / (one + ((cv(2) / v2 + cv(3)) / v2 + cv(4)) / v2)
c = log(c * r * g * h)
```

```
c
c      Computing integral
c      Given a row k, the procedure starts at the midpoint and works
c      outward (index j) in calculating the probability at nodes
c      symmetric about the midpoint.  The rows (index k) are also
c      processed outwards symmetrically about the midpoint.  The
c      centre row is unpaired.
c
```

```
20 gstep = g
```

```

    qw(1) = -one
    qw(jmax + 1) = -one
    pk1 = one
    pk2 = one
    do 28 k = 1, kmax
      gstep = gstep - g
21   gstep = -gstep
      gk = gmid + gstep
      pk = zero
      if (pk2 .le. pcutk .and. k .gt. kmin) goto 26
      w0 = c - gk * gk * half
      pz = alnorm(gk, .true.)
      x = alnorm(gk - q, .true.) - pz
      if (x .gt. zero) pk = exp(w0 + r1 * log(x))
      if (v .gt. vmax) goto 26
c
      jump = -jmax
22   jump = jump + jmax
      do 24 j = 1, jmax
        jj = j + jump
        if (qw(jj) .gt. zero) goto 23
        hj = h * j
        if (j .lt. jmax) qw(jj + 1) = -one
        ehj = exp(hj)
        qw(jj) = q * ehj
        vw(jj) = v * (hj + half - ehj * ehj * half)
c
23   pj = zero
        x = alnorm(gk - qw(jj), .true.) - pz
        if (x .gt. zero) pj = exp(w0 + vw(jj) + r1 * log(x))
        pk = pk + pj
        if (pj .gt. pcutj) goto 24
        if (jj .gt. jmin .or. k .gt. kmin) goto 25
24   continue
25   h = -h
        if (h .lt. zero) goto 22
c
26   prtrng = prtrng + pk
        if (k .gt. kmin .and. pk .le. pcutk .and. pk1 .le. pcutk) goto 99
        pk2 = pk1
        pk1 = pk
        if (gstep .gt. zero) goto 21
28   continue
c
99   return
    end
c
c
double precision function qtrng(p, v, r, ifault)
implicit double precision (a-h, o-z)
c
c   Algorithm AS 190.1 Appl. Statist. (1983) Vol.32, No. 2
c
c   Approximates the quantile p for a studentized range
c   distribution having v degrees of freedom and r samples
c   for probability p, p.ge.0.90 .and. p.le.0.99.
c
c   Uses functions alnorm, ppnd, prtrng and qtrng0 -
c   Algorithms AS 66, AS 111, AS 190 and AS 190.2
c
double precision p, v, r, pcut, p75, p80, p90, p99, p995

```

```
double precision p175, one, two, five
double precision q1, p1, q2, p2, e1, e2
double precision eps
data jmax, pcut, p75, p80, p90, p99, p995, p175, one, two, five
# /8, 0.001d0, 0.75d0, 0.80d0, 0.90d0, 0.99d0, 0.995d0, 1.75d0,
# 1.0d0, 2.0d0, 5.0d0/
data eps/1.0d-4/

c
c      Check input parameters
c
      ifault = 0
      nfault = 0
      if (v .lt. one .or. r.lt. two) ifault = 1
      if (p .lt. p90 .or. p .gt. p99) ifault = 2
      if (ifault .ne. 0) goto 99

c
c      Obtain initial values
c
      q1 = qtrng0(p, v, r, nfault)
      if (nfault .ne. 0) goto 99
      p1 = prtrng(q1, v, r, nfault)
      if (nfault .ne. 0) goto 99
      qtrng = q1
      if (abs(p1-p) .lt. pcut) goto 99
      if (p1 .gt. p) p1 = p175 * p - p75 * p1
      if (p1 .lt. p) p2 = p + (p - p1) * (one - p) / (one - p1) * p75
      if (p2 .lt. p80) p2 = p80
      if (p2 .gt. p995) p2 = p995
      q2 = qtrng0(p2, v, r, nfault)
      if (nfault .ne. 0) goto 99

c
c      Refine approximation
c
      do 14 j = 2, jmax
         p2 = prtrng(q2, v, r, nfault)
         if (nfault .ne. 0) goto 99
         e1 = p1 - p
         e2 = p2 - p
         qtrng = (q1 + q2) / two
         d = e2 - e1
         if (abs(d) .gt. eps) qtrng = (e2 * q1 - e1 * q2) / d
         if(abs(e1) .lt. abs(e2)) goto 12
         q1 = q2
         p1 = p2
12      if (abs(p1 - p) .lt. pcut * five) goto 99
         q2 = qtrng
14 continue

c
99 if (nfault .ne. 0) ifault = 9
   return
end

c
c      double precision function qtrng0(p, v, r, ifault)
c      implicit double precision (a-h, o-z)

c
c      Algorithm AS 190.2 Appl. Statist. (1983) Vol.32, No.2
c
c      Calculates an initial quantile p for a studentized range
c      distribution having v degrees of freedom and r samples
c      for probability p, p.gt.0.80 .and. p.lt.0.995.
```

```
c
c      Uses function ppnd - Algorithm AS 111
c
double precision p, v, r, q, t, vmax, half, one, four, c1, c2, c3
double precision c4, c5
data vmax, half, one, four, c1, c2, c3, c4, c5 / 120.0d0, 0.5d0,
# 1.0d0, 4.0d0, 0.8843d0, 0.2368d0, 1.214d0, 1.208d0, 1.4142d0/
c
t=ppnd(half + half * p,ifault)
if (v .lt. vmax) t = t + (t * t* t + t) / v / four
q = c1 - c2 * t
if (v .lt. vmax) q = q - c3 / v + c4 * t / v
qtrng0 = t * (q * log(r - one) + c5)
return
end
```

```
      subroutine sarmas(z, nz, n, beta, nbeta, ip, iq, ips, iqs, isea,
+         iqap, maxit, a, s, sm, w, nw, ifault)
c
c   ALGORITHM AS 191  APPL. STATIST. (1983) VOL. 32, NO. 2
c
      double precision z(nz), a(nz), w(nw), beta(nbeta), s, sm
c
c   Local variables
c
      logical switch
      double precision zero, one, oneneg, etol, sprev, detm, detms,
+         relerr, temp
c
c   Initialize numerical constants
c
      data zero/0.d0/, one/1.d0/, oneneg/-1.d0/
c
c   ETOL = error tolerance in convergence criterion
c
      data etol/1.d-10/
c
      iter = 0
      switch = .false.
      sprev = zero
      ipq = ip + iq
      ipqps = ipq + ips
      ipsts = ips + isea
      ipsts1 = ipsts + 1
      iqsts = iqs + isea
      iqsts1 = iqsts + 1
      ipsqs = ips + iqs
      iqap2 = iqap
      if (ip .eq. 0 .and. ips .eq. 0) iqap2 = min(iqap, iq + iqsts)
      maxit2 = maxit
      if (iq .eq. 0 .and. iqs .eq. 0) maxit2 = 0
      if (maxit2 .eq. 0) switch = .true.
      nby2 = n / 2
c
c   Input validation
c
      ifault = 0
      ir = max(iq + iqsts, ip + ipsts)
      if (ir .ge. n) ifault = 5
      if (maxit .gt. 0 .and. ir .gt. iqap) ifault = 7
      if (ipq + ipsqs .gt. nbeta) ifault = 4
      if (n + iqap2 .gt. nz) ifault = 4
      if (nw .lt. max(nz, 1 + ipq * (ipq + 3)/2,
+         1 + ipsqs * (ipsqs + 3)/2)) ifault = 4
      if (min(ip, iq, ips, iqs, isea, iqap, maxit) .lt. 0) ifault = 6
      if (ifault .ge. 1) return
c
c   Obtain necessary determinants.
c   Check for stationarity/invertibility
c
      detm = one
      detms = one
      ier = 0
      if (ipq .ne. 0) call dtarma(beta, ipq, ip, iq, w, nw, detm, ier)
      if (ier .gt. 0) go to 340
      if (ipsqs .eq. 0) go to 20
      ii = ipq
```



```
do 10 i = 1, ipsqs
  ii = ii + 1
  a(i) = beta(ii)
10 continue
call dtarma(a, ipsqs, ips, iqs, w, nw, detms, ier)
if (ier .gt. 0) go to 340
c
c   If IQAP2 = 0, use conditional sum of squares method
c
20 if (iqap2 .eq. 0) go to 200
c
c   If no seasonal component and no moving-average component, proceed
c   directly to back-forecasting step (Y and E-series not needed)
c
  if (ipsqs .eq. 0 .and. iq .eq. 0) go to 110
c
c   Calculate Y-series, use W-vector
c
do 60 i = 1, n
  w(i) = zero
  if (i .le. ip) go to 60
  w(i) = z(i)
  if (ip .eq. 0) go to 40
  do 30 j = 1, ip
    iii = i - j
    w(i) = w(i) - beta(j) * z(iii)
30  continue
40  l = min(iq, i - 1)
  if (l .eq. 0) go to 60
  do 50 j = 1, l
    jj = ip + j
    iii = i - j
    w(i) = w(i) + beta(jj) * w(iii)
50  continue
60  continue
c
c   Calculate E-series, use A-vector
c
lqs = iqs
do 100 i = 1, n
  a(i) = zero
  if (i .le. ipsts) go to 100
  a(i) = w(i)
  if (ips .eq. 0) go to 80
  iii = i
  jj = ipq
  do 70 j = 1, ips
    iii = iii - isea
    jj = jj + 1
    a(i) = a(i) - beta(jj) * w(iii)
70  continue
80  if (iqs .eq. 0) go to 100
  if (i .le. iqsts1) lqs = (i - 1) / isea
  if (lqs .eq. 0) go to 100
  iii = i
  do 90 j = 1, lqs
    iii = iii - isea
    jj = ipqps + j
    a(i) = a(i) + beta(jj) * a(iii)
90  continue
100 continue
```

```
c
c      Back-forecast Y-series, use w(n+1), w(n+2), ...
c
110 do 150 i = 1, iqap2
      npi = n + i
      w(npi) = zero
      a(npi) = zero
      if (i .gt. iqsts) go to 130
      iii = npi
      do 120 j = 1, iqs
        iii = iii - isea
        jj = ipqps + j
        w(npi) = w(npi) - beta(jj) * a(iii)
120  continue
130  if (ips .eq. 0) go to 150
      iii = npi
      do 140 j = 1, ips
        iii = iii - isea
        jj = ipq + j
        w(npi) = w(npi) + beta(jj) * w(iii)
140  continue
150  continue
c
c      Back-forecast Z-series, use z(n+1), z(n+2), ...
c
      do 190 i = 1, iqap2
        npi = n + i
        z(npi) = w(npi)
        if (iq .eq. 0) go to 170
        do 160 j = 1, iq
          npimj = npi - j
          jj = ip + j
          z(npi) = z(npi) - beta(jj) * w(npimj)
160  continue
170  if (ip .eq. 0) go to 190
        do 180 j = 1, ip
          npij = npi - j
          z(npi) = z(npi) + beta(j) * z(npij)
180  continue
190  continue
c
c      Calculate X-series, use W-vector
c
200  npqap = n + iqap2
      ii = npqap + 1
      do 240 i = 1, npqap
        ii = ii - 1
        w(ii) = z(ii)
        iml = i - 1
        l = min(iml, ip)
        if (l .eq. 0) go to 220
        iii = ii
        do 210 j = 1, l
          iii = iii + 1
          w(ii) = w(ii) - beta(j) * z(iii)
210  continue
220  l = min(iml, iq)
        if (l .eq. 0) go to 240
        iii = ii
        do 230 j = 1, l
          iii = iii + 1
```

```
        jj = ip + j
        w(ii) = w(ii) + beta(jj) * w(iii)
230  continue
240  continue
c
c  Calculate A-series, use A-vector
c
  ii = npqap + 1
  do 280 i = 1, npqap
    ii = ii - 1
    a(ii) = w(ii)
    if (isea .eq. 0) go to 280
    if (i .le. ipsts1) lps = (i - 1) / isea
    if (lps .eq. 0) go to 260
    iii = ii
    do 250 j = 1, lps
      iii = iii + isea
      jj = ipq + j
      a(ii) = a(ii) - beta(jj) * w(iii)
250  continue
260  if (i .le. iqsts1) lqs = (i - 1) / isea
    if (lqs .eq. 0) go to 280
    iii = ii
    do 270 j = 1, lqs
      iii = iii + isea
      jj = ipqps + j
      a(ii) = a(ii) + beta(jj) * a(iii)
270  continue
280  continue
c
c  Calculate the sum of squares
c
  s = zero
  do 300 i = 1, npqap
300  s = s + a(i) * a(i)
c
c  Test for convergence
c
  if (iqap2 .eq. 0) go to 330
  if (switch) go to 310
  ifault = 0
  relerr = (s - sprev) / s
  if (abs(relerr) .le. etol) go to 330
c
c  Convergence not obtained
c
310  ifault = 1
    if (iter .ge. maxit2) go to 330
c
c  Reverse the series and proceed to the forecasting step.
c
  sprev = s
  ii = n
  do 320 i = 1, nby2
    temp = w(ii)
    w(ii) = w(i)
    w(i) = temp
    temp = a(ii)
    a(ii) = a(i)
    a(i) = temp
    temp = z(ii)
```

```
        z(ii) = z(i)
        z(i) = temp
        ii = ii - 1
320 continue
    if (switch) iter = iter + 1
    switch = .not. switch
    go to 110
c
c    Modified sum of squares
c
330 temp = oneneg / float(n)
    sm = s * detm**temp * detms**(float(isea) * temp)
    if (maxit2 .eq. 0) ifault = 0
    return
c
c    Model is nonstationary or noninvertible
c
340 ifault = ier + 1
    return
end
c
c
c
    subroutine dtarma(beta, nbeta, ip, iq, ws, nws, detm, ifault)
c
c    ALGORITHM AS 191.1 APPL. STATIST. (1983) VOL. 32, NO. 2
c
c    double precision beta(nbeta), ws(nws), detm
c
c    Local variables
c
c    double precision zero, one, oneneg, det, det1
c    data zero/0.d0/, one/1.d0/, oneneg/-1.d0/
c
c    ifault = 0
c    if (nbeta .lt. ip + iq) go to 140
c    nwchek = 1 + nbeta * (nbeta + 3)/2
c    if (nwchek .gt. nws) go to 140
c    det = one
c    det1 = one
c    ir = ip + iq
c    irs = nws - ir - 1
c    irspl = irs + 1
c    ws(irspl) = oneneg
c    isw = 0
c    if (ip .eq. 0) isw = 1
c    iloop = ip
10 if (isw .eq. 1) iloop = iq
    if (iloop .eq. 0) go to 120
    if (isw .eq. 2) go to 30
    do 20 i = 1, iloop
        irspi = irs + i + 1
        ippi = isw * ip + i
        ws(irspi) = beta(ippi)
20 continue
    go to 60
30 if (ip .eq. 0) go to 120
    iloop = ir
c
c
c    Multiply the autoregressive and moving-average operators to obtain
c    coefficients in the left-adjoint AR(ip+iq) model
```

```
c
do 50 i = 1, ir
  ii = irs + 1 + i
  ws(ii) = zero
  imiq = i - iq
  j1 = max(0, imiq) + 1
  j2 = min(i, ip) + 1
  do 40 j = j1, j2
    jm1 = j - 1
    if (j .eq. 1) then
      bj = oneneg
    else
      bj = beta(jm1)
    end if
    imj = i - j + 1
    ippimj = ip + imj
    if (imj .eq. 0) then
      bi = oneneg
    else
      bi = beta(ippimj)
    end if
    ws(ii) = ws(ii) - bi * bj
  40 continue
50 continue

c
c   Form the Schur matrix
c
60 m = 0
  iend = iloop + 1
  do 90 i = 1, iloop
    do 80 j = 1, i
      m = m + 1
      ws(m) = zero
      l = min(i, j)
      do 70 k = 1, l
        irsi = irs + i - k + 1
        irsj = irs + j - k + 1
        irspi = irs + iend - i + k
        irspj = irs + iend - j + k
        ws(m) = ws(m) + ws(irsi) * ws(irsj)
        ws(m) = ws(m) - ws(irspi) * ws(irspj)
      70 continue
    80 continue
  90 continue

c
c   Calculate the determinant using the modified Cholesky
c   decomposition
c
  call mchol(ws, nws, iloop, det, ifault)
  if (ifault .gt. 0) go to 130

c
  if (isw .ge. 1) go to 110
  isw = 1
  det1 = det * det
  go to 10

c
110 if (isw .eq. 2) go to 120
  isw = 2
  det1 = det1 * det * det
  go to 10

c
```

```
120 detm = det1 / det
    return
c
130 ifault = isw + 1
    return
140 ifault = 3
    return
end

c
c
c
subroutine mchol(a, na, n, det, ifault)
c
c   Algorithm AS 191.2  Appl. Statist. (1983) Vol. 32, No. 2
c
c   This algorithm performs the modified Cholesky decomposition
c   A=LDL' where L is lower triangular and D is diagonal.  This
c   form of decomposition avoids the square-root computation of
c   the standard decomposition.
c
c   Parameters:-
c
c   a      Double precision array (na)
c           input:  Positive definite matrix stored in
c                   symmetric mode as a11, a21, a22,...
c                   amm.
c           output: Modified Cholesky decomposition
c                   stored as a one-dimensional array
c                   as d11,l21,d22,l31,l32,d33,.....,
c                   lm1,lm2,...,lmm-1,dmm.
c   na     Integer      input:  m*(m+1)/2
c   n      Integer      input:  m, order of input matrix
c   det    Double precision output: Determinant of a
c   ifault Integer      output: Fault Indicator
c                               =1 if na or n is invalid
c                               =2 if matrix a is not positive-definite
c                               =0 otherwise
c
c   double precision a(na), eta, one, det, w, t, tt
c   data one /1.0d0/
c
c   eta - largest number such that 1.0 + eta = 1.0
c   (depends upon machine precision)
c
c   data eta /1.0d-14/
c
c   ifault = 1
c   det = one
c   if (n .le. 0) goto 70
c   if (na .lt. n*(n+1)/2) goto 70
c   ifault = 2
c   j = 1
c   k = 0
c   do 60 irow = 1,n
c     l = 0
c     do 20 icol = 1,irow
c       k = k+1
c       w = a(k)
c       m = j
c       if (irow .eq. icol) goto 30
c       do 10 i = 1,icol
```

```
        l = l+1
        if (i .eq. icol) goto 20
        w = w-a(l)*a(m)
        m = m+1
10     continue
20     a(k) = w
c
30     ii = 0
    do 40 i = 1,icol
        if(i .eq. icol) goto 50
        ii = ii+i
        t = a(m)
        tt = a(m) / a(ii)
        w = w - t * tt
        a(m) = tt
        m = m+1
40     continue
50     if (w .lt. eta*abs(a(k))) goto 70
        a(k) = w
        det = det*w
        j = j+irow
60     continue
    ifault = 0
70     return
    end
```

```
SUBROUTINE pearsn(xbar, sd, itype, rbl, b2, bndry, sigpt, ifault)
```

```
! Code converted using TO_F90 by Alan Miller
```

```
! Date: 1999-09-25 Time: 16:22:51
```

```
! N.B. Array a has been removed from the list of arguments,  
! and replaced with a PARAMETER statement in this routine.
```

```
! ALGORITHM AS 192 APPL. STATIST. (1983) VOL.32, NO.3
```

```
! Computes approximate significance points of a Pearson curve with given  
! first four moments, or first three moments and left or right boundary.
```

```
! Error codes
```

```
! IFAULT = 0 successful completion
```

```
! = 1 SD < 0.0
```

```
! = 2 ITYPE < 1 or > 3
```

```
! = 3 | RB1 | > 2.0
```

```
! = 4 XBAR value impossible with the value entered for BNDRY
```

```
! = 5 B2 cannot be computed for the first 3 moments + left boundary
```

```
! = 6 B2 out of range, that is:
```

```
! If | RB1 | <= 1.0 then
```

```
! B2 < 1.5 * | RB1 | + 1.5 or B2 > 0.2 * | RB1 | + 10.8
```

```
! If | RB1 | > 1.0 then
```

```
! B2 < 3.9 * | RB1 | - 0.9 or B2 > 4.8 * | RB1 | + 6.2
```

```
IMPLICIT NONE
```

```
REAL, INTENT(IN) :: xbar
```

```
REAL, INTENT(IN) :: sd
```

```
INTEGER, INTENT(IN) :: itype
```

```
REAL, INTENT(IN) :: rbl
```

```
REAL, INTENT(IN OUT) :: b2
```

```
REAL, INTENT(IN) :: bndry
```

```
REAL, INTENT(OUT) :: sigpt(:)
```

```
INTEGER, INTENT(OUT) :: ifault
```

```
REAL :: b(9), rbeta1, ca, ca2, carbl, denom, absca, bnd1, bnd2, sgn, &  
pi1, pi2
```

```
INTEGER :: i, j, k, l
```

```
REAL, PARAMETER :: zero = 0.0, point2 = 0.2, rthalf = 0.70710678, &  
point9 = 0.9, one = 1.0, onept5 = 1.5, two = 2.0, &  
three = 3.0, thrpt9 = 3.9, four = 4.0, forpt8 = 4.8, &  
sixpt2 = 6.2, tenpt8 = 10.8
```

```
REAL, PARAMETER :: a(418) = (/ &  
-1.9336, -1.6061, 2.6955, -1.7036, 1.7236, -1.3209, -2.5464, 1.6812, -0.11812, &  
0.050875, 0.16042, -1.0616, 0.43929, &  
-0.35799, 0.51040, 1.0958, -0.63453, 0.053175, -0.019945, 0.25597, 0.32520, &  
-0.094571, 2.0418, -2.5786, 0.61148, -0.64242, &  
1.1968, -0.33145, 0.015508, -4.1444, 0.13884, 4.6625, 0.37661, -0.20447, &  
-1.9508, -0.20214, 0.11921, -0.0085268, &
```

```
-1.6453, -1.8494, 2.3915, -1.5844, 1.8290, -1.1167, -3.6091, 2.7150, -0.45857, &  
0.048102, 0.89117, -1.2700, 0.37653, &  
-0.81542, 0.56815, 1.6562, -1.1908, 0.24574, -0.024375, -1.5063, 4.4876, &  
-0.60765, -6.5584, 2.8944, -0.42381, 2.2664, &  
-1.3425, 0.25806, -0.010421, -1.9526, 0.21332, 2.1317, -1.1996, 0.21033, &  
-0.52154, 0.53597, -0.12355, 0.0060658, &
```

```
-1.1044, -1.1300, 1.7681, 0.10947, 0.30566, -0.90598, -0.98814, 0.49355, &  
0.30625, -0.018707, 0.74941, -1.3174, 0.23974, &  
-0.12433, 0.59105, 0.85714, -0.47292, -0.16028, 0.012684, -1.4645, 4.5349, &
```



-0.71053, -7.9213, 4.0018, -0.61932, 2.7320, &  
-1.7752, 0.35919, -0.014944, -2.0999, 0.30754, 3.6865, -2.3140, 0.39961,  
-1.1530, 1.0257, -0.22981, 0.011032, &  
  
-0.85842, 0.78929, 1.2196, -0.55088, -0.96385, -0.57312, -0.076974, 0.34882,  
0.47311, -0.056120, -0.63153, -1.2697, 0.64649, &  
0.92712, 0.49088, 0.48118, -0.46407, -0.39753, 0.052413, -0.92873, 2.2039,  
0.25828, 0.74312, -2.4307, 0.49934, 0.029833, &  
0.68249, -0.19687, 0.0068136, -2.9758, -0.050738, 0.067069, 2.0835, -0.45211,  
-0.28149, -0.58012, 0.17621, -0.0067195, &  
  
-2.4031, -1.4891, 0.75590, -2.3309, 9.2314, -3.8930, -7.0192, 2.3648, 0.44308,  
-0.029437, 16.616, -4.9826, 1.0626, &  
-18.888, 7.2830, 14.642, -2.6394, -1.2739, 0.060862, -1.6092, 0.81385,  
-0.059847, -0.18180, 1.2679, -0.36205, 0.29683, &  
-0.83310, 0.26630, -0.015081, 0.43536, 0.27965, 1.2516, -3.0536, 0.65936,  
-1.0579, 1.7886, -0.47962, 0.025311, &  
  
-2.0711E-4, 0.0068277, -7.5482E-6, 0.47086, -0.21213, 1.1003E-4, -0.22462,  
0.11733, -0.079682, -1.0565E-5, 2.5087, -2.6169, &  
0.94103, -2.3261, 1.6482, 2.3024, -1.4821, -0.020294, 9.9168E-4, -0.097078,  
0.58192, -0.019936, -0.7025, 0.11526, 0.0013959, &  
0.1595, -0.062382, 0.01338, 1.8557E-4, -1.8383, -0.54124, 0.68041, 1.7654,  
-0.37606, -1.113, 0.044447, 0.042456, -0.0017448, &  
  
0.39672, -0.17140, -0.74246, 0.48553, 0.19650, 0.58942, -1.5768, 0.37082,  
-0.32481, 0.025296, -0.60818, -1.9005, 0.45451, &  
0.79612, 1.0544, -1.9010, 0.29849, -0.51728, 0.050926, 0.45223, -2.4004,  
0.38372, 3.6817, -1.0796, 0.016619, -1.6829, &  
0.81147, -0.10376, 0.0052116, -4.3837, 0.67456, 6.3029, -1.8042, 0.023516,  
-2.9320, 1.4537, -0.20680, 0.010634, &  
  
0.77212, 0.028272, -1.3932, 0.95628, -0.37918, 0.85487, 0.38225, -1.3009,  
0.42400, -0.051933, 0.17133, -1.5330, 1.2721, &  
-0.58446, 0.78993, 0.33412, -1.2988, 0.39155, -0.046683, 2.2548, -1.7005,  
-0.65377, -2.9256, 2.1397, 0.093244, 3.2094, &  
-2.2896, 0.24580, -0.0020536, 0.30478, -0.58544, -4.0524, 1.8239, 0.083952,  
3.4072, -2.0163, 0.20345, -7.5748E-4, &  
  
1.1504, 0.22674, -1.7407, 1.1356, -0.58596, 0.88839, 0.34743, -1.2531, 0.42319,  
-0.014362, 0.17074, -1.2892, 1.1653, &  
-0.46699, 0.58479, 0.33975, -1.0005, 0.25271, -0.0091547, 2.1265, -8.7599,  
2.3560, 8.0491, -3.3844, -0.028416, -4.3522, &  
3.9741, -0.92840, 0.055908, -5.5206, 1.6024, 6.1077, -2.4508, -0.012514,  
-3.7719, 2.8877, -0.59134, 0.034299, &  
  
1.5989, 1.5353, -2.2124, 0.83145, -1.2543, 0.92247, 2.2076, -1.4147, 0.053879,  
0.058513, 0.42581, -1.1636, 0.67165, &  
-0.47849, 0.46159, 0.97601, -0.61165, -0.054400, 0.029952, 10.803, -5.6739,  
-8.3559, -12.404, 29.846, -7.7439, -6.2673, &  
-1.3612, 1.3966, -0.22122, 2.8678, -3.0580, -14.864, 16.489, -4.0334, -0.49139,  
-1.7927, 0.98545, -0.10118, &  
  
2.4201, -1.9281, -3.3357, 2.3720, 1.7318, 1.4149, -0.64616, -2.7558, 0.28474,  
-0.034471, -0.078628, -1.2092, 0.43924, &  
0.43093, 0.53223, 0.34235, -1.0741, 0.080494, -0.013004, -15.787, -3.9798,  
23.933, 24.332, -46.762, 6.0862, 15.874, &  
5.2360, -2.4644, 0.28404, -14.830, 8.5161, 23.701, -19.419, 2.4239, -1.8457,  
4.8007, -1.2525, 0.099997 /)

! Check for invalid input arguments

```
ifault = 1
IF (sd <= zero) RETURN
ifault = 2
IF (itype < 1 .OR. itype > 3) RETURN
rbeta1 = ABS(rb1)
ifault = 3
IF (rbeta1 > two) RETURN
IF (itype == 1) GO TO 10

!      Compute B2 using XBAR, SD, RB1, and the known boundary

ifault = 4
IF ((itype == 2 .AND. xbar <= bndry) .OR. (itype == 3 .AND. xbar >= bndry)) &
    RETURN
ifault = 5
ca = sd / (xbar - bndry)
ca2 = ca * ca
carb1 = ca * rb1
denom = four * ca2 - carb1 + two
IF (denom <= zero) RETURN
absca = ABS(ca)
bnd1 = (ca2 - one) / ca
IF (absca <= rthalf) THEN
    bnd2 = four * ca / (one - ca2)
ELSE
    bnd2 = four * ca + two / ca
END IF
IF ((itype == 2 .AND. (rb1 < bnd1 .OR. rb1 > bnd2)) .OR. &
    (itype == 3 .AND. (rb1 < bnd2 .OR. rb1 > bnd1))) RETURN
b2 = three * (carb1 * (carb1 + one) + rb1 * rb1 + two) / denom

10 ifault = 6
IF ((rbeta1 <= one .AND. (b2 < onept5 * rbeta1 + onept5 .OR. &
    b2 > point2 * rbeta1 + tenpt8)) .OR. (rbeta1 > one .AND. &
    (b2 < thrpt9 * rbeta1 - point9 .OR. b2 > forpt8 * rbeta1 + sixpt2))) RETURN
ifault = 0

!      Initialization

b(1) = rbeta1
b(2) = b2
b(3) = rbeta1 * rbeta1
b(4) = rbeta1 * b2
b(5) = b2 * b2
b(6) = b(3) * rbeta1
b(7) = b(3) * b2
b(8) = b(5) * rbeta1
b(9) = b(5) * b2

!      Significance point computation

k = -19
IF (rbeta1 > one) k = 0
sgn = one
IF (rb1 < zero) sgn = -one
DO i = 1, 11
    l = i
    IF (rb1 < zero) l = 12 - i
    k = k + 20
    pil = a(k)
```

```
DO j = 1, 9
  k = k + 1
  pi1 = pi1 + a(k) * b(j)
END DO
pi2 = one
DO j = 1, 9
  k = k + 1
  pi2 = pi2 + a(k) * b(j)
END DO

!      Compute significance point

  sigpt(1) = xbar + sd * sgn * pi1 / pi2
END DO
RETURN
END SUBROUTINE pearsn

PROGRAM test_as192
IMPLICIT NONE

INTERFACE
  SUBROUTINE pearsn(xbar, sd, itype, rb1, b2, bndry, sigpt, ifault)
    IMPLICIT NONE
    REAL, INTENT(IN)      :: xbar
    REAL, INTENT(IN)      :: sd
    INTEGER, INTENT(IN)   :: itype
    REAL, INTENT(IN)      :: rb1
    REAL, INTENT(IN OUT)  :: b2
    REAL, INTENT(IN)      :: bndry
    REAL, INTENT(OUT)     :: sigpt(:)
    INTEGER, INTENT(OUT)  :: ifault
  END SUBROUTINE pearsn
END INTERFACE

INTEGER :: itype, ifault
REAL    :: xbar, sd, rb1, b2, bndry, sigpt(11)

DO

  WRITE(*, '(a)', ADVANCE='NO') ' Enter mean & st.devn.: '
  READ(*, *) xbar, sd
  WRITE(*, *) 'ITYPE = 1  4 moments used'
  WRITE(*, *) 'ITYPE = 2  3 moments + left boundary used'
  WRITE(*, *) 'ITYPE = 3  3 moments + right boundary used'
  WRITE(*, '(a)', ADVANCE='NO') ' Enter ITYPE: '
  READ(*, *) itype
  WRITE(*, '(a)', ADVANCE='NO') ' Enter root(beta1) with sign of beta1: '
  READ(*, *) rb1
  IF (itype == 1) THEN
    WRITE(*, '(a)', ADVANCE='NO') ' Enter beta2: '
    READ(*, *) b2
  END IF
  IF (itype > 1) THEN
    WRITE(*, '(a)', ADVANCE='NO') ' Enter boundary: '
    READ(*, *) bndry
  END IF

  CALL pearsn(xbar, sd, itype, rb1, b2, bndry, sigpt, ifault)
  IF (ifault /= 0) THEN
```

```
        WRITE(*, *) 'IFFAULT = ', ifault
    ELSE
        WRITE(*, '(" Percentage points"/ " ", 11f7.2)') sigpt
    END IF

END DO

STOP
END PROGRAM test_as192
```

```
      subroutine spect(a, m, bigt, mu, nusq, lognu, u, iu, v, iv, z,
+          ifault)
c
c   Algorithm AS 193  Appl. Statist. (1983) vol. 32, no. 3
c
c   A revised algorithm for the spectral test
c
      integer bigt, iu, iv, t, t1, ifault
      double precision a, m, mu(bigt), nusq(bigt), lognu(bigt),
+          u(iu, bigt), v(iv, bigt), z(bigt)
      double precision h, hprime, mmax, mmax2, msq, p, pi, pprime, q,
+          vprod
      data zero/0.d0/, one/1.d0/, two/2.d0/, four/4.d0/
c
c   Suitable values for
c   1) IBM REAL*8
c   data mmax/33554432.d0/
c   2) IBM REAL*16
c
c   data mmax/9007199254740992.d0/
c
c   3) CDC 7600 Double precision
c   data mmax/35184372088832.d0/
c
c   Test the validity of the input parameters
c
      mmax2 = mmax + mmax
      ifault = 0
      if (bigt .lt. 2) ifault = 1
      if (a .ge. m .or. a .le. zero .or. m .le. zero) ifault = 2
      if (m .gt. mmax) ifault = 3
      if (ifault .gt. 0) return
c
c   Check that A and M are relatively prime.
c   Needs valid A and M.  Uses Euclid's algorithm.
c
      h = a
      hprime = m
10  r = mod(hprime, h)
      if (r .eq. zero) go to 20
      hprime = h
      h = r
      go to 10
20  if (h .ne. one) then
      ifault = 4
      return
      end if
      msq = m * m
c
c   All steps refer to those in Knuth's algorithm.
c   Step 1 - initialization.
c
      h = a
      hprime = m
      p = one
      pprime = zero
      r = a
      s = one + a * a
c
c   Step 2 - Euclidean step
c
```

```
30 q = int(hprime / h)
   uc = hprime - q * h
   vc = pprime - q * p
   w = uc * uc + vc * vc
   if (w .ge. s) go to 40
   s = w
   hprime = h
   h = uc
   pprime = p
   p = vc
   go to 30
c
c   Step 3 - compute nu(2)
c
40 uc = uc - h
   vc = vc - p
   w = uc * uc + vc * vc
   if (w .ge. s) go to 50
   s = w
   hprime = uc
   pprime = vc
50 nusq(2) = s
c
c   Initialize U and V matrices.
c   N.B. We store by columns whereas Knuth stores by rows.
c
   t = 2
   u(1,1) = -h
   u(1,2) = -hprime
   u(2,1) = p
   u(2,2) = pprime
   sign = one
   if (pprime .gt. zero) sign = -one
   v(1,1) = sign * pprime
   v(1,2) = -sign * p
   v(2,1) = sign * hprime
   v(2,2) = -sign * h
c
c   Step 4 - advance T
c
60 if (t .eq. bigt) go to 200
   t1 = t
   t = t + 1
   r = mod(a*r, m)
   u(1,t) = -r
   u(t,t) = one
   u(t,1) = zero
   v(1,t) = zero
   v(t,t) = m
   do 70 i = 2, t1
     u(i,t) = zero
     u(t,i) = zero
     v(i,t) = zero
70 continue
   do 90 i = 1, t1
     qtemp = v(1,i) * r
     q = nint(qtemp / m)
     v(t,i) = qtemp - q * m
     do 80 i2 = 1, t
70   u(i2, t) = u(i2, t) + q * u(i2, i)
90 continue
```

```

    s = min(s, vprod(u(1,t), u(1,t), t))
    k = t
    j = 1
c
c   Step 5 - transform
c
100 do 120 i = 1, t
    if (i .eq. j) go to 120
    vij = vprod(v(1,i), v(1,j), t)
    vjj = vprod(v(1,j), v(1,j), t)
    if (two * abs(vij) .le. vjj) go to 120
    q = nint(vij / vjj)
    do 110 i2 = 1, t
        v(i2, i) = v(i2, i) - q * v(i2, j)
        u(i2, j) = u(i2, j) + q * u(i2, i)
110 continue
    k = j
120 continue
c
c   Step 6 - examine new bound
c
    if (k .eq. j) s = min(s, vprod(u(1,j), u(1,j), t))
c
c   Step 7 - advance J
c
    j = j + 1
    if (j .eq. t + 1) j = 1
    if (j .ne. k) go to 100
c
c   Step 8 - prepare for search
c
c   MU and LOGNU are used to store Knuth's X and Y respectively
c
    do 130 i = 1, t
        mu(i) = zero
        lognu(i) = zero
        qtemp = vprod(v(1,i), v(1,i), t)
        if (qtemp .gt. mmax2) go to 240
        qtemp = qtemp / msq
        z(i) = int(sqrtdble((int(qtemp * s))))
130 continue
    k = t
c
c   Step 9 - advance XK
c
140 if (mu(k) .eq. z(k)) go to 190
    mu(k) = mu(k) + one
    do 150 i = 1, t
150 lognu(i) = lognu(i) + u(i,k)
c
c   Step 10 - advance K
c
160 k = k + 1
    if (k .gt. t) go to 180
    mu(k) = -z(k)
    do 170 i = 1, t
170 lognu(i) = lognu(i) - two * z(k) * u(i,k)
    go to 160
180 s = min(s, vprod(lognu, lognu, t))
c
c   Step 11 - decrease K

```

```
c
190 k = k - 1
    if (k .ge. 1) go to 140
    nusq(t) = s
    go to 60
c
c    Calculate NU and log(NU)
c
200 do 210 i = 2, bigt
    mu(i) = sqrt(nusq(i))
    lognu(i) = log(mu(i)) / log(two)
210 continue
c
c    Calculate transformed MU values
c
    pi = four * atan(one)
    q = one
    do 220 t = 2, bigt, 2
        q = q * pi * two / t
        mu(t) = q * mu(t) ** t / m
220 continue
    if (bigt .eq. 2) return
    q = two
    do 230 t = 3, bigt, 2
        q = q * pi * two / t
        mu(t) = q * mu(t) ** t / m
230 continue
    return
c
240 ifault = 5
    return
end
c
c
    double precision function vprod(u, v, t)
c
c    Algorithm AS 193.1 Appl. Statist. (1983) vol.32, no.3
c
c    Auxiliary function to calculate the inner product of vectors
c    U and V of length T.
c    N.B. Equivalent to DDOT from LINPACK.
c
    integer t
    double precision u(t), v(t), zero
    data zero/0.d0/
c
    vprod = zero
    do 10 i = 1, t
10 vprod = vprod + u(i) * v(i)
    return
end
```



```

SUBROUTINE BREJ(MM, NT, ERR, N, ALPHA, LP, BETA, LQ, OM, NOM, WKA,
* WKB, NMIN, WKC, W, NW, Q, IFAULT)

```

```

C
C   ALGORITHM AS 194  APPL. STATIST. (1983) VOL.32, NO.3
C

```

```

C   COMPUTES A TEST STATISTIC FOR GOODNESS OF FIT FOR TIME SERIES
C   AUTOREGRESSIVE MOVING AVERAGE PROCESSES.
C

```

```

C   Auxiliary routines required: AS6 & AS7
C

```

```

C   DIMENSION ERR(N), ALPHA(LP), BETA(LQ), OM(NOM, NOM), WKA(NMIN),
*   WKB(NMIN), WKC(NW), W(NW)
C

```

```

C   DATA TOL, ITMAX /0.001, 50/
C

```

```

C   K = LP + LQ - 2
C   LK = K + 1
C   MN = NT - K
C   N22 = MN * (MN + 1) / 2
C   LMLE = NT - MM - K
C

```

```

C   ELEMENTARY CHECKING OF INPUT PARAMETERS.
C

```

```

C   IF (NMIN .LT. N22 + K * K .OR. NW .LT. 2 * NT .OR. NOM .LT. MN)
*   IFAULT = 5
C   IF (LMLE .LE. 0) IFAULT = 4
C   IF (IFAULT .GT. 0) RETURN
C

```

```

C   CALCULATE CORRELATION COEFFICIENTS USING ESTIMATED RESIDUALS
C   IN ARRAY ERR.  STORE COEFFICIENTS IN THE LATTER PART OF WKC.
C

```

```

C   ESS = 0.0
C   DO 10 I = 1, N
10  ESS = ESS * ERR(I) * ERR(I)
C   DO 30 I = 1, NT
C     IPT = I + NT
C     NMI = N - I
C     TEMP = 0.0
C     DO 20 J = 1, NMI
C       JPI = J + I
C       TEMP = TEMP + ERR(J) * ERR(JPI)
20  CONTINUE
C     WKC(IPT) = TEMP / ESS
30  CONTINUE
C

```

```

C   CALCULATE PHI-S OF GODOLPHIN (1980) UPTO NT-1 AND STORE
C   THEM IN WKC.
C

```

```

C   SUBROUTINE FOLD CALCULATES THE COEFFICIENTS OF A POLYNOMIAL
C   WHICH IS THE PRODUCT OF TWO POLYNOMIALS, SEE ROBINSON (1967),
C   PAGE 29.
C

```

```

C   SUBROUTINE ZERO IS DEFINED ON PAGE 16, AND CALLED ALSO BY
C   SUBROUTINE FOLD.
C

```

```

C   CALL FOLD(LP, ALPHA, LQ, BETA, LK, WKA)
C   CALL ZERO(NT, WKC)
C

```

```

C   THE COEFFICIENTS OF THE INVERSE POLYNOMIAL WHICH ARE THE
C   PHI-S ARE STORED IN WKC.
C

```

```

C   WKC(1) = -WKA(2)

```

```

      IF (K .EQ. 1) GOTO 60
      DO 50 J = 2, K
        TEMP = WKC(J)
        JJ = J - 1
        DO 40 JS = 1, JJ
          JMJSP1 = J - JS + 1
          TEMP = TEMP - WKA(JMJSP1) * WKC(JS)
40      CONTINUE
        WKC(J) = TEMP - WKA(J + 1)
50      CONTINUE
60      DO 80 J = LK, NT
        TEMP = WKC(J)
        DO 70 JS = 1, K
          JMJS = J - JS
          TEMP = TEMP - WKA(JS + 1) * WKC(JMJS)
70      CONTINUE
        WKC(J) = TEMP
80      CONTINUE
C
C      FORM THE INVERSE OF THE FIRST K ROWS OF THE DESIGN MATRIX
C      AND STORE THIS TEMPORARILY IN THE LATTER PART OF WKB.
C      THAT IS, FORM  $X(K)^*(-1)$ , WHICH IS LOWER TRIANGULAR.
C
      KK = K * LK / 2 + N22
      CALL ZERO(KK, WKB)
      NP22 = N22 + 1
      WKB(NP22) = 1.0
      IF (K .EQ. 1) GOTO 110
      DO 100 I = 2, K
        IM1 = I - 1
        IIP1 = I * (I - 1) / 2 + 1 + N22
        TEMP = WKB(IIP1)
        DO 90 J = 1, IM1
          J1 = J * (J - 1) / 2 + 1 + N22
          IMJ = I - J
          TEMP = TEMP - WKB(J1) * WKC(IMJ)
90      CONTINUE
        WKB(IIP1) = TEMP
        DO 100 J = 2, I
          IJ = I * (I - 1) / 2 + J + N22
          IJ11 = IM1 * (IM1 - 1) / 2 + J - 1 + N22
          WKB(IJ) = WKB(IJ11)
100     CONTINUE
C
C      FORM THE PRODUCT OF  $X(K)^*(-1)$  AND ITS TRANSPOSE, AND STORE
C      THIS IN THE LATTER PART OF WKA.
C
110     DO 130 I = 1, K
        DO 130 J = 1, I
          TEMP = 0.0
          DO 120 L = 1, J
            IL = I * (I - 1) / 2 + L + N22
            JL = J * (J - 1) / 2 + L + N22
            TEMP = TEMP + WKB(IL) * WKB(JL)
120     CONTINUE
          IKJ = (I - 1) * K + J + N22
          JIK = (J - 1) * K + I + N22
          WKA(IKJ) = TEMP
          WKA(JIK) = TEMP
130     CONTINUE
C

```

```
C      THE SECTION DOWN TO STATEMENT LABELLED 190 EVALUATES
C      SEQUENTIALLY THE ROWS OF THE MATRIX GIVEN BY FORMULA (1.2)
C      AND STORES THIS UPPER TRIANGULAR MATRIX IN THE ARRAY WKA.
C
DO 190 I = LK, NT
    TEMP = 0.0
C
C      THE DIAGONAL ELEMENT OF THE MATRIX (4.2) IS EVALUATED
C      AND STORED IN WKA.
C
DO 140 J = 1, K
    IMJ = I - J
    T1 = WKC(IMJ)
    DO 140 L = 1, K
        LJ = (L - 1) * K + J + N22
        IML = I - L
        TEMP = TEMP + WKC(IML) * T1 * WKA(LJ)
140    CONTINUE
    TEMP = TEMP + 1.0
    IKIK = (I - K) * (I - K + 1) / 2
    WKA(IKIK) = SQRT(TEMP)
    IMKP1 = I - K + 1
    IF (I .EQ. NT) GOTO 190
C
C      THE LOOP INVOLVING STATEMENT LABELLED 180 SIMULTANEOUSLY
C      UPDATES THE MATRIX STORED IN THE LATTER PART OF WKA
C      AND EVALUATES THE ROW OF THE UPPER TRIANGULAR MATRIX
C      THAT IS STORED IN WKA.  THE UPDATING IS DONE VIA THE
C      FORMULA ON PAGE 152 OF BROWN, DURBIN AND EVANS (1975).
C
DO 180 J = IMKP1, MN
    DO 160 L = 1, K
        S0 = 0.0
        DO 150 IC = 1, K
            LIC = (L - 1) * K + IC + N22
            IMIC = I - IC
            S0 = S0 + WKA(LIC) * WKC(IMIC)
150        CONTINUE
        W(L) = S0
160    CONTINUE
    S0 = 0.0
    DO 170 L = 1, K
        T1 = W(L)
        KPJML = K + J - L
        DO 170 M = 1, K
            LM = (L - 1) * K + M + N22
            WKA(LM) = WKA(LM) - (T1 * W(M)) / TEMP
            IMM = I - M
            S0 = S0 + WKC(KPJML) * WKA(LM) * WKC(IMM)
170    CONTINUE
    JIMK = J * (J - 1) / 2 + I - K
    WKA(JIMK) = S0 * WKA(IKIK)
180    CONTINUE
190    CONTINUE
C
C      IN THE LOOP ENDING AT STATEMENT LABELLED 220 THE INVERSE
C      OF THE UPPER TRIANGULAR MATRIX C* IS STORED IN WKB.
C
DO 200 I = 1, MN
    II = I * (I + 1) / 2
    WKB(II) = 1.0 / WKA(II)
```

```
200 CONTINUE
    MNM1 = MN - 1
    DO 220 L = 1, MNM1
        I = MN - L
        II = I * (I + 1) / 2
        T1 = WKB(II)
        IP1 = I + 1
        DO 220 J = IP1, MN
            JMI = J - I
            TEMP = 0.0
            DO 210 JJ = 1, JMI
                IJJI = (I + JJ) * (I + JJ - 1) / 2 + I
                IJMI = (I + JMI) * (I + JMI - 1) / 2 + I + JJ
                TEMP = TEMP - WKA(IJJI) * WKB(IJMI)
210 CONTINUE
            JI = J * (J - 1) / 2 + I
            WKB(JI) = TEMP * T1
220 CONTINUE
C
C     THE TRANSFORMED RESIDUAL SERIAL CORRELATIONS ARE CALCULATED
C     IN TWO STEPS.  THE COMPONENT OF W FORMED FROM C* BY X* BY
C     X(K)**(-1) BY THE VECTOR OF SERIAL CORRELATIONS IS CALCULATED
C     IN THE LOOP OF STATEMENT LABELLED 260 AND THEN SUBTRACTED
C     FROM THE COMPONENT FORMED FROM C* BY THESE CORRELATIONS,
C     STORED IN THE LATTER PART OF ARRAY WKC.
C
    DO 260 L = 1, K
        L12 = L + N22
        DO 240 I = 1, MN
            TEMP = 0.0
            DO 230 J = I, MN
                JI = J * (J - 1) / 2 + I
                KPJML = K + J - L
                TEMP = TEMP + WKB(JI) * WKC(KPJML)
230 CONTINUE
            OM(I, L) = TEMP
240 CONTINUE
            TEMP = 0.0
            DO 250 J = 1, L
                JPT = J + NT
                LJ = L * (L - 1) / 2 + J + N22
                TEMP = TEMP + WKB(LJ) * WKC(JPT)
250 CONTINUE
            WKA(L12) = TEMP
260 CONTINUE
            DO 290 I = 1, MN
                TEMP = 0.0
                DO 270 J = 1, K
                    J12 = J + N22
                    TEMP = TEMP + OM(I, J) * WKA(J12)
270 CONTINUE
                IPMN = I + MN
                W(IPMN) = TEMP
                TEMP = 0.0
                DO 280 J = I, MN
                    JI = J * (J - 1) / 2 + I
                    KPJPT = K + J + NT
                    TEMP = TEMP + WKB(JI) * WKC(KPJPT)
280 CONTINUE
                W(IPMN) = TEMP - W(IPMN)
290 CONTINUE
```

```

C
C      FIND THE APPROXIMATE MAXIMUM LIKELIHOOD ESTIMATE OF THE
C      NON-ZERO RESIDUAL SERIAL CORRELATIONS
C
      CALL MLE(W, NW, MN, OM, NOM, WKA, WKB, NMIN, LMLE, WKC, MM, TOL,
*      ITMAX, IFAULT)
      IF (IFAULT .GT. 0) RETURN
C
      EVALUATE THE INVERSE OF THE MATRIX
      OM11 - OM12 * OM22 ** (-1) * (OM12 PRIME).
      STORE THIS MATRIX IN WKA AND ITS INVERSE IN WKB.
C
DO 330 I = 1, MM
  DO 310 J = 1, LMLE
    JPM = J + MM
    TEMP = 0.0
    DO 300 M = 1, LMLE
      M3 = M + MM
      T1 = OM(I, M3)
      LMJ = M * (M - 1) / 2 + J
      IF (J .LE. M) GOTO 300
      LMJ = J * (J - 1) / 2 + M
      TEMP = TEMP + T1 * WKB(LMJ)
300    CONTINUE
      OM(JPM, I) = TEMP
310    CONTINUE
      DO 330 J = 1, I
        IJ = I * (I - 1) / 2 + J
        TEMP = 0.0
        DO 320 M = 1, LMLE
          M3 = M + MM
          TEMP = TEMP + OM(M3, I) * OM(J, M3)
320        CONTINUE
          WKA(IJ) = OM(I, J) - TEMP
330    CONTINUE
      CALL SYMINV(WKA, MM, WKB, WKC, NULLTY, IFAULT)
      IF (IFAULT .GT. 0) RETURN
C
      EVALUATE THE QUADRATIC FORM (3.2) OF GODOLPHIN (1980).
C
      Q = 0.0
      DO 350 I = 1, MM
        TEMP = W(I)
        DO 340 J = 1, I
          IJ = I * (I - 1) / 2 + J
          Q = Q + TEMP * W(J) * WKB(IJ) * 2.0
340        CONTINUE
          II = I * (I + 1) / 2
          Q = Q - TEMP * TEMP * WKB(II)
350        CONTINUE
      Q = Q * FLOAT(N)
      RETURN
      END
C
      SUBROUTINE MLE(W, NW, MN, OM, NOM, X, XI, NMIN, L, PHI, MM, TOL,
*      ITMAX, IFAULT)
C
      ALGORITHM AS 194.1  APPL. STATIST. (1983) VOL.32, NO.3
C
      EVALUATES THE APPROXIMATE MAXIMUM LIKELIHOOD ESTIMATE BY
      ITERATING THE TRANSFORMED RESIDUAL SERIAL CORRELATIONS

```

```

C      AS IN (3.1) OF GODOLPHIN (1980).  THESE ARE STORED IN ARRAY W.
C
C      VALUES RETURNED ARE,
C      W(I), I=1,...,MM,          MLE OF NON-ZERO CORRELATION.
C      OM          THE FINAL ESTIMATE OF OMEGA STORED IN MATRIX FORM.
C      XI          THE INVERSE OF OMEGA22 STORED AS AN ARRAY.
C
DIMENSION W(NW), OM(NOM, NOM), X(NMIN), XI(NMIN), PHI(NW)
IT = 1
CALL ZERO(MN, W)
DO 10 I = 1, MM
MNPI = MN + I
W(I) = W(MNPI)
10   CONTINUE
C
C      THE MATRIX OM IS SET UP FROM THE CURRENT ITERATION OF THE
C      APPROXIMATE MAXIMUM LIKELIHOOD ESTIMATES OF THE NON-ZERO
C      CORRELATIONS, THAT IS THE NON-ZERO COMPONENTS OF THE
C      EXPECTATION OF THE VECTOR W UNDER THE ALTERNATIVE
C      HYPOTHESIS, USING THE ALGORITHM ON PAGE 245 OF GODOLPHIN
C      (1977).  IT IS AN APPROXIMATION TO THE COVARIANCE MATRIX
C      OF W.
C
C      FIRSTLY, AN AUXILIARY VECTOR, PHI, BASED ON THE CURRENT
C      ITERATION STORED IN W(I), I=1,...,M IS SET, BEGINNING
C      WITH PHI(1).
C
20   TEMP = 1.0
DO 30 I = 1, MM
TEMP = TEMP + 2.0 * W(I) * W(I)
PHI(I + 1) = 0.0
30   CONTINUE
PHI(1) = TEMP
M2 = 2 * MN + 1
DO 40 I = MM, M2
40   PHI(I + 1) = 0.0
C
C      SECOND STAGE OF ALGORITHM FOR PHI.
C
DO 50 I = 1, MM
PHI(I + 1) = PHI(I + 1) + 2.0 * W(I)
PHI(2 * I + 1) = PHI(2 * I + 1) + W(I) * W(I)
50   CONTINUE
IF (MM .EQ. 1) GOTO 70
C
C      FINAL STAGE OF ALGORITHM FOR SETTING PHI.
C
LMM = MM - 1
DO 60 I = 1, LMM
LI = I + 1
DO 60 J = LI, MM
JPIP1 = J + I + 1
JMIP1 = J - I + 1
TEMP = 2.0 * W(I) * W(J)
PHI(JPIP1) = PHI(JPIP1) + TEMP
PHI(JMIP1) = PHI(JMIP1) + TEMP
60   CONTINUE
70   TP1 = PHI(1)
C
C      THE FOLLOWING FORMULA, (2.6) IN GODOLPHIN (1977), USES
C      THE ELEMENTS OF VECTOR PHI AND THE CURRENT ITERATIONS

```

```

C      FOR THE CORRELATIONS STORED IN W.
C      THIS DEFINES THE ELEMENTS OF MATRIX OM.
      DO 80 I = 1, MN
      TWI = W(I)
      TPI1 = PHI(I + 1)
      DO 80 J = I, MN
      JMIP1 = J - I + 1
      JPIP1 = J + I + 1
      OM(I, J) = PHI(JMIP1) + PHI(JPIP1) + 2.0 * (TWI * W(J) * TP1 -
* TWI * PHI(J + 1) - W(J) * TPI1)
      OM(J, I) = OM(I, J)
80     CONTINUE
C
C      THE INVERSE OF THE LAST QUADRANT OF THE COVARIANCE MATRIX
C      OM IS EVALUATED USING AS6/7 ALGORITHMS.
C
      DO 90 I = 1, L
      II = I * (I - 1) / 2
      IPMM = I + MM
      DO 90 J = 1, I
      IIPJ = II + J
      JPMM = J + MM
      X(IIPJ) = OM(IPMM, JPMM)
90     CONTINUE
      CALL SYMINV(X, L, XI, PHI, NULLTY, IFAULT)
      IF (IFAULT .GE. 1) RETURN
      T = 0.0
C
C      THE NEXT ITERATION FOR THE APPROXIMATE MAXIMUM LIKELIHOOD
C      ESTIMATE OF CORRELATION IS MADE USING FORMULA (3.1) OF
C      GODOLPHIN (1980).
C
      DO 130 J = 1, MM
      S = 0.0
      DO 120 I = 1, L
      II = I * (I - 1) / 2
      Y = 0.0
      DO 100 K = 1, I
      IK = II + K
      MMK = MM + K + MN
      Y = Y + XI(IK) * W(MMK)
100     CONTINUE
      DO 110 K = I, L
      KI = K * (K - 1) / 2 + I
      MMK = MM + K + MN
      Y = Y + XI(KI) * W(MMK)
110     CONTINUE
      MMI = MM + I
      MMIN = MMI + MN
      II = I * (I + 1) / 2
      Y = Y - XI(II) * W(MMIN)
      S = S + OM(J, MMI) * Y
120     CONTINUE
      JPMN = J + MN
      T = T + ABS(W(J) - W(JPMN) + S)
      W(J) = W(JPMN) - S
130     CONTINUE
C
C      TEST FOR CONVERGENCE OF ITERATION.
C
      IF (IT .GT. ITMAX) IFAULT = 3

```

```
IT = IT + 1
IF (T .GT. TOL .AND. IT .LE. ITMAX) GOTO 20
RETURN
END
```

C  
C The following subroutines are from the book by E.A. Robinson  
C

```
SUBROUTINE ZERO(LX, X)
INTEGER LX
REAL X(LX)
```

C  
C Local variable  
C

```
INTEGER I
```

C  
DO 10 I = 1, LX  
10 X(I) = 0.0  
RETURN  
END

C  
SUBROUTINE FOLD(LA, A, LB, B, LC, C)  
INTEGER LA, LB, LC  
REAL A(LA), B(LB), C(LC)

C  
C Local variables  
C

```
INTEGER I, J, K
```

C  
LC = LA + LB - 1  
CALL ZERO(LC, C)  
DO 20 I = 1, LA  
DO 10 J = 1, LB  
K = I + J - 1  
C(K) = C(K) + A(I)\*B(J)  
10 CONTINUE  
20 CONTINUE  
RETURN  
END



```

c This file contains two versions of the algorithm. The first is that
c published in the journal, including several auxiliary routines which
c are not in the journal, but converted to double precision.
c The second version is one which calls IMSL routines.
c
c      subroutine mulnor(a, b, sig, eps, n, inf, prob, bound, ifault)
c
c      Algorithm AS 195  appl. statist. (1984) vol.33, no.1
c
c      Computes multivariate normal distribution function and computes
c      the probability that a multivariate normal vector falls in a
c      rectangle in n-space with error less than eps.
c
c      Auxiliary routines required: BIVNOR (CACM algorithm 462) which
c      needs DERF, PPND = AS111 (or PPND7 or PPND16 from AS241), and
c      SYMINV = AS7 which calls CHOL = AS6. BIVNOR and DERF are
c      included in this file.
c
c      double precision
c      *      a(*), b(*), sig(*), c(7), d(7), co(25), sd(2), coef(5, 3),
c      *      binc(7, 5), bl(7, 5), br(7, 35, 5), r(36, 5), s(5, 27),
c      *      xss(6, 6), pr2(6), prep(6), preb(6), cv(5, 15), sinv(28),
c      *      cond1(5), xm(5), cond(5), beta(5, 5), bh(5), fe(5), sigma(28),
c      *      ep(5), del(3, 5), bou4(5), bou5(5), ans(6), fact(5), prod(5),
c      *      bint(6), bcs(5), bcn(7), eo(13), do(25)
c      integer inf(7), intvl(5), ind(5), ksa(5), num(5), itype(5)
c      logical simps, ipr
c      double precision eps, bound, prob, cons2, cons3, cons4, epsmin,
c      +      epssim, zero, p05, p15, half, one, two, three, six, eight,
c      +      ten, twelve, fifteen, forty5, ninety, nine45, bou1, bou2, bou3,
c      +      cup, det, eplos, epsi, ept, fac, fsa, rho, sigc, t, tem, temb,
c      +      temp, wb, wl, wt, wu, x1, x2, xs, y1, y2, z
c      double precision alnorm, bivnor, f2, f3, f4, f5, f6, ppnd, phi, x,
c      +      y
c      data coef
c      * /0.3111111111111111D0, 1.4222222222222222D0, 0.5333333333333333D0,
c      * 1.4222222222222222D0, 0.3111111111111111D0, 0.3333333333333333D0,
c      * 0.0D0, 1.3333333333333333D0, 0.0D0, 0.3333333333333333D0, 0.5D0,
c      * 0.0D0, 0.0D0, 0.0D0, 0.5D0/
c      data bcs /1.0D0, 4.0D0, 6.0D0, 4.0D0, 1.0D0/
c      data bcn /1.0D0, 6.0D0, 15.0D0, 20.0D0, 15.0D0, 6.0D0, 1.0D0/
c      data do /-3.75043972D0,-3.3242574D0, -2.85697D0, -2.36675941D0,
c      * -2.3344142D0, -1.8891759D0, -1.7320508D0, -1.3556262D0,
c      * -1.15440539D0, -1.0D0, -0.74196378D0, -0.61670659D0,0.0D0,
c      * 0.61670659D0, 0.74196378D0, 1.0D0, 1.15440539D0,1.3556262D0,
c      * 1.7320508D0, 1.8891759D0, 2.3344142D0, 2.36675941D0, 2.85697D0,
c      * 3.3242574D0,3.75043972D0/
c      data eo / -2.85697D0, -2.3344142D0, -1.7320508D0, -1.3556262D0,
c      * -1.0D0, -0.74196378D0, 0.0D0, 0.74196378D0, 1.0D0, 1.3556262D0,
c      * 1.7320508D0, 2.3344142D0, 2.85697D0/
c      data cons2 /6.879833D0/, cons3 /4.517004D0/, cons4 /76.371214D0/,
c      * epsmin /1.0d-8/, epssim /6.0d-5/
c      data zero, p05, p15, half, one, two, three, six, eight, ten,
c      * twelve, fifteen, forty5, ninety, nine45 /0.0D0, 0.05D0, 0.15D0,
c      * 0.5D0, 1.0D0, 2.0D0, 3.0D0, 6.0D0, 8.0D0, 10.0D0, 12.0D0,
c      * 15.0D0, 45.0D0, 90.D0, 945.D0/
c
c      Functions needed to calculate the first six derivatives of
c      the normal density
c
c      f2(x, y) = abs((x * x - one) / (y * y))

```

```

f3(x, y) = abs(-x * (x * x - three) / (y * y * y))
f4(x, y) = abs((three + x * x * (-six + x * x)) / (y ** 4))
f5(x, y) = abs(x * (-fifteen + x * x * (ten - x * x))) / (y ** 5)
f6(x, y) = abs(-fifteen + x * x * (forty5 - x * x * (-fifteen +
* x * x))) / (y ** 6)

```

```

c     Checking for faulty data

```

```

c

```

```

ifault = 0
if (eps .le. epsmin) ifault = 2
if (n .le. 0 .or. n .gt. 7) ifault = 3
if (ifault .ne. 0) return
do 1 i = 1, n
1 if (inf(i) .eq. 2 .and. a(i) .lt. b(i)) ifault = 100 + i
if (ifault .ne. 0) return
bound = eps

```

```

c     Finding z such that p(n(0,1).gt.z) .lt. 0.15*eps/n
c     co will contain the roots of the first 5 or 7 Hermite
c     polynomials

```

```

ept = eps * p15 / float(n)
z = -ppnd(ept, ifault) + epsmin
if (ifault .ne. 0) return
cup = alnorm(z, .true.)

```

```

c

```

```

c     inverting sig and the n-2 lower right hand principal minors

```

```

c

```

```

ik = 0
ij = 0
do 3 i = 1, n
  do 3 j = 1, i
    ik = ik + 1
    if (i .eq. j) goto 2
    ij = ij + 1
    sigma(ik) = sig(ij)
    goto 3
2  sigma(ik) = one
3  continue
if (n .le. 2) goto 4
call invert(sigma, sinv, cv, n, det, ifault)
if (ifault .ne. 0) return
simps = .true.
if (det .lt. p05 .or. eps .le. epssim) simps = .false.
prob = zero
det = sinv(1) * sinv(3) - sinv(2) * sinv(2)
sd(1) = sqrt(sinv(3) / det)
sd(2) = sqrt(sinv(1) / det)
rho = -sinv(2) / (sd(1) * sd(2) * det)
if (abs(rho) .gt. one) goto 400
4 nm2 = n - 2
  nm1 = n - 1

```

```

c

```

```

c     checking whether upper and lower endpoints are too big

```

```

c

```

```

eplos = zero
do 6 l = 1, n
  c(l) = max(b(l), -z)
  d(l) = min(a(l), z)
  if (inf(l) .eq. 0) d(l) = z
  if (inf(l) .eq. 1) c(l) = -z
  if (a(l) .gt. z .or. inf(l) .eq. 0) eplos = eplos + cup
  if (b(l) .lt. -z .or. inf(l) .eq. 1) eplos = eplos + cup
  if (c(l) .ge. d(l)) return

```

```
6 continue
  if (n .eq. 1) goto 350
  fac = one
  ipr = .false.
  if (inf(1) .ne. 1 .or. inf(2) .ne. 1) goto 7
  ipr = .true.
  eplos = eplos - two * cup
  goto 8
7 if (inf(1) .ne. 0 .or. inf(2) .ne. 0) goto 8
  fac = -one
  ipr = .true.
  d(1) = c(1)
  d(2) = c(2)
  eplos = eplos - two * cup
8 if (n .eq. 2) goto 360
  ifault = 5
  epsi = (eps - eplos) / float(nm2)
c   Finding regression coefficients (beta,bh) and bounds on the
c   conditional integrals (binc)
c   cond(1)=conditional variance of variable n-1+1 given later
c   variables
c
do 15 l = 1, nm2
  cond(1) = one / sqrt(cv(1, 1))
  condl(1) = log(cond(1))
  do 10 i = 1, l
    beta(1, i) = zero
    do 10 j = 1, l
      jk = (1 - i + 1) * (1 - i) / 2 + j
      if (j .gt. 1 - i + 1) jk = j * (j - 1) / 2 + 1 - i + 1
      jn = (n - 1 + j) * (n - 1 + j - 1) / 2 + n - 1
      beta(1, i) = beta(1, i) + sigma(jn) * cv(1, jk)
10  continue
    k = n - 1 - 1
    bh(k + 1) = beta(1, l)
    do 11 i = 1, k
      bh(i) = zero
      do 11 j = 1, l
        jn = (j + n - 1) * (j + n - 1 - 1) / 2 + n - 1
        ijk = 1 + j * (j - 1) / 2
        bh(i) = bh(i) + sigma(jn) * cv(1, ijk)
11  continue
    k = 0
    sigc = zero
    do 12 j = 1, l
      do 12 i = 1, j
        k = k + 1
        sigc = sigc + bh(i) * bh(j) * sinv(k)
12  continue
    binc(1, l) = one
    binc(2, l) = sqrt(sigc)
    binc(3, l) = two * sigc
    binc(4, l) = cons2 * sigc * binc(2, l)
    binc(5, l) = twelve * sigc * sigc
    if (simps) goto 13
    binc(6, l) = sigc * sigc * binc(1, l) * cons3
    binc(7, l) = (sigc ** 3) * cons4
13  if (l .lt. nm2) goto 15
    do 14 i = 1, nm2
      bh(i) = zero
      do 14 j = 1, nm2
```

```

        jk = (1 - i + 1) * (1 - i) / 2 + j
        if (j .gt. 1 - i + 1) jk = j * (j - 1) / 2 + 1 - i + 1
        jn = (2 + j) * (1 + j) / 2 + 1
        bh(i) = bh(i) + sigma(jn) * cv(1, jk)
14  continue
15  continue
    l = 1
c
c      co will contain the roots of the first 5 or 7 Hermite
c      polynomials
c
    if (simps) goto 50
    do 40 i = 1, 25
40  co(i) = do(i)
    iend = 25
    ien = 7
    goto 60
50  do 55 i = 1, 13
55  co(i) = eo(i)
    iend = 13
    ien = 5
c
c      Initialising values.  xss contains partial sums used for
c      calculating conditional means.
c
60  do 70 i = 1, nm1
70  xss(i, 1) = zero
    xm(1) = zero
    prod(1) = one
    pr2(1) = one
    do 80 i = 1, nm2
        ni = n - i + 1
        pr2(i + 1) = pr2(i) * (d(ni) - c(ni))
80  continue
c
c      bint(1) is a bound on the error accumulated at levels 1 and
c      deeper.
c      ans(1) is the accumulated integral at level 1.
c      prep(1) contains the integrand at level 1.
c      preb(1) bounds the error accumulated at levels deeper than 1.
c
    bint(nm1) = zero
90  intvl(1) = 2
    ans(1) = zero
    bou4(1) = zero
    bint(1) = zero
    prep(1) = zero
    preb(1) = zero
    k = 1
c
c      Finding which of the co are in the current interval.
c      s(1,.) are the endpoints of intervals on which the integrand
c      at level 1 and its derivatives are monotone.
c      num(1) is the number of such intervals.
c
    nl = n - 1 + 1
    s(1, 1) = c(nl) - xm(1)
    s(1, iend + 2) = d(nl) - xm(1)
    num(1) = iend + 2
    do 91 i = 1, iend
        njs = i

```

```

        if (s(l, 1) .lt. co(i) * cond(l)) goto 92
        num(l) = num(l) - 1
91 continue
92 if (num(l) .eq. 2) goto 99
   do 94 i = njs, iend
      mjs = iend - i + njs
      if (s(l, iend + 2) .ge. co(mjs) * cond(l)) goto 96
      num(l) = num(l) - 1
94 continue
96 if (num(l) .eq. 2) goto 99
   do 98 i = njs, mjs
      inj = i - njs + 2
      s(l, inj) = co(i) * cond(l)
98 continue
99 numl = num(l)
   s(l, numl) = s(l, iend + 2)
c
c      ep(l)  is an upper limit on the allowable error at level l.
c      r(k,l) is the right end-point of the current sub-interval.
c      fe(l)  is the left end-point of the current sub-interval.
c      ind(l)-1 indicates which point of the Newton-Cotes formula
c      we are dealing with.
c
c      ep(l) = epsi / pr2(l + 1)
c      r(1, 1) = s(1, 2)
c      ind(l) = 6
c
c      Bounding derivatives at left end-point of current interval.
c      bl(i,l) is a bound on the ith derivative of the normal
c      density at level l at the left end-point.
c
c      fe(l) = s(l, 1)
c      t = fe(l) / cond(l)
c      bl(1, 1) = phi(t, condl(l))
c      bl(2, 1) = bl(1, 1) * abs(t / cond(l))
c      bl(3, 1) = bl(1, 1) * f2(t, cond(l))
c      bl(4, 1) = bl(1, 1) * f3(t, cond(l))
c      bl(5, 1) = bl(1, 1) * f4(t, cond(l))
c      if (simps) goto 100
c      bl(6, 1) = bl(1, 1) * f5(t, cond(l))
c      bl(7, 1) = bl(1, 1) * f6(t, cond(l))
c      Bounding derivatives at right end-point of sub-interval.
c      br(i,l) is a bound on the ith derivative of the normal
c      density at level l at the right end-point.
c
c      100 t = r(k, 1) / cond(l)
c      br(1, k, 1) = phi(t, condl(l))
c      br(2, k, 1) = br(1, k, 1) * abs(t / cond(l))
c      br(3, k, 1) = br(1, k, 1) * f2(t, cond(l))
c      br(4, k, 1) = br(1, k, 1) * f3(t, cond(l))
c      br(5, k, 1) = br(1, k, 1) * f4(t, cond(l))
c      if (simps) goto 104
c      br(6, k, 1) = br(1, k, 1) * f5(t, cond(l))
c      br(7, k, 1) = br(1, k, 1) * f6(t, cond(l))
c      104 r(k + 1, 1) = (fe(l) + r(k, 1)) * half
c      bou5(l) = ep(l) * (r(k, 1) - s(l, 1))
c      del(2, 1) = r(k + 1, 1) - fe(l)
c
c      Checking the bound for the trapezoidal rule
c
c      del(3, 1) = two * del(2, 1)

```

```

    bou1 = max(br(1, k, 1), bl(1, 1)) * binc(3, 1) +
*   two * max(br(2, k, 1), bl(2, 1)) * binc(2, 1) +
*   max(br(3, k, 1), bl(3, 1)) * binc(1, 1)
    bou3 = bou4(1) + bou1 * (del(3, 1) ** 3) * prod(1) / twelve
    itype(1) = 3
    if (bou3 .le. bou5(1)) goto 200
c
c     Checking the bound for Simpsons rule.
c
    bou1 = zero
    do 110 ij = 1, 5
        jk = 6 - ij
        bou2 = max(br(ij, k, 1), bl(ij, 1))
        bou1 = bou1 + bou2 * binc(jk, 1) * bcs(ij)
110 continue
    bou3 = bou4(1) + bou1 * (del(2, 1) ** 5) * prod(1) / ninety
    itype(1) = 2
    if (bou3 .le. bou5(1)) goto 200
    if (simps) goto 130
c
c     Checking the bound for boules rule, if necessary.
c
    del(1, 1) = half * del(2, 1)
    bou1 = zero
    itype(1) = 1
    do 120 ij = 1, 7
        jk = 8 - ij
        bou2 = max(br(ij, k, 1), bl(ij, 1))
        bou1 = bou1 + bou2 * binc(jk, 1) * bcn(ij)
120 continue
    bou3 = bou4(1) + bou1 * (del(1, 1) ** 7) * prod(1) * eight /
*   nine45
    if (bou3 .le. bou5(1)) goto 200
c
c     Sub-dividing further at level 1 when the bound is too big.
c
130 k = k + 1
    if (k .gt. 35) return
    goto 100
200 bint(1) = bint(1) + bou3 - bou4(1)
    bou4(1) = bou3
    ksa(1) = k
    if (ind(1) .eq. 6) goto 202
    if (itype(1) - 2) 205, 206, 210
c
c     The next 30 lines condition on the value xs and go to level l+1
c
202 ind(1) = 5
    xs = fe(1)
    fact(1) = bl(1, 1)
203 xss(nm1, 1 + 1) = xss(nm1, 1) + bh(1) * (xs + xm(1))
    do 204 ll = 1, nm2
204 xss(ll, 1 + 1) = xss(ll, 1) + beta(ll, 1) * (xs + xm(1))
    if (l .eq. nm2) goto 300
c
c     xm is the mean of the next variable given those fixed so far.
c
    xm(1 + 1) = xss(1, 1 + 1)
    prod(1 + 1) = prod(1) * fact(1)
    l = l + 1
    goto 90

```

```

205 ind(l) = 4
    k = ksa(l)
    xs = half * (fe(l) + r(k + 1, l))
    goto 207
206 ind(l) = 3
    k = ksa(l)
    xs = r(k + 1, l)
207 t = xs / cond(l)
    fact(l) = phi(t, condl(l))
    goto 203
208 ind(l) = 2
    k = ksa(l)
    xs = half * (r(k, l) + r(k + 1, l))
    goto 207
210 ind(l) = 1
    k = ksa(l)
    xs = r(k, l)
    fact(l) = br(1, k, l)
    goto 203
c
c     Evaluate conditional bivariate probabilities at deepest level
c
300 x1 = fac * (xss(nm1, nm1) - d(1)) / sd(1)
    x2 = fac * (xss(nm2, nm1) - d(2)) / sd(2)
    l = nm1
    ans(l) = bivnor(x1, x2, rho)
    if (ipr) goto 310
    y1 = (xss(nm1, nm1) - c(1)) / sd(1)
    y2 = (xss(nm2, nm1) - c(2)) / sd(2)
    wu = bivnor(y1, y2, rho)
    wt = bivnor(x1, y2, rho)
    wb = bivnor(y1, x2, rho)
    ans(l) = ans(l) + wu - wt - wb
310 if (l .eq. 1) goto 340
    l = l - 1
c
c     Advancing the integration at the current level
c
    indl = ind(l)
    numl = num(l)
    ity = itype(l)
    temp = fact(l) * ans(l + 1)
    temb = bint(l + 1)
    fsa = one
    if (indl .ne. 1) goto 315
    tem = temp
    temp = temp + prep(l)
    temb = temb + preb(l)
    prep(l) = tem
    preb(l) = bint(l + 1)
    fsa = two
315 ans(l) = ans(l) + coef(indl, ity) * temp * del(ity, l)
    bint(l) = bint(l) + coef(indl, ity) * temb * del(ity, l)
c
c     Making use of the error which did not accumulate at level l+1
c
    ep(l) = ep(l) + del(ity, l) * coef(indl, ity) * (fsa * float(nm2 -
* 1) * epsi / pr2(l + 1) - temb) / (s(l, numl) - s(l, 1))
    if (indl .eq. 1) goto 320
    igo = indl - (1 + (itye(l) * (itye(l) - 1)) / 2)
    goto (210, 208, 206, 205), igo

```

```
c
c      Un-subdividing at level 1.
320 k = ksa(1)
    do 322 i = 1, ien
322 bl(i, 1) = br(i, k, 1)
    ind(1) = 5
    fe(1) = r(k, 1)
    if (k .eq. 1) goto 326
    k = k - 1
    goto 104
326 if (intvl(1) .eq. num(1)) goto 310
    intvl(1) = intvl(1) + 1
    intl = intvl(1)
    r(1, 1) = s(1, intl)
    goto 100

c
c      Completion of integration and bounding.
c
340 ifault = 0
    prob = ans(1)
    bound = bint(1) + eplos
    return

c
c      special cases --
c      label 350 - n=1
c      label 360 - n=2
c
350 prob = alnorm(d(1), .false.) - alnorm(c(1), .false.)
    return
360 rho = sigma(2)
    if (abs(rho) .gt. one) goto 400
    y1 = -d(1) * fac
    y2 = -d(2) * fac
    prob = bivnor(y1, y2, rho)
    if (ipr) return
    x1 = -c(1)
    x2 = -c(2)
    w1 = bivnor(x1, x2, rho)
    wt = bivnor(x1, y2, rho)
    wb = bivnor(y1, x2, rho)
    prob = w1 - wt - wb + prob
    return

c
c      Error return for covariance not positive definite.
c
400 ifault = 4
    return
end

c
c
c
c      double precision function phi(x, y)
c
c      algorithm as 195.1  appl. statist. (1984) vol.33, no.1
c
c      computes univariate normal density
c      xlow=log(smallest floating point number)
c      sq2p=log(sqrt(two*pi))
c
c      double precision arg, half, sq2p, x, xlow, y, zero
c
```



```

data xlow /-87.0D0/, sq2p /0.91893853320467274D0/, zero /0.D0/,
* half /0.5D0/
phi = zero
arg = -half * x * x - sq2p - y
if (arg .gt. xlow) phi = exp(arg)
return
end

```

C  
C  
C

```
DOUBLE PRECISION FUNCTION BIVNOR(AH, AK, R)
```

C  
C BIVNOR is a controlled precision Fortran function to calculate  
C the bivariate normal upper right area, viz. the probability for  
C two normal variates X and Y whose correlation is R, that X > AH  
C and Y > AK.  
C The accuracy is specified as the number of decimal digits, IDIG.

C  
C Reference:  
C Donnelly, T.G. (1973) Algorithm 462, Bivariate normal  
C distribution, Comm. A.C.M., vol.16, p. 638.

C  
C Corrected for the case AH = 0, AH non-zero by reversing AH & AK  
C in such cases.

C  
C DOUBLE PRECISION AH, AK, R

C  
C Local variables

```

DOUBLE PRECISION TWOPI, B, XAH, XAK, GH, GK, RR, GAUSS, DERF, H2,
+ A2, H4, EX, W2, AP, S2, SP, S1, SN, SGN, SQR, CON, WH, WK, GW,
+ T, G2, CONEX, CN, TWO, ZERO, ONE, FOUR, QUART, HALF, EXPLIM
INTEGER IDIG, IS
DATA TWO/2.D0/, ZERO/0.D0/, ONE/1.D0/, FOUR/4.D0/, QUART/0.25D0/,
+ HALF/0.5D0/
GAUSS(T) = (ONE + DERF(T/SQRT(TWO)))/TWO

```

C  
C GAUSS is a univariate lower normal tail area calculated here from  
C the central error function, DERF.  
C It may be replaced by the algorithm in Hill, I.D. and Joyce, S.A.  
C Algorithm 304, Normal curve integral (S15), Comm. A.C.M. (10),  
C (June 1967), p.374 or with Applied Statistics algorithm AS66.  
C Source: Owen, D.B. Ann. Math. Statist., vol.27 (1956), p.1075.

C  
C DATA TWOPI/6.2831 85307 17958 7D0/, IDIG/15/, EXPLIM/80.D0/

C  
C B = ZERO  
C IF (AH .EQ. ZERO) THEN  
C     XAH = AK  
C     XAK = AH  
C ELSE  
C     XAH = AH  
C     XAK = AK  
C END IF

```

GH = GAUSS(-XAH) / TWO
GK = GAUSS(-XAK) / TWO
IF (R .EQ. ZERO) THEN
  B = FOUR * GH * GK
  GO TO 350
END IF

```

```

RR = ONE - R*R
IF (RR .LT. ZERO) THEN
  WRITE(*, *)'Error in BIVNOR, R = ', R
  GO TO 390
END IF
IF (RR .GT. ZERO) GO TO 100
C
C R^2 = 1.0
C
IF (R .GE. ZERO) GO TO 70
IF (XAH + XAK .GE. ZERO) GO TO 350
B = TWO * (GH + GK) - ONE
GO TO 350
70 IF (XAH - XAK .LT. ZERO) THEN
  B = TWO * GK
ELSE
  B = TWO * GH
END IF
GO TO 350
C
C Regular case, R^2 < 1
C
100 SQR = SQRT(RR)
IF (IDIG .EQ. 15) THEN
  CON = TWOPI * 1.D-15 / TWO
ELSE
  CON = TWOPI / TWO / 10**IDIG
END IF

IF (XAH .NE. ZERO) GO TO 170
IF (XAK .NE. ZERO) GO TO 190
B = ATAN(R/SQR) / TWOPI + QUART
GO TO 350
170 B = GH

IF (XAH*XAK) 180, 200, 190
180 B = B - HALF
190 B = B + GK
200 WH = -XAH
WK = (XAK/XAH - R)/SQR
GW = TWO * GH
IS = -1
210 SGN = -ONE
T = ZERO
IF (WK .EQ. ZERO) GO TO 320
IF (ABS(WK) - ONE) 270, 230, 240
230 T = WK * GW * (ONE - GW) / TWO
GO TO 310
240 SGN = -SGN
WH = WH * WK
G2 = GAUSS(WH)
WK = ONE / WK
IF (WK .LT. ZERO) B = B + HALF
B = B - (GW + G2)/TWO + GW*G2
270 H2 = WH * WH
A2 = WK * WK
H4 = H2 / TWO
IF (H4 .LT. EXPLIM) THEN
  EX = EXP(-H4)
ELSE

```

```

      EX = ZERO
      END IF
      W2 = H4 * EX
      AP = ONE
      S2 = AP - EX
      SP = AP
      S1 = ZERO
      SN = S1
      CONEX = ABS(CON / WK)
      GO TO 290

```

```

280 SN = SP
      SP = SP + ONE
      S2 = S2 - W2
      W2 = W2 * H4 / SP
      AP = -AP*A2
290 CN = AP * S2 / (SN + SP)
      S1 = S1 + CN
      IF (ABS(CN) - CONEX .GT. ZERO) GO TO 280

```

```

      T = (ATAN(WK) - WK*S1) / TWOPI
310 B = B + SGN*T
320 IF (IS .GE. 0) GO TO 350
      IF (XAK .NE. ZERO) THEN
          WH = -XAK
          WK = (XAH/XAK - R) / SQR
          GW = TWO * GK
          IS = 1
          GO TO 210
      END IF

```

```

350 IF (B .LT. ZERO) B = ZERO
      IF (B .GT. ONE) B = ONE
390 BIVNOR = B

```

C

```

      RETURN
      END

```

C

C

C

```

SUBROUTINE INVERT(A, AINV, C, N, DET, IFAULT)

```

C

C

C

C

C

C

C

```

      Invert the NxN symmetric matrix, A, of which only the lower
      triangle is stored by rows.  The inverse is returned in AINV.
      The inverse of the last I rows and columns, for I = 1, 2, ...,
      N-2, is returned in C(I,*).  DET = the determinant of A.
      IFAULT = 4 if A is not positive definite.

```

C

```

      DOUBLE PRECISION A(*), AINV(*), C(5,*), DET
      INTEGER N, IFAULT

```

C

C

C

```

      Local variables

```

```

      DOUBLE PRECISION ONE, WK(15), W(7)
      INTEGER NULLTY, NN, I, ROW1, WKPOS, ROW, APOS, COL
      DATA ONE/1.D0/

```

C

```

      DO 50 I = 1, N-2

```

C

C

```

      Copy the last I rows and columns of A into WK.

```

```

C
  NN = I * (I + 1) / 2
  ROW1 = N + 1 - I
  WKPOS = 1
  DO 20 ROW = ROW1, N
    APOS = ROW * (ROW - 1) / 2 + ROW1
    DO 10 COL = ROW1, ROW
      WK(WKPOS) = A(APOS)
      WKPOS = WKPOS + 1
      APOS = APOS + 1
10    CONTINUE
20  CONTINUE
C
C  Call SYMINV to invert WK in situ.
C
  CALL SYMINV(WK, I, NN, WK, W, NULLTY, IFAULT)
  IF (IFAULT .NE. 0) GO TO 70
C
C  Copy the inverse into the I-th row of C.
C
  DO 40 APOS = 1, NN
40  C(I, APOS) = WK(APOS)
50 CONTINUE
C
C  Use AS6 (CHOL) to calculate the determinant.
C  This is inefficient as AS7 will call AS6 again to repeat the same
C  calculations.  AS6/7 can easily be converted to calculate the
C  determinant.
C
  NN = N * (N + 1) / 2
  CALL CHOL(A, N, NN, AINV, NULLTY, IFAULT)
  IF (IFAULT .NE. 0) GO TO 70
  DET = ONE
  APOS = 1
  DO 60 ROW = 1, N
    DET = DET * AINV(APOS)
    APOS = APOS + ROW + 1
60 CONTINUE
  DET = DET * DET
C
C  Invert the full matrix.
C
  CALL SYMINV(A, N, NN, AINV, W, NULLTY, IFAULT)
  IF (IFAULT .EQ. 0) RETURN
C
70 IFAULT = 4
  RETURN
  END
C
C
C  SUBROUTINE CALERF(ARG,RESULT,JINT)
C-----
C
C  THIS PACKET COMPUTES THE ERROR AND COMPLEMENTARY ERROR FUNCTIONS
C  FOR REAL ARGUMENTS ARG.  IT CONTAINS TWO FUNCTION TYPE
C  SUBPROGRAMS, ERF AND ERFC (OR DERF AND DERFC), AND ONE
C  SUBROUTINE TYPE SUBPROGRAM, CALERF.  THE CALLING STATEMENTS
C  FOR THE PRIMARY ENTRIES ARE
C
C
C          Y=ERF(X)      (OR   Y=DERF(X) )

```

```

C   AND
C           Y=ERFC(X)   (OR   Y=DERFC(X) ).
C
C   THE ROUTINE CALERF IS INTENDED FOR INTERNAL PACKET USE ONLY,
C   ALL COMPUTATIONS WITHIN THE PACKET BEING CONCENTRATED IN THIS
C   ROUTINE. THE FUNCTION SUBPROGRAMS INVOKE CALERF WITH THE
C   STATEMENT
C           CALL CALERF(ARG,RESULT,JINT)
C   WHERE THE PARAMETER USAGE IS AS FOLLOWS
C
C           FUNCTION           PARAMETERS FOR CALERF
C           CALL               ARG           RESULT           JINT
C   ERF(ARG)           ANY REAL ARGUMENT   ERF(ARG)           0
C   ERFC(ARG)          ABS(ARG) .LT. XMAX   ERFC(ARG)          1
C
C   THE MAIN COMPUTATION EVALUATES NEAR MINIMAX APPROXIMATIONS
C   FROM "RATIONAL CHEBYSHEV APPROXIMATIONS FOR THE ERROR FUNCTION"
C   BY W. J. CODY, MATH. COMP., 1969, PP. 631-638. THIS
C   TRANSPORTABLE PROGRAM USES RATIONAL FUNCTIONS THAT THEORETICALLY
C   APPROXIMATE ERF(X) AND ERFC(X) TO AT LEAST 18 SIGNIFICANT
C   DECIMAL DIGITS. THE ACCURACY ACHIEVED DEPENDS ON THE ARITHMETIC
C   SYSTEM, THE COMPILER, THE INTRINSIC FUNCTIONS, AND PROPER
C   SELECTION OF THE MACHINE-DEPENDENT CONSTANTS.
C
C*****
C EXPLANATION OF MACHINE-DEPENDENT CONSTANTS
C
C   XSMALL = ARGUMENT BELOW WHICH ERF(X) MAY BE REPRESENTED
C           BY 2*X/SQRT(PI) AND ABOVE WHICH X*X WILL
C           NOT UNDERFLOW. A CONSERVATIVE VALUE IS THE
C           LARGEST X SUCH THAT 1.0 + X = 1.0 TO MACHINE
C           PRECISION.
C   XMAX   = LARGEST ARGUMENT ACCEPTABLE TO ERFC; SOLUTION TO
C           EQUATION: W(X) * (1-0.5/X**2) = XMIN, WHERE
C           W(X) = EXP(-X*X)/(X*SQRT(PI)), AND XMIN IS THE
C           SMALLEST POSITIVE MACHINE NUMBER (SEE TABLE BELOW).
C
C   APPROXIMATE VALUES FOR SOME IMPORTANT MACHINES ARE:
C
C           XSMALL           XMAX           XMIN
C   IBM 195      (D.P.)    1.39D-17    13.306    5.40D-79
C   CDC 7600     (S.P.)    7.11E-15    25.922    3.13E-294
C   CRAY-1       (S.P.)    7.11E-15    75.326    4.58E-2467
C   UNIVAC 1108 (D.P.)    1.73D-18    26.582    2.78D-309
C   VAX 11/780  (S.P.)    5.96E-8     9.269     2.94E-39
C   VAX 11/780  (D.P.)    1.39D-17    9.269     2.94D-39
C   IBM PC       (S.P.)    5.96E-8     9.194     1.18E-38
C   IBM PC       (D.P.)    1.11D-16    26.543    2.23D-308
C
C*****
C ERROR RETURNS
C
C   THE PROGRAM RETURNS ERFC = 0 FOR ARG .GT. XMAX.
C
C   OTHER SUBPROGRAMS REQUIRED (SINGLE PRECISION VERSION)
C
C   ABS, EXP

```

```

C
C OTHER SUBPROGRAMS REQUIRED (DOUBLE PRECISION VERSION)
C
C     DABS, DEXP
C
C
C AUTHOR: W. J. CODY
C     MATHEMATICS AND COMPUTER SCIENCE DIVISION
C     ARGONNE NATIONAL LABORATORY
C     ARGONNE, IL 60439
C
C LATEST MODIFICATION: JANUARY 8, 1985
C
C-----
C     INTEGER I,JINT
CS     REAL           A, ARG, B, C, D, FOUR, HALF, P, ONE, Q, RESULT, SQRPI,
CS     1             TWO, THRESH, X, XMAX, XDEN, XNUM, XSMALL, Y, YSQ, ZERO
C     DOUBLE PRECISION A, ARG, B, C, D, FOUR, HALF, P, ONE, Q, RESULT, SQRPI,
C     1             TWO, THRESH, X, XMAX, XDEN, XNUM, XSMALL, Y, YSQ, ZERO
C     DIMENSION A(5),B(4),C(9),D(8),P(6),Q(5)
C-----
C     MATHEMATICAL CONSTANTS
C-----
CS     DATA FOUR,ONE,HALF,TWO,ZERO/4.0E0,1.0E0,0.5E0,2.0E0,0.0E0/
CS     DATA SQRPI/5.6418958354775628695E-1/,THRESH/0.46875E0/
C     DATA FOUR,ONE,HALF,TWO,ZERO/4.0D0,1.0D0,0.5D0,2.0D0,0.0D0/
C     DATA SQRPI/5.6418958354775628695D-1/,THRESH/0.46875D0/
C-----
C     MACHINE-DEPENDENT PARAMETERS
C-----
CS     DATA XSMALL/4.2E-16/, XMAX/9.269E0/
C     DATA XSMALL/4.2D-16/, XMAX/9.269D0/
C-----
C     COEFFICIENTS FOR APPROXIMATION TO DERF IN FIRST INTERVAL
C-----
CS     DATA A/3.16112374387056560E00,1.13864154151050156E02,
CS     1         3.77485237685302021E02,3.20937758913846947E03,
CS     2         1.85777706184603153E-1/
C     DATA B/2.36012909523441209E01,2.44024637934444173E02,
CS     1         1.28261652607737228E03,2.84423683343917062E03/
C     DATA A/3.16112374387056560D00,1.13864154151050156D02,
CS     1         3.77485237685302021D02,3.20937758913846947D03,
CS     2         1.85777706184603153D-1/
C     DATA B/2.36012909523441209D01,2.44024637934444173D02,
CS     1         1.28261652607737228D03,2.84423683343917062D03/
C-----
C     COEFFICIENTS FOR APPROXIMATION TO DERFC IN SECOND INTERVAL
C-----
CS     DATA C/5.64188496988670089E-1,8.88314979438837594E0,
CS     1         6.61191906371416295E01,2.98635138197400131E02,
CS     2         8.81952221241769090E02,1.71204761263407058E03,
CS     3         2.05107837782607147E03,1.23033935479799725E03,
CS     4         2.15311535474403846E-8/
C     DATA D/1.57449261107098347E01,1.17693950891312499E02,
CS     1         5.37181101862009858E02,1.62138957456669019E03,
CS     2         3.29079923573345963E03,4.36261909014324716E03,
CS     3         3.43936767414372164E03,1.23033935480374942E03/
C     DATA C/5.64188496988670089D-1,8.88314979438837594D0,
CS     1         6.61191906371416295D01,2.98635138197400131D02,
CS     2         8.81952221241769090D02,1.71204761263407058D03,
CS     3         2.05107837782607147D03,1.23033935479799725D03,

```

```

4      2.15311535474403846D-8/
DATA D/1.57449261107098347D01,1.17693950891312499D02,
1      5.37181101862009858D02,1.62138957456669019D03,
2      3.29079923573345963D03,4.36261909014324716D03,
3      3.43936767414372164D03,1.23033935480374942D03/

```

C-----

C COEFFICIENTS FOR APPROXIMATION TO DERFC IN THIRD INTERVAL

C-----

```

CS     DATA P/3.05326634961232344E-1,3.60344899949804439E-1,
CS     1      1.25781726111229246E-1,1.60837851487422766E-2,
CS     2      6.58749161529837803E-4,1.63153871373020978E-2/
CS     DATA Q/2.56852019228982242E00,1.87295284992346047E00,
CS     1      5.27905102951428412E-1,6.05183413124413191E-2,
CS     2      2.33520497626869185E-3/
DATA P/3.05326634961232344D-1,3.60344899949804439D-1,
1      1.25781726111229246D-1,1.60837851487422766D-2,
2      6.58749161529837803D-4,1.63153871373020978D-2/
DATA Q/2.56852019228982242D00,1.87295284992346047D00,
1      5.27905102951428412D-1,6.05183413124413191D-2,
2      2.33520497626869185D-3/

```

C-----

```

X = ARG
CS     Y = ABS(X)
      Y = DABS(X)
      IF (Y .GT. FOUR) GO TO 200
      IF (Y .GT. THRESH) GO TO 100

```

C-----

C EVALUATE ERF FOR ABS(X) .LE. 0.46875

C-----

```

      YSQ = ZERO
      IF (Y .GT. XSMALL) YSQ = Y * Y
      XNUM = A(5)*YSQ
      XDEN = YSQ
      DO 20 I = 1, 3
        XNUM = (XNUM + A(I)) * YSQ
        XDEN = (XDEN + B(I)) * YSQ
20 CONTINUE
      RESULT = X * (XNUM + A(4)) / (XDEN + B(4))
      IF (JINT .NE. 0) RESULT = ONE - RESULT
      GO TO 800

```

C-----

C EVALUATE ERFC FOR 0.46875 .LT. ABS(X) .LE. 4.0

C-----

```

100 YSQ = Y * Y
      XNUM = C(9)*Y
      XDEN = Y
      DO 120 I = 1, 7
        XNUM = (XNUM + C(I)) * Y
        XDEN = (XDEN + D(I)) * Y
120 CONTINUE
CS     RESULT = EXP(-YSQ) * (XNUM + C(8)) / (XDEN + D(8))
      RESULT = DEXP(-YSQ) * (XNUM + C(8)) / (XDEN + D(8))
      GO TO 300

```

C-----

C EVALUATE ERFC FOR ABS(X) .GT. 4.0

C-----

```

200 RESULT = ZERO
      IF (Y .GE. XMAX) GO TO 300
220 YSQ = ONE / (Y * Y)
      XNUM = P(6)*YSQ
      XDEN = YSQ

```

```
      DO 240 I = 1, 4
          XNUM = (XNUM + P(I)) * YSQ
          XDEN = (XDEN + Q(I)) * YSQ
240 CONTINUE
      RESULT = YSQ *(XNUM + P(5)) / (XDEN + Q(5))
CS      RESULT = (EXP(-Y*Y) / Y) * (SQRPI - RESULT)
      RESULT = (DEXP(-Y*Y) / Y) * (SQRPI - RESULT)
C-----
C  FIX UP FOR NEG. ARG., ERF, ETC.
C-----
      300 IF (JINT .EQ. 0) GO TO 350
          IF (X .LT. ZERO) RESULT = TWO - RESULT
          GO TO 800
      350 RESULT = (HALF - RESULT) + HALF
          IF (X .LT. ZERO) RESULT = -RESULT
C-----
      800 RETURN
C----- LAST CARD OF CALERF -----
      END
```

```
CS      REAL FUNCTION ERF(X)
      DOUBLE PRECISION FUNCTION DERF(X)
C-----
C
C  PROGRAM TO COMPUTE THE ERROR FUNCTION
C
C  AUTHOR - W. J. CODY
C
C  DATE - JANUARY 8, 1985
C
C-----
      INTEGER JINT
CS      REAL          X, RESULT
      DOUBLE PRECISION X, RESULT
C-----
      JINT = 0
      CALL CALERF(X,RESULT,JINT)
CS      ERF = RESULT
      DERF = RESULT
      RETURN
C----- LAST CARD OF DERF -----
      END
```

```
CS      REAL FUNCTION ERFC(X)
      DOUBLE PRECISION FUNCTION DERFC(X)
C-----
C
C  PROGRAM TO COMPUTE THE COMPLEMENTARY ERROR FUNCTION
C
C  AUTHOR - W. J. CODY
C
C  DATE - JANUARY 8, 1985
C
C-----
      INTEGER JINT
```



```

CS      REAL          X, RESULT
        DOUBLE PRECISION X, RESULT
C-----
        JINT = 1
        CALL CALERF(X,RESULT,JINT)
CS      ERFC = RESULT
        DERFC = RESULT
        RETURN
C----- LAST CARD OF DERFC -----
        END
c
c-----
c
        subroutine mulnor(a, b, sig, eps, n, inf, prob, bound, ifault)
c
c      algorithm as 195  appl. statist. (1984) vol.33, no.1
c
c      computes multivariate normal distribution function and computes
c      the probability that a multivariate normal vector falls in a
c      rectangle in n-space with error less than eps.
c
c      Auxiliary functions required: ANORDF, ANORIN, BNRDF, LFDRG, LFTRG
c      and LINRG from the IMSL Stat/Library.
c
        dimension
*      a(*), b(*), sig(*), c(7), d(7), co(25), sd(2), coef(5, 3),
*      binc(7, 5), bl(7, 5), br(7, 35, 5), r(36, 5), s(5, 27),
*      xss(6, 6), pr2(6), prep(6), preb(6), cv(5, 15), sinv(28),
*      cond1(5), xm(5), cond(5), beta(5, 5), bh(5), fe(5), sigma(28),
*      ep(5), del(3, 5), bou4(5), bou5(5), ans(6), fact(5), prod(5),
*      bint(6), bcs(5), bcn(7), eo(13), do(25)
        dimension inf(7), intvl(5), ind(5), ksa(5), num(5), itype(5)
        logical simps, ipr
        data coef(1, 1), coef(2, 1), coef(3, 1), coef(4, 1), coef(5, 1),
*      coef(1, 2), coef(2, 2), coef(3, 2), coef(4, 2), coef(5, 2),
*      coef(1, 3), coef(2, 3), coef(3, 3), coef(4, 3), coef(5, 3)
*      /0.3111111111111111, 1.4222222222222222, 0.5333333333333333,
*      1.4222222222222222, 0.3111111111111111, 0.3333333333333333, 0.0,
*      1.3333333333333333, 0.0, 0.3333333333333333, 0.5, 0.0, 0.0, 0.0,
*      0.5/
        data bcs(1), bcs(2), bcs(3), bcs(4), bcs(5) /1.0, 4.0, 6.0, 4.0,
*      1.0/
        data bcn(1), bcn(2), bcn(3), bcn(4), bcn(5), bcn(6), bcn(7)
*      /1.0, 6.0, 15.0, 20.0, 15.0, 6.0, 1.0/
        data do(1), do(2), do(3), do(4), do(5), do(6), do(7), do(8),
*      do(9), do(10), do(11), do(12), do(13), do(14), do(15), do(16),
*      do(17), do(18), do(19), do(20), do(21), do(22), do(23), do(24),
*      do(25) / - 3.75043972, -3.3242574, -2.85697, -2.36675941,
*      -2.3344142, -1.8891759, -1.7320508, -1.3556262, -1.15440539, -1.,
*      -0.74196378, -0.61670659, 0.0,
*      0.61670659, 0.74196378, 1.0, 1.15440539, 1.3556262, 1.7320508,
*      1.8891759, 2.3344142, 2.36675941, 2.85697, 3.3242574, 3.75043972/
        data eo(1), eo(2), eo(3), eo(4), eo(5), eo(6), eo(7), eo(8),
*      eo(9), eo(10), eo(11), eo(12), eo(13) / - 2.85697, -2.3344142,
*      -1.7320508, -1.3556262, -1.0, -0.74196378, 0.0, 0.74196378, 1.0,
*      1.3556262, 1.7320508, 2.3344142, 2.85697/
        data cons2 /6.879833/, cons3 /4.517004/, cons4 /76.371214/,
*      epsmin /1.0e-8/, epssim /6.0e-5/
        data zero, p05, p15, half, one, two, three, six, eight, ten,
*      twelve, fifteen, forty5, ninety, nine45 /0.0, 0.05, 0.15, 0.5,
*      1.0, 2.0, 3.0, 6.0, 8.0, 10.0, 12.0, 15.0, 45.0, 90, 945/

```

```

c
c      functions needed to calculate the first six derivatives of
c      the normal density
c
f2(x, y) = abs((x * x - one) / (y * y))
f3(x, y) = abs(-x * (x * x - three) / (y * y * y))
f4(x, y) = abs((three + x * x * (-six + x * x)) / (y ** 4))
f5(x, y) = abs(x * (-fifteen + x * x * (ten - x * x))) / (y ** 5)
f6(x, y) = abs(-fifteen + x * x * (forty5 - x * x * (-fifteen +
* x * x))) / (y ** 6)
c      checking for faulty data
c
ifault = 0
if (eps .le. epsmin) ifault = 2
if (n .le. 0 .or. n .gt. 7) ifault = 3
if (ifault .ne. 0) return
do 1 i = 1, n
1 if (inf(i) .eq. 2 .and. a(i) .lt. b(i)) ifault = 100 + i
if (ifault .ne. 0) return
bound = eps
c      finding z such that p(n(0,1).gt.z).lt. 0.15*eps/n
c      co will contain the roots of the first 5 or 7 hermite
c      polynomials
ifault=0.
ept = eps * p15 / float(n)
z = -anorin(ept) + epsmin
cup=1-anordf(z)
c
c      inverting sig and the n-2 lower right hand principal minors
c
ik = 0
ij = 0
do 3 i = 1, n
  do 3 j = 1, i
    ik = ik + 1
    if (i .eq. j) goto 2
    ij = ij + 1
    sigma(ik) = sig(ij)
    goto 3
2  sigma(ik) = one
3 continue
if (n .le. 2) goto 4
call invert(sigma, sinv, cv, n, det, ifault)
if (ifault .ne. 0) return
simps = .true.
if (det .lt. p05 .or. eps .le. epssim) simps = .false.
prob = zero
det = sinv(1) * sinv(3) - sinv(2) * sinv(2)
sd(1) = sqrt(sinv(3) / det)
sd(2) = sqrt(sinv(1) / det)
rho = -sinv(2) / (sd(1) * sd(2) * det)
if (abs(rho) .gt. one) goto 400
4 nm2 = n - 2
  nm1 = n - 1
c
c      checking whether upper and lower endpoints are too big
c
eplos = zero
do 6 l = 1, n
  c(l) = max(b(l), -z)
  d(l) = min(a(l), z)

```

```

        if (inf(1) .eq. 0) d(1) = z
        if (inf(1) .eq. 1) c(1) = -z
        if (a(1) .gt. z .or. inf(1) .eq. 0) eplos = eplos + cup
        if (b(1) .lt. -z .or. inf(1) .eq. 1) eplos = eplos + cup
        if (c(1) .ge. d(1)) return
5 continue
  if (n .eq. 1) goto 350
  fac = one
  ipr = .false.
  if (inf(1) .ne. 1 .or. inf(2) .ne. 1) goto 7
  ipr = .true.
  eplos = eplos - two * cup
  goto 8
7 if (inf(1) .ne. 0 .or. inf(2) .ne. 0) goto 8
  fac = -one
  ipr = .true.
  d(1) = c(1)
  d(2) = c(2)
  eplos = eplos - two * cup
8 if (n .eq. 2) goto 360
  ifault = 5
  epsi = (eps - eplos) / float(nm2)
c    finding regression coefficients (beta,bh) and bounds on the
c    conditional integrals (binc)
c    cond(1)=conditional variance of variable n-1+1 given later
c    variables
c
do 15 l = 1, nm2
  cond(1) = one / sqrt(cv(1, 1))
  condl(1) = log(cond(1))
  do 10 i = 1, l
    beta(1, i) = zero
    do 10 j = 1, l
      jk = (1 - i + 1) * (1 - i) / 2 + j
      if (j .gt. 1 - i + 1) jk = j * (j - 1) / 2 + 1 - i + 1
      jn = (n - 1 + j) * (n - 1 + j - 1) / 2 + n - 1
      beta(1, i) = beta(1, i) + sigma(jn) * cv(1, jk)
10 continue
  k = n - 1 - 1
  bh(k + 1) = beta(1, l)
  do 11 i = 1, k
    bh(i) = zero
    do 11 j = 1, l
      jn = (j + n - 1) * (j + n - 1 - 1) / 2 + n - 1
      ijk = 1 + j * (j - 1) / 2
      bh(i) = bh(i) + sigma(jn) * cv(1, ijk)
11 continue
  k = 0
  sigc = zero
  do 12 j = 1, l
    do 12 i = 1, j
      k = k + 1
      sigc = sigc + bh(i) * bh(j) * sinv(k)
12 continue
  binc(1, 1) = one
  binc(2, 1) = sqrt(sigc)
  binc(3, 1) = two * sigc
  binc(4, 1) = cons2 * sigc * binc(2, 1)
  binc(5, 1) = twelve * sigc * sigc
  if (simps) goto 13
  binc(6, 1) = sigc * sigc * binc(1, 1) * cons3

```

```

    binc(7, 1) = (sigc ** 3) * cons4
13  if (l .lt. nm2) goto 15
    do 14 i = 1, nm2
        bh(i) = zero
        do 14 j = 1, nm2
            jk = (1 - i + 1) * (1 - i) / 2 + j
            if (j .gt. 1 - i + 1) jk = j * (j - 1) / 2 + 1 - i + 1
            jn = (2 + j) * (1 + j) / 2 + 1
            bh(i) = bh(i) + sigma(jn) * cv(1, jk)
14  continue
15  continue
    l = 1
c
c      co will contain the roots of the first 5 or 7 hermite
c      polynomials
c
    if (simps) goto 50
    do 40 i = 1, 25
40  co(i) = do(i)
    iend = 25
    ien = 7
    goto 60
50  do 55 i = 1, 13
55  co(i) = eo(i)
    iend = 13
    ien = 5
c
c      initialising values.  xss contains partial sums used for
c      calculating conditional means.
c
60  do 70 i = 1, nm1
70  xss(i, 1) = zero
    xm(1) = zero
    prod(1) = one
    pr2(1) = one
    do 80 i = 1, nm2
        ni = n - i + 1
        pr2(i + 1) = pr2(i) * (d(ni) - c(ni))
80  continue
c
c      bint(1) is a bound on the error accumulated at levels 1 and
c      deeper.
c      ans(1) is the accumulated integral at level 1.
c      prep(1) contains the integrand at level 1.
c      preb(1) bounds the error accumulated at levels deeper than 1.
c
    bint(nm1) = zero
90  intvl(1) = 2
    ans(1) = zero
    bou4(1) = zero
    bint(1) = zero
    prep(1) = zero
    preb(1) = zero
    k = 1
c
c      finding which of the co are in the current interval.
c      s(1,.) are the endpoints of intervals on which the integrand
c      at level 1 and its derivatives are monotone.
c      num(1) is the number of such intervals.
c
    nl = n - 1 + 1

```

```

    s(1, 1) = c(nl) - xm(1)
    s(1, iend + 2) = d(nl) - xm(1)
    num(1) = iend + 2
    do 91 i = 1, iend
        njs = i
        if (s(1, 1) .lt. co(i) * cond(1)) goto 92
        num(1) = num(1) - 1
91 continue
92 if (num(1) .eq. 2) goto 99
    do 94 i = njs, iend
        mjs = iend - i + njs
        if (s(1, iend + 2) .ge. co(mjs) * cond(1)) goto 96
        num(1) = num(1) - 1
94 continue
96 if (num(1) .eq. 2) goto 99
    do 98 i = njs, mjs
        inj = i - njs + 2
        s(1, inj) = co(i) * cond(1)
98 continue
99 num1 = num(1)
    s(1, num1) = s(1, iend + 2)
c
c     ep(1)  is an upper limit on the allowable error at level 1.
c     r(k,1) is the right end-point of the current sub-interval.
c     fe(1)  is the left end-point of the current sub-interval.
c     ind(1)-1 indicates which point of the newton-cotes formula
c     we are dealing with.
c
    ep(1) = epsi / pr2(1 + 1)
    r(1, 1) = s(1, 2)
    ind(1) = 6
c
c     bounding derivatives at left end-point of current interval.
c     bl(i,1) is a bound on the ith derivative of the normal
c     density at level 1 at the left end-point.
c
    fe(1) = s(1, 1)
    t = fe(1) / cond(1)
    bl(1, 1) = phi(t, cond(1))
    bl(2, 1) = bl(1, 1) * abs(t / cond(1))
    bl(3, 1) = bl(1, 1) * f2(t, cond(1))
    bl(4, 1) = bl(1, 1) * f3(t, cond(1))
    bl(5, 1) = bl(1, 1) * f4(t, cond(1))
    if (simps) goto 100
    bl(6, 1) = bl(1, 1) * f5(t, cond(1))
    bl(7, 1) = bl(1, 1) * f6(t, cond(1))
c     bounding derivatives at right end-point of sub-interval.
c     br(i,1) is a bound on the ith derivative of the normal
c     density at level 1 at the right end-point.
c
100 t = r(k, 1) / cond(1)
    br(1, k, 1) = phi(t, cond(1))
    br(2, k, 1) = br(1, k, 1) * abs(t / cond(1))
    br(3, k, 1) = br(1, k, 1) * f2(t, cond(1))
    br(4, k, 1) = br(1, k, 1) * f3(t, cond(1))
    br(5, k, 1) = br(1, k, 1) * f4(t, cond(1))
    if (simps) goto 104
    br(6, k, 1) = br(1, k, 1) * f5(t, cond(1))
    br(7, k, 1) = br(1, k, 1) * f6(t, cond(1))
104 r(k + 1, 1) = (fe(1) + r(k, 1)) * half
    bou5(1) = ep(1) * (r(k, 1) - s(1, 1))

```

```

    del(2, 1) = r(k + 1, 1) - fe(1)
c
c     checking the bound for the trapezoidal rule
c
    del(3, 1) = two * del(2, 1)
    bou1 = max(br(1, k, 1), bl(1, 1)) * binc(3, 1) +
*   two * max(br(2, k, 1), bl(2, 1)) * binc(2, 1) +
*   max(br(3, k, 1), bl(3, 1)) * binc(1, 1)
    bou3 = bou4(1) + bou1 * (del(3, 1) ** 3) * prod(1) / twelve
    itype(1) = 3
    if (bou3 .le. bou5(1)) goto 200
c
c     checking the bound for simpsons rule.
c
    bou1 = zero
    do 110 ij = 1, 5
        jk = 6 - ij
        bou2 = max(br(ij, k, 1), bl(ij, 1))
        bou1 = bou1 + bou2 * binc(jk, 1) * bcs(ij)
110 continue
    bou3 = bou4(1) + bou1 * (del(2, 1) ** 5) * prod(1) / ninety
    itype(1) = 2
    if (bou3 .le. bou5(1)) goto 200
    if (simps) goto 130
c
c     checking the bound for boules rule, if necessary.
c
    del(1, 1) = half * del(2, 1)
    bou1 = zero
    itype(1) = 1
    do 120 ij = 1, 7
        jk = 8 - ij
        bou2 = max(br(ij, k, 1), bl(ij, 1))
        bou1 = bou1 + bou2 * binc(jk, 1) * bcn(ij)
120 continue
    bou3 = bou4(1) + bou1 * (del(1, 1) ** 7) * prod(1) * eight /
*   nine45
    if (bou3 .le. bou5(1)) goto 200
c
c     sub-dividing further at level 1 when the bound is too big.
c
130 k = k + 1
    if (k .gt. 35) return
    goto 100
200 bint(1) = bint(1) + bou3 - bou4(1)
    bou4(1) = bou3
    ksa(1) = k
    if (ind(1) .eq. 6) goto 202
    if (itype(1) - 2) 205, 206, 210
c
c     the next 30 lines condition on the value xs and go to level l+1
c
202 ind(1) = 5
    xs = fe(1)
    fact(1) = bl(1, 1)
203 xss(nm1, 1 + 1) = xss(nm1, 1) + bh(1) * (xs + xm(1))
    do 204 ll = 1, nm2
204 xss(ll, 1 + 1) = xss(ll, 1) + beta(ll, 1) * (xs + xm(1))
    if (l .eq. nm2) goto 300
c
c     xm is the mean of the next variable given those fixed so far.

```

```

c
  xm(l + 1) = xss(l, l + 1)
  prod(l + 1) = prod(l) * fact(l)
  l = l + 1
  goto 90
205 ind(l) = 4
  k = ksa(l)
  xs = half * (fe(l) + r(k + 1, l))
  goto 207
206 ind(l) = 3
  k = ksa(l)
  xs = r(k + 1, l)
207 t = xs / cond(l)
  fact(l) = phi(t, condl(l))
  goto 203
208 ind(l) = 2
  k = ksa(l)
  xs = half * (r(k, l) + r(k + 1, l))
  goto 207
210 ind(l) = 1
  k = ksa(l)
  xs = r(k, l)
  fact(l) = br(l, k, l)
  goto 203

c
c   evaluate conditional bivariate probabilities at deepest level
c
300 x1 = fac * (xss(nm1, nm1) - d(1)) / sd(1)
  x2 = fac * (xss(nm2, nm1) - d(2)) / sd(2)
  l = nm1
  ans(l) = bivnor(x1, x2, rho)
  if (ipr) goto 310
  y1 = (xss(nm1, nm1) - c(1)) / sd(1)
  y2 = (xss(nm2, nm1) - c(2)) / sd(2)
  wu = bivnor(y1, y2, rho)
  wt = bivnor(x1, y2, rho)
  wb = bivnor(y1, x2, rho)
  ans(l) = ans(l) + wu - wt - wb
310 if (l .eq. 1) goto 340
  l = l - 1

c
c   advancing the integration at the current level
c
  indl = ind(l)
  numl = num(l)
  ity = itype(l)
  temp = fact(l) * ans(l + 1)
  temb = bint(l + 1)
  fsa = one
  if (indl .ne. 1) goto 315
  tem = temp
  temp = temp + prep(l)
  temb = temb + preb(l)
  prep(l) = tem
  preb(l) = bint(l + 1)
  fsa = two
315 ans(l) = ans(l) + coef(indl, ity) * temp * del(ity, l)
  bint(l) = bint(l) + coef(indl, ity) * temb * del(ity, l)

c
c   making use of the error which did not accumulate at level l+1
c

```

```
    ep(1) = ep(1) + del(ity, 1) * coef(indl, ity) * (fsa * float(nm2 -
* 1) * epsi / pr2(1 + 1) - temb) / (s(1, num1) - s(1, 1))
    if (indl .eq. 1) goto 320
    igo = indl - (1 + (itype(1) * (itype(1) - 1)) / 2)
    goto (210, 208, 206, 205), igo
c
c      un-subdividing at level 1.
320 k = ksa(1)
    do 322 i = 1, ien
322 bl(i, 1) = br(i, k, 1)
    ind(1) = 5
    fe(1) = r(k, 1)
    if (k .eq. 1) goto 326
    k = k - 1
    goto 104
326 if (intvl(1) .eq. num(1)) goto 310
    intvl(1) = intvl(1) + 1
    intl = intvl(1)
    r(1, 1) = s(1, intl)
    goto 100
c
c      completion of integration and bounding.
c
340 ifault = 0
    prob = ans(1)
    bound = bint(1) + eplos
    return
c
c      special cases --
c      label 350 - n=1
c      label 360 - n=2
c
350 prob=anordf(d(1))-anordf(c(1))
    return
360 rho = sigma(2)
    if (abs(rho) .gt. one) goto 400
    y1 = -d(1) * fac
    y2 = -d(2) * fac
    prob = bivnor(y1, y2, rho)
    if (ipr) return
    x1 = -c(1)
    x2 = -c(2)
    w1 = bivnor(x1, x2, rho)
    wt = bivnor(x1, y2, rho)
    wb = bivnor(y1, x2, rho)
    prob = w1 - wt - wb + prob
    return
c
c      error return for covariance not positive definite.
c
400 ifault = 4
    return
end
c
c
c      function phi(x, y)
c
c      algorithm as 195.1 appl. statist. (1984) vol.33, no.1
c
c      computes univariate normal density
```



```
c      xlow=log(smallest floating point number)
c      sq2p=log(sqrt(two*pi))
c
c      real arg, half, sq2p, x, xlow, y, zero
c
c      real exp
c
c      data xlow /-87.0/, sq2p /0.91893853320467274/, zero /0.0/,
* half /0.5/
c      phi = zero
c      arg = -half * x * x - sq2p - y
c      if (arg .gt. xlow) phi = exp(arg)
c      return
c      end
```

```
c
c
c
c      real function bivnor(x,y,r)
c      data range/25.0/
c
c      xx=max(-range,min(range,x))
c      yy=max(-range,min(range,y))
c      bivnor=1+bnrdf(xx,yy,r)-anordf(xx)-anordf(yy)
c      return
c      end
```

```
c
c
c
c      subroutine invert(a,ai,c,n,det,ier)
c      dimension a(*),ai(*),c(5,1),s(5,5),ipiv(20),aa(5,5)
```

```
c
c      l=0
c      do 3 i=1,n
c          do 3 j=1,i
c              l=l+1
c              aa(i,j)=a(l)
3      aa(j,i)=aa(i,j)
c      call linrg(n,aa,5,s,5)
c      l=0
c      do 4 i=1,n
c          do 4 j=1,i
c              l=l+1
4      ai(l)=s(i,j)
c      do 1 nm=1,(n-2)
c          ii=n+1-nm
c          l1=0
c          do 2 i=ii,n
c              l1=l1+1
c              l2=0
c              do 2 j=ii,n
c                  l2=l2+1
2      s(l1,l2)=aa(i,j)
c      call linrg(nm,s,5,s,5)
c      l=0
c      do 1 i=1,l1
c          do 1 j=1,i
c              l=l+1
1      c(nm,l)=s(i,j)
c      call lftrg(n,aa,5,aa,5,ipiv)
c      call lfdrg(n,aa,5,ipiv,det1,det2)
c      det=det1*10.0**det2
```

```
ier=0  
return  
end
```

```
c  
c  
c
```

```
subroutine matinv(a,nd,n,ifault)  
dimension a(nd,1)
```

```
c
```

```
ifault=0  
call linrg(n,a,nd,a,nd)  
return  
end
```

```

SUBROUTINE LOGCCH(NS, NCA, NCT, NIMAX, NMAX, NMAX1, NVMAX, NVMAX1,
* NV, Z, IVAR, COVI, CNTR, W, WB, WDB, WD2B, U, INS, DB, D2B, DL,
* B, COV, CHI2, ST, IFAULT)

```

```

C
C     ALGORITHM AS 196 APPL. STATIST. (1984) VOL.33, NO.1
C

```

```

C     LOGISTIC ANALYSIS OF CASE-CONTROL STUDIES
C

```

```

c     *** WARNING This file has been input using a scanner and may
c             contain errors.
c

```

```

C
C     INTEGER NCA(NS), NCT(NS), IVAR(NVMAX), INS(NS)
C     REAL Z(NVMAX, NIMAX), COVI(NVMAX1), CNTR(NVMAX, NS), W(NVMAX),
*     WB(NMAX1), WDB(NVMAX, NMAX1), WD2B(NVMAX1, NMAX1), U(NMAX),
*     DB(NVMAX), D2B(NVMAX1), DL(NVMAX), B(NVMAX), COV(NVMAX1)

```

```

C
C     REAL CHI2, EPS, ZERO, ONE, TWO, BMN, CONST, C1, FM, RLIK, RLIKP,
*     RLIKS, ST, T, TTT

```

```

C
C     REAL ABS, ALGFAC, ALOG, FLOAT

```

```

C
C     DATA MAXIT /20/, EPS /0.00001/, ZERO /0.0/, ONE /1.0/, TWO /2.0/

```

```

C
C     INITIAL SETTINGS
C

```

```

C
C     RLIKP = ONE
C     IFAULT = 0
C     ITS = 0
C     IF (NV .GT. NVMAX) GOTO 21
C     IF (NVMAX * (NVMAX + 1) / 2 .GT. NVMAX1) GOTO 21
C     IF (NMAX + 1 .GT. NMAX1) GOTO 21
C     INS(1) = 0
C     IF (NCA(1) + NCT(1) .GT. NMAX .OR. NCA(1) + NCT(1) .GT. NIMAX)
*     GOTO 21
C     IF (NS .EQ. 1) GOTO 2
C     DO 1 I = 2, NS
C     IF (NCA(I) + NCT(I) .GT. NMAX) GOTO 21
C     I1 = I - 1
C     INS(I) = NCA(I1) + NCT(I1) + INS(I1)
1 CONTINUE
C     IF (INS(NS) + NCA(NS) + NCT(NS) .GT. NIMAX) GOTO 21

```

```

C
C     CENTRE THE INDEPENDENT VARIABLES ABOUT THE MEAN OF THE
C     COVARIATES FOR THE CASES (C.F. S.HOWARDS COMMENT TO COX (1972))
C

```

```

2 DO 6 I = 1, NS
C     IF (NCA(I) * NCT(I) .EQ. 0) GOTO 6
C     M = NCA(I)
C     N = M + NCT(I)
C     FM = 1.0 / FLOAT(M)
C     I1 = INS(I)
C     DO 5 K = 1, NV
C     CNTR(K, I) = ZERO
C     K1 = IVAR(K)
C     J1 = I1
C     DO 3 J = 1, M
C     J1 = J1 + 1
C     CNTR(K, I) = CNTR(K, I) + Z(K1, J1)
3 CONTINUE
C     CNTR(K, I) = CNTR(K, I) * FM
C     J1 = I1

```

```

      DO 4 J = 1, N
      J1 = J1 + 1
      Z(K1, J1) = Z(K1, J1) - CNTR(K, I)
4 CONTINUE
5 CONTINUE
6 CONTINUE
7 ITS = ITS + 1
  IF (ITS .GT. MAXIT) GOTO 23
  RLIK = ZERO
  K = 0
  DO 8 J = 1, NV
  DL(J) = ZERO
  DO 8 JJ = 1, J
  K = K + 1
  COVI(K) = ZERO
8 CONTINUE

C
C      LOOP THROUGH STRATA
C
      DO 14 I = 1, NS
      IF (NCA(I) * NCT(I) .EQ. 0) GOTO 14
      M = NCA(I)
      N = M + NCT(I)
      NID = INS(I)

C
C      FIND U(J)=EXP(Z(J)*BETA) FOR EACH INDIVIDUAL J IN THE STRATA.
C      ALSO, FIHD TTT, THE TOTAL OF THE (Z(J)*BETA)S.
C
      TTT = ZERO
      DO 10 J = 1, N
      J1 = J + NID
      T = ZERO
      DO 9 K = 1, NV
      L = IVAR(K)
      T = T + B(K) * Z(L, J1)
9 CONTINUE
      TTT = TTT + T
      U(J) = EXP(T)
10 CONTINUE

C
C      CALC LATE THE CONSTANT CONST=
C      ((N(C)M) * EXP(M*BETA*XBAR))**(1/M)
C      WHERE XBAR IS THE MEAN OF THE COVARIATES OVER THE CASES AND
C      CONTROLS, AHD DIVIDE EACH U(J) BY THIS CONSTANT.
C      THIS KEEPS THE SUMS CALCULATED BY SUBROUTINE HOWARD FROM
C      BECOMING TOO LARGE IN ABSOLUTE VALUE.
C      NOTE - ALGFAC(X)=LN((X)FACTORIAL)
C
      C1 = ALGFAC(N) - (ALGFAC(M) + ALGFAC(N - M)) + TTT * FLOAT(M) /
*      FLOAT(N)
      CONST = EXP(-C1 / FLOAT(M))
      DO 11 J = 1, N
11 U(J) = U(J) * CONST

C
C      CALL TO HOWARD TO CALCULATE SUM(EXP(S(L)*BETA)) OVER ALL
C      COMBINATIONS OF N LABELS TAKEN M AT A TIME, AND ITS FIRST AND
C      SECOND DERIVATIVES WITH RESPECT TO BETA.
C      NOTE - THE VALUE FOR THE SUM AND ITS DERIVATIVES RETURNED BY
C      HOWARD ARE THE TRUE VALUES DIVIDED BY THE CONSTANT CONST**M.
C      THEREFORE RLIK IS CORRECTED FOR THIS CONSTANT SO THAT THE
C      LIKELIHOOD RATIO TEST STATISTIC WILL BE CORRECT.

```

```

C          NOTE - SC=BETA*(SUM(Z(J)) OVER THE CASES) = 0 BY DEFINITION.
C
CALL HOWARD(M, N, U, Z, NID, IVAR, NVMAX, NIMAX, NMAX, NVMAX1, NV,
*  NMAX1, WB, WDB, WD2B, DB, D2B, BMN)
RLIK = RLIK - ALOG(BMN) - C1
L = 0
IR = 1
IS = 0

C
C          CALCULATE THE CUMULATIVE SCORE UP TO THIS STRATUM.
C
DO 13 K = 1, NV
DL(K) = DL(K) - DB(K) / BMN
DO 13 KK = 1, K
L = L + 1
IS = IS + 1
IF (IS .LE. IR) GOTO 12
IR = IR + 1
IS = 1

C
C          CALCULATE THE CUMULATIVE INFORMATION UP TO THIS STRATUM.
C
12 COVI(L) = COVI(L) + D2B(L) / BMN - DB(IR)
13 CONTINUE
14 CONTINUE
IF (ITS .EQ. 1) RLIKS = RLIK

C
C          CALCULATE THE INVERSE OF THE INFORMATION MATRIX
C
CALL SYMINV(COVI, NV, COV, W, NULLTY, IFAULT, NVMAX1)
IF (IFAULT .NE. 0) GOTO 22

C
C          CALCULATE NEW PARAMETER ESTIMATES
C
DO 17 I = 1, NV
W(I) = ZERO
I2 = I * (I - 1) / 2
DO 15 J = 1, I
K = I2 + J
W(I) = W(I) + DL(J) * COV(K)
15 CONTINUE
I1 = I + 1
IF (I1 .GT. NV) GOTO 17
DO 16 K = I1, NV
J = K * (K - 1) / 2 + I
W(I) = W(I) + DL(K) * COV(J)
16 CONTINUE
17 CONTINUE
DO 18 I = 1, NV
18 B(I) = B(I) + W(I)
IF (ITS .NE. 1) GOTO 20

C
C          CALCULATE THE TEST SCORE
C
ST = ZERO
DO 19 I = 1, NV
19 ST = ST + W(I) * DL(I)

C
C          TEST FOR CONVERGENCE
C
20 RLIK = RLIK - RLIKS

```

```
        IF (ABS(RLIKP - RLIK) .LE. EPS) GOTO 24
        RLIKP = RLIK
        GOTO 7
21 IFAULT = 1
        GOTO 25
22 IFAULT = 2
        GOTO 25
23 IFAULT = 3
        GOTO 25
24 CHI2 = TWO * RLIK
C
C        RETURN MATRIX Z TO THE FORM IT WAS IN WHEN LOGCCH WAS CALLED
C
25 DO 27 I = 1, NS
        IF (NCA(I) * NCT(I) .EQ. 0) GOTO 27
        N = NCA(I) + NCT(I)
        I1 = INS(I)
        DO 26 K = 1, NV
            K1 = IVAR(K)
            J1 = I1
            DO 26 J = 1, N
                J1 = J1 + 1
                Z(K1, J1) = Z(K1, J1) + CNTR(K, I)
26 CONTINUE
27 CONTINUE
        RETURN
        END
C
C        SUBROUTINE HOWARD(M, N, U, Z, NID, IVAR, NVMAX, NIMAX, NMAX,
*      NVMAX1, NV, NMAX1, WB, WDB, WD2B, DB, D2B, BMN)
C
C        ALGORITHM AS 122.1 APPL. STATIST. (1984) VOL.33, NO.1
C
C        INTEGER IVAR(NVMAX)
C        REAL U(NMAX), Z(NVMAX, NIMAX), WB(NMAX1), WDB(NVMAX, NMAX1),
*      WD2B(NVMAX1, NMAX1), DB(NVMAX), D2B(NVMAX1)
C
C        REAL BMN, ZERO, ONE
C
C        DATA ZERO /0.0/, ONE /1.0/
C
C        NV1 = NV * (NV + 1) / 2
C
C        INITIALISE THE REQUIRED MATRICES AND VECTORS FOR THE RECURSION
C
        WB(1) = ONE
        I = 0
        DO 1 L = 1, NV
            WDB(L, 1) = ZERO
            DO 1 LL = 1, L
                I = I + 1
                WD2B(I, 1) = ZERO
1 CONTINUE
        M1 = M + 1
        IF (M .EQ. 0) GOTO 9
        DO 3 J = 2, M1
            WB(J) = ZERO
            I = 0
            DO 2 L = 1, NV
                WDB(L, J) = ZERO
            DO 2 LL = 1, L
```

```
      I = I + 1
      WD2B(I, J) = ZERO
2 CONTINUE
3 CONTINUE
      NMMP1 = N - M + 1
      DO 8 IM = 1, NMMP1
      DO 7 J = 1, M
      J1 = J + 1
      I = J + IM - 1
      I1 = I + NID
      IR = 1
      IS = 0
      DO 5 L = 1, NV1
      IS = IS + 1
      IS1 = IVAR(IS)
      IR1 = IVAR(IR)
      IF (IS .LE. IR) GOTO 4
      IR = IR + 1
      IS = 1
      IS1 = IVAR(IS)
      IR1 = IVAR(IR)
C
C      CALCULATE SUM(EXP(S(L)*BETA)) OVER ALL COMBINATIONS OF N
C      LABELS TAKEN M AT A TIME?  AND ITS FIRST AND SECOND DERIVATIVES
C      WITH RESPECT TO BETA.
C      NOTE - THE VALUES RETURNED BT THIS ROUTINE ARE THE TRUE VALUES
C      OF THE SUMS DIVIDED BY TME CONSTANT CONST**M, WHERE CONST
C      IS AS CALCULATED IN 2UBROUTINE LOGCCH.
C
4 WD2B(L, I1) = WD2B(L, J1) + U(I) * WD2B(L, J) + Z(IR1, I1) *
  * Z(IS1, I1) * U(I) * WB(J) + Z(IR1, I1) * U(I) * WDB(IS, J) +
  * Z(IS1, I1) * U(I) * WDB(IR, J)
5 CONTINUE
      DO 6 L = 1, NV
      L1 = IVAR(L)
      WDB(L, J1) = WDB(L, J1) + U(I) * WDB(L, J) + Z(L1, I1) * U(I) *
  * WB(J)
6 CONTINUE
      WB(J1) = WB(J1) + U(I) * WB(J)
7 CONTINUE
8 CONTINUE
9 BMN = WB(M1)
      I = 0
      DO 10 L = 1, NV
      DB(L) = WDB(L, M1)
      DO 10 LL = 1, L
      I = I + 1
      D2B(I) = WD2B(I, M1)
10 CONTINUE
      RETURN
      END

      REAL FUNCTION ALGFAC(I)
C
C      ALGORITHM AS 196.2 APPL. STATIST. (1984) VOL.33, NO.1
C
C      EVALUATES THE NATURAL LOGARITHM OF GAMMA(I+1)=LN(I-FACTOREIAL)
C      (FORTRAN VERSION OF ACM291 - M.C.PIKE AND I.D.HILL,CACM,9,1966)
C
      REAL HALF, CONST, ONE, TWELVE, TREE60, AA, AK, B
C
```

```
REAL ALOG, FLOAT
C
DATA HALF, CONST, ONE, TWELVE, TREE60 /0.5, 0.9189385333, 1.0,
* 12.0, 360.0/

IF (I .GT. 7) GOTO 3
B = ONE
IF (I .LE. 1) GOTO 2
DO 1 K = 2, I
1 B = B * FLOAT(K)
2 ALGFAC = ALOG(B)
RETURN
3 AA = FLOAT(I)
AK = ONE / AA
ALGFAC = (AA + HALF) * ALOG(AA) + AK * (ONE / TWELVE - (AK * AK)
* / TREE60) - AA + CONST
RETURN
END
```



```

SUBROUTINE FLIKAM(P,MP,Q,MQ,W,E,N,SUMSQ,FACT,VW,VL,
*           MRP1,VK,MR,TOLER,IFAU)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)

C
C   ALGORITHM AS 197  APPLIED STATISTICS (1984) VOL.33, NO.1
C
C   COMPUTES THE LIKELIHOOD FUNCTION OF AN AUTOREGRESSIVE-MOVING
C   AVERAGE PROCESS, EXPRESSED AS FACT * SUMSQ.
C
C   3/96 CAC  FROM STATLIB; CONVERTED TO DOUBLE PRECISION, NO TABS,
C   UPPERCASE, MIN --> MIN0, MAX --> MAX0 TO AGREE WITH JOURNAL
C   LISTING.  FIXED 4 BUGS (SEE COMMENTS WITH ORIGINAL BELOW).
C
C   TESTED SUCCESSFULLY ON THE FOLLOWING MODELS AND BENCHMARK RESULTS:
C   MA(1)  BOX-JENKINS(1976) SERIES A  -  ARIMA(0,1,1).
C   MA(2)  OSBORN(1976) USING 28-OBS SECTIONS OF B-J SERIES C
C   ARMA(1,1)  BOX-JENKINS(1976) SERIES A  (MEAN REMOVED FIRST).
C   ARMA(2,1)  DAVID CUSHMAN'S SERIES.  COMPARED WITH TSP PROC CODE
C             THAT IMPLEMENTED NEWBOLD(1974) METHOD.
C   ARMA(3,1), ARMA(4,1), ARMA(5,1)  COMPARED WITH GAUSS RESULTS USING
C             ANSLEY(1979) METHOD, WHICH IS NOT COMPLETELY EXACT ML
C             (IS MISSING THE QUADRATIC FORM IN THE INITIAL RESIDUALS
C             MENTIONED IN JUDGE, ET AL (1980) THEORY AND PRACTICE).
C
C   ORIGINAL CODE FROM STATLIB USED P(MP),Q(MQ) BELOW, BUT THIS
C   FAILS ON COMPUTERS LIKE VAX/VMS WHEN MP OR MQ ARE ZERO.
C   DIMENSION P(1),Q(1),W(N),E(N),VW(MRP1),VL(MRP1),VK(MR)

C
DATA EPSIL1 /1.D-10/
DATA ZERO, P0625, ONE, TWO, FOUR, SIXTEN /
*   0.D0, 0.0625D0, 1.D0, 2.D0, 4.D0, 16.D0/

C
FACT = ZERO
DETMAN = ONE
DETCAR = ZERO
SUMSQ = ZERO
MXPQ = MAX0(MP, MQ)
MXPQP1 = MXPQ + 1
MQP1 = MQ + 1
MPP1 = MP + 1

C
C   CALCULATION OF THE AUTOCOVARANCE FUNCTION OF A PROCESS WITH
C   UNIT INNOVATION VARIANCE (VW) AND THE COVARIANCE BETWEEN THE
C   VARIABLE AND THE LAGGED INNOVATIONS (VL).
C
CALL TWACF(P,MP,Q,MQ,VW,MXPQP1,VL,MXPQP1,VK,MXPQ,IFAU)
IF (MR .NE. MAX0(MP, MQP1)) IFAU = 6
IF (MRP1 .NE. MR + 1) IFAU = 7
IF (IFAU .GT. 0) RETURN

C
C   COMPUTATION OF THE FIRST COLUMN OF MATRIX P (VK)
C
VK(1) = VW(1)
IF (MR .EQ. 1) GO TO 150
DO 140 K = 2, MR
  VK(K) = ZERO
  IF (K .GT. MP) GO TO 120
  DO 110 J = K, MP
    JP2MK = J + 2 - K
C
C   ORIGINAL CODE FROM STATLIB
C   VK(K) = VK(K) + P(J) + VW(JP2MK)

```

```

C          FIXED TO AGREE WITH JOURNAL LISTING AND EQN (10.2)
          VK(K) = VK(K) + P(J) * VW(JP2MK)
110      CONTINUE
120      IF (K .GT. MQP1) GO TO 140
          DO 130 J = K, MQP1
              JP1MK = J + 1 - K
              VK(K) = VK(K) - Q(J-1) * VL(JP1MK)
130      CONTINUE
140      CONTINUE

C
C          COMPUTATION OF THE INITIAL VECTORS L AND K (VL, VK).
C
150      R = VK(1)
          VL(MR) = ZERO
          DO 160 J = 1, MR
              VW(J) = ZERO
              IF (J .NE. MR) VL(J) = VK(J+1)
              IF (J .LE. MP) VL(J) = VL(J) + P(J) * R
              VK(J) = VL(J)
160      CONTINUE

C
C          INITIALIZATION
C
          LAST = MPP1 - MQ
          LOOP = MP
          JFROM = MPP1
          VW(MPP1) = ZERO
          VL(MXPQP1) = ZERO

C
C          EXIT IF NO OBSERVATION, ELSE LOOP ON TIME.
C
          IF (N .LE. 0) GO TO 500
          DO 290 I = 1, N

C
C          TEST FOR SKIPPED UPDATING
C
          IF (I .NE. LAST) GO TO 170
          LOOP = MIN0(MP, MQ)
          JFROM = LOOP + 1

C
C          TEST FOR SWITCHING
C
          IF (MQ .LE. 0) GO TO 300
170      IF (R .LE. EPSIL1) GO TO 400
          IF (DABS(R - ONE) .LT. TOLER .AND. I .GT. MXPQ) GO TO 300

C
C          UPDATING SCALARS
C
          DETMAN = DETMAN * R
190      IF (DABS(DETMAN) .LT. ONE) GO TO 200
          DETMAN = DETMAN * P0625
          DETCAR = DETCAR + FOUR
          GO TO 190
200      IF (DABS(DETMAN) .GE. P0625) GO TO 210
          DETMAN = DETMAN * SIXTEN
          DETCAR = DETCAR - FOUR
          GO TO 200
210      VW1 = VW(1)
          A = W(I) - VW1
          E(I) = A / DSQRT(R)
          AOR = A / R

```

```

SUMSQ = SUMSQ + A * AOR
VL1 = VL(1)
ALF = VL1 / R
R = R - ALF * VL1
IF (LOOP .EQ. 0) GO TO 230
C
C   UPDATING VECTORS
C
DO 220 J = 1, LOOP
  FLJ = VL(J+1) + P(J) * VL1
  VW(J) = VW(J+1) + P(J) * VW1 + AOR * VK(J)
  VL(J) = FLJ - ALF * VK(J)
  VK(J) = VK(J) - ALF * FLJ
220 CONTINUE
230 IF (JFROM .GT. MQ) GO TO 250
DO 240 J = JFROM, MQ
  VW(J) = VW(J+1) + AOR * VK(J)
  VL(J) = VL(J+1) - ALF * VK(J)
  VK(J) = VK(J) - ALF * VL(J+1)
240 CONTINUE
250 IF (JFROM .GT. MP) GO TO 270
DO 260 J = JFROM, MP
260 VW(J) = VW(J+1) + P(J) * W(I)
270 CONTINUE
290 CONTINUE
GO TO 390
C
C   QUICK RECURSIONS
C
300 NEXTI = I
  IFAULT = -NEXTI
DO 310 I = NEXTI, N
310 E(I) = W(I)
  IF (MP .EQ. 0) GO TO 340
DO 330 I = NEXTI, N
  DO 320 J = 1, MP
    IMJ = I - J
    E(I) = E(I) - P(J) + W(IMJ)
320 CONTINUE
330 CONTINUE
340 IF (MQ .EQ. 0) GO TO 370
DO 360 I = NEXTI, N
  DO 350 J = 1, MQ
    IMJ = I - J
    E(I) = E(I) + Q(J) * E(IMJ)
350 CONTINUE
360 CONTINUE
C
C   RETURN SUM OF SQUARES AND DETERMINANT
C
370 DO 380 I = NEXTI, N
380 SUMSQ = SUMSQ + E(I) * E(I)
C
C   CODE FOR CONDITIONAL SUM OF SQUARES.
C   REPLACES ALL EXECUTABLE UP TO AND INCLUDING THAT LABELLED 380.
C
C   FACT = ZERO
C   DETMAN = ONE
C   DETCAR = ZERO
C   SUMSQ = ZERO
C   MXPQ = MAX0(MP, MQ)

```

```

C          DO 380 I = MXPQ, N
C          E(I) = W(I)
C          IF (MP .LE. 0) GO TO 340
C          DO 320 J = 1, MP
C             IMJ = I - J
C             E(I) = E(I) - P(J) * W(IMJ)
C          320      CONTINUE
C          340      IF (MQ .LE. 0) GO TO 380
C          DO 350 J = 1, MQ
C             IMJ = I - J
C             E(I) = E(I) + Q(J) * E(IMJ)
C          350      CONTINUE
C          380      SUMSQ = SUMSQ + E(I) * E(I)
C
C 390 FN = N
C     FACT = DETMAN ** (ONE / FN) * TWO ** (DETCAR / FN)
C     RETURN
C
C     EXECUTION ERRORS
C
C 400 IFAULT = 8
C     RETURN
C 500 IFAULT = 9
C     RETURN
C     END
C-----
C     SUBROUTINE TWACF(P,MP,Q,MQ,ACF,MA,CVLI,MXPQP1,ALPHA,MXPQ,IFAU
C     IMPLICIT DOUBLE PRECISION(A-H,O-Z)
C
C     ALGORITHM AS 197.1 APPLIED STATISTICS (1984) VOL.33, NO. 1
C
C     IMPLEMENTATION OF THE ALGORITHM OF G. TUNNICLIFFE WILSON
C     (J. STATIST. COMPUT. SIMUL. 8, 1979, 301-309) FOR THE COMPUTATION
C     OF THE AUTOCOVARIANCE FUNCTION (ACF) OF AN ARMA PROCESS OF ORDER
C     (MP, MQ) AND UNIT INNOVATION VARIANCE.  THE AUTOREGRESSIVE AND
C     MOVING AVERAGE COEFFICIENTS ARE STORED IN VECTORS P AND Q, USING
C     BOX AND JENKINS NOTATION.  ON OUTPUT, VECTOR CVLI CONTAINS THE
C     COVARIANCES BETWEEN THE VARIABLE AND THE (K-1)-LAGGED INNOVATION
C     FOR K = 1, ..., MQ+1.
C
C     ORIGINAL CODE FROM STATLIB USED P(MP),Q(MQ) BELOW, BUT THIS
C     FAILS ON COMPUTERS LIKE VAX/VMS WHEN MP OR MQ ARE ZERO.
C     DIMENSION P(1), Q(1), ACF(MA), CVLI(MXPQP1), ALPHA(MXPQ)
C
C     DATA EPSIL2 /1.D-10/
C     DATA ZERO, HALF, ONE, TWO /0.D0, 0.5D0, 1.D0, 2.D0/
C
C     IFAULT = 0
C     IF (MP .LT. 0 .OR. MQ .LT. 0) IFAULT = 1
C     IF (MXPQ .NE. MAX0(MP, MQ)) IFAULT = 2
C     IF (MXPQP1 .NE. MXPQ + 1) IFAULT = 3
C     IF (MA .LT. MXPQP1) IFAULT = 4
C     IF (IFAU
C
C     INITIALIZATION, AND RETURN IF MP = MQ = 0
C
C     ACF(1) = ONE
C     CVLI(1) = ONE
C     IF (MA .EQ. 1) RETURN
C     DO 10 I = 2, MA
C 10 ACF(I) = ZERO

```

```

      IF (MXPQP1 .EQ. 1) RETURN
      DO 20 I = 2, MXPQP1
20   CVLI(I) = ZERO
      DO 90 K = 1, MXPQ
90   ALPHA(K) = ZERO
C
C     COMPUTATION OF THE A.C.F. OF THE MOVING AVERAGE PART,
C     STORED IN ACF.
C
      IF (MQ .EQ. 0) GO TO 180
      DO 130 K = 1, MQ
          CVLI(K+1) = -Q(K)
          ACF(K+1) = -Q(K)
          KC = MQ - K
          IF (KC .EQ. 0) GO TO 120
          DO 110 J = 1, KC
              JPK = J + K
              ACF(K+1) = ACF(K+1) + Q(J) * Q(JPK)
110   CONTINUE
120   ACF(1) = ACF(1) + Q(K) * Q(K)
130   CONTINUE
C
C     INITIALIZATION OF CVLI = T.W.-S PHI -- RETURN IF MP = 0.
C
180  IF (MP .EQ. 0) RETURN
      DO 190 K = 1, MP
          ALPHA(K) = P(K)
          CVLI(K) = P(K)
190  CONTINUE
C
C     COMPUTATION OF T.W.-S ALPHA AND DELTA (DELTA STORED IN ACF
C     WHICH IS GRADUALLY OVERWRITTEN).
C
      DO 290 K = 1, MXPQ
          KC = MXPQ - K
          IF (KC .GE. MP) GO TO 240
          DIV = ONE - ALPHA(KC+1) * ALPHA(KC+1)
          IF (DIV .LE. EPSIL2) GO TO 700
          IF (KC .EQ. 0) GO TO 290
          DO 230 J = 1, KC
              KCP1MJ = KC + 1 - J
              ALPHA(J) = (CVLI(J) + ALPHA(KC+1) * CVLI(KCP1MJ)) / DIV
230   CONTINUE
240   IF (KC .GE. MQ) GO TO 260
          J1 = MAX0(KC + 1 - MP, 1)
          DO 250 J = J1, KC
              KCP1MJ = KC + 1 - J
C
C             ORIGINAL CODE FROM STATLIB
C             ACF(J+1) = ACF(J+1) + ACF(K+2) * ALPHA(KCP1MJ)
C             FIXED TO AGREE WITH JOURNAL LISTING
              ACF(J+1) = ACF(J+1) + ACF(KC+2) * ALPHA(KCP1MJ)
250   CONTINUE
260   IF (KC .GE. MP) GO TO 290
          DO 270 J = 1, KC
              CVLI(J) = ALPHA(J)
270   CONTINUE
290   CONTINUE
C
C     COMPUTATION OF T.W.-S NU (NU IS STORED IN CVLI, COPIED INTO
C     ACF).
C
      ACF(1) = HALF * ACF(1)

```

```
DO 330 K = 1, MXPQ
  IF (K .GT. MP) GO TO 330
  KP1 = K + 1
  DIV = ONE - ALPHA(K) * ALPHA(K)
  DO 310 J = 1, KP1
    KP2MJ = K + 2 - J
    CVLI(J) = (ACF(J) + ALPHA(K) * ACF(KP2MJ)) / DIV
310 CONTINUE
  DO 320 J = 1, KP1
320 ACF(J) = CVLI(J)
330 CONTINUE
C
C COMPUTATION OF ACF (ACF IS GRADUALLY OVERWRITTEN).
C
DO 430 I = 1, MA
  MIIM1P = MIN0(I-1, MP)
  IF (MIIM1P .EQ. 0) GO TO 430
  DO 420 J = 1, MIIM1P
    IMJ = I - J
    ACF(I) = ACF(I) + P(J) * ACF(IMJ)
420 CONTINUE
430 CONTINUE
ACF(1) = ACF(1) * TWO
C
C COMPUTATION OF CVLI - RETURN WHEN MQ = 0.
C
CVLI(1) = ONE
IF (MQ .LE. 0) GO TO 600
DO 530 K = 1, MQ
  CVLI(K+1) = -Q(K)
  IF (MP .EQ. 0) GO TO 530
  MIKP = MIN0(K, MP)
  DO 520 J = 1, MIKP
    KP1MJ = K + 1 - J
    CVLI(K+1) = CVLI(K+1) + P(J) * CVLI(KP1MJ)
520 CONTINUE
530 CONTINUE

600 RETURN
C
C EXECUTION ERROR DUE TO (NEAR) NON-STATIONARITY.
C
700 IFAULT = 5
RETURN
END
```

```

SUBROUTINE PROBS(K, W, P, IFAULT)
C
C     ALGORITHM AS 198 APPL. STATIST. (1984) VOL.33,NO.1
C
C     CALCULATION OF THE PROBABILITIES P(L,K) FOR THE CASE OF
C     SIMPLE ORDER.
C
C     Auxiliary functions required: PR1 & F1 from AS 158
C
C     DIMENSION W(20), P(20), Q(20, 20), CH(20, 20)
C     REAL ZERO, HALF
C     DATA C1 /1.0E-6/, ZERO/0.0/, HALF/0.5/
C
C     CHECK THAT K .GE. 3 AND .LE. 20
C
C     IFAULT = 2
C     IF (K .LT. 3 .OR. K .GT. 20) RETURN
C
C     CHECK THAT THE WEIGHTS ARE POSITIVE
C
C     IFAULT = 1
C     DO 1 I = 1, K
C     IF (W(I) .LE. ZERO) RETURN
1 CONTINUE
C
C     CHECK WEIGHTS FOR EQUALITY
C
C     IFAULT = 0
C     WW = W(1)
C     DO 2 I = 2, K
C     IF (ABS(WW - W(I)) .GT. C1) GOTO 7
2 CONTINUE
C
C     EQUAL WEIGHTS
C
C     CALL CHASE(K, Q, .TRUE.)
C     DO 3 J = 1, K
3 P(J) = A(J, K)
RETURN
C
C     UNEQUAL WEIGHTS
C
7 IF (K .GT. 5) GOTO 11
K2 = K - 2
GOTO (8, 9, 10), K2
8 P(1) = PR1(1, 3, W)
P(2) = HALF
P(3) = HALF - P(1)
RETURN
9 P(1) = PR1(1, 4, W)
P(4) = PR1(4, 4, W)
P(2) = HALF - P(4)
P(3) = HALF - P(1)
RETURN
10 P(5) = PR1(5, 5, W)
P(4) = PR1(4, 5, W)
P(2) = HALF - P(4)
P(1) = PR1(1, 5, W)
P(3) = HALF - P(1) - P(5)
RETURN
11 CALL CHASE(K, CH, .FALSE.)

```

```

      CALL CHASE(K, Q, .TRUE.)
      CALL PAPRX(K, W, CH, Q, P)
      RETURN
      END

```

```

C
      SUBROUTINE PAPRX(K, W, CH, P, PA)
C
C      ALGORITHM AS 198.1 APPL. STATIST. (1984) VOL.33, NO.1
C
C      THIS SUBROUTINE COMPUTES THE APPROXIMATE PLK-S.
C
      REAL W(20), CH(20, 20), P(20, 20), PA(20), PB(20), PBP(20),
*     SUMS(2), ZERO, ONE, THREE, PT65, PT35
      INTEGER INDEX(20), A, B
      DATA ZERO/0.0/, ONE/1.0/, THREE/3.0/, PT65/0.65/, PT35/0.35/
C
      ALPHA = ONE / THREE
C
      INITIALISE PA,PB,PBP
C
      DO 10 I = 1, 20
         PA(I) = ZERO
         PB(I) = ZERO
         PBP(I) = ZERO
10     CONTINUE
C
      DETERMINE MASIMUM AND MINIMUM OF WEIGHTS
C
      WMAX = W(1)
      WMIN = W(1)
      DO 20 I = 2, K
         WW = W(I)
         IF (WW .LT. WMIN) WMIN = WW
         IF (WW .LT. WMAX) WMAX = WW
20     CONTINUE
      CUT = PT65 * WMIN + PT35 * WMAX
C
      DETERMINE THE INDICES OF THE WEIGHTS AND THE NUMBER OF
      LARGE WEIGHTS (M)
C
      M = 0
      DO 40 I = 1, K
         IF (W(I) .LT. CUT) GOTO 30
         INDEX(I) = 1
         M = M + 1
         GOTO 40
30     INDEX(I) = 0
40     CONTINUE
C
      IF A=0 AND B=0 SET PB=PLM
C
      N = INDEX(1) + INDEX(K)
      IF (N .NE. 2) GO TO 90
      DO 80 L = 1, M
80     PB(L) = P(L, M)
         GOTO 240
C
      DETERMINE A,B
C
90     A = 1
      B = 1

```



```
      DO 100 I = 1, K
        IF (INDEX(I) .NE. 0) GOTO 110
        A = A + 1
100 CONTINUE
110 DO 120 I = 1, K
      J = K - I + 1
      IF (INDEX(J) .NE. 0) GOTO 130
      B = B + 1
120 CONTINUE
130 IF (N .EQ. 0) GOTO 190
      N = MAX0(A, B)
      DO 180 L = 1, K
        SUM = ZERO
        DO 170 I = 1, L
          J = L - I + 1
          SUM = SUM + P(I, M) * CH(J, N)
170 CONTINUE
        PB(L) = SUM
180 CONTINUE
      GOTO 240
190 DO 210 L = 1, K
      SUM = ZERO
      DO 200 I = 1, L
        J = L - I + 1
        SUM = SUM + CH(I, A) * CH(J, B)
200 CONTINUE
      PBP(L) = SUM
210 CONTINUE
      DO 230 L = 1, K
      SUM = ZERO
      DO 220 I = 1, L
        J = L - I + 1
        SUM = SUM + PBP(I) * P(J, M)
220 CONTINUE
      PB(L) = SUM
230 CONTINUE
C
C      DETERMINE R
C
240 SUMS(1) = ZERO
      SUMS(2) = ZERO
      DO 250 I = 1, K
        J = INDEX(I) + 1
        SUMS(J) = SUMS(J) + W(I)
250 CONTINUE
      X = K - M
      Y = M
      R = SUMS(2) * X / (SUMS(1) * Y)
      RI = ONE / R ** ALPHA
      DO 260 L = 1, K
260 PA(L) = (ONE - RI) * PB(L) + RI * P(L, K)
      RETURN
      END
C
      SUBROUTINE CHASE(K, CH, EQUAL)
C
C      ALGORITHM AS 198.2 APPL. STATIST. (1984) VOL.33, NO.1
C
C      THIS SUBROUTINE COMPUTES CHASE PLK-S IF EQUAL=.FALSE.
C      OR EQUAL WEIGHT PROBABILITIES IF EQUAL=.TRUE.
C
```

```
LOGICAL EQUAL
REAL ZERO, HALF, ONE, CH(20, 20)
DATA ZERO/0.0/, HALF/0.5/, ONE/1.0/
```

C

```
DO 20 J = 1, K
  DO 10 I = 1, K
10  CH(I, J) = ZERO
20  CONTINUE
  CH(1, 1) = ONE
  CH(1, 2) = HALF
  CH(2, 2) = HALF
  KM = K - 1
  DO 60 J = 1, KM
    J1 = J + 1
    IF (EQUAL) GOTO 30
    X = J + J - 1
    Y = J + J
    GOTO 40
30  X = J
    Y = J1
40  Y1 = ONE / Y
    CH(1, J1) = X * Y1 * CH(1, J)
    CH(J1, J1) = Y1 * CH(J, J)
    DO 50 I = 2, J
      CH(I, J1) = Y1 * CH(I - 1, J) + X * Y1 * CH(I, J)
50  CONTINUE
60  CONTINUE
  RETURN
END
```

```
      SUBROUTINE BAB(N, M, SI, T, S, A, MAX, CRIT, BEST, NEVAL, IFAULT)
C
C   ALGORITHM AS 199 APPL. STATIST. (1984) VOL.33, NO.2
C
C   Efficient branch and bound algorithm for determining the optimal
C   feature subset of given size.
C
C   Incorporates a corrected version of the corrections in ASR 67.
C   The second of those corrections caused a jump into a DO loop.
C
      REAL SI(N,N), T(N), S(N,N,N), CRIT, ZERO, D
      INTEGER A(N), MAX(M), BEST(M), NEVAL(N), AI8, AJ8, OMIT
      LOGICAL SKIP
C
      DATA ZERO /0.0/
C
C   Check for invalid values of M and N
C
      IFAULT = 1
      IF (M .LT. 2 .OR. N .LE. M) RETURN
      IFAULT = 0
C
C   Initialize arrays - A holds current M-subset, MAX holds upper
C   limit for possible member features in M-subset.
C   Initial optimal criterion is CRIT = 0
C   SKIP = .FALSE. indicates that current position on solution tree
C   follows consecutively in enumeration sequence rather than a jump
C   from a rejected branch.
C
      DO 4 I = 1, N
        DO 3 J = 1, N
3       S(I,J,N) = SI(I,J)
        NEVAL(I) = 0
4      CONTINUE
      SKIP = .FALSE.
      CRIT = ZERO
      DO 5 I = 1, M
        A(I) = I
        MAX(I) = N - M + I
        BEST(I) = 0
5      CONTINUE
10     K1 = A(M)
        K2 = MAX(M)
        DO 30 I = K1, K2
C
C   Enumerate members of next subset
C
          DO 13 J = I, N
            JJ = M - I + J
            A(JJ) = J
13          CONTINUE
          MM = M + N - I
C
C   If subset of size N, skip to calculation of criterion for
C   subsequent descendent subsets.
C   If consecutive enumeration (SKIP = .FALSE.) next feature omitted
C   is A(M).
C   If following jump in enumeration sequence (SKIP = .TRUE.) next
C   feature omitted is A(M-L).
C
          IF (MM .EQ. N) GO TO 22
```

```

        OMIT = M
        IF (.NOT. SKIP) GO TO 15
        OMIT = M - L
        SKIP = .FALSE.
C
C   Evaluate criterion function for current subset from that of
C   previous subset, excluding feature A(OMIT).
C
15   M9 = MM + 1
        D = ZERO
        DO 17 I8 = 1, MM
            I9 = I8
            AI8 = A(I8)
            IF (I8 .GE. OMIT) I9 = I8 + 1
            DO 16 J8 = 1, MM
                J9 = J8
                AJ8 = A(J8)
                IF (J8 .GE. OMIT) J9 = J8 + 1
                S(I8,J8,MM) = S(I9,J9,M9) - S(OMIT,I9,M9) * S(OMIT,J9,M9) /
*                   S(OMIT,OMIT,M9)
                D = D + T(AI8) * T(AJ8) * S(I8,J8,MM)
16   CONTINUE
17   CONTINUE
        NEVAL(MM) = NEVAL(MM) + 1
C
C   Check criteria of current subset, D, relative to optimal value
C   CRIT.
C
        IF (D .GT. CRIT .AND. MM .EQ. M) GO TO 28
        IF (D .GT. CRIT) GO TO 22
C
C   Optimal value not exceeded, so abandon downward search of branch.
C   Prepare for return to next lower level branching mode not yet
C   explored.  SKIP = .TRUE. indicates jump to lower level before
C   termination of branch.
C
60   M1 = M - 1
        DO 18 L = 1, M1
            ML = M - L
            IF (A(ML) .LT. A(ML+1) - 1) GO TO 19
18   CONTINUE
        L = M
19   DO 20 LL = 1, L
            ML = M - LL + 1
            A(ML) = MAX(ML)
20   CONTINUE
        SKIP = .TRUE.
        GO TO 35
C
C   Optimal value CRIT exceeded by lower level subset.  Reduce by
C   one feature at a time until either criterion falls below CRIT or
C   subset size reaches M.
C
22   MX = MM - M
        DO 27 MO = 1, MX
            D = ZERO
            M8 = MM - MO
            M9 = M8 + 1
            DO 24 I8 = 1, M8
                I9 = I8
                IF (I8 .GT. M) I9 = I8 + 1

```

```

        A(I8) = A(I9)
        DO 23 J8 = 1, M8
            J9 = J8
            IF (J8 .GT. M) J9 = J8 + 1
            S(I8,J8,M8) = S(I9,J9,M9) - S(M+1,I9,M9) * S(M+1,J9,M9) /
*
                S(M+1,M+1,M9)
23     CONTINUE
24     CONTINUE
        DO 26 I8 = 1, M8
            AI8 = A(I8)
            DO 25 J8 = 1, M8
                AJ8 = A(J8)
                D = D + T(AI8) * T(AJ8) * S(I8,J8,M8)
25     CONTINUE
26     CONTINUE
            NEVAL(M8) = NEVAL(M8) + 1
            IF (D .LE. CRIT) GO TO 30
27     CONTINUE
C
C     Update optimal criterion function, CRIT, and corresponding
C     M-subset BEST(.).
C
28     CRIT = D
        DO 29 L1 = 1, M
            BEST(L1) = A(L1)
            IF (I .EQ. K2) GO TO 60
30     CONTINUE
C
C     Update feature subset required for return to lower level branching
C     mode of tree.  Search complete if first member A(1) has taken all
C     its possible feature values.
C
35     DO 50 I = 2, M
        II = M - I + 1
        IF (A(II) .EQ. MAX(II)) GO TO 50
        A(II) = A(II) + 1
        I1 = II + 1
        DO 40 J = I1, M
40     A(J) = A(J-1) + 1
        GO TO 10
50     CONTINUE
C
C     Successful completion of search
C
        RETURN
        END
```

```

SUBROUTINE SUMSQ(N, APPROX, BL, BU, IFAULT)
C
C   ALGORITHM AS 200  APPL. STATIST. (1984) VOL.33, NO.2
C
C   Approximates the sum of squares of normal scores and gives bounds
C   for the truncation error involved in the approximation.
C
C   Coefficients SA(K) are the squares of the Fourier coefficients
C   A(2*K-1).
C
C   REAL APPROX, BL, BU, SA(14), ZERO, ONE, PROD, RI, RK, RN, SUM1,
*     SUM2
C
C   DATA SA/
*   0.95492 96583, 0.03349 20160, 0.00667 47227, 0.00227 80925,
*   0.00101 63627, 0.00053 26443, 0.00031 08437, 0.00019 58978,
*   0.00013 08187, 0.00009 13941, 0.00006 63703, 0.00004 96799,
*   0.00004 11471, 0.00003 49349/
C   DATA ZERO/0.0/, ONE/1.0/, NMAX/27/
C
C   Value of zero is arbitrarily given in case of failure
C
C   APPROX = ZERO
C   BL = ZERO
C   BU = ZERO
C
C   Check consistency of input parameter
C
C   IFAULT = 1
C   IF (N .LE. 1) RETURN
C   IFAULT = 0
C
C   RN = N
C   NM = NMAX - 2
C   IF (N .GT. NMAX) GO TO 1
C   M = N / 2
C   NM = 2 * M - 1
1  SUM1 = ZERO
   SUM2 = ZERO
   KK = 0
   DO 3 K = 1, NM, 2
     RK = K
     PROD = ONE
     DO 2 I = 1, K
       RI = I
       PROD = PROD * (RN - RI) / (RN + RK - RI + ONE)
2  CONTINUE
     KK = KK + 1
     PROD = PROD * RN
     SUM1 = SUM1 + SA(KK) * PROD
     SUM2 = SUM2 + SA(KK)
3  CONTINUE
C
C   Approximate value is computed
C
C   APPROX = SUM1
C   IF (N .LE. NMAX) RETURN
C   PROD = ONE
C   DO 4 I = 1, NMAX
     RI = I
     PROD = PROD * (RN - RI) / (RN + RI)

```

```
4 CONTINUE
  PROD = PROD * RN
C
C Lower & upper bounds for the truncation error are computed
C
  BL = PROD * SA(14)
  BU = PROD * (ONE - SUM2)
C
  RETURN
  END
```

```
      SUBROUTINE COMICS(ALP, NP, P, TOL, PI, CPI, CP, SP, IFAULT)
C
C   ALGORITHM AS 201  APPL. STATIST. (1984) VOL.33, NO.2
C
C   Subroutine to combine predictions about a statistic based on the
C   orderings of a set of means with an F-test to test for differences
C   between the means.
C
      INTEGER NP, IFAULT, I, J
      REAL ALP, P(NP), TOL, PI(NP), CPI(NP), CP(NP), SP(NP), ZERO, ONE,
*      CUM, PIJ, X, XALP, ABS
C
      DATA ZERO /0.0/, ONE /1.0/
C
      Test ALP
C
      IFAULT = 1
      IF (ALP .LE. ZERO .OR. ALP .GE. ONE) RETURN
C
      Compute cumulative distribution of statistic
C
      IFAULT = 2
      CP(1) = P(1)
      IF (P(1) .LE. ZERO) RETURN
      DO 10 I = 2, NP
         IF (P(I) .LE. ZERO) RETURN
         CP(I) = CP(I-1) + P(I)
10  CONTINUE
C
      Check that distribution sums to one
C
      IFAULT = 3
      IF (ABS(CP(NP) - ONE) .GT. TOL) RETURN
      IFAULT = 0
C
      Compute distribution of combined likelihoods (PI) and cumulative
      combined distribution (CPI)
C
      CUM = ZERO
      DO 30 J = 1, NP
         PIJ = ZERO
         DO 20 I = J, NP
20      PIJ = PIJ + P(I) / CP(I)
         PI(J) = P(J) * PIJ
         CUM = CUM + PI(J)
         CPI(J) = CUM
30  CONTINUE
C
      Determine criteria for significance on combined dist X
C
      DO 40 I = 1, NP
         IF (CPI(I) .GT. ALP) GO TO 50
40  CONTINUE
      I = NP
50  XALP = CPI(I) - ALP
      X = -XALP * P(I) / PI(I) + CP(I)
C
      Determine significance level required of F
C
      DO 60 I = 1, NP
         SP(I) = X / CP(I)
```



```
        IF (SP(I) .GT. ONE) SP(I) = ONE  
60 CONTINUE  
C  
    RETURN  
    END
```

```

      SUBROUTINE MODLIK(NN, NNP2, Y, DEL, ALPHA, BETA, DELTA1, DELTA2,
*   NGR, K, INK, NK, NFAIL, H, A, VML, CUMCEN, DAT, IFAULT)
C
C   ALGORITHM AS 202  APPL. STATIST. (1984) VOL.33, NO.2
C
C   MODLIK uses cross-validation to select parameters for the
C   3-parameter nonparametric hazard estimator.
C
      INTEGER NN, NNP2, DEL(NN), NGR, K, INK, NK, NFAIL, CUMCEN(NN),
*   IFAULT, I, IM, ITEST, J, JM, JM1, JP1, KTH, KTH2, LKTH, MAXIT,
*   NJ1, NT
      REAL Y(NN), ALPHA, BETA, DELTA1, DELTA2, H(NN,NN), A(NN,NN), VML,
*   DAT(NNP2), ZERO, EPS2, BIG, ALEPH1, ALEPH2, ALEPH3, BET1, BET2,
*   BET3, DHAA, FMAB, FMAX, SS, TEST
C
      DATA ZERO, EPS2, BIG /0.0, 1.0E-04, 1.0E25/, MAXIT/10/
C
      NT = NN - 1
C
      Check for input faults
C
      NFAIL = 0
      IFAULT = 1
      IF (NN .LE. 0 .OR. ALPHA .LE. ZERO .OR. BETA .LE. ZERO .OR.
*   DELTA1 .LE. ZERO .OR. DELTA2 .LE. ZERO .OR. NGR .LE. 0 .OR.
*   K .LE. 0 .OR. INK .LE. 0 .OR. NK .LE. 0 .OR. NNP2 .NE. NN+2)
*   RETURN
      IFAULT = 2
      DO 25 I = 1, NN
         J = DEL(I)**2
         IF (Y(I) .LT. ZERO .OR. J .NE. DEL(I)) RETURN
         NFAIL = NFAIL + DEL(I)
25  CONTINUE
      DHAA = NFAIL
      IFAULT = 3
      DO 30 I = 1, NT
         IF (Y(I) .GT. Y(I+1)) RETURN
30  CONTINUE
      IFAULT = 4
      LKTH = K + (NK-1)*INK
      ITEST = NFAIL - LKTH - 1
      IF (ITEST .LE. 0) RETURN
      IM = 1
      JM = 2
      DO 55 I = 1, NT
         KTH = 0
35      IF (Y(IM) .LT. Y(JM) .OR. DEL(IM) .LT. DEL(JM)) GO TO 45
         IF (DEL(IM) .GT. DEL(JM)) RETURN
         IF (DEL(JM) .LT. 1) GO TO 45
         KTH = KTH + 1
         IF (K .LE. KTH) RETURN
         IF (JM .GE. NN) GO TO 60
         JM = JM + 1
         GO TO 35
45      IM = JM
         IF (JM .GE. NN) GO TO 60
         JM = JM + 1
55  CONTINUE
C
C   Set up the A matrix
C

```

```

60 SS = DEL(1) / FLOAT(NN-1)
   DO 65 J = 2, NN
       NJ1 = NN - J + 1
       A(1,J) = SS
       A(NN,NJ1) = DEL(NN)
65 CONTINUE
   DO 95 J = 2, NT
       SS = DEL(J) / FLOAT(NN-J)
       JP1 = J + 1
       DO 75 I = JP1, NN
95   A(J,I) = SS
       JM1 = J - 1
       SS = DEL(J) / FLOAT(NN-JM1)
       DO 85 I = 1, JM1
85   A(J,I) = SS
95 CONTINUE
   DO 99 J = 1, NN
99   A(J,J) = ZERO
C
C   Locate the maximizer of the log-likelihood function.
C   For a given value of K, evaluate the log-modified likelihood
C   function over a grid of alpha and beta points, then use the
C   maximizer as the starting point for the N-R algorithm.
C
   FMAB = - BIG
   DO 250 KTH = K, LKTH, INK
       CALL KTHNN(NN, NNP2, DEL, Y, KTH, NFAIL, 1, H, CUMCEN, DAT)
       FMAX = - BIG
       DO 150 IM = 1, NGR
           ALEPH1 = ALPHA + (IM - 1) * DELTA1
           DO 100 JM = 1, NGR
               BET1 = BETA + (JM - 1) * DELTA2
               CALL EVDER(NN, DEL, Y, A, H, 0, ALEPH1, BET1, DHAA, VML,
*                   TEST, IFAULT)
               IF (VML .LT. FMAX .OR. IFAULT .GT. 0) GO TO 100
               FMAX = VML
               ALEPH2 = ALEPH1
               BET2 = BET1
100          CONTINUE
150          CONTINUE
C
C   This loop controls the maximum number (MAXIT) of N-R iterations.
C
   DO 175 IM = 1, MAXIT
       CALL EVDER(NN, DEL, Y, A, H, 1, ALEPH2, BET2, DHAA, VML, TEST,
*           IFAULT)
C
C   The following IF statement tests for non-positive values of alpha
C   and beta.  If the condition is true, user must specify another
C   grid search for this value of K.  Irrespective of the outcome of
C   this test, the program proceeds to a larger (valid) value of K.
C
       IF (IFAUULT .EQ. 5) GO TO 250
C
C   Test if the algorithm has converged.
C
       IF (TEST .LT. EPS2) GO TO 200
175  CONTINUE
C
C   Convergence achieved or maximum number of iterations performed.
C   Compare with previous maximizer vector.  Update vector if nec.

```

```
C
200  IF (VML .LT. FMAB) GO TO 250
      FMAB = VML
      KTH2 = KTH
      ALEPH3 = ALEPH2
      BET3 = BET2
250  CONTINUE
      K = KTH2
      ALPHA = ALEPH3
      BETA = BET3
      VML = FMAB

C
      RETURN
      END

C
C
      SUBROUTINE KTHNN(NN, NNP2, DEL, Y, K, NFAIL, IKTH, H, CUMCEN, DAT)
C
C      ALGORITHM AS 202.1  APPL. STATIST. (1984) VOL.33, NO.2
C
C      KTHNN computes the matrix H of K-th nearest neighbour distances.
C
      INTEGER NN, NNP2, DEL(NN), K, NFAIL, IKTH, CUMCEN(NN), CENTRE,
*      FSD, I, IDUM, J, K1, KP1, LOW, NJ1, NR
      REAL Y(NN), H(NN,NN), DAT(NNP2), ZERO, BIG, DIFF, KNN, KP1NN

C
      DATA ZERO, BIG /0.0, 1.0E25/

C
      CENTRE = 2
      LOW = 2
      DAT(1) = - BIG
      DAT(NFAIL+2) = BIG
      KP1 = K + 1
      NR = NN
      IF (IKTH .LT. 1) NR = 1

C
C      Collapse the observation vector, but record the cumulative number
C      of censored observations between failures.
C
      J = 0
      K1 = 0
      DO 150 I = 1, NFAIL
50    J = J + 1
      IF (DEL(J) .GT. 0) GO TO 100
      K1 = K1 + 1
      GO TO 50
100   DAT(I+1) = Y(J)
      CUMCEN(I) = K1
150  CONTINUE

C
C      This loop moves the point of interest to the right.
C
      DO 750 I = 1, NFAIL

C
C      Move the window to the right.
C
180   IDUM = LOW + K + 1
      DIFF = (DAT(IDUM) - DAT(CENTRE)) - (DAT(CENTRE) - DAT(LOW))
      IF (DIFF .GT. ZERO) GO TO 250
      LOW = LOW + 1
      GO TO 180
```

```

C
C   Determine which edge is the K-th nearest neighbour.
C
250   IDUM = LOW + K
      DIFF = (DAT(IDUM) - DAT(CENTRE)) - (DAT(CENTRE) - DAT(LOW))
      KNN = DAT(IDUM)
      IF (DIFF .LE. ZERO) KNN = DAT(LOW)
      IF (IKTH .GT. 0) GO TO 400
      H(I,1) = ABS(KNN - DAT(CENTRE))
      GO TO 725
400   FSD = LOW + CUMCEN(LOW-1) - 1
C
C   Find the K+1st nearest neighbour.
C
      IDUM = LOW + K + 1
      DIFF = (DAT(IDUM) - DAT(CENTRE)) - (DAT(CENTRE) - DAT(LOW-1))
      KP1NN = DAT(IDUM)
      IF (DIFF .GT. ZERO) KP1NN = DAT(LOW-1)
C
C   Compute the K-th nearest neighbour matrix H.  A typical row
C   consists of three segments - pre-window, window and post-window.
C
      DIFF = ABS(KNN - DAT(CENTRE))
      IF (FSD .LE. 1) GO TO 625
      K1 = FSD - 1
      DO 600 J = 1, K1
600   H(I,J) = DIFF
625   K1 = 1
      DO 650 J = FSD, NN
          IF (DEL(J) .GT. 0) GO TO 635
          H(I,J) = DIFF
          GO TO 650
635   H(I,J) = ABS(KP1NN - DAT(CENTRE))
          K1 = K1 + 1
          IF (K1 .GT. KP1) GO TO 675
650   CONTINUE
675   IF (J .GE. NN) GO TO 725
          K1 = J + 1
          DO 700 J = K1, NN
700   H(I,J) = DIFF
725   IF (CENTRE .LE. NFAIL) CENTRE = CENTRE + 1
750 CONTINUE
C
C   Expand the H matrix.
C
      J = 0
      DO 850 K1 = 1, NFAIL
775   J = J + 1
          NJ1 = NN - J + 1
          IF (DEL(NJ1) .LT. 1) GO TO 775
          IDUM = NFAIL - K1 + 1
          DO 800 I = 1, NR
800   H(NJ1,I) = H(IDUM,I)
850 CONTINUE
          DO 950 I = 1, NN
              IF (DEL(I) .GT. 0) GO TO 950
              DO 900 J = 1, NR
900   H(I,J) = ZERO
950 CONTINUE
          IF (IKTH .LT. 1) GO TO 990
          DO 975 I = 1, NN

```

```
975 H(I,I) = ZERO
990 RETURN
END
```

C  
C

```
SUBROUTINE EVDER(NN, DEL, Y, A, H, IFLAG, ALPHA, BETA, DHAA, VML,
* TEST, IFAULT)
```

C  
C

```
ALGORITHM AS 202.2 APPL. STATIST. (1984) VOL.33, NO.2
```

C  
C  
C  
C  
C

```
EVDER evaluates the log-modified-likelihood function (ML) and its
gradient vector and Hessian matrix. If FLAG = 1, an N-R step is
performed.
```

C  
C

```
INTEGER NN, DEL(NN), IFLAG, IFAULT, I, J, KM
REAL Y(NN), A(NN,NN), H(NN,NN), ALPHA, BETA, DHAA, VML, TEST,
* ZERO, EPS1, ONFI, ONTH, TWTH, FS, ONE, TWO, THREE, FF, FOUR,
* FIVE, TBIG, BIG, A1, B1, CT, D1, D0K, D1K, D2K, DHB, D2HB, DSA,
* G1, G2, SK, SDK, SD2K, T, T1, T2, X1, X3, X5
```

C  
C

```
DATA ZERO /0.0/, EPS1 /1.0E-4/, ONFI /0.2/, ONTH /0.3333333333/,
* TWTH /0.6666666667/, FS /0.9375/, ONE /1.0/, TWO /2.0/, THREE
* /3.0/, FF /3.75/, FOUR /4.0/, FIVE /5.0/, TBIG /350.0/, BIG
* /1.0E25/
```

C  
C

```
IFAULT = 5
D0K = ZERO
D1K = ZERO
D2K = ZERO
DHB = ZERO
D2HB = ZERO
VML = ZERO
```

C  
C  
C

```
Delete each observation, one at a time.
```

```
DO 150 KM = 1, NN
SK = ZERO
SDK = ZERO
SD2K = ZERO
```

C  
C

```
Compute the contribution of the deleted point to ML and its
first two derivatives for fixed values of alpha and beta.
```

C  
C

```
DO 100 I = 1, NN
IF (A(I,KM) .LE. ZERO) GO TO 100
T = BETA * H(I,KM)
T2 = MIN(Y(KM), Y(I) + T)
T1 = MAX(ZERO, Y(I) - T)
IF (T1 .GT. T2) GO TO 100
A1 = (T2 - Y(I)) / T
B1 = (T1 - Y(I)) / T
X1 = A1 - B1
X3 = A1**3 - B1**3
X5 = A1**5 - B1**5
D0K = D0K + (X1 - X3*TWTH + X5*ONFI) * A(I,KM)
IF (IFLAG .LT. 1) GO TO 50
D1K = D1K + (X3*ONTH - X5*ONFI) * A(I,KM)
D2K = D2K + (X5 - X3) * A(I,KM)
50 IF (DEL(KM) .LT. 1) GO TO 100
A1 = (Y(KM) - Y(I)) / T
A1 = A1**2
```

```

        IF (A1 .GT. ONE) GO TO 100
        SK = SK + (ONE - A1)**2 / H(I,KM) * A(I,KM)
        IF (IFLAG .LT. 1) GO TO 100
        SDK = SDK + (ONE - A1) * A1 / H(I,KM) * A(I,KM)
        SD2K = SD2K + (FIVE*A1 - THREE) * A1 / H(I,KM) * A(I,KM)
100    CONTINUE
        IF (DEL(KM) .LT. 1) GO TO 150
C
C    If SK <= 0 restart the N-R algorithm.
C
        IF (SK .LE. ZERO) RETURN
        VML = VML + LOG(SK * FS / ALPHA)
        IF (IFLAG .LT. 1) GO TO 150
        DHB = DHB + SDK / SK
        D2HB = D2HB + SD2K/SK - (SDK/SK)**2 * FOUR
150    CONTINUE
        DSA = D0K * FS * BETA / ALPHA**2
        VML = VML - DSA * ALPHA
        IF (IFLAG .LT. 1) GO TO 300
C
C    Compute the gradient vector (G1, G2), the Hessian matrix
C    (H11=A1, H12=H21=B1, H22=D1), and update alpha and beta.
C
        G1 = -DHAA/ALPHA + DSA
        G2 = -D1K*FF/ALPHA + DHB*FOUR/BETA
        A1 = DHAA/ALPHA**2 - D0K*FS*BETA*TWO/ALPHA**3
        B1 = D1K*FF/ALPHA**2
        D1 = D2HB*FOUR/BETA**2 - D2K*FF/(ALPHA*BETA)
        CT = A1*D1 - B1**2
        ALPHA = ALPHA - (G1*D1 - G2*B1)/CT
        BETA = BETA + (G1*B1 - G2*A1)/CT
        TEST = SQRT(G1**2 + G2**2)
C
C    Test for negative alpha and beta values.
C    If condition is true, the algorithm is diverging.
C    Also test for unbounded increase of beta.
C
        IF (BETA .LT. EPS1 .OR. ALPHA .LT. EPS1) RETURN
        IF (BETA .LT. TBIG) GO TO 300
C
C    If beta is large, compute alpha and VML analytically.
C
        SD2K = ZERO
        VML = ZERO
        DO 250 I = 1, NN
            SDK = ZERO
            DO 200 J = 1, NN
200        IF (A(J,I) .GT. ZERO) SDK = SDK + A(J,I)/H(J,I)
            IF (DEL(I) .GT. 0) VML = VML + LOG(SDK * FS)
            SD2K = SD2K + SDK*Y(I)
250    CONTINUE
        ALPHA = FS * SD2K / DHAA
        BETA = BIG
        VML = -DHAA - DHAA*LOG(ALPHA) + VML
        TEST = ZERO
C
300    IFAULT = 0
        RETURN
        END

```

```
subroutine mixture(a, k, m, c, x, n, alpha, mean, sd, tol, nobvs,  
+   logl, counter, putout, ifault)
```

c

c Translation from Algol 60 by Alan Miller of AS 203.

c

c ALGORITHM AS 203 APPL. STATIST. (1984) VOL.33, NO. 3

c

c This algorithm calculates the maximum likelihood estimates of the  
c parameters of a mixture of normal or exponential or Poisson or  
c binomial distributions. These parameters are the mixing  
c proportions, the means and (in the normal distribution case)  
c standard deviations. It also calculates the log-likelihood  
c function and the number of iterations taken to satisfy the  
c tolerance value.

c

c Users must provide their own routine `putout' which prints the  
c estimated parameter values after each iteration. The form of  
c this routine is:

```
subroutine putout(k, alpha, mean, sd, logl)  
integer k  
real alpha(k), mean(k), sd(k), logl
```

c

c Notes:

c The original (Algol) variable names have been retained. This  
c means that some variable names have more than 6 characters, such  
c as `counter', `newalpha', etc.

c The authors treat the normal distribution as if it were a discrete  
c distribution.

c In Fortran 77 it is necessary to give explicit dimensions to some  
c of the temporary arrays which are not passed as arguments.

c Maximum values have been set for k and m (kmax and mmax) in the  
c parameter statement under `Local variables' below.

c

```
integer a, k, m, c, n(m), nobvs, counter, ifault  
real x(m), alpha(k), mean(k), sd(k), tol, logl  
external putout
```

c

c Local variables

c

```
integer kmax, mmax, i, j  
parameter (kmax = 20, mmax = 100)  
logical test  
real sumalpha, part, oldlogl, newalpha(kmax), newmean(kmax),  
+   newsd(kmax), dt(kmax), nt(kmax), vt(kmax), g(mmax),  
+   f(mmax, kmax), zero, one, half  
data zero /0.0/, one /1.0/, half /0.5/
```

c

```
if (a .lt. 1 .or. a .gt. 4) then  
  ifault = 1  
  return  
else  
  ifault = 0  
end if
```

```
do 10 i = 1, m-1  
  if (x(i) .gt. x(i+1)) then  
    ifault = 5  
    return  
  end if
```

```
10 continue
```



```
    if (nobvs .lt. 2 * m) then
      ifault = 6
      return
    end if

    do 20 i = 1, m
      if (n(i) .lt. 0) then
        ifault = 6
        return
      end if
      if (a .ne. 1) then
        if (x(i) .lt. zero) then
          ifault = 7
          return
        end if
      end if
    20 continue

    oldlogl = zero
    counter = 0

c
c   Start of iterative cycle
c
  30 counter = counter + 1
  do 40 j = 1, k
    if (alpha(j) .gt. one .or. alpha(j) .lt. zero) then
      ifault = 2
      return
    end if
    if (mean(j) .ge. x(m) .or. mean(j) .le. x(1)) then
      ifault = 3
      return
    end if
    if (a .eq. 1) then
      if (sd(j) .le. zero) then
        ifault = 4
        return
      end if
    end if
  40 continue

  do 60 i = 1, k-1
    do 50 j = i+1, k
      if (mean(i) .eq. mean(j)) then
        if (a .eq. 1) then
          if (sd(i) .eq. sd(j)) then
            ifault = 9
            return
          end if
        else
          ifault = 8
          return
        end if
      end if
    50 continue
  60 continue

  logl = zero
  do 80 i = 1, m
    g(i) = zero
    do 70 j = 1, k
```

```

c
c   a = 1 denotes normal mixture
c   a = 2 denotes exponential mixture
c   a = 3 denotes Poisson mixture
c   a = 4 denotes binomial mixture
c
      if (a .eq. 1) then
        f(i,j) = exp(-half*((x(i) - mean(j))/sd(j))**2) / sd(j)
      else if (a .eq. 2) then
        f(i,j) = exp(-x(i)/mean(j)) / mean(j)
      else if (a .eq. 3) then
        if (x(i) .eq. x(1)) then
          f(i,j) = exp(-mean(j)) * mean(j)**x(i)
        else
          f(i,j) = f(i-1,j) * mean(j)
        end if
      else
        if (x(i) .eq. x(1)) then
          f(i,j) = (one - mean(j) / x(m))**x(m) * (mean(j) /
+             (x(m) - mean(j)))**x(i)
        else
          f(i,j) = f(i-1,j) * (mean(j) / (x(m) - mean(j)))
        end if
      end if
      g(i) = g(i) + alpha(j) * f(i,j)
70  continue
      logl = logl + n(i) * log(g(i))
80  continue
c
c   Calculation of the probability densities of the sub-populations
c   which form the mixture, and the log-likelihood function.
c
      test = .false.
      sumalpha = zero
      do 100 j = 1, k
        nt(j) = zero
        dt(j) = zero
        vt(j) = zero
        do 90 i = 1, m
          part = f(i,j) * n(i) / g(i)
          dt(j) = dt(j) + part
          nt(j) = nt(j) + part * x(i)
          if (a .eq. 1) vt(j) = vt(j) + part * (x(i) - mean(j))**2
90  continue
c
c   Calculation of denominators and numerators of new estimates.
c
      newmean(j) = nt(j) / dt(j)
      if (j .ne. k) then
        newalpha(j) = alpha(j) * dt(j) / nobvs
        sumalpha = sumalpha + newalpha(j)
      else
        newalpha(k) = one - sumalpha
      end if
      if (a .eq. 1) newsd(j) = sqrt(vt(j) / dt(j))
c
c   Convergence test.
c
      if (abs(oldlogl - logl) .gt. tol) test = .true.
      oldlogl = logl
      alpha(j) = newalpha(j)

```

```
        mean(j) = newmean(j)
        if (a .eq. 1) sd(j) = newsd(j)
100 continue
c
  if (c .gt. 0) then
    if ((counter/c)*c .eq. counter) then
      call putout(k, alpha, mean, sd, logl)
    end if
  end if

  if (test) go to 30
return
end
```

This version of AS204 is in Pascal. It does not use AS 66 for the calculation of normal probabilities, but one of Hastings' algorithms.

(\* Program description: Journal of the Royal Statistical Society (Series C) Vol 33 No 3 1984, R.W. Farebrother, Algorithm AS204, pp 332 - 339

Use of Rubin's (1962) method to evaluate the expression  $\Pr\{d k(i) K\}(m(i),k(i)) < c\}$  where  $k(i)$  and  $c$  are positive constants, and where  $K\}(m(i),k(i))$  represents an independent chi-squared random variable with  $m(j)$  degrees of freedom and non-centrality parameter  $k(i)$ .

n = number of chi-squared terms  
c = Critical chi-squared value  
maxit = maximum number of iterations = 500 in Vol 33 No. 3 1984  
eps = degree of accuracy

This includes an auxiliary algorithm, Function 26.2.17 from 'Handbook of Mathematical Functions', (1968), p 932, to obtain probabilities for the standard normal distribution.

The program returns the cumulative probability value at the point  $c$  in the distribution.

```
*)
CONST
  n = 3;          (* number of terms in equation *)
  maxit = 500;   (* maximum number of iterations in eq. 3 of algorithm *)
  eps = 0.0001;  (* desired level of accuracy *)
  mode = 0.90625; (* as in AS 204A *)
```

```
VAR
  RUBEN, tol, beta, ao, aoinv : Real;
  c, dnsty, z, rz             : Real;
  eps2, hold, hold2, sum, sum1 : Real;
  dans, lans, pans ,prbty, temp : Real;
  ifault, itemp, i, j, k, m   : Integer;
  lambda, delta               : Array[1..n] of Real;
  mult                         : Array[1..n] of Integer;
  gamma, theta                : Array[1..n] of Real;
  a, b                         : Array[1..maxit] of Real;
  exit, L                      : Boolean;
```

```
Procedure centnorm(VAR x,prob: Real);
```

```
const
  p = 0.2316419;
  b1 = 0.319381530;
  b2 = -0.356563782;
  b3 = 1.781477937;
  b4 = -1.821255978;
  b5 = 1.330274429;
```

```
var
  constant, Z, t, Q : real;
  (*
    x      standardised value
    Z      N(0,1) function value at x
    Q      P(X > abs(x)) where X is N(0,1)
    prob   P(-x < z < x) *)
```

```
Begin
```

```
constant := 1/sqrt(2*pi);
If abs(x) < 4.5 then
Begin
  if x < 0 then
    x := -x;
  Z := exp(-x*x/2)*constant;
  t := 1/(1+p*x);
  Q := (((b5*t+b4)*t+b3)*t+b2)*t+b1)*t*Z;
end
else
  Q := 0;
prob := 1 - 2 * Q;
End; (* centnorm *)
```

BEGIN

```
(* RUBEN evaluates the probability that a positive definite quadratic
form in Normal variates is less than a given value *)
```

```
c := 1.0;
For i := 1 to n do
  delta[i] := 0.0;
lambda[1] := 6;
lambda[2] := 3;
lambda[3] := 1;
For i := 1 to n do
  mult[i] := 1;

exit := false;
L := false;
If (n < 1) OR (c <= 0.0) OR (maxit < 1) OR (eps <= 0.0) then
Begin
  RUBEN := -2.0;
  ifault := 2;
End
Else
Begin
  tol := -200.0;
  (* preliminaries *)
  beta := lambda[1];
  sum := lambda[1];
  For i := 1 to n do
  Begin
    hold := lambda[i];
    If (hold <= 0.0) OR (mult[i] < 1) OR (delta[i] < 0.0) then
    Begin
      RUBEN := -7.0;
      ifault := -i;
      exit := true;
      i := n;
    End;
    If beta > hold then beta := hold;
    If sum < hold then sum := hold;
  End;
  End;
  If exit = false then
  Begin
    If mode > 0.0 then
    Begin
      temp := mode * beta;
      beta := temp;
    End
  Else
```

```
Begin
  temp := 2.0/(1.0/beta + 1.0/sum);
  beta := temp;
End;
k := 0;
sum := 1.0;
sum1 := 0.0;
for i := 1 to n do
Begin
  hold := beta/lambda[i];
  gamma[i] := 1.0 - hold;
  temp := 1;
  for j := 1 to mult[i] do
    temp := temp * hold;
  sum := sum * temp;
  sum1 := sum1 + delta[i];
  k := k + mult[i];
  theta[i] := 1.0;
End;
Writeln;
ao := EXP(0.5 * (LN(sum) - sum1));
If ao <= 0.0 then
Begin
  RUBEN := 0.0;
  dnsty := 0.0;
  ifault := 1;
End
Else
Begin
  z := c/beta;
  (* evaluate probability and density of chi-squared on
    k degrees of freedom. The constant 0.22579135264473
    is ln(sqrt(pi/2)) *)
  itemp := (k DIV 2) * 2;
  If k = itemp then
  Begin
    i := 2;
    lans := -0.5 * z;
    dans := EXP(lans);
    pans := 1.0 - dans;
  end
  Else
  Begin
    i := 1;
    lans := -0.5 * (z + LN(z)) - 0.22579135264473;
    dans := EXP(lans);
    rz := SQRT(z);
    centnorm(rz,pans);
    (* centnorm(x) will be a procedure or function to
      evaluate the probability that a standard normal
      variable lies in the interval [-x,x]
      Algorithm AS66 recommended *)
  End;
  k := k - 2;
  While i <= k do
  Begin
    If lans < tol then
    Begin
      lans := lans + LN(z/i);
      dans := EXP(lans);
    End
  End;
End;
```

```

Else
Begin
    temp := dans;
    dans := temp * z/i;
End;
temp := pans;
pans := temp - dans;
i := i + 2;
End;
{ evaluate successive terms of expansion }
prbty := pans;
dnsty := dans;
eps2 := eps/ao;
aoinv := 1.0/ao;
sum := aoinv - 1.0;
For m := 1 to maxit do
Begin
    sum1 := 0.0;
    For i := 1 to n do
    Begin
        hold := theta[i];
        theta[i] := hold * gamma[i];
        hold2 := theta[i];
        temp := hold2 * mult[i] + m * delta[i] * (hold -
hold2);

        sum1 := sum1 + temp;
    End;
    b[m] := 0.5 * sum1;
    sum1 := b[m];
    itemp := m - 1;
    (* itemp = 0 when m = 1 !!! *)
    If itemp > 0 then
    For i := itemp downto 1 do
        sum1 := sum1 + b[i] * a[m-i];
    a[m] := sum1/m;
    sum1 := a[m];
    k := k + 2;
    If lans < tol then
    Begin
        lans := lans + LN(z/k);
        dans := EXP(lans);
    End
    Else
    Begin
        temp := dans;
        dans := temp * z/k;
    End;
    pans := pans - dans;
    sum := sum - sum1;
    temp := dnsty;
    dnsty := temp + dans * sum1;
    temp := sum1;
    sum1 := pans * temp;
    temp := prbty;
    prbty := temp + sum1;
    If prbty < -aoinv then
    Begin
        RUBEN := -3.0;
        ifault := 3;
        exit := true;
        m := maxit;

```

```
End;
If exit = false then
Begin
  temp := ABS(pans* sum);
  If temp < eps2 then
  Begin
    temp := ABS(sum1);
    If temp < eps2 then
    Begin
      ifault := 0;
      L := true;
      m := maxit;
    End;
  end;
end;
End; { m }
If L = false then ifault := 4;
If exit = false then
Begin
  temp := dnsty;
  dnsty := ao * temp/(beta + beta);
  temp := prbty;
  prbty := ao * temp;
  If (prbty < 0.0) OR (prbty > 1.0) then
    ifault := ifault + 5
  Else
    If dnsty < 0.0 then ifault := ifault + 6;
  RUBEN := prbty;
end;
end;
End;
End;
Writeln('probability = ',RUBEN:10:6);
Writeln('fault code = ',ifault:3);
END.
```



```

SUBROUTINE ENUM(R,C,N,M,IFAU)
C
C
C   ALGORITHM AS 205 APPL. STATIST. (1984) VOL 33, NO. 3.
C   ENUMERATES ALL R*C CONTINGENCY TABLES WITH GIVEN ROW TOTALS N(I)
C   AND COLUMN TOTALS M(J) AND CALCULATES THE HYPERGEOMETRIC
C   PROBABILITY OF EACH TABLE.
C
C   FOR TABLES HAVING TWO OR MORE ROW SUMS REPEATED, EQUIVALENT
C   TABLES DIFFERING ONLY BY A ROW PERMUTATION ARE NOT SEPARATELY
C   ENUMERATED. A REPRESENTATIVE OF EACH EQUIVALENCE CLASS IS ENUMERATED
C   AND THE MULTIPLICITY OF EACH CLASS CALCULATED.
C
C   FOR EACH TABLE ENUMERATED, SUBROUTINE EVAL IS CALLED TO CARRY OUT
C   CALCULATIONS ON THE TABLE.
C
INTEGER R,C,N(10),M(10),IFAU
INTEGER TABLE(10,10),BOUND(10,10),Z(10)
INTEGER REPS(10),MULT(10),REPSR,REpsc,MULTR,MULTC,ONE
INTEGER NTOTAL,NTOT,MAX,NMAX,RM,CM,LEFT,ROWBND,ROWSUM
INTEGER I,J,II,JJ,IIP,IIM,JP,KEEP
REAL PROB(10,10),FLOGM(201),FACTLM(201),ZERO
REAL PROB0
LOGICAL REPT(10),REPTC(10),IEQIM
C
C   LOCAL VARIABLES -
C   TABLE(I,J)   - (I,J)-TH ENTRY OF CURRENT TABLE
C   NTOTAL        - TOTAL OF TABLE ENTRIES
C   BOUND(I,J)    - CURRENT UPPER BOUND ON TABLE(I,J) TO SATISFY
C                   ROW AND COLUMN TOTALS
C   REPT(I)       - LOGICAL = TRUE IF ROW TOTALS N(I), N(I-1) ARE EQUAL
C                   = FALSE OTHERWISE
C   REPS(I)       - NUMBER OF PREVIOUS ROWS EQUAL TO ROW I
C   MULT(I)       - MAXIMUM NUMBER OF EQUIVALENT TABLES
C                   GIVEN FIRST I ROWS
C   Z(J)          - LOWER BOUND ON SUM OF ENTRIES USED BY ALGORITHM C
C   PROB(I,J)     - PARTIAL SUM OF TERMS IN LOG(P)
C
C
DATA MAX/10/ , NMAX/201/ , ZERO/0.0E0/ , ONE/1/
C
C   MAX - MAXIMUM DIMENSION OF TABLE
C   NMAX - MAXIMUM NUMBER OF OBSERVATIONS + 1
C
C   CHECK INPUT VALUES
C
IFAU=1
IF(R.GT.MAX .OR. C.GT.MAX .OR. R.LE.0 .OR. C.LE.0) RETURN
C
IFAU=3
NTOTAL=0
DO 10 I=1,R
  IF(N(I) .LE. 0) RETURN
  NTOTAL=NTOTAL+N(I)
10 CONTINUE
NTOT=0
DO 20 J=1,C
  IF (M(J) .LE. 0) RETURN
  NTOT=NTOT+M(J)
20 CONTINUE

```

```
      IFAULT=2
      IF (NTOT.NE.NTOTAL) RETURN
C
      IFAULT=4
      IF (NTOTAL.GE.NMAX) RETURN
C
      IFAULT=0
C
      INITIALISE FLOGM(K)=LOG(K-1), FACTLM(K)=LOG(K-1 FACTORIAL)
C
      FLOGM(1)=ZERO
      FACTLM(1)=ZERO
      DO 50 K=1,NTOTAL
        FLOGM(K+1)=ALOG(FLOAT(K))
        FACTLM(K+1)=FACTLM(K)+FLOGM(K+1)
50    CONTINUE
C
      CONSTANTS
C
      RM=R-1
      CM=C-1
C
      SORT ROWS AND COLUMNS INTO ASCENDING ORDER
C
      DO 60 I=1,RM
        IP=I+1
        DO 60 II=IP,R
          IF (N(I).LE.N(II)) GOTO 60
          KEEP=N(I)
          N(I)=N(II)
          N(II)=KEEP
60    CONTINUE
C
      DO 70 J=1,CM
        JP=J+1
        DO 70 JJ=JP,C
          IF(M(J).LE.M(JJ))GOTO 70
          KEEP=M(J)
          M(J)=M(JJ)
          M(JJ)=KEEP
70    CONTINUE
C
      CALCULATE MULTIPLICITIES OF ROWS AND COLUMNS
C
      REPTC(J) = .TRUE. IF COLUMNS J AND J-1 HAVE THE SAME TOTAL
      REPT(I)  = .TRUE. IF ROWS I AND I-1 HAVE THE SAME TOTAL
C
      MULTC=ONE
      REPSC=ONE
      REPTC(1)=.FALSE.
      DO 80 J=2,C
        REPTC(J) = (M(J).EQ.M(J-1))
        IF(REPTC(J)) GOTO 79
        REPSC=ONE
        GOTO 80
79      REPSC=REPSC+ONE
        MULTC=MULTC*REPSC
80    CONTINUE
C
      MULTR=ONE
      REPSR=ONE
```

```
      REPT(1)=.FALSE.
      DO 85 I=2,R
        REPT(I)=(N(I).EQ.N(I-1))
        IF(REPT(I))GOTO 84
        REPSR=ONE
        GOTO 85
84      REPSR=REPSR+ONE
        MULTR=MULTR*REPSR
85      CONTINUE
C
C      IF COLUMN MULTIPLICITY EXCEEDS ROW MULTIPLICITY TRANSPOSE TABLE
C
      IF (MULTR.GE.MULTC) GOTO 100
      MAXRC=MAX0(R,C)
      DO 90 IJ=1,MAXRC
        KEEP=N(IJ)
        N(IJ)=M(IJ)
        M(IJ)=KEEP
90      CONTINUE
      KEEP=R
      R=C
      C=KEEP
      RM=R-1
      CM=C-1
      DO 95 I=1,R
65      REPT(I)=REPTC(I)
      MULTR=MULTC
C
C      SET UP INITIAL TABLE
C
C      MAXIMUM MULTIPLICITY
C
100     MULT(1)=MULTR
      REPS(1)=ONE
C
C      CONSTANT TERM IN PROBABILITY
C
      PROB0=-FACTLM(NTOTAL+1)
      DO 105 I=1,R
        II=N(I)
        PROB0=PROB0+FACTLM(II+1)
105     CONTINUE
      DO 106 J=1,C
        JJ=M(J)
        PROB0=PROB0+FACTLM(JJ+1)
106     CONTINUE
C
C      CALCULATE BOUNDS ON ROW 1
C
      DO 110 J=1,C
110     BOUND(1,J) = M(J)
C
C      FOR EACH I FIND GREATEST I-TH ROW SATISFYING BOUNDS
C
      DO 150 I=1,R
        IF (I.NE.1) PROB0=PROB(I-1,C)
        LEFT=N(I)
C
C      ELEMENTS OF ROW I
C
      IEQIM = REPT(I)
```

```
DO 120 J=1,CM
IJ=MIN0(LEFT,BOUND(I,J))
TABLE(I,J) = IJ
IF (J.EQ.1) PROB(I,J) = PROB0 - FACTLM(IJ+1)
IF (J.NE.1) PROB(I,J) = PROB(I,J-1) - FACTLM(IJ+1)
LEFT=LEFT - TABLE(I,J)
IF (I.LT.R) BOUND(I+1,J) = BOUND(I,J) - TABLE(I,J)
IF (LEFT.EQ.0) GOTO 121
IF (IEQIM) IEQIM=TABLE(I,J).EQ.TABLE(I-1,J)
120 CONTINUE
TABLE(I,C)=LEFT
PROB(I,C)=PROB(I,CM)-FACTLM(LEFT+1)
IF (I.LT.R) BOUND(I+1,C)=BOUND(I,C)-LEFT
GOTO 123
121 JP=J+1
DO 122 JJ=JP,C
TABLE(I,JJ)=0
PROB(I,JJ)=PROB(I,JJ-1)
BOUND(I+1,JJ)=BOUND(I,JJ)
122 CONTINUE
123 IF(I.EQ.1) GOTO 150
MULT(I)=MULT(I-1)
REPS(I)=ONE
IF (.NOT.IEQIM) GOTO 150
REPS(I)=REPS(I-1)+ONE
MULT(I)=MULT(I)/REPS(I)
C
150 CONTINUE
C
C
C CALL EVAL FOR TABLE 1
C
CALL EVAL(TABLE,R,C,N,M,PROB(R,C),MULT(R))
C
C COMMENCE ENUMERATION OF REMAINING TABLES
C START OF MAIN LOOP
C
200 I=R
210 I=I-1
C
C IF I = 0 NO MORE TABLES ARE POSSIBLE
C
IF (I.EQ.0) RETURN
C
C J=CM
LEFT=TABLE(I,C)
ROWBND=BOUND(I,C)
C
C TRY TO DECREASE ELEMENT (I,J)
C
220 IF (TABLE(I,J).GT.0 .AND. LEFT.LT.ROWBND) GOTO 230
C
C ELEMENT (I,J) CANNOT BE DECREASED - TRY (I,J-1)
C
IF(J.EQ.1) GOTO 210
LEFT=LEFT+TABLE(I,J)
ROWBND=ROWBND+BOUND(I,J)
J=J-1
GOTO 220
C
C DECREASE ELEMENT (I,J)
```

```
C
230     IJ=TABLE(I,J)
      PROB(I,J)=PROB(I,J)+FLOGM(IJ+1)
      TABLE(I,J)=TABLE(I,J)-1
      BOUND(I+1,J)=BOUND(I+1,J)+1

C
C     IF ROW I WAS THE SAME AS ROW I-1 IT IS NO LONGER
C
      IF (REPS(I).EQ.ONE) GOTO 270
      REPS(I)=ONE
      MULT(I)=MULT(I-1)

C
C     COMPLETE ROW I WITH THE LARGEST POSSIBLE VALUES
C
270    II=I
      IIP=II+1
      IIM=II-1
      JNEXT=J+1
      LEFT=LEFT+1
      GOTO 380

C
C     FILL UP REMAINING ROWS
C
300    II=II+1
C
C     THE LAST ROW IS TREATED SEPARATELY
C
      IF (II.EQ.R) GOTO 400
      IIP=II+1
      IIM=II-1
      IF (REPT(II)) GOTO 310

C
C     ROW TOTAL N(II) IS NOT A REPEAT - MAKE ROW II AS LARGE AS POSSIBLE
C
      LEFT=N(II)
      JNEXT=1
      GOTO 380

C
C     REPEATED ROW TOTALS
C
C     (I) IF ROW II-1 SATISFIES THE BOUNDS ON ROW II REPEAT IT
C
310    DO 320 J=1,C
      IF (TABLE(IIM,J).GT.BOUND(II,J)) GOTO 330
      IJ=TABLE(IIM,J)
      TABLE(II,J)=IJ
      BOUND(IIP,J)=BOUND(II,J)-TABLE(II,J)
      IF (J.EQ.1) PROB(II,J) = PROB(IIM,C) - FACTLM(IJ+1)
      IF (J.NE.1) PROB(II,J) = PROB(II,J-1) - FACTLM(IJ+1)
320    CONTINUE

C
C     ROW II IS A REPEAT OF ROW II-1
C
      REPS(II)=REPS(IIM)+ONE
      MULT(II)=MULT(IIM)/REPS(II)
      GOTO 300

C
C     ELEMENT J OF ROW II-1 WAS TOO BIG
C
C     CONSTRUCT THE SEQUENCE Z(J) OF LOWER BOUNDS
C
```

```
330 IF (J.GT.1) GOTO 331
C
C     IF J=1 THE BOUNDS ARE SATISFIED AUTOMATICALLY
C
      IJ=BOUND(II,1)
      TABLE(II,1)=IJ
      PROB(II,1)=PROB(IIM,C)-FACTLM(IJ+1)
      JNEXT=2
      LEFT=N(II)-TABLE(II,1)
      BOUND(IIP,1)=0
      GOTO 380
331 Z(J)=N(II)
      JM=J-1
      IF (J.EQ.C) GOTO 336
      JP=J+1
      DO 335 JJ=JP,C
335 Z(J)=Z(J)-BOUND(II,JJ)
336 DO 340 JJM=1,JM
      JJ=J-JJM
      Z(JJ)=Z(JJ+1)-BOUND(II,JJ+1)
340 CONTINUE
C
C     (II) IF THE CUMULATIVE TOTALS OF ROW II-1 ALL EXCEED THE BOUNDS Z(J)
C           MAKE ELEMENT (II,J) EQUAL TO ITS BOUND
C
      ROWSUM=0
      JKEEP=0
      DO 350 JJ=1,JM
        ROWSUM=ROWSUM+TABLE(IIM,JJ)
        IF ( ROWSUM.LT.Z(JJ) ) GOTO 360
        IF ( ROWSUM.GT.Z(JJ) .AND. TABLE(IIM,JJ).GT.0 ) JKEEP=JJ
350 CONTINUE
      TABLE(II,J)=BOUND(II,J)
      BOUND(IIP,J)=0
      IJ=TABLE(II,J)
      PROB(II,J) = PROB(II,JM) - FACTLM(IJ+1)
      REPS(II)=ONE
      MULT(II)=MULT(IIM)
C
C     COMPLETE ROW II WITH THE LARGEST POSSIBLE ELEMENTS
C
      JNEXT=JP
      LEFT=N(II)
      DO 355 JJ=1,J
355 LEFT=LEFT-TABLE(II,JJ)
      GOTO 380
C
C     (III) THE CUMULATIVE SUMS VIOLATE THE BOUNDS
C           IF NO ELEMENT OF ROW II-1 CAN BE CHANGED TO SATISFY THE BOUNDS
C           NO SUITABLE ROW II IS POSSIBLE
C           IN THAT CASE GO BACK AND TRY DECREASING ROW II-1
C
360 IF (JKEEP.NE.0) GOTO 370
      I=II
      GOTO 210
C
C     ELEMENT (II,JKEEP) CAN BE DECREASED
C
370 BOUND(IIP,JKEEP)=BOUND(IIP,JKEEP) + 1
      IJ=TABLE(II,JKEEP)
      PROB(II,JKEEP)=PROB(II,JKEEP)+FLOGM(IJ+1)
```

```

TABLE(II,JKEEP)=TABLE(II,JKEEP) - 1
C
C   COMPLETE THE ROW
C
JNEXT=JKEEP+1
LEFT=N(II)
DO 375 JJ=1,JKEEP
375 LEFT=LEFT-TABLE(II,JJ)
C
C   ROW II IS COMPLETE UP TO ELEMENT JNEXT-1
C   MAKE THE REMAINING ELEMENTS AS LARGE AS POSSIBLE
C   (THIS SECTION OF CODE IS USED FOR EVERY ROW, REPEATED OR NOT)
C
380 IF (JNEXT.EQ.C) GOTO 390
C
DO 385 J=JNEXT,CM
TABLE(II,J)=MIN0(LEFT,BOUND(II,J))
LEFT=LEFT-TABLE(II,J)
BOUND(IIP,J)=BOUND(II,J)-TABLE(II,J)
IJ=TABLE(II,J)
IF (J.EQ.1) PROB(II,J) = PROB(IIM,C) - FACTLM(IJ+1)
IF (J.NE.1) PROB(II,J)=PROB(II,J-1)-FACTLM(IJ+1)
IF (LEFT.EQ.0) GOTO 391
385 CONTINUE
390 TABLE(II,C)=LEFT
PROB(II,C)=PROB(II,CM)-FACTLM(LEFT+1)
BOUND(IIP,C)=BOUND(II,C)-LEFT
GOTO 393
391 JP=J+1
DO 392 JJ=JP,C
TABLE(II,JJ)=0
PROB(II,JJ) = PROB(II,JJ-1)
BOUND(IIP,JJ)=BOUND(II,JJ)
392 CONTINUE
393 REPS(II)=ONE
IF (II.GT.1) MULT(II)=MULT(IIM)
GOTO 300
C
C   THE FINAL ROW
C
400 IF (REPT(R)) GOTO 420
C
C   NOT A REPEAT - SET ROW R EQUAL TO ITS BOUNDS
C
IJ=BOUND(R,1)
TABLE(R,1) = IJ
PROB(R,1) = PROB(RM,C) - FACTLM(IJ+1)
DO 410 J=2,C
IJ=BOUND(R,J)
TABLE(R,J)=IJ
PROB(R,J) = PROB(R,J-1) - FACTLM(IJ+1)
410 CONTINUE
MULT(R)=MULT(RM)
GOTO 500
C
C   ROW TOTAL R IS A REPEAT - ENSURE THAT IT IS LESS THAN ROW R-1
C
420 DO 430 J=1,C
IF (BOUND(R,J).GT.TABLE(RM,J)) GOTO 440
IJ=BOUND(R,J)
TABLE(R,J)=IJ

```

```
      IF (J.EQ.1) PROB(R,J) = PROB(RM,C) - FACTLM(IJ+1)
      IF (J.NE.1) PROB(R,J) = PROB(R,J-1) - FACTLM(IJ+1)
      IF (TABLE(R,J).NE.TABLE(RM,J)) GOTO 450
430  CONTINUE
      C
      C      ROW R IS A REPEAT OF ROW R-1
      C
      REPS(R)=REPS(RM)+ONE
      MULT(R)=MULT(RM)/REPS(R)
      GOTO 500
      C
      C      IF ROW R WOULD BE BIGGER THAN ROW R-1 GO BACK AND TRY
      C      DECREASING ROW R-2
      C
440  I=RM
      GOTO 210
      C
      C      ROW R IS ALREADY LESS THEN ROW R-1 SO NO MORE CHECKS ARE NEEDED
      C
450  JP=J+1
      DO 460 JJ=JP,C
          IJ=BOUND(R,JJ)
          TABLE(R,JJ)=IJ
          PROB(R,JJ) = PROB(R,JJ-1) - FACTLM(IJ+1)
460  CONTINUE
      MULT(R)=MULT(RM)
      C
      C      THE TABLE IS COMPLETE - CALL SUBROUTINE EVAL
      C
500  CALL EVAL(TABLE,R,C,N,M,PROB(R,C),MULT(R))
      C
      C
      C      END OF MAIN LOOP
      C
      GOTO 200
      C
      C
      END
      C
      SUBROUTINE EVAL(TABLE,R,C,N,M,PROB,MULT)
      INTEGER TABLE(10,10),R,C,N(10),M(10),MULT
      C
      RETURN
      END
```



```
      SUBROUTINE SMOOTH(NROW, NCOL, NDIM, X, W, A, B, NCYCLE, ICYCLE, G,  
*      EPS, IFAULT)  
C  
C      ALGORITHM AS 206  APPL. STATIST. (1984) VOL.33, NO.3  
C  
C      Subroutine to order a two-dimensional array using an algorithm of  
C      Dykstra & Robertson (1982).  The ordering is done so that the  
C      regression function is increasing in each independent variable.  
C  
C      Incorporates corrections from Applied Statistics vol.35(3),  
C      vol.36(1) and vol.40(1).  
C  
      REAL X(NROW,NCOL), W(NROW,NCOL), A(NROW,NCOL,4), B(NDIM,5),  
*      G(NROW,NCOL), EPS, ZERO, DELTA, DELC, DELR, ORD, WW, FRACT  
      DATA ZERO/0.0/, DELTA/0.00001/, FRACT/0.5/  
C  
      IFAULT = 0  
C  
C      Check that there are at least 2 rows and columns  
C  
      IF (NROW .LT. 2 .OR. NCOL .LT. 2) GO TO 120  
C  
C      Check that weights are positive or zero  
C  
      WSUM = ZERO  
      WXSUM = ZERO  
      WMIN = 1.0E+08  
      DO 3 I = 1, NROW  
        DO 3 J = 1, NCOL  
          WW = W(I,J)  
          IF (WW .LT. ZERO) GO TO 110  
          IF (WW .LT. DELTA) GO TO 3  
          WSUM = WSUM + WW  
          WXSUM = WXSUM + WW * X(I,J)  
          IF (WW .LT. WMIN) WMIN = WW  
3 CONTINUE  
      IF (WSUM .LT. DELTA) GO TO 130  
      WMEAN = WXSUM / WSUM  
C  
      DO 5 I = 1, NROW  
        DO 5 J = 1, NCOL  
          WW = W(I,J)  
          A(I,J,3) = WW  
          A(I,J,4) = X(I,J)  
          IF (WW .GE. DELTA) GO TO 5  
          A(I,J,3) = FRACT * WMIN  
          A(I,J,4) = WMEAN  
          ICT = ICT + 1  
          IFAULT = 4  
5 CONTINUE  
C  
C      Initialize R and C to zero, and set up workspace  
C  
      IFLAG = 0  
      DELR = ZERO  
      DELC = ZERO  
      ITIC = 0  
8 ITIC = ITIC + 1  
      DO 10 I = 1, NROW  
        DO 10 J = 1, NCOL  
          G(I,J) = A(I,J,4)
```

```

        A(I,J,2) = ZERO
        A(I,J,1) = ZERO
10 CONTINUE
C
C   Initialize counter for number of cycles
C
        ICOUNT = 0
        IF (IFLAG .EQ. 1) GO TO 55
        IF (ITIC .EQ. 3 .AND. DELC .GT. DELR) GO TO 55
C
C   Smooth over rows
C
25 JCOUNT = 0
        DO 50 I = 1, NROW
            DO 30 J = 1, NCOL
                B(J,1) = G(I,J) - A(I,J,1)
                B(J,2) = A(I,J,3)
30 CONTINUE
C
        CALL PAV(NCOL, B, 1, B(1,2), B(1,3))
C
        KCOUNT = 0
        DO 40 J = 1, NCOL
            ORD = B(J,3)
            A(I,J,1) = ORD - B(J,1)
            IF (ABS(ORD - G(I,J)) .LT. EPS) KCOUNT = KCOUNT + 1
            G(I,J) = ORD
40 CONTINUE
C
C   Determine if there is no change in the Ith row from the previous
C   iteration
C
        IF (KCOUNT .EQ. NCOL) JCOUNT = JCOUNT + 1
50 CONTINUE
C
        ICOUNT = ICOUNT + 1
        IF (ICOUNT .EQ. 2 .AND. IFLAG .EQ. 1)
*       CALL DIST(A(1,1,1), NROW, NCOL, DELR, IFLAG)
        IF (ICOUNT .EQ. 2 .AND. IFLAG .EQ. 2 .AND. ITIC .EQ. 2) GO TO 8
        IF (ICOUNT .EQ. 1) GO TO 55
        IF (NCYCLE .EQ. ICOUNT) GO TO 100
C
C   Determine if there has been no change in all rows from the
C   previous iteration
C
        IF (JCOUNT .EQ. NROW) GO TO 90
C
C   Smooth over columns
C
55 LCOUNT = 0
        DO 80 J = 1, NCOL
            DO 60 I = 1, NROW
                A(I,J,2) = G(I,J) - A(I,J,2)
60 CONTINUE
C
        CALL PAV(NROW, A(1,J,2), 1, A(1,J,3), B(1,3))
C
        MCOUNT = 0
        DO 70 I = 1, NROW
            ORD = B(I,3)
            A(I,J,2) = ORD - A(I,J,2)
            IF (ABS(ORD - G(I,J)) .LT. EPS) MCOUNT = MCOUNT + 1

```

```
      G(I,J) = ORD
70  CONTINUE
C
C  Determine if there is no change in the Jth column from the
C  previous iteration
C
      IF (MCOUNT .EQ. NROW) LCOUNT = LCOUNT + 1
80  CONTINUE
C
      ICOUNT = ICOUNT + 1
      IF (ICOUNT .EQ. 2 .AND. IFLAG .EQ. 0)
*     CALL DIST(A(1,1,2), NROW, NCOL, DELC, IFLAG)
      IF (ICOUNT .EQ. 2 .AND. IFLAG .EQ. 1) GO TO 8
      IF (ICOUNT .EQ. 1) GO TO 25
C
C  Determine if there is has been no change in any column from the
C  previous iteration
C
      IF (LCOUNT .EQ. NCOL) GO TO 90
C
C  Check if number of cycles has been reached
C
      IF (NCYCLE .EQ. ICOUNT) GO TO 100
      GO TO 25
90  ICYCLE = ICOUNT
      RETURN
C
100 ICYCLE = ICOUNT
      IFAULT = IFAULT + 1
      RETURN
110 IFAULT = 2
      RETURN
120 IFAULT = 3
      RETURN
130 IFAULT = 6
      RETURN
      END

      SUBROUTINE PAV(K, X, IORDER, W, FINALX)
C
C  ALGORITHM AS 206.1  APPL. STATIST. (1984) VOL.33, NO.3
C
C  Apply pool adjacent violators theorem
C
      INTEGER NW(20)
      REAL X(20), W(20), FINALX(20), FX(20), PW(20), W1(20), WT(20), EPS
C
      DATA EPS/1.0E-06/
C
C  Set up workspace
C
      NWC = K
      DO 10 I = 1, K
          NW(I) = 1
          FX(I) = X(I)
          IF (IORDER .EQ. 0) FX(I) = -FX(I)
          WT(I) = W(I)
          PW(I) = WT(I) * FX(I)
          W1(I) = W(I)
10  CONTINUE
```

```
      IBEL = K - 1
20  I = 0
30  I = I + 1
35  IF (I .GT. IBEL) GO TO 50
      I1 = I + 1
C
C   Determine if pooling is required
C
      IF (FX(I) - FX(I1) .LE. EPS) GO TO 30
C
C   Pool the adjacent values
C
      PW(I) = PW(I) + PW(I1)
      W1(I) = W1(I) + W1(I1)
      FX(I) = PW(I) / W1(I)
      NW(I) = NW(I) + NW(I1)
      NWC = NWC - 1
      IF (I1 .GT. IBEL) GO TO 45
      DO 40 J = I1, IBEL
          J1 = J + 1
          PW(J) = PW(J1)
          W1(J) = W1(J1)
          FX(J) = FX(J1)
          NW(J) = NW(J1)
40  CONTINUE
45  IBEL = IBEL - 1
      GO TO 35
50  ICOUNT = 0
      IF (IBEL .LE. 0) GO TO 70
C
C   Determine if all values are ordered
C
      DO 60 L = 1, IBEL
60  IF (FX(L) - FX(L+1) .LE. EPS) ICOUNT = ICOUNT + 1
      IF (ICOUNT .NE. IBEL) GO TO 20
C
C   Recover final ordered values
C
70  J = 1
      JL = 1
      JU = NW(1)
80  DO 90 L = JL, JU
90  FINALX(L) = FX(J)
      J = J + 1
      IF (J .GT. NWC) GO TO 100
      JL = JU + 1
      JU = JU + NW(J)
      GO TO 80
100 IF (IORDER .EQ. 1) RETURN
      DO 110 I = 1, K
110 FINALX(I) = -FINALX(I)
      RETURN
      END

      SUBROUTINE DIST(A1, NROW, NCOL, DEL, IFLAG)
C
C   ALGORITHM AS 206.2  APPL. STATIST. (1984) VOL.33, NO.3
C
      REAL A1(NROW,NCOL), ZERO, DEL
C
```

```
DATA ZERO/0.0/
```

```
C
```

```
DEL = ZERO
```

```
DO 20 I = 1, NROW
```

```
  DO 20 J = 1, NCOL
```

```
    DEL = DEL + A1(I,J) * A1(I,J)
```

```
20 CONTINUE
```

```
IFLAG = IFLAG + 1
```

```
RETURN
```

```
END
```

```
      subroutine gllm(ni, nid, nj, nk, nkp, ji, y, c, conv, w, v, e, f,
*   cspr, csrlr, ifault)
c
c   algorithm as 207 appl. statist. (1984) vol.33, no.3
c
c   fitting a generalized log-linear model
c   to fully or partially classified frequencies.
c
c   integer ji(ni)
c   double precision y(nj), c(nid, nkp), w(4, ni), v(2, nkp), e(ni),
*   f(nj), eps, zero, one, cmin, conv, csrlr, cspr, csum, ctmx, ff,
*   yy
c   logical lconv
c   data eps, zero, one/0.00001d0, 0.0d0, 1.0d0/
c
c   ifault = 1
c
c   check the ji array
c
c   do 100 i = 1, ni
c   if (ji(i) .lt. 1 .or. ji(i) .gt. nj) return
100 continue
c   ifault = 0
c
c   initialize
c
c   do 110 i = 1, ni
110 e(i) = one
c   do 120 j = 1, nj
120 w(3, j) = zero
c
c   standardize the c matrix
c
c
c   cmin = zero
c   do 130 i = 1, ni
c   do 130 k = 1, nk
c   cmin = min(cmin, c(i, k))
130 continue
c   if (cmin .eq. zero) goto 150
c   do 140 i = 1, ni
c   do 140 k = 1, nk
c   c(i, k) = c(i, k) - cmin
140 continue
150 ctmx = zero
c   do 170 i = 1, ni
c   csum = zero
c   do 160 k = 1, nk
160 csum = csum + c(i, k)
c   ctmx = max(ctmx, csum)
c   w(4, i) = csum
170 continue
c   if (ctmx .gt. eps) goto 180
c   ifault = 2
c   return
180 if (abs(ctmx - one) .le. eps) goto 200
c   do 190 i = 1, ni
c   do 190 k = 1, nk
c   c(i, k) = c(i, k) / ctmx
190 continue
c   goto 150
200 do 210 i = 1, ni
```

```

        if (abs(w(4, i) - one) .gt. eps) goto 220
210 continue
    nkk = nk
    goto 300
220 nkk = nkp
    do 230 i = 1, ni
230 c(i, nkk) = one - w(4, i)
c
c     enter the em algorithm
c
300 do 310 j = 1, nj
310 f(j) = zero
    do 320 i = 1, ni
        j = ji(i)
        f(j) = f(j) + e(i)
320 continue
c
c     check for convergence
c
    lconv = .true.
    do 330 j = 1, nj
        if (abs(f(j) - w(3, j)) .gt. conv) lconv = .false.
        w(3, j) = f(j)
330 continue
    if (lconv) goto 500
c
    do 340 i = 1, ni
        j = ji(i)
        w(1, i) = y(j)
        if (f(j) .gt. eps) w(1, i) = e(i) * y(j) / f(j)
340 continue
    do 360 k = 1, nkk
        v(1, k) = zero
        do 350 i = 1, ni
350 v(1, k) = v(1, k) + c(i, k) * w(1, i)
360 continue
c
c     enter the ipf algorithm
c
400 do 410 i = 1, ni
410 w(2, i) = e(i)
    do 440 k = 1, nkk
        v(2, k) = zero
        do 420 i = 1, ni
420 v(2, k) = v(2, k) + c(i, k) * e(i)
        do 430 i = 1, ni
430 if (c(i, k) .gt. eps .and. v(2, k) .gt. eps)
    * e(i) = e(i) * (v(1, k) / v(2, k)) ** c(i, k)
440 continue
        do 450 i = 1, ni
            if (abs(e(i) - w(2, i)) .gt. conv) goto 400
450 continue
        goto 300
c
c     calculate the goodness-of-fit statistics
c
500 cspr = zero
    cslr = zero
    do 530 j = 1, nj
        yy = y(j)
        ff = f(j)

```

```
        if (ff .le. eps) goto 530
        cspr = cspr + (yy - ff) ** 2 / ff
        if (yy .le. eps) goto 530
        cslr = cslr + yy * log(yy / ff)
530 continue
    cslr = 2.0d0 * cslr
    return
end
```



```

SUBROUTINE LGSTN(ZM, ZP, TOL, IFAULT)
C
C     ALGORITHM AS 208  APPL. STATIST. (1985) VOL.34, NO.1
C
C     FITS LOGISTIC NORMAL FOR 3 DIMENSIONAL CASE, USING
C     MOMENTS OF FIRST AND SECOND ORDER
C
REAL DJ(5, 5), EPS, ONE, R(5), SS, TOL, TWO, WW, WW0, WW1, WW2,
* WW3, ZERO, ZM(5), ZM1, ZM2, ZP(5)
INTEGER IP(5)
DATA ZERO, ONE, TWO, EPS, ITMAX / 0.0, 1.0, 2.0, 0.01, 20/
C
C     FIND STARTING VALUES
C
IFAULT = 0
N = 5
R(1) = ZM(3) - ZM(1) ** 2
R(2) = ZM(5) - ZM(2) ** 2
R(3) = ZM(4) - ZM(1) * ZM(2)
ZM1 = ONE - ZM(1)
ZM2 = ONE - ZM(2)
WW = ONE - ZM(1) - ZM(2)
WW0 = ZM1 * ZM2 + ZM(1) * ZM(2)
WW1 = R(1) * ZM2 ** 2 + R(2) * ZM(1) ** 2 + TWO * R(3) * ZM2 *
* ZM(1)
WW2 = R(1) * ZM(2) * ZM2 + R(2) * ZM1 * ZM(1) + R(3) * WW0
WW3 = R(1) * ZM(2) ** 2 + R(2) * ZM1 ** 2 + TWO * R(3) * ZM1 *
* ZM(2)
C
C     CHECK THAT MOMENTS ARE IN RANGE
C
IF (AMIN1(R(1), R(2), ZM(1), ZM(2), WW, WW1, WW3) .LE. ZERO)
* IFAULT = 1
IF (IFAULT .NE. 0) RETURN
WW1 = SQRT(ONE / WW1)
WW3 = SQRT(ONE / WW3)
ZP(1) = ALOG(ZM(1) / WW)
ZP(2) = ALOG(ZM(2) / WW)
ZP(3) = ZM(1) * WW * WW1
ZP(4) = ZM(2) * WW * WW3
C
C     FIND INITIAL VALUE FOR ZP(5) THAT IS INSIDE ALLOWED RANGE
ZP(5) = AMIN1(AMAX1(WW1 * WW2 * WW3, -ONE + EPS), ONE - EPS)
C
C     INITIAL VALUES IN ZP SO START ITERATION CYCLE
C
IT = 0
100 IT = IT + 1
C
C     FIND MOMENTS AND DERIVATIVES GIVEN LATEST PARAMETER VALUES
C
CALL LSQ2(ZM, ZP, R, DJ, SS, IER)
IF (IER .NE. 0) IFAULT = 4
IF (IFAULT .NE. 0) RETURN
C
C     DECOMPOSE 2ND DERIVATIVE MATRIX
C
CALL DECOMP(N, N, DJ, IP)
IF (IP(N) .EQ. 0) IFAULT = 3
IF (IFAULT .NE. 0) RETURN
C

```

```

C          SOLVE LINEAR EQUATION
C
C          CALL SOLVE(N, N, DJ, R, IP)
C
C          FIND UPDATED PARAMETER ESTIMATES
C
C          ZP(1) = ZP(1) - R(1)
C          ZP(2) = ZP(2) - R(2)
C          ZP(3) = ZP(3) * EXP(-R(3))
C          ZP(4) = ZP(4) * EXP(-R(4))
C          WW = EXP(-R(5)) * (ONE + ZP(5)) / (ONE - ZP(5))
C          ZP(5) = (WW - ONE) / (WW + ONE)
C          IF (SS .LE. TOL) RETURN
C          IF (IT .EQ. ITMAX) IFAULT = 2
C          IF (IFAULT .NE. 0) RETURN
C          GOTO 100
C          END
C
C          SUBROUTINE LSQ2(ZM, ZP, R, DJ, SS, IER)
C
C          ALGORITHM AS 208.1  APPL. STATIST. (1985) VOL.34, NO.1
C
C          LSQ2 FINDS SS AND DERIVATIVES FOR FITTING LOGISTIC NORMAL
C          FOR S2 BY MOMENTS
C
C          REAL D(5, 5, 6), DC, DJ(5, 5), DR, DT, D34, EPS, EPS1, HALF, ONE,
*          R(5), SS, ZERO, ZI, ZJ, ZM(5), ZMOM(5, 5), ZP(5)
C          INTEGER IMAP(6), KMAP(6)
C          DATA KMAP(1), KMAP(2), KMAP(3), KMAP(4), KMAP(5), KMAP(6)
*          /0, 1, 2, 1, 4, 2/
C          DATA IMAP(1), IMAP(2), IMAP(3), IMAP(4), IMAP(5), IMAP(6)
*          /0, 4, 3, 4, 3, 3/
C          DATA ZERO, HALF, ONE, EPS, EPS1 /0.0, 0.5, 1.0, 7.7, 18.0/
C
C          IER = 0
C
C          CHECK THAT PARAMETERS ARE IN RANGE
C
C          IF (AMIN1(ZP(3), ZP(4)) .LE. ZERO) IER = 1
C          IF (IER .NE. 0) RETURN
C          IF (ABS(ZP(5)) .GT. ONE) IER = 2
C          IF (AMAX1(EPS / ZP(3) + ABS(ZP(1)), EPS / ZP(4) + ABS(ZP(2))))
*          .GT. EPS1) IER = 3
C          IF (IER .NE. 0) RETURN
C
C          GET MOMENTS
C
C          CALL MOM2(ZP, ZMOM)
C
C          INITIALISE D WITH MOMENTS OR ZEROS
C
C          DO 100 K = 2, 4, 2
C          DO 100 I = 1, 5
C          J = 6 - I
100      D(I, J, K) = ZERO
C          DO 120 I = 1, 5
C          J0 = 6 - I
C          DO 120 J = 1, J0
120      D(I, J, 1) = ZMOM(I, J)
C
C          DO DIFFERENCING ON D TO GET DERIVATIVES

```

```

C          KMPA AND IMAP TELL WHICH DIFFERENCES TO USE
C
DO 200 K = 2, 6
K0 = KMAP(K)
I0 = IMAP(K)
DO 200 I = 1, I0
ZI = I - 1
J0 = I0 - I + 1
DO 200 J = 1, J0
ZJ = J - 1
IF (K .LE. 3) D(I, J, K) = ZI * D(I, J, K0) - (ZI + ZJ) *
* D(I + 1, J, K0)
IF (K .GT. 3) D(I, J, K) = ZJ * D(I, J, K0) - (ZI + ZJ) *
* D(I, J + 1, K0)
200      CONTINUE
L = 0
SS = ZERO
D34 = ONE / (ZP(3) * ZP(4))
DC = HALF * (ONE - ZP(5) ** 2) * D34
DR = ZP(3) / ZP(4)
DO 400 I = 2, 3
DO 400 J = 1, I
K = I - J + 1
L = L + 1
C
C          FIND SS, RESIDUALS AND DERIVATIVES W.R.T. PARAMETERS
C          D(K,J,1) CONTAINS FITTED MOMENT CORRESPONDING TO ZM(L)
C
R(L) = D(K, J, 1) - ZM(L)
SS = SS + R(L) ** 2
DT = ZP(5) * D(K, J, 6)
DJ(L, 1) = D(K, J, 2)
DJ(L, 2) = D(K, J, 4)
DJ(L, 3) = -D34 * (D(K, J, 3) / DR + DT)
DJ(L, 4) = -D34 * (D(K, J, 5) * DR + DT)
DJ(L, 5) = DC * D(K, J, 6)
400      CONTINUE
RETURN
END
C
SUBROUTINE MOM2(ZP, A)
C
C          ALGORITHM AS 208.2 APPL. STATIST. (1985) VOL.34, NO.1
C
C          MOM2 CALCULATES E((X**(I-1))(Y**(J-1))) I,J=1 TO 5
C          =A(I,J) FOR LOGISTIC NORMAL
C          I+J LESS THAN 6
C          USING (20,20) POINT HERMITIAN INTEGRATION
C
REAL A(5, 5), AB(10), CON, ONE, W, WT(10), W0, X, Y, Z, ZERO,
* ZP(5), Z1, Z10, Z2, Z20, Z3
C
C          WT AND AB CONTAIN THE WEIGHTS AND ABCISSAS FOR THE
C          HERMITIAN INTEGRATION
C
DATA WT(1), WT(2), WT(3), WT(4), WT(5), WT(6), WT(7), WT(8),
* WT(9), WT(10)
* /0.2607930634495549E18, 0.161739333984E18,
* 0.6150637206397691E17,0.13997837447101E17,
* 0.1830103131080493E16, 0.1288262799619294E15,
* 0.4402121090230853E13, 0.6127490259982946E11,

```

```
* 0.2482062362315179E9, 0.1257800672437927E6/  
DATA AB(1), AB(2), AB(3), AB(4), AB(5), AB(6), AB(7), AB(8),  
* AB(9), AB(10)  
* /0.34696415708135593, 1.04294534880275103, 1.74524732081412671,  
* 2.45866361117236775, 3.18901481655338941, 3.94396735065731627,  
* 4.73458133404605532, 5.57873880589320117, 6.51059015701365447,  
* 7.61904854167975829/  
DATA ZERO, ONE, CON /0.0, 1.0, 1.0E-36/  
  
C  
Z = SQRT(ONE - ZP(5) ** 2)  
  
C  
C INITIALIZE A() TO ZERO  
C  
DO 100 J = 1, 5  
J0 = 6 - J  
DO 100 J1 = 1, J0  
100 A(J, J1) = ZERO  
DO 500 I = 1, 10  
X = AB(I)  
W0 = WT(I)  
DO 500 J = 1, 10  
Y = AB(J)  
W = W0 * WT(J)  
  
C  
C GIVEN (X,Y)= GRID POINT AND W= WEIGHT DO FOR (+-X,+Y)  
C  
DO 500 I1 = 1, 2  
DO 400 J1 = 1, 2  
Z10 = W  
Z1 = EXP(X / ZP(3) + ZP(1))  
Z2 = EXP((Y * Z + ZP(5) * X) / ZP(4) + ZP(2))  
Z3 = ONE / (ONE + Z1 + Z2)  
Z1 = Z1 * Z3  
Z2 = Z2 * Z3  
DO 150 I0 = 1, 5  
Z20 = Z10  
J10 = 6 - I0  
DO 140 J0 = 1, J10  
A(I0, J0) = A(I0, J0) + Z20  
Z20 = Z20 * Z2  
140 CONTINUE  
Z10 = Z10 * Z1  
150 CONTINUE  
Y = -Y  
400 CONTINUE  
X = -X  
500 CONTINUE  
C  
C RESCALE MOMENTS TO AVOID UNDERFLOW  
C  
DO 600 J = 1, 5  
J0 = 6 - J  
DO 600 J1 = 1, J0  
600 A(J, J1) = A(J, J1) * CON  
RETURN  
END
```

```
SUBROUTINE PKURT(B2, N, P, ZP, IFAULT)
```

```

C
C     ALGORITHM AS209  APPL. STATIST. (1985) VOL. 34, NO. 1
C
C     EVALUATES P VALUE FOR COEFFICIENT OF KURTOSIS B2.
C     N IS SAMPLE SIZE, N GE 5.
C     ZP IS NORMAL EQUIVALENT DEVIATE FOR P.
C     BASED ON SIMULATIONS OF DISTRIBUTION OF B2 APPROXIMATED
C     BY MODIFIED SU. USES FIRST ORDER APPROXIMATION TO MEAN AND SD
C     OF TRANSFORMED B2 FOR N GT 5000.
C     APPROXIMATION ACCURATE TO ABOUT +/- 0.05 FOR ZP IN RANGE -3.1
C     LT ZP LT 3.1.
C
C     IFAULT = 0    OK
C     1    B2 LT 0
C     2    N LT 15
C     3    P(B2) LT 0.0001 (WHEN NLT15) : P RETURNED AS 0.0001
C     4    P(B2) GT 0.9999 (WHEN NLT15) : P RETURNED AS 0.9999
C     5,6  INTERNAL ERROR IN COMPUTING B-SPLINE INTERPOLANT
C     7    B2 BELOW EXTRAPOLATED SIMULATION LIMIT: P AND ZP RETURNED
C     AS 0
C
C     INTEGER N1(22), N2(19)
C     REAL LAMDA, CSL1(22), CI1(22), CSL2(19), CI2(19), KNOT(24)
C     REAL PERC(20, 10), PWRK(20), COEF(24), PERZ(20)
C
C     WRK IS WORKING ARRAY OF DIM LWRK = (NO. OF POINTS)*6 + 16 =
C     136 FOR 20.
C
C     REAL WRK(136), LOWP, LOWZ
C     LOGICAL LOWER
C     DATA MSMALL /22/, MBIG /19/, M /20/, LWRK /136/, I5000 /5000/,
*   I100 /100/
C     DATA LOWP /0.0001/, LOWZ /-3.71902/
C     DATA ZERO /0.0E0/, ONE /1.0E0/, TWO /2.0E0/, THREE /3.0E0/, FIVE /
*   5.0E0/
C     DATA TWENT4 /24.0E0/, HUNDRD /100.0E0/, LOWER /.FALSE./
C
C     DATA N1(1), N1(2), N1(3), N1(4), N1(5) /15, 15, 15, 15, 17/
C     DATA N1(6), N1(7), N1(8), N1(9), N1(10) /18, 19, 20, 22, 25/
C     DATA N1(11), N1(12), N1(13), N1(14), N1(15) /30, 35, 40, 45, 50/
C     DATA N1(16), N1(17), N1(18), N1(19), N1(20) /60, 70, 80, 100, 100/
C     DATA N1(21), N1(22) /100, 100/
C
C     DATA N2(1), N2(2), N2(3), N2(4), N2(5) /100, 100, 100, 100, 140/
C     DATA N2(6), N2(7), N2(8), N2(9), N2(10) /160, 180, 200, 250, 300/
C     DATA N2(11), N2(12), N2(13), N2(14), N2(15) /400, 500, 600, 800,
*   1000/
C     DATA N2(16), N2(17), N2(18), N2(19) /5000, 5000, 5000, 5000/
C
C     DATA CSL1(1), CSL1(2), CSL1(3) /0.130608, 0.130309, 0.130799/
C     DATA CSL1(4), CSL1(5), CSL1(6) /0.131271, 0.130269, 0.131037/
C     DATA CSL1(7), CSL1(8), CSL1(9) /0.133146, 0.131201, 0.131552/
C     DATA CSL1(10), CSL1(11), CSL1(12) /0.134288, 0.136172, 0.139247/
C     DATA CSL1(13), CSL1(14), CSL1(15) /0.145013, 0.153807, 0.167036/
C     DATA CSL1(16), CSL1(17), CSL1(18) /0.191936, 0.217312, 0.246664/
C     DATA CSL1(19), CSL1(20), CSL1(21), CSL1(22) /0.0, 0.0, 0.0, 0.0/
C
C     DATA CI1(1), CI1(2), CI1(3) /0.991947, 0.984242, 0.981813/
C     DATA CI1(4), CI1(5), CI1(6) /0.967821, 0.962803, 0.951360/
C     DATA CI1(7), CI1(8), CI1(9) /0.934610, 0.909853, 0.873722/

```

DATA CI1(10), CI1(11), CI1(12) /0.823252, 0.772149, 0.716999/  
DATA CI1(13), CI1(14), CI1(15) /0.639262, 0.531453, 0.375579/  
DATA CI1(16), CI1(17), CI1(18) /0.141451, -0.096974, -0.316306/  
DATA CI1(19), CI1(20), CI1(21), CI1(22) /0.0, 0.0, 0.0, 0.0/

C

DATA CSL2(1), CSL2(2), CSL2(3) /0.246227, 0.242238, 0.264287/  
DATA CSL2(4), CSL2(5), CSL2(6) /0.290128, 0.307728, 0.316642/  
DATA CSL2(7), CSL2(8), CSL2(9) /0.322317, 0.304390, 0.284983/  
DATA CSL2(10), CSL2(11), CSL2(12) /0.267009, 0.240296, 0.221648/  
DATA CSL2(13), CSL2(14), CSL2(15) /0.162402, 0.111749, 0.092712/  
DATA CSL2(16), CSL2(17), CSL2(18), CSL2(19) /0.0, 0.0, 0.0, 0.0/

C

DATA CI2(1), CI2(2), CI2(3) /-0.320361, -0.338391, -0.439550/  
DATA CI2(4), CI2(5), CI2(6) /-0.592816, -0.678397, -0.754728/  
DATA CI2(7), CI2(8), CI2(9) /-0.794209, -0.800182, -0.788895/  
DATA CI2(10), CI2(11), CI2(12) /-0.765971, -0.760544, -0.746093/  
DATA CI2(13), CI2(14), CI2(15) /-0.733140, -0.724729, -0.719960/  
DATA CI2(16), CI2(17), CI2(18), CI2(19) /0.0, 0.0, 0.0, 0.0/

C

DATA PERC(1, 1), PERC(2, 1), PERC(3, 1), PERC(4, 1), PERC(5, 1)  
\* /1.170, 1.173, 1.177, 1.196, 1.212/  
DATA PERC(6, 1), PERC(7, 1), PERC(8, 1), PERC(9, 1), PERC(10, 1)  
\* /1.244, 1.278, 1.348, 1.497, 1.808/  
DATA PERC(11, 1), PERC(12, 1), PERC(13, 1), PERC(14, 1), PERC(15,  
\* 1) /2.133, 2.465, 2.694, 2.875, 3.003/  
DATA PERC(16, 1), PERC(17, 1), PERC(18, 1), PERC(19, 1), PERC(20,  
\* 1) /3.110, 3.162, 3.219, 3.230, 3.244/

C

DATA PERC(1, 2), PERC(2, 2), PERC(3, 2), PERC(4, 2), PERC(5, 2)  
\* /1.016, 1.042, 1.059, 1.136, 1.189/  
DATA PERC(6, 2), PERC(7, 2), PERC(8, 2), PERC(9, 2), PERC(10, 2)  
\* /1.287, 1.382, 1.488, 1.598, 1.867/  
DATA PERC(11, 2), PERC(12, 2), PERC(13, 2), PERC(14, 2), PERC(15,  
\* 2) /2.211, 2.667, 2.993, 3.281, 3.516/  
DATA PERC(16, 2), PERC(17, 2), PERC(18, 2), PERC(19, 2), PERC(20,  
\* 2) /3.746, 3.875, 4.047, 4.084, 4.138/

C

DATA PERC(1, 3), PERC(2, 3), PERC(3, 3), PERC(4, 3), PERC(5, 3)  
\* /1.116, 1.139, 1.155, 1.213, 1.252/  
DATA PERC(6, 3), PERC(7, 3), PERC(8, 3), PERC(9, 3), PERC(10, 3)  
\* /1.329, 1.416, 1.533, 1.699, 1.949/  
DATA PERC(11, 3), PERC(12, 3), PERC(13, 3), PERC(14, 3), PERC(15,  
\* 3) /2.277, 2.779, 3.188, 3.544, 3.872/  
DATA PERC(16, 3), PERC(17, 3), PERC(18, 3), PERC(19, 3), PERC(20,  
\* 3) /4.227, 4.443, 4.775, 4.868, 5.010/

C

DATA PERC(1, 4), PERC(2, 4), PERC(3, 4), PERC(4, 4), PERC(5, 4)  
\* /1.077, 1.131, 1.162, 1.265, 1.315/  
DATA PERC(6, 4), PERC(7, 4), PERC(8, 4), PERC(9, 4), PERC(10, 4)  
\* /1.391, 1.469, 1.581, 1.753, 2.032/  
DATA PERC(11, 4), PERC(12, 4), PERC(13, 4), PERC(14, 4), PERC(15,  
\* 4) /2.340, 2.853, 3.316, 3.722, 4.110/  
DATA PERC(16, 4), PERC(17, 4), PERC(18, 4), PERC(19, 4), PERC(20,  
\* 4) /4.560, 4.851, 5.351, 5.491, 5.770/

C

DATA PERC(1, 5), PERC(2, 5), PERC(3, 5), PERC(4, 5), PERC(5, 5)  
\* /1.132, 1.180, 1.208, 1.297, 1.350/  
DATA PERC(6, 5), PERC(7, 5), PERC(8, 5), PERC(9, 5), PERC(10, 5)  
\* /1.439, 1.524, 1.634, 1.801, 2.089/  
DATA PERC(11, 5), PERC(12, 5), PERC(13, 5), PERC(14, 5), PERC(15,  
\* 5) /2.408, 2.910, 3.398, 3.844, 4.263/

```
DATA PERC(16, 5), PERC(17, 5), PERC(18, 5), PERC(19, 5), PERC(20,  
* 5) /4.807, 5.156, 5.801, 6.013, 6.371/
```

C

```
DATA PERC(1, 6), PERC(2, 6), PERC(3, 6), PERC(4, 6), PERC(5, 6)  
* /1.145, 1.217, 1.247, 1.338, 1.390/  
DATA PERC(6, 6), PERC(7, 6), PERC(8, 6), PERC(9, 6), PERC(10, 6)  
* /1.476, 1.565, 1.679, 1.844, 2.133/  
DATA PERC(11, 6), PERC(12, 6), PERC(13, 6), PERC(14, 6), PERC(15,  
* 6) /2.458, 2.963, 3.467, 3.943, 4.419/  
DATA PERC(16, 6), PERC(17, 6), PERC(18, 6), PERC(19, 6), PERC(20,  
* 6) /4.981, 5.389, 6.183, 6.448, 6.925/
```

C

```
DATA PERC(1, 7), PERC(2, 7), PERC(3, 7), PERC(4, 7), PERC(5, 7)  
* /1.189, 1.239, 1.273, 1.372, 1.428/  
DATA PERC(6, 7), PERC(7, 7), PERC(8, 7), PERC(9, 7), PERC(10, 7)  
* /1.513, 1.600, 1.718, 1.888, 2.178/  
DATA PERC(11, 7), PERC(12, 7), PERC(13, 7), PERC(14, 7), PERC(15,  
* 7) /2.505, 3.009, 3.506, 4.002, 4.492/  
DATA PERC(16, 7), PERC(17, 7), PERC(18, 7), PERC(19, 7), PERC(20,  
* 7) /5.110, 5.547, 6.411, 6.760, 7.304/
```

C

```
DATA PERC(1, 8), PERC(2, 8), PERC(3, 8), PERC(4, 8), PERC(5, 8)  
* /1.198, 1.272, 1.303, 1.401, 1.457/  
DATA PERC(6, 8), PERC(7, 8), PERC(8, 8), PERC(9, 8), PERC(10, 8)  
* /1.545, 1.635, 1.753, 1.925, 2.212/  
DATA PERC(11, 8), PERC(12, 8), PERC(13, 8), PERC(14, 8), PERC(15,  
* 8) /2.539, 3.045, 3.544, 4.043, 4.542/  
DATA PERC(16, 8), PERC(17, 8), PERC(18, 8), PERC(19, 8), PERC(20,  
* 8) /5.178, 5.663, 6.645, 7.050, 7.750/
```

C

```
DATA PERC(1, 9), PERC(2, 9), PERC(3, 9), PERC(4, 9), PERC(5, 9)  
* /1.230, 1.301, 1.337, 1.431, 1.486/  
DATA PERC(6, 9), PERC(7, 9), PERC(8, 9), PERC(9, 9), PERC(10, 9)  
* /1.577, 1.665, 1.784, 1.955, 2.246/  
DATA PERC(11, 9), PERC(12, 9), PERC(13, 9), PERC(14, 9), PERC(15,  
* 9) /2.570, 3.075, 3.575, 4.085, 4.602/  
DATA PERC(16, 9), PERC(17, 9), PERC(18, 9), PERC(19, 9), PERC(20,  
* 9) /5.294, 5.802, 6.817, 7.242, 8.037/
```

C

```
DATA PERC(1, 10), PERC(2, 10), PERC(3, 10), PERC(4, 10), PERC(5,  
* 10) /1.249, 1.321, 1.354, 1.457, 1.510/  
DATA PERC(6, 10), PERC(7, 10), PERC(8, 10), PERC(9, 10), PERC(10,  
* 10) /1.602, 1.694, 1.814, 1.985, 2.274/  
DATA PERC(11, 10), PERC(12, 10), PERC(13, 10), PERC(14, 10),  
* PERC(15, 10) /2.597, 3.095, 3.589, 4.088, 4.602/  
DATA PERC(16, 10), PERC(17, 10), PERC(18, 10), PERC(19, 10),  
* PERC(20, 10) /5.282, 5.769, 6.861, 7.296, 8.166/
```

C

```
DATA PERZ(1), PERZ(2), PERZ(3) /-3.71902, -3.29053, -3.09023/  
DATA PERZ(4), PERZ(5), PERZ(6) /-2.57583, -2.32635, -1.95996/  
DATA PERZ(7), PERZ(8), PERZ(9) /-1.64485, -1.28155, -0.84162/  
DATA PERZ(10), PERZ(11), PERZ(12) /-0.25335, 0.25335, 0.84162/  
DATA PERZ(13), PERZ(14), PERZ(15) /1.28155, 1.64485, 1.95996/  
DATA PERZ(16), PERZ(17), PERZ(18) /2.32635, 2.57583, 3.09023/  
DATA PERZ(19), PERZ(20) /3.29053, 3.71902/
```

C

C

C

C

```
DEFINE FUNCTIONS OF SAMPLE SIZE FOR THE MEAN AND VARIANCE OF  
B2.
```

```
EB2(AN) = THREE * (AN - ONE) / (AN + ONE)
```

```
VB2(AN) = TWENTY4 * AN * (AN - TWO) * (AN - THREE) / ((AN + ONE)
```

```
      * * (AN + ONE) * (AN + THREE) * (AN + FIVE) )
C
C      SET SMALLEST ARGUMENT FOR EXP
C
      ENEG = X02AEF(DUMMY)
C
      P = ZERO
      ZP = ZERO
      IFAULT = 2
      IF (N .LT. 5) RETURN
      IFAULT = 1
      IF (B2 .LT. ZERO) RETURN
      IFAULT = 0
      IF (N .GT. 14) GOTO 20
C
      VERY SMALL SAMPLES. USE SPLINE APPROX TO SIMULATION PERCENTAGE
      POINTS.
      TRANSFER APPROPRIATE PERCENTILES TO WORKING ARRAY
C
      N4 = N - 4
      IFAULT = 3
      P = LOWP
      ZP = LOWZ
      IF (B2 .LT. PERC(1, N4)) RETURN
      IFAULT = 4
      P = ONE - LOWP
      ZP = -LOWZ
      IF (B2 .GT. PERC(M, N4)) RETURN
      IFAULT = 0
      P = ZERO
      ZP = ZERO
      DO 10 I = 1, 20
10 PWRK(I) = PERC(I, N4)
      M4 = M + 4
      IFAIL = 0
      CALL E01BAF(M, PWRK, PERZ, KNOT, COEF, M4, WRK, LWRK, IFAIL)
      IF (IFAIL .GT. 0) IFAULT = IFAIL + 5
      IF (IFAIL .GT. 0) RETURN
      IFAIL = 0
      CALL E02BBF(M4, KNOT, COEF, B2, ZP, IFAIL)
      IF (IFAIL .GT. 0) IFAULT = IFAIL + 5
      IF (IFAIL .GT. 0) RETURN
      P = ALNORM(ZP, LOWER)
      RETURN
C
      N GT 14
C
20 AN = FLOAT(N)
      X = ALOG(AN / HUNDRD)
C
      SMOOTHED VALUE FOR LOCATION PARAMETER (XI).
C
      DENOM = ONE
      ARG = -0.02687 * (AN - HUNDRD)
      IF (ARG .GE. ENEG) DENOM = ONE + EXP(ARG)
      XI = 0.8 + 2.2 / DENOM
C
      IF (N .GE. HUNDRD) GOTO 30
C
      FIND LAMDA AND A FOR N LT 100
C
```



```

      LAMDA = 0.17162 * EXP(AN * 0.02253)
      A = 0.3155 - 1.1555 * X * (1.0 + X * (0.6143 + 0.3423 * X))
C
C      ASSIGN KNOTS FOR INTERPOLATING SPLINE
C
      DO 25 I = 1, MSMALL
25 KNOT(I) = ALOG(FLOAT(N1(I)) / HUNDRD)
C
C      GET THETA AND ETA USING B-SPLINE INTERPOLATION FUNCTIONS
C
      IFAIL = 0
      CALL E02BBF(MSMALL, KNOT, CSL1, X, THETA, IFAIL)
      IF (IFAIL .NE. 0) IFAULT = IFAIL + 5
      IF (IFAILT .GT. 0) RETURN
      IFAIL = 0
      CALL E02BBF(MSMALL, KNOT, CI1, X, ETA, IFAIL)
      IF (IFAIL .NE. 0) IFAULT = IFAIL + 5
      IF (IFAILT .GT. 0) RETURN
      GOTO 60
C
C      FIND LAMDA AND A FOR N GE 100
C
30 LAMDA = EXP( - 0.06174 + 0.711 / (1.0 + EXP(2.0581 * (X - 0.6374))
* ) )
      A = 0.3155 - 0.31287 * (EXP(-2.295 * X) - ONE)
      IF (N.GT. I5000) GOTO 60
C
C      ASSIGN KNOTS FOR INTERPOLATING SPLINE
C
      DO 40 I = 1, MBIG
40 KNOT(I) = ALOG(FLOAT(N2(I)) / HUNDRD)
C
C      GET THETA AND ETA USING B-SPLINE INTERPOLATION FUNCTIONS
C
      IFAIL = 0
      CALL E02BBF(MBIG, KNOT, CSL2, X, THETA, IFAIL)
      IF (IFAIL .NE. 0) IFAULT = IFAIL + 5
      IF (IFAILT .GT. 0) RETURN
      IFAIL = 0
      CALL E02BBF(MBIG, KNOT, CI2, X, ETA, IFAIL)
      IF (IFAIL .NE. 0) IFAULT = IFAIL + 5
      IF (IFAILT .GT. 0) RETURN
C
C      A IS SHAPE, XI IS LOCATION, LAMDA IS SCALE
C
60 Y = (B2 - XI) / LAMDA
      H = A + Y + SQRT(ONE + Y * Y)
      IF (H .GT. ONE) GOTO 65
C
C      B2 BELOW LIMIT OF MODIFIED JOHNSON CURVE (I.E. ILLEGAL).
C
61 IFAULT = 7
      RETURN
65 IF (N .LE. I5000) GOTO 70
C
C      GET EXPECTED VALUE (ETA) AND SD (THETA) OF TRANSFORMED B2 (=H).
C      (USES LOW ORDER APPROX EVALUATED AT EXPECTED VALUE OF B2)
C
      YE = (EB2(AN) - XI) / LAMDA
      HE = A + YE + SQRT(ONE + YE * YE)
      IF (HE .LE. ONE) GOTO 61

```

```

ETA = ALOG(ALOG(HE))
THETA = SQRT(VB2(AN)) * ABS((HE - A) / (LAMDA * HE * ALOG(HE)
* * (HE - A - YE)) )
70 ZP = (ALOG(ALOG(H)) - ETA) / THETA
P = ALNORM(ZP, LOWER)
RETURN
END

C
SUBROUTINE PSKEW(B1, N, P, ZP, IFAULT)

C
C     ALGORITHM AS209.1  APPL. STATIST. (1985) VOL. 34, NO. 1
C
C     EVALUATES P VALUE FOR COEFFICIENT OF SKEWNESS (SQRT(BETA.1))
C     IN NORMAL SAMPLES. ASSUMES A SU APPROXIMATION AS WORKED OUT BY
C     D'AGOSTINO,
C     BIOMETRIKA, 1970, 57,679-681.
C     N = SAMPLE SIZE, ZP = NORMAL EQUIVALENT DEVIATE FOR B1, P = P
C     VALUE
C
C     IFAULT = 0, SUCCESS
C     1, N LT 10

LOGICAL LOWER
REAL NINE
DATA ZERO /0.0E0/, ONE /1.0E0/, TWO /2.0E0/, THREE /3.0E0/, FIVE /
* 5.0E0/
DATA SIX /6.0E0/, SEVEN /7.0E0/, NINE /9.0E0/, TWENTY7 /27.0E0/
DATA SEVNTY /70.0E0/, LOWER /.FALSE./
ZP = ZERO
P = ZERO
IFAULT = 1
IF (N .LT. 10) RETURN
IFAULT = 0
AN = N
AN1 = AN + ONE
AN3 = AN + THREE
ANM2 = AN - TWO
Y = B1 * SQRT(AN1 * AN3 / (SIX * ANM2) )
BETA2 = THREE * (AN * AN + TWENTY7 * AN - SEVNTY) * AN1 * AN3 /
* (ANM2 * (AN + FIVE) * (AN + SEVEN) * (AN + NINE) )
W2 = SQRT(TWO * BETA2 - TWO) - ONE
DELTA = ONE / SQRT(ALOG(W2) / TWO)
ALPHA = SQRT(TWO / (W2 - ONE))
Y1 = Y / ALPHA
ZP = DELTA * ALOG(Y1 + SQRT(ONE + Y1 * Y1))
P = ALNORM(ZP, LOWER)
RETURN
END
REAL FUNCTION ALNORM(Z, UPPER)
LOGICAL UPPER
IF (UPPER) CALL STAT8(Z, ALNORM, DUMMY)
IF (.NOT.UPPER) CALL STAT8(Z, DUMMY, ALNORM)
RETURN
END

```

```

      SUBROUTINE SBFIT1(N, XL, XU, XBAR, SD, RB1, ZP, TOL, SS, RVRS,
*   IFAULT)
C
C   ALGORITHM AS 210  APPL. STATIST. (1985) VOL.34, NO.1
C
C   FITS 5-PARAMETER JOHNSON SB-CURVE TO MOMENTS
C   DELTA=ZP(1), GAMMA= ZP(2), ALPHA=ZP(3)
C
      REAL A(9), AL, AL1, C, C0, C1,  C00, C10, EPS, FOUR, ONE, ONE5,
*   R(3), RB1, RB10, SD, SIG, SS, THREE, TOL, TWO, WD, XBAR, XL,
*   XU, ZERO, ZM(3), ZMA, ZMB, ZP(3)
      INTEGER IP (3)
      LOGICAL RVRS
      DATA ZERO, ONE, ONE5, TWO, THREE, FOUR
*   / 0.0, 1.0, 1.5, 2.0, 3.0, 4.0/
      DATA EPS, ITMAX /1.0E-3, 20/
      IFAULT = 0
C
C   TRANSFORM TO (0,1)
C
      WD = XU - XL
      IF (WD .LE. ZERO .OR. N .LT. 2 .OR. N .GT. 3) IFAULT = 1
      IF (SD .LE. ZERO) IFAULT = 2
      IF (IFAILT .NE. 0) RETURN
      ZM(1) = (XBAR - XL) / WD
      SIG = SD / WD
      ZM(2) = SIG * SIG + ZM(1) ** 2
      IF (ZM(2) .GE. ZM(1)) IFAULT = 2
      IF (IFAILT .NE. 0) RETURN
      AL = ONE
      RVRS = .FALSE.
      ZMA = ZM(1)
      IF (N .EQ. 2) GOTO 30
      RB10 = RB1
      ZM(3) = ZM(1) ** 3 + SIG * SIG * (THREE * ZM(1) + RB1 * SIG)
      IF (ZM(3) .GE. ZM(2) .OR. ZM(3) .LE. ZM(2) ** ONE5) IFAULT = 2
      IF (IFAILT .NE. 0) RETURN
C
C   FIND STARTING VALUE FOR ALPHA
C
      C = RB10 / (THREE * SIG)
      C0 = ONE / (ONE + C * (ONE - ZM(1)))
      C1 = ONE / (ONE - C * ZM(1))
      C00 = (C0 - ZM(1) * (ONE + C0)) / (ZM(1) + ALOG(ONE - ZM(1)))
      C10 = (ZM(1) * (ONE + C1) - ONE) / (ONE - ZM(1) + ALOG(ZM(1)))
C
C   IF NECESSARY, REVERSE
C
      IF (C00 .GE. C10) GOTO 10
      RB10 = -RB10
      ZM(3) = ONE - THREE * (ZM(1) - ZM(2)) - ZM(3)
      ZM(2) = ONE - TWO * ZM(1) + ZM(2)
      ZM(1) = ONE - ZM(1)
      RVRS = .TRUE.
      C1 = C0
      ZMA = ONE - ZMA
10   IF (C00 .GE. ZERO .AND. C10 .GE. ZERO) GOTO 30
20   C00 = AL - ZMA * (AL + C1)
      C10 = ALOG(ZM(1)) + AL * (ONE - ZMA)
      C0 = AMAX1(-FOUR, AMIN1(FOUR, C00 / C10))
      AL = AL * EXP(-C0)

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      ZMA = ZM(1) ** (ONE / AL)
      IF (ABS(CO) .GT. EPS) GOTO 20
C
C      FIND STARTING VALUES FOR DELTA AND GAMMA
C
30     ZMB = ONE - ZMA
      AL1 = AL + ONE
      ZP(1) = AL * ZM(1) * ZMB /SIG + (AL ** 2 - AL1 * ZMA * (TWO *
* AL1 - (AL + THREE) * ZMA)) / (FOUR * AL * ZM(1) * ZMB / SIG)
      ZP(2) = ZP(1) + ALOG(ZMB / ZMA) + (AL - AL1 * ZMA) / (TWO * ZP(1))
      ZP(3) = AL
C
C      START ITERATION CYCLE
C
      I = 0
40     I = I + 1
      CALL LSQ1(N, ZM, ZP, R, A, SS, IFL)
      IF (IFL .NE. 0) IFAULT = 3
      IF (IFault .NE. 0) RETURN
      CALL DECOMP(N, N, A, IP)
      IF (IP(N) .EQ. 0) IFAULT = 4
      IF (IFault .NE. 0) RETURN
      CALL SOLVE(N, N, A, R, IP)
      DO 50 I0 = 1, N
50     ZP(I0) = ZP(I0) - R(I0)
      IF (SS .LE. TOL) RETURN
      IF (I .EQ. ITMAX) IFAULT = 5
      IF (IFault .NE. 0) RETURN
      GOTO 40
      END
C
      SUBROUTINE LSQ1(N, ZM, ZP, R, AA, SS, IFL)
C
C      ALGORITHM AS 210.1 APPL. STATIST. (1985) VOL.34, NO.1
C
C      FINDS THE SUM-OF-SQUARES AND DERIVATIVES FOR FITTING
C      A 5-PARAMETER JOHNSON SC-CURVE
C
      REAL A1(3), A2(3), A3(3), A4(3), AA(N, N), EPS, EPS1, HUN, ONE,
* PT1, PT01, R(3), SS, TEN, TWO, X, X1, ZERO, ZM(3), ZP(3)
      DATA ZERO, ONE, TWO, TEN, PT1, PT01, HUN, EPS, EPS1
* / 0.0, 1.0, 2.0, 10.0, 0.1, 0.01, 100.0, 7.7, 34.0/
      IFL = 0
C
C      IF PARAMETER VALUES ARE OUT OF RANGE,
C      RETURN WITH ERROR MESSAGE
C
      IF (ZP(1) .LE. ZERO) IFL = 1
      IF (ZP(3) .LT. PT01 .OR. ZP(3) .GT. HUN) IFL = 2
      IF (IFL .NE. 0) RETURN
      IF ((EPS + ABS(ZP(2))) / ZP(1) .GT. EPS1) IFL = 3
      IF (IFL .NE. 0) RETURN
C
C      FIND MOMENTS GIVEN LATEST ESTIMATES
C
      CALL MOM1(N, ZP, A1, A2, A3, A4)
      SS = ZERO
      DO 10 I = 1, N
      R(I) = A1(I) - ZM(I)
      SS = SS * R(I) ** 2
      X = I

```

```

X1 = X * ZP(3)
AA(I, 1) = X1 * (A2(I) * ZP(2) + (A3(I) - X1 * (A2(I) - A3(I)))
* / ZP(1)) / ZP(1) ** 2
AA(I, 2) = -X1 * A2(I) / ZP(1)
IF (N .EQ. 3) AA(I, 3) = X * A4(I)
10 CONTINUE
RETURN
END

C
SUBROUTINE MOM1(N, ZP, A1, A2, A3, A4)

C
C ALGORITHM AS 210.2 APPL. STATIST. (1985) VOL.34, NO.1
C
C FINDS FITTED MOMENTS FOR 5-PARAMETER SB-CURVE
C LET AL=I*ALPHA, THEN
C A1(I)=E(X**AL)
C A2(I)=E(X**AL-X**(AL+ONE))
C A3(I)=E(X**(AL+ONE)-X**(AL+TWO))
C A4(I)=E(LOG(X)*X**AL)
C WHERE E() MEANS EXPECTED VALUE
C
REAL A1(N), A2(N), A3(N), A4(N), AB(10), CON, ONE, X, WT(10),
* Z, Z0, Z1, Z2, Z3, Z4, ZERO, ZP(3)

C
C WT AND AB ARE WEIGHTS AND ABSCISSAS FOR HERMITIAN INTEGRATION
C
DATA WT(1), WT(2), WT(3), WT(4), WT(5),
* WT(6), WT(7), WT(8), WT(9), WT(10)
* /0.2607930634495549E36, 0.161739333984E36,
* 0.6150637206397691E35, 0.13997837447101E35,
* 0.1830103131080493E34, 0.1288262799619294E33,
* 0.4402121090230853E31, 0.6127490259982946E29,
* 0.2482062362315179E27, 0.1257800672438E24/
DATA AB(1), AB(2), AB(3), AB(4), AB(5),
* AB(6), AB(7), AB(8), AB(9), AB(10)
* /0.34696415708135593, 1.04294534880275103,
* 1.74524732081412671, 2.45866361117236775,
* 3.18901481655338941, 3.94396735065731627,
* 4.73458133404605532, 5.57873880589320117,
* 6.51059015701365447, 7.61904854167975829/
DATA CON, ZERO, ONE /1.0E-36, 0.0, 1.0/
DO 10 I = 1, N
A1(I) = ZERO
A2(I) = ZERO
A3(I) = ZERO
A4(I) = ZERO
10 CONTINUE
DO 40 I = 1, 10
X = AB(I)
DO 30 I1 = 1, 2
Z = EXP((ZP(2) + X) / ZP(1))
Z0 = ONE / (Z + ONE)
Z1 = Z * Z0
Z2 = Z0 ** ZP(3)
Z3 = WT(I)
Z4 = ALOG(Z0)
DO 20 I2 = 1, N
Z3 = Z3 * Z2
A1(I2) = A1(I2) + Z3
Z = Z3 * Z1
A2(I2) = A2(I2) + Z

```

```
      A3(I2) = A3(I2) + Z * Z0
      A4(I2) = A4(I2) + Z3 * Z4
20     CONTINUE
      X = -X
30     CONTINUE
40     CONTINUE
      DO 50 I = 1, N
      A1(I) = A1(I) * CON
      A2(I) = A2(I) * CON
      A3(I) = A3(I) * CON
      A4(I) = A4(I) * CON
50     CONTINUE
      RETURN
      END
```

c This file includes ASR 71 and ASR 74 which provide replacements for  
c subroutines FALG and GALG respectively. The replacements have been  
c placed at the end.

```
c
      SUBROUTINE FGALG(A, RN, B, IP, K, IFAULT, NF)
C
C      ALGORITHM AS211 APPL. STATIST. (1985) VOL. 34, NO. 2
C      F-G DIAGONALIZATION ALGORITHM
C
      REAL A(5, 10, 10), H(5, 10, 10), RN(5), B(10, 10)
      REAL ZERO, ONE, P8, P6, G1, G2
      DATA ZERO /0.0/, ONE /1.0/, P8 /0.8/, P6 /0.6/
C
      CHECK INPUT PARAMETERS
C
      IFAULT = 1
      IF (K .LT. 1 .OR. K .GT. 5) RETURN
      IFAULT = 2
      IF (IP .LT. 2 .OR. IP .GT. 10) RETURN
      IFAULT = 3
      DO 3 I = 1, K
      IF (RN(I) .LE. ZERO) RETURN
3 CONTINUE
      DO 4 I = 1, K
      IFAULT = -I
      DO 4 L = 2, IP
      JEND = L - 1
      DO 4 J = 1, JEND
      IF (A(I, L, J) .NE. A(I, J, L)) RETURN
4 CONTINUE
      IFAULT = 0
C
      DO 5 L = 1, IP
      DO 5 J = 1, IP
      B(L, J) = ZERO
      IF (L .EQ. J) B(L, J) = ONE
5 CONTINUE
C
      DO 7 I = 1, K
      DO 7 L = 1, IP
      DO 7 J = 1, IP
7 H(I, L, J) = A(I, L, J)
      CALL FALG(A, RN, B, IP, K, IFAULT, NF)
      IF (IFAULT .NE. 0 .OR. NF .GT. 1) RETURN
C
      IF F-ALGORITHM STOPPED AFTER ONLY 1 ITERATION, TRY
C      ANOTHER INITIAL APPROXIMATION TO THE ORTHOGONAL MATRIX B.
C
      DO 8 I = 1, K
      DO 8 L = 1, IP
      DO 8 J = 1, IP
8 A(I, L, J) = H(I, L, J)
      IP1 = IP - 1
      DO 6 L = 1, IP1
      DO 6 J = 1, IP
      G1 = P8 * B(L, J) + P6 * B(L + 1, J)
      G2 = P8 * B(L + 1, J) - P6 * B(L, J)
      B(L, J) = G1
      B(L + 1, J) = G2
6 CONTINUE
      CALL FALG(A, RN, B, IP, K, IFAULT, NF)
```

```
RETURN  
END
```

C

```
SUBROUTINE FALG(A, RN, B, IP, K, IFAULT, NF)  
REAL A(5, 10, 10), RN(5), B(10, 10), BOLD(10, 10)  
REAL AUX(10, 10), T(5, 2, 2), Q(2, 2), G(10, 10)  
REAL EPS, EPSF, DIFF, ZERO  
DATA ZERO /0.0/, EPSF /0.0001/, MAXF /15/
```

C

```
NF = 0  
IFAULT = 0  
IP1 = IP - 1
```

C

C

C

```
START ITERATION STEP OF F-ALGORITHM
```

```
5 NF = NF + 1  
DO 6 L = 1, IP  
DO 6 J = 1, IP  
6 BOLD(L, J) = B(L, J)  
DO 7 L = 1, IP1  
JSTART = L + 1  
DO 7 J = JSTART, IP  
DO 8 M = 1, IP  
G(M, 1) = B(M, L)  
8 G(M, 2) = B(M, J)  
DO 9 I = 1, K  
DO 10 M1 = 1, IP  
DO 10 M2 = 1, IP  
10 AUX(M1, M2) = A(I, M1, M2)  
CALL MULT(AUX, G, IP, 2)  
T(I, 1, 1) = AUX(1, 1)  
T(I, 2, 1) = AUX(2, 1)  
T(I, 1, 2) = AUX(1, 2)  
T(I, 2, 2) = AUX(2, 2)  
9 CONTINUE
```

C

```
CALL GALG(T, Q, RN, K, IFAULT)  
IF (IFAULT .NE. 0) RETURN
```

C

```
DO 7 M = 1, IP  
B(M, L) = G(M, 1) * Q(1, 1) + G(M, 2) * Q(2, 1)  
B(M, J) = G(M, 1) * Q(1, 2) + G(M, 2) * Q(2, 2)  
7 CONTINUE  
EPS = ZERO  
DO 11 L = 1, IP  
DO 11 J = 1, IP  
DIFF = ABS(B(L, J) - BOLD(L, J))  
IF (DIFF .GT. EPS) EPS = DIFF  
11 CONTINUE  
IF (EPS .GE. EPSF .AND. NF .LT. MAXF) GOTO 5  
IF (EPS .GE. EPSF) IFAULT = 4  
DO 12 I = 1, K  
DO 13 L = 1, IP  
DO 13 J = 1, IP  
13 AUX(L, J) = A(I, L, J)  
CALL MULT(AUX, B, IP, IP)  
DO 12 L = 1, IP  
DO 12 J = 1, IP  
A(I, L, J) = AUX(L, J)  
12 CONTINUE  
RETURN
```



```

        END
C
        SUBROUTINE GALG(T, Q, RN, K, IFAULT)
        REAL T(5, 2, 2), Q(2, 2), RN(5), DELTA(5, 2), COEF(5), U(2, 2)
        REAL EPSG, ZERO, ONE, TWO, CO, SI, CO2, SI2, COSI, SINOLD, CP
        DATA ZERO /0.0/, ONE /1.0/, TWO /2.0/, EPSG /0.0001/
        MAXG = 5
C
        IF (K .EQ. 1) MAXG = 1
        CO = ONE
        SI = ZERO
C
        START ITERATION STEP OF G-ALGORITHM
C
        DO 1 NG = 1, MAXG
        SINOLD = SI
        CO2 = CO * CO
        SI2 = SI * SI
        COSI = TWO * CO * SI
C
        DO 2 I = 1, K
        DELTA(I, 1) = CO2 * T(I, 1, 1) + SI2 * T(I, 2, 2) + COSI *
        * T(I, 1, 2)
        DELTA(I, 2) = CO2 * T(I, 2, 2) + SI2 * T(I, 1, 1) - COSI *
        * T(I, 2, 1)
        IF (DELTA(I, 1) .GT. ZERO .AND. DELTA(I, 2) .GT. ZERO) GOTO 4
        IFAULT = -I
        RETURN
4 COEF(I) = RN(I) * (DELTA(I, 1) - DELTA(I, 2)) / (DELTA(I, 1)
        * * DELTA(I, 2))
2 CONTINUE
        DO 3 L = 1, 2
        DO 3 J = 1, 2
        U(L, J) = ZERO
        DO 3 I = 1, K
        U(L, J) = U(L, J) + COEF(I) * T(I, L, J)
3 CONTINUE
C
        CALL EIGVEC(U, Q)
C
        REORDER MATRIX Q AND/OR MULTIPLY COLUMN(S) BY -1 IF
        NECESSARY, SUCH THAT Q IS A ROTATION, AND Q(1,1) IS
        THE LARGEST ELEMENT
C
        INDEX = 1
        IF(ABS(Q(1, 1)) .LT. ABS(Q(1, 2))) INDEX = 2
        CP = Q(1, INDEX)
        CO = ABS(CP)
        SI = Q(2, INDEX)
        IF (CP .LT. ZERO) SI = -SI
        Q(1, 1) = CO
        Q(2, 1) = SI
        Q(1, 2) = -SI
        Q(2, 2) = CO
        IF (ABS(SI - SINOLD) .LT. EPSG) RETURN
1 CONTINUE
        RETURN
        END
C
        SUBROUTINE EIGVEC(U, Q)
        REAL U(2, 2), Q(2, 2)

```

```

REAL ZERO, ONE, TWO, ROOT, DENOM, EP
DATA ZERO /0.0/, ONE /1.0/, TWO /2.0/, EP /1 .E - 10/

```

```

C
ROOT = (U(1, 1) + U(2, 2)) / TWO
ROOT = ROOT + SQRT(((U(1, 1) - U(2, 2)) / TWO) ** 2 + U(1, 2)
* ** 2)
DENOM = SQRT((ROOT - U(1, 1)) ** 2 + U(1, 2) ** 2)
Q(1, 1) = ONE
Q(2, 1) = ZERO
IF (DENOM .LT. EP) GOTO 1
Q(1, 1) = U(1, 2) / DENOM
Q(2, 1) = (ROOT - U(1, 1)) / DENOM
1 Q(1, 2) = -Q(2, 1)
Q(2, 2) = Q(1, 1)
RETURN
END

```

```

C
SUBROUTINE MULT(A, B, IP, IQ)
REAL A(10, 10), B(10, 10), H(10, 10)
REAL ZERO
DATA ZERO /0.0/

```

```

C
DO 1 I = 1, IQ
DO 1 J = 1, IP
H(I, J) = ZERO
DO 1 K = 1, IP
H(I, J) = H(I, J) + B(K, I) * A(K, J)
1 CONTINUE
DO 2 I = 1, IQ
DO 2 J = 1, I
A(I, J) = ZERO
DO 3 K = 1, IP
3 A(I, J) = A(I, J) + H(I, K) * B(K, J)
A(J, I) = A(I, J)
2 CONTINUE
RETURN
END

```

```

C
C-----
C

```

```

SUBROUTINE FALG(A, RN, B, IP, K, IFAULT, NF)
C
C ASR 71 (REMARK ON AS 211) APPL. STATIST. (1988) VOL. 37, NO. 1
C
INTEGER I, IFAULT, IP, IP1, J, JSTART, K, L, M, NF, MAXF
REAL A(5, 10, 10), AUX(10, 10), B(10, 10), B1, B2, BOLD(10, 10)
REAL C, C2, DIFF, EPS, EPSF, Q(2, 2), R1, RN(5), S, T(5, 2, 2)
REAL T1, T2, ZERO, ONE, TWO
DATA ZERO /0.0/, ONE /1.0/, TWO /2.0/, EPSF /0.0001/, MAXF /15/

```

```

C
NF = 0
IFAULT = 0
IP1 = IP - 1
C
C INITIAL MULTIPLICATION
C
DO 2 I = 1, K
DO 1 L = 1, IP
DO 1 J = 1, IP
1 AUX(L, J) = A(I, L, J)
CALL MULT(AUX, B, IP, IP)

```

```
      DO 2 L = 1, IP
      DO 2 J = 1, IP
2     A(I, L, J) = AUX(L, J)
C
C       START ITERATION STEP OF F-ALGORITHM
C
4     NF = NF + 1
      DO 5 L = 1, IP
      DO 5 J = 1, IP
5     BOLD(L, J) = B(L, J)
      DO 8 L = 1, IP1
      JSTART = L + 1
      DO 8 J = JSTART, IP
      DO 6 I = 1, K
      T(I, 1, 1) = A(I, L, L)
      T(I, 1, 2) = A(I, L, J)
      T(I, 2, 1) = A(I, J, L)
      T(I, 2, 2) = A(I, J, J)
6     CONTINUE
C
C       GET ROTATION SINE AND COSINE
C
      CALL GALG(T, Q, RN, K, IFAULT)
      IF (IFAULT .NE. 0) RETURN
C
C       ROTATE B
C
      C = Q(1, 1)
      S = Q(2, 1)
      R1 = S / (ONE + C)
      DO 7 M = 1, IP
      B1 = B(M, L)
      B2 = B(M, J)
      B(M, L) = B1 + S * (B2 - R1 * B1)
      B(M, J) = B2 - S * (B1 + R1 * B2)
7     CONTINUE
C
C       UPDATE THE A MATRICES
C
      T1 = S / C
      T2 = T1 * T1
      C2 = C * C
      DO 8 I = 1, K
      A(I, L, L) = C2 * (T(I, 1, 1) + TWO * T1 * T(I, 1, 2) + T2 *
* T(I, 2, 2))
      A(I, J, J) = C2 * (T2 * T(I, 1, 1) - TWO * T1 * T(I, 1, 2)
* + T(I, 2, 2))
      A(I, L, J) = C2 * (T1 * (T(I, 2, 2) - T(I, 1, 1)) + (ONE - T2)
* * T(I, 1, 2))
      A(I, J, L) = A(I, L, J)
      DO 8 M = 1, IP
      IF (M .EQ. J .OR. M .EQ. L) GOTO 8
      B1 = A(I, M, L)
      B2 = A(I, M, J)
      A(I, M, L) = B1 + S * (B2 - R1 * B1)
      A(I, M, J) = B2 - S * (B1 + R1 * B2)
      A(I, L, M) = A(I, M, L)
      A(I, J, M) = A(I, M, J)
8     CONTINUE
C
C       CHECK FOR CONVERGENCE
```

```
C
  EPS = ZERO
  DO 9 L = 1, IP
  DO 9 J = 1, IP
  DIFF = ABS(B(L, J) - BOLD(L, J))
  IF (DIFF .GT. EPS) EPS = DIFF
9 CONTINUE
  IF (EPS .GE. EPSF .AND. NF .LT. MAXF) GOTO 4
  IF (EPS .GE. EPSF) IFAULT = 4
  RETURN
  END

C
C-----
C
C This is ASR 74
C
  SUBROUTINE GALG (T, Q, RN, K, IFAULT)
  REAL C, CO, EIGHT, EPSG, FMG, FOUR, H, ONE, PI, Q(2,2), RN(5), SI,
&      T(5,2,2), THETA, TMP, TWO, U, WT, ZERO
C
  DATA EPSG/1.0E-8/, ZERO/0.0/, ONE/1.0/, TWO/2.0/, FOUR/4.0/,
&      EIGHT/8.0/, PI/3.141592653589793238/
C
  FMG = ZERO
  H = ZERO
C
C          COMPUTE ITERATION CONSTANTS
  DO 1 I=1, K
  U = (T(I,2,2)-T(I,1,1))/TWO
  C = T(I,1,2)
  WT = RN(I)
  FMG = FMG + WT*(U*U-C*C)
1 H = H + WT*U*C
C
C          CHECK FOR DEGENERATE CASES
  IF (ABS(H) .LT. EPSG .OR. ABS(FMG) .LT. EPSG) GOTO 2
C
C          NODEGENERATE CASES (NO. 1 TO 4)
C
  THETA = ATAN(-TWO*H/FMG)/FOUR
C
C          CASES 2 AND 4
  IF (H .GT. ZERO .AND. FMG .LT. ZERO) THETA = THETA - PI/FOUR
  IF (H .LT. ZERO .AND. FMG .LT. ZERO) THETA = THETA + PI/FOUR
  GO TO 3
C
C          DEGENERATE CASES (NO. 5 TO 9)
C
2 THETA = ZERO
  IF (FMG .LE. -EPSG) THETA = -PI/FOUR
  IF (H .GE. EPSG) THETA = -PI/EIGHT
  IF (H .LE. -EPSG) THETA = PI/EIGHT
C
C          GET COSINES AND SINES FROM ANGLE
3 SI      = SIN(THETA)
  CO      = COS(THETA)
  Q(1,1) = CO
  Q(1,2) = -SI
  Q(2,1) = SI
  Q(2,2) = CO
  RETURN
  END
```

```

SUBROUTINE EXPFIT(N, X, Y, W, IC, CV, P, RSS, Z, IFAULT)
C
C     ALGORITHM AS 212  APPL.STATIST. (1985) VOL.34, NO.2
C
C     FITS EXPONENTIAL CURVE  $E(Y) = G_0 + G_1(1 - \exp(P \cdot X))/P$  USING
C     MODIFIED NEWTON ITERATIONS ON P AFTER ELIMINATING G0 AND G1
C
REAL X(N), Y(N), W(N), Z(N), CV(4), P(3), RSS
INTEGER IC(3)
REAL EPS1, EPS2, EXPMAX, ZERO, ONE, TWO, HALF, FIVE, XMAXP, XMINP,
* XMAXO, XMINO, XLOC, STEPMX, POWMAX, SY, POWNEW, YLOC, ZBAR,
* YBAR, SZZ, SZY, SW, BXCX0, BXCX1, BXCX2, D, ZDIF, YDIF, C, B1,
* B0, RSSNEW, RSSMAX, RSSMIN, POWMIN, DP, DPDP, D2ZDP2, ERR, WT,
* T, PLIM, PSTEP, DPDB0, DPDB1, XSC, DZDP
C
C     CONSTANTS - EXPMAX IS MACHINE DEPENDENT
C
DATA EPS1 /1.0E-6/, EPS2 /1.0E-4/, MAXIT /20/, EXPMAX /300.0/
DATA ZERO /0.0/, ONE /1.0/, TWO /2.0/, HALF /0.5/, FIVE /5.0/
C
C     CHECK FOR VALID PARAMETERS, FIND OVERALL MIN AND MAX OF X, ...
C
NDIFX = 0
IF (N .LE. 0) GOTO 30
IFAULT = 5
XMAXO = X(1)
XMINO = XMAXO
DO 20 I = 1, N
IF (W(I) .LT. ZERO) RETURN
XMAXO = AMAX1(X(I), XMAXO)
XMINO = AMIN1(X(I), XMINO)
IF (W(I) .EQ. ZERO) GOTO 20
C
C     ... ACCUMULATE MIN AND MAX WITH NON-ZERO WEIGHTS AND CHECK FOR
C     ENOUGH DISTINCT VALUES OF THIS TYPE
C
IF (NDIFX .NE. 0) GOTO 10
XMAXP = X(I)
XMINP = XMAXP
NDIFX = 1
GOTO 20
10 IF (X(I) .NE. XMINP .AND. X(I) .NE. XMAXP) NDIFX = NDIFX + 1
XMAXP = AMAX1(X(I), XMAXP)
XMINP = AMIN1(X(I), XMINP)
20 CONTINUE
30 IFAULT = 4
NPAR = 3
DO 40 I = 1, 3
IF (IC(I) .NE. 0) NPAR = NPAR - 1
40 CONTINUE
IF (NDIFX .LT. MAX0(NPAR, 2)) RETURN
C
STEPMX = FIVE / (XMAXP - XMINP)
IF (IC(2) .EQ. 0) GOTO 50
XMAXP = CV(2)
XMINP = XMAXP
50 POWMAX = HALF * EXPMAX / AMAX1(XMAXP - XMINO, XMAXO, XMINP, XMAXP,
* -XMINP)
IFAULT = 3
POWNEW = ZERO
IF (IC(3) .EQ. 0) GOTO 60

```

```

        POWNEW = CV(4)
        IF (ABS(POWNEW) .GT. POWMAX) RETURN
60 YLOC = ZERO
        IF (IC(2) .NE. 0) YLOC = CV(3)
        IF (IC(1) .NE. 0) YLOC = CV(1)
        SYY = ZERO
        IFAULT = 0
C
C        MAIN LOOP OF ALGORITHM
C
        DO 240 ITER = 1, MAXIT
C
C        FIND LSE OF LINEAR PARAMS FOR FIXED POWER P BY ....
C
70 ZBAR = ZERO
        YBAR = ZERO
        SZZ = ZERO
        SZY = ZERO
        SW = ZERO
        XLOC = XMINP
        IF (POWNEW .GT. ZERO) XLOC = XMAXP
C
C        ... FINDING TRANSFORMED Z VARIABLES AND ACCUMULATING SSQS ...
C
        DO 110 I = 1, N
        IF (IC(1) .EQ. 0) GOTO 80
        Z(I) = EXP((X(I) - XLOC) * POWNEW)
        GOTO 90
80 Z(I) = BXCX0((X(I) - XLOC), POWNEW)
C
90 D = W(I)
        IF (D .LE. ZERO) GOTO 110
        ZDIF = Z(I)
        YDIF = Y(I) - YLOC
        IF (IC(1) .NE. 0 .OR. IC(2) .NE. 0) GOTO 100
        SW = SW + D
        C = D / SW
        D = D * (ONE - C)
        ZDIF = ZDIF - ZBAR
        YDIF = YDIF - YBAR
        ZBAR = ZBAR + ZDIF * C
        YBAR = YBAR + YDIF * C
100 SZZ = SZZ + ZDIF * ZDIF * D
        SZY = SZY + ZDIF * YDIF * D
        IF (ITER .EQ. 1) SYY = SYY + YDIF * YDIF * D
110 CONTINUE
C
C        ... AND FROM THESE FINDING ESTIMATES, FITTED VALUES AND RSS(P)
C
        B1 = SZY / SZZ
        IF (IC(1) * IC(2) .NE. 0) B1 = CV(3) - CV(1)
        B0 = YBAR - B1 * ZBAR + YLOC
        IF (IC(1) * IC(2) .NE. 0) GOTO 120
        RSSNEW = SYY - B1 * SZY
        GOTO 130
120 RSSNEW = SYY + B1 * B1 * SZZ - TWO * B1 * SZY
130 DO 140 I = 1, N
140 Z(I) = B0 + B1 * Z(I)
        IF (IC(3) .GT. 0 .OR. RSSNEW .LE. ZERO) GOTO 1000
        IF (ITER .NE. 1) GOTO 150
        RSSMAX = RSSNEW

```

```

      GOTO 170
C
C      TEST FOR CONVERGENCE, TOO MANY ITERATIONS OR WHETHER RSS(P)
C      HAS INCREASED
C
150 IF (ABS(RSSNEW - RSSMIN) .LE. EPS1 * RSSMAX .AND. ABS(POWMIN -
      * POWNEW) .LE. EPS2 * ABS(POWMIN) .AND. DPDP .GE. ZERO) GOTO 1000
      IF (RSSNEW .LE. RSSMIN) GOTO 160
      POWNEW = (POWNEW + POWMIN) * HALF
      GOTO 70
160 IF (ITER .LT. MAXIT) GOTO 170
      IFAULT = 1
      GOTO 1000
170 RSSMIN = RSSNEW
      POWMIN = POWNEW
C
C      FIND DERIVATIVES OF RSS(P) W.R.T. POWER P BY ....
C
      DP = ZERO
      DPDP = ZERO
      DPDB0 = ZERO
      DPDB1 = ZERO
      DO 200 I = 1, N
C
C      ... FINDING DERIVATIVES OF EACH TRANSFORMED Z ...
C
      WT = W(I)
      IF (WT .LE. ZERO) GOTO 200
      XSC = X(I) - XLOC
      IF (IC(1) .EQ. 0) GOTO 180
      DZDP = XSC * EXP(XSC * POWMIN)
      D2ZDP2 = DZDP * XSC
      GOTO 190
180 DZDP = BXCX1(XSC, POWMIN)
      D2ZDP2 = BXCX2(XSC, POWMIN)
C
C      ... ACCUMULATING PARTIAL DERIVATIVES OF RSS W.R.T. ALL
C      PARAMETERS ...
C
190 ERR = Y(I) - Z(I)
      DP = DP + ERR * DZDP * WT
      DPDP = DPDP + (B1 * DZDP * DZDP - ERR * D2ZDP2) * WT
      DPDB1 = DPDB1 + (Y(I) - B0 - TWO * ERR) * DZDP * WT
      DPDB0 = DPDB0 + DZDP * WT
200 CONTINUE
      DP = -TWO * B1 * DP
      DPDP = TWO * B1 * DPDP
      DPDB1 = TWO * DPDB1
      DPDB0 = TWO * B1 * DPDB0
C
C      ... AND FROM THESE OBTAINING THE FULL DERIVATIVES W.R.T. P
C
      IF (IC(1) * IC(2) .NE. 0) GOTO 210
      T = DPDB1 - ZBAR * DPDB0
      DPDP = DPDP - HALF * T * T / SZZ
      IF (IC(1) .EQ. 0 .AND. IC(2) .EQ. 0) DPDP = DPDP - HALF * DPDB0 *
      * DPDB0 / SW
C
C      FIND MODIFIED NEWTON STEP FOR P, ENSURING THAT NEITHER THE
C      STEP NOR RESULTING POWER IS TOO LARGE
C

```

```

210 PLIM = STEPMX * FLOAT(ITER)
    IF (DPDP .NE. ZERO) GOTO 220
    PSTEP = SIGN(PLIM, DP)
    GOTO 230
220 PSTEP = DP / ABS(DPDP)
    IF (PSTEP .LT. -PLIM) PSTEP = -PLIM
    IF (PSTEP .GT. PLIM) PSTEP = PLIM
230 POWNEW = POWMIN - PSTEP
    IF (ITER .EQ. MAXIT - 1 .AND. ABS(PSTEP) * FLOAT(ITER) .GT. HALF *
* ABS(POWNEW) .OR. ABS(POWNEW) .GT. POWMAX) POWNEW = SIGN(POWMAX,
* -PSTEP)
    IF (POWMIN * POWNEW .GE. POWMAX * POWMAX) GOTO 1000
240 CONTINUE
C
C     FINALLY RETURN PARAMETER ESTIMATES
C
1000 RSS = AMAX1(RSSNEW, ZERO)
    IF (ABS(POWNEW) .GE. POWMAX) IFAULT = 2
    P(3) = POWNEW
    IF (IC(1) .EQ. 0) GOTO 1010
    T = B1 * EXP( - POWNEW * XLOC)
    P(1) = B0 + T
    P(2) = T * POWNEW
    RETURN
1010 P(2) = B1 * EXP( - XLOC * POWNEW)
    P(1) = B0 + B1 * BXCX0( - XLOC, POWNEW)
    RETURN
    END
C
REAL FUNCTION BXCX0(X, P)
C
C     ALGORITHM AS 212.1 APPL.STATIST. (1985) VOL.34, NO.2
C
C     EVALUATES (EXP(X*P) - 1)/P
C
REAL X, P
REAL EPS, ONE, XP, TERM, SERIES, AI
C
C     CONSTANTS - EPS IS MACHINE DEPENDENT
C
DATA EPS /1.0E-10/
DATA ONE /1.0/
C
XP = X * P
IF (ABS(XP) .LT. ONE) GOTO 10
BXCX0 = (EXP(XP) - ONE) / P
RETURN
10 TERM = ONE
SERIES = ONE
AI = ONE
20 AI = AI + ONE
TERM = TERM * XP / AI
SERIES = SERIES + TERM
IF (ABS(TERM) .GT. EPS) GOTO 20
BXCX0 = SERIES * X
RETURN
    END
C
REAL FUNCTION BXCX1(X, P)
C
C     ALGORITHM AS 212.2 APPL. STATIST. (1985) VOL.34, NO.2

```



```
C
C      EVALUATES DERIVATIVE OF (EXP(X*P) - 1)/P
C      WITH RESPECT TO P
C
REAL X, P
REAL EPS, HALF, ONE, TWO, XP, TERM, SERIES, AI
C
C      CONSTANTS - EPS IS MACHINE DEPENDENT
C
DATA EPS /1.0E-10/
DATA HALF /0.5/, ONE /1.0/, TWO /2.0/
C
XP = X * P
IF (ABS(XP) .LT. ONE) GOTO 10
BXCX1 = ((XP - ONE) * EXP(XP) + ONE) / (P * P)
RETURN
10 TERM = HALF
   SERIES = HALF
   AI = ONE
20 TERM = TERM * (AI + ONE) / AI / (AI + TWO) * XP
   SERIES = SERIES + TERM
   AI = AI + ONE
   IF (ABS(TERM) .GT. EPS) GOTO 20
   BXCX1 = SERIES * (X * X)
   RETURN
END
C
REAL FUNCTION BXCX2(X, P)
C
C      ALGORITHM AS 212.3 APPL. STATIST. (1985) VOL.34, NO.2
C
C      EVALUATES SECOND DERIVATIVE OF (EXP(X*P) - 1)/P
C      WITH RESPECT TO P
C
REAL X, P
REAL EPS, ONE, TWO, THREE, XP, TERM, SERIES, AI
C
C      CONSTANTS - EPS IS MACHINE DEPENDENT
C
DATA EPS /1.0E-10/
DATA ONE /1.0/, TWO /2.0/, THREE /3.0/
C
XP = X * P
IF (ABS(XP) .LT. ONE) GOTO 10
BXCX2 = (((XP - TWO) * XP + TWO) * EXP(XP) - TWO) / (P * P * P)
RETURN
10 TERM = ONE / THREE
   SERIES = TERM
   AI = ONE
20 TERM = TERM * (AI + TWO) / AI / (AI + THREE) * XP
   SERIES = SERIES + TERM
   AI = AI + ONE
   IF (ABS(TERM) .GT. EPS) GOTO 20
   BXCX2 = SERIES * (X * X * X)
   RETURN
END
```

```

SUBROUTINE RPCORM(NX, N, D, C, U, A, M, ISEED, IFAULT)
C
C     ALGORITHM AS213 APPL. STATIST. (1985) VOL. 34, NO. 2.
C     THIS ALGORITHM RANDOMLY SELECTS A CORRELATION MATRIX FROM THE
C     CLASS OF ALL CORRELATION MATRICES WITH SPECIFIED EIGENVALUES
C
REAL D(NX), C(NX, NX), U(NX), A(NX, NX)
INTEGER M(NX, 3)
DATA EPS /0.00001/
DATA ZERO, ONE, TWO, FOUR, ZP25, ZP5 /0.0, 1.0, 2.0, 4.0, 0.25,
* 0.5/
C
IFAULT = 0
IF(N .GT. 0) GOTO 40
10 IFAULT = 1
RETURN
20 IFAULT = 2
RETURN
30 IFAULT = 3
RETURN
40 IF(N .GT. NX) GOTO 10
TT = ZERO
DO 60 I = 1, N
IF(D(I) .LT. ZERO) GOTO 10
TT = TT + D(I)
DO 50 J = 1, N
50 A(I, J) = ZERO
A(I, I) = ONE
60 CONTINUE
IF (ABS(TT - FLOAT(N)) .GT. EPS * FLOAT(N)) GOTO 10
C
C     GENERATE AN ORTHOGONAL MATRIX A FROM THE INVARIANT MEASURE ON
C     THE GROUP OF ORTHOGONAL MATRICES.  CONSTRUCT A ONE COLUMN AT
C     A TIME.
C
DO 300 L = 1, N
NMLP1 = N - L + 1
CALL GGNOR(ISEED, NMLP1, U(L))
IF(L .EQ. N) GOTO 260
SS = ZERO
DO 120 I = L, N
120 SS = SS + U(I) * U(I)
UL = SQRT(SS)
IF(UL .EQ. ZERO) GOTO 20
C
C     CALCULATE LENGTH OF U AND STORE IT IN UL.  RANDOMLY CHOSE
C     SIGN OF UL TO PREVENT LOSS OF SIGNIFICANCE IN VL.
C
UL = SIGN(UL, -U(L))
C
C     PROJECT U ONTO ORTHOGONAL COMPLEMENT OF FIRST L-1 COLUMNS OF
C     A, NORMALIZE AND STORE THE PROJECTION IN L-TH COLUMN OF A.
C     CALCULATE PROJECTION MATRIX FOR ORTHOGONAL COMPLEMENT OF
C     FIRST L COLUMNS OF A AND STORE IT IN LAST N-L COLUMNS OF A.
C
LP1 = L + 1
VL = UL - U(L)
DO 250 I = 1, N
TT = ZERO
DO 230 J = L, N
230 TT = TT + A(I, J) * U(J)

```

```

      HV = TT / UL
      HW = (HV - A(I, L)) / VL
      A(I, L) = HV
      DO 240 J = LP1, N
240  A(I, J) = A(I, J) - HW * U(J)
250  CONTINUE
C
C      ASSIGN RANDOM ORIENTATION TO L-TH COLUMN OF A.
C
260  IF(U(L) .GT. ZERO) GOTO 300
      DO 270 I = 1, N
270  A(I, L) = -A(I, L)
300  CONTINUE
C
C      COMPUTE RANDOM COVARIANCE MATRIX C=ADA'
C
      DO 310 J = 1, N
      DO 310 I = J, N
      C(I, J) = ZERO
      DO 305 K = 1, N
305  C(I, J) = C(I, J) + A(I, K) * D(K) * A(J, K)
310  CONTINUE
      DO 315 J = 2, N
      JM1 = J - 1
      DO 315 I = 1, JM1
      C(I, J) = C(J, I)
315  CONTINUE
C
C      RANDOMLY SELECT TWO DIAGONAL ELEMENTS OF C, ONE GREATER THAN
C      ONE AND THE OTHER LESS THAN ONE, THEN CONSTRUCT THE APPRO-
C      PRIATE 2X2 ROTATIONAL MATRIX WHICH SETS ONE DIAGONL ELEMENT
C      EQUAL TO ONE WHILE MAINTAINING THE STRUCTURE OF EIGENVALUES
C
      NK = 0
      DO 320 I = 1, N
      IF(ABS(C(I, I) - ONE) .GT. EPS) GOTO 320
      NK = NK + 1
      M(NK, 1) = I
320  CONTINUE
      NM = N - NK - 1
      IF(NM .EQ. -1) RETURN
      IF(NM .EQ. 0) GOTO 30
      SUM = ZERO
      DO 400 NN = 1, NM
      IG = 0
      IL = 0
      DO 350 K = 1, N
C
C      M(.,1), M(.,2) AND M(.,3) STORE INDICES OF DIAGONAL ELEMENTS
C      OF C WHICH ARE .EQ. ONE, .GT. ONE, AND .LT. ONE RESPECTIVELY
C
      DO 330 KK = 1, NK
      IF (K .EQ. M(KK, 1)) GOTO 350
330  CONTINUE
      IF (C(K, K) .GT. (ONE + EPS)) GOTO 340
      IL = IL + 1
      M(IL, 3) = K
      GOTO 350
340  IG = IG + 1
      M(IG, 2) = K
350  CONTINUE

```

```

      IF (IL * IG .EQ. 0) GOTO 30
      II = INT(GGUBF(ISEED) * IG) + 1
      JJ = INT(GGUBF(ISEED) * IL) + 1
      I1 = M(II, 2)
      J1 = M(JJ, 3)
      I = MIN0(I1, J1)
      J = MAX0(I1, J1)
      IF (ABS(C(I, I) - ONE) .LE. EPS) GOTO 390
C
C      SOLVE THE QUADRATIC EQUATION AND DETERMINE THE ROTATION ANGLE
C
      CII = C(I, I)
      CIJ = C(I, J)
      CJJ = C(J, J)
      CIIMJJ = CII - CJJ
      CIIPJJ = CII + CJJ - TWO
      CIJIJ = CIJ * CIJ
      CA = CIJIJ + ZP25 * CIIMJJ * CIIMJJ
      CB = ZP5 * CIIPJJ * CIIMJJ
      CC = ZP25 * CIIPJJ * CIIPJJ - CIJIJ
      DT = SQRT(CB * CB - FOUR * CA * CC)
C
C      RANDOMLY SELECT ONE OF THE TWO POSSIBLE SOLUTIONS
C
      IF (GGUBF(ISEED) .GE. ZP5) DT = -DT
      THETA = ARCOS(ZP5 * (-CB + DT) / CA) / TWO
      CS = COS(THETA)
      SN = SIN(THETA)
C
C      CHOOSE THE CORRECT DIRECTION OF ROTATION
C
      IF (ABS(CS * CS * CII + SN * SN * CJJ + TWO * CS * SN * CIJ - ONE)
* .GT. EPS) SN = -SN
C
C      COMPUTE C=PCP' USING THE FACT THAT P IS A ROTATIONAL
C      MATRIX WITH THE ROTATION BEING OPERATED BY 2 X 2 MATRIX
C      (CS SN) / (-SN CS). ONLY ELEMENTS OF I AND J-TH ROWS
C      (HENCE COLUMNS) OF C ARE CHANGED BY THE ROTATION.
C
      DO 360 II = 1, N
      DO 360 JJ = 1, N
360 A(II, JJ) = C(II, JJ)
      A(I, I) = CS * CS * CII + SN * SN * CJJ + TWO * CS * SN * CIJ
      IF(ABS(A(I, I) - ONE) .GT. EPS) GOTO 30
      M(NN, 1) = I
      NK = NK + 1
      A(J, J) = CS * CS * CJJ + SN * SN * CII - TWO * CS * SN * CIJ
      A(J, I) = (CS * CS - SN * SN) * CIJ + CS * SN * (CJJ - CII)
      A(I, J) = A(J, I)
      DO 370 L = 1, N
      IF(L .EQ. I .OR. L .EQ. J) GOTO 370
      A(I, L) = CS * C(I, L) + SN * C(J, L)
      A(J, L) = -SN * C(I, L) + CS * C(J, L)
      A(L, I) = A(I, L)
      A(L, J) = A(J, L)
370 CONTINUE
      DO 380 II = 1, N
      DO 380 JJ = 1, N
380 C(II, JJ) = A(II, JJ)
390 SUM = SUM + C(I, I)
400 CONTINUE

```

```
C
C      SET THE REMAINING DIAGONAL ELEMENT TO BE (N-SUM) AND
C      SEE IF IT IS WITHIN THE SPECIFIED PRECISION LIMIT
C
C(N, N) = FLOAT(N) - SUM
IF(ABS(C(N, N) - ONE) .GT. EPS) GOTO 30
RETURN
END
```

```

    subroutine monte(est, conf, nsims, simval, ordval, lsb, sbound,
# lbb, bbound, alow, ahi, blow, bhi, clow, chi, dlow, dhi,
# ifault)
    implicit double precision (a-h,o-z)

c
c     Algorithm AS214 Appl. Statistics. (1985) vol. 34, no. 3
c
c     Sets up monte carlo confidence intervals
c     uses function ppnd - algorithm AS 111 (see also AS241)
c
    logical lsb, lbb
    dimension simval(nsims), ordval(nsims)
    data least /5/
    data zero, half, one, two, hun, big /0.0d0,
# 0.5d0, 1.0d0, 2.0d0, 1.0d2, 1.0d20 /

c
    ifault = 0
    sbnd = sbound
    bbnd = bbound
    if (conf .ge. hun) ifault = 6
    if (conf .le. zero) ifault = 7
    if (ifault .gt. 0) return

c
c     Symmetric mci
c
c     Find mean and variance
c
    v1 = zero
    v2 = zero
    do 10 j = 1, nsims
        fj = float(j)
        v2 = v2 + (fj - one) * (simval(j) - v1) ** 2 / fj
        v1 = (simval(j) + (fj - one) * v1) / fj
10    continue
    stderr = zero
    if (v2 .gt. zero) stderr = sqrt(v2 / float(nsims - 1))
    alpha = half * (hun - conf) / hun
    z = -ppnd(alpha, ifault)
    if (ifault .eq. 0) goto 20
    ifault = 6
    return
20    ahi = z * stderr
        alow = est - ahi
        ahi = est + ahi

c
c     Calculate bias adjustment, so that the number of values that
c     must be ordered is known
c
    call biasad(est, nsims, simval, z, limit1, limit2, ifault)
    limit1 = alpha * float(nsims + 1) + half
    limitu = (one-alpha) * float(nsims + 1) + half
    if (limit1 .lt. least) ifault = 5
    if (limit1 .eq. limitu) ifault = 7
    if (ifault .gt. 0) return
    l1 = max0(limit1, 2 * limit1)
    l2 = min0(limit2, 2 * limitu - nsims - 1)
    if (lsb) sbnd = -big
    if (lbb) bbn = big

c
c     Select and order the l1 smallest and the nsims+1-l2 largest
c     values

```

```
c
    call order(simval,ordval, nsims, 11, 12)
    if (sbnd .le. ordval(1)) goto 40
    if (lsb) goto 30
    ifault = 1
    return
30  sbnd = ordval(1) * two
    if (sbnd .gt. zero) sbnd = -sbnd
40  if (bbnd .ge. ordval(nsims)) goto 60
    if (lbb) goto 50
    ifault = 2
    return
50  bbnd = ordval(nsims) * two
    if (bbnd .lt. zero) bbnd = -bbnd
c
c      Equal tails mci ( percentile method )
c
60  blow = ordval(limitl)
    bhi = ordval(limitu)
c
c      Bias-corrected percentile method
c
    clow = sbnd
    if (limit1 .gt. 0) clow = ordval(limit1)
    chi = bbnd
    if (limit2 .le. nsims) chi = ordval(limit2)
c
c      Minimum lenght mci
c
    call lmin(ordval, nsims, sbnd, bbnd, limitl, limitu, dlow, dhi)
    return
end
c
c
c
c
c
c
c      subroutine biasad(est, nsims, simval, z, limit1, limit2, ifault)
c      implicit double precision (a-h,o-z)
c
c      Finds adjustment required to implement bias corrected
c      percentile method
c
c      Uses functions alnorm and ppnd -
c      algorithms AS 66 and AS 111
c
c      dimension simval(nsims)
c      data half, two/0.5d0, 2.0d0/
c
c      j = 0
c      k = 0
c
c      m = (number of values less than est)+(half the number equal to est),
c      rounded up if not integral
c
c      do 30 m = 1, nsims
c          if (simval(m) - est) 10, 20, 30
10      j = j + 1
20      k = k + 1
30      continue
    m = (j + k + 1) / 2
```

```
    if (m .eq. 0) ifault = 3
    if (m .eq. nsims) ifault = 4
    if (ifault .gt. 0) return
    zed = two * ppnd(float(m) / float(nsims), ifail)
c
c ifail cannot exceed 0 since m .ge. 1 and m .le. (nsims-1)
c
    fn1 = float(nsims + 1)
    limit1 = fn1 * alnorm(zed - z, .false.) + half
    limit2 = fn1 * alnorm(zed + z, .false.) + half
    return
end
c
c
c
c
c
c
    subroutine order(simval, ordval, nsims, l1, l2)
    implicit double precision (a-h, o-z)
c
c     Orders the smallest and largest values from simval and
c     puts them in ordval
c
    dimension simval(nsims), ordval(nsims)
c
    ordval(1) = simval(1)
    ordval(nsims) = ordval(1)
    lm1 = 1
    lm2 = nsims
    do 100 j = 2, nsims
        if (simval(j) .lt. ordval(lm1)) goto 10
        if (lm1 .eq. 11) goto 50
        lm1 = lm1 + 1
        ordval(lm1) = simval(j)
        goto 50
10     if (lm1 .lt. 11) lm1 =lm1 +1
        if (lm1 .eq. 2) goto 30
        l1 =lm1 -2
        do 20 k = 1, l1
            kk = lm1 - k
            ordval(kk + 1) = ordval(kk)
            if (ordval(kk-1) .le. simval(j)) goto 40
20     continue
30     ordval(2) = ordval(1)
        kk=1
40     ordval(kk) = simval(j)
50     if (simval(j) .gt. ordval(lm2)) goto 60
        if (lm2 .eq. 12) goto 100
        lm2 = lm2 - 1
        ordval(lm2) = simval(j)
        goto 100
60     if (lm2 .gt. 12) lm2 = lm2 - 1
        if (lm2 .eq. nsims - 1) goto 80
        l1 = nsims - 2
        do 70 k = lm2, l1
            kk = k + 1
            ordval(k) = ordval(kk)
            if (ordval(kk + 1) .ge. simval(j)) goto 90
70     continue
80     kk = nsims
```



```
ordval(kk -1) = ordval(kk)
90 ordval(kk) = simval(j)
100 continue
return
end

c
c
c
subroutine lmin(ordval, nsims, sbnd, bbnd, limitl, limitu,
#dlow,dhi)
implicit double precision (a-h, o-z)

c
c Finds the interval with minimum length
c
dimension ordval(nsims)
length = limitu - limitl
numb = nsims - length
diff = ordval(nsims) - ordval(1)
l = 0
do 10 k = 1, numb
kk = k + length
if (diff .le. ordval(kk) - ordval(k)) goto 10
l = k
diff = ordval(kk) - ordval(k)
10 continue
dlow = ordval(l)
l = l + length
dhi = ordval(l)
l = numb + 1
if (dhi - dlow .le. bbnd - ordval(l)) goto 20
dlow = ordval(l)
dhi = bbnd
20 l = length
if (dhi - dlow .le. ordval(l) -sbnd) return
dlow = sbnd
dhi = ordval (l)
return
end
```

```
SUBROUTINE MLEGEV(X, N, PARA, VCOV, MONIT, IFAULT)
```

```
C      ALGORITHM AS215  APPL. STATIST. (1985) VOL. 34, NO. 3
C      Modifications in AS R76 (1989) have been incorporated.
```

```
C      Additional modifications by J. R. M. Hosking, August 1994:
C      Modify steepest-ascent step so that it is invariant to
C      rescaling the data. Improves chance of convergence from
C      poor initial values.
```

```
C      MAXIMUM-LIKELIHOOD ESTIMATION OF GENERALIZED EXTREME-VALUE
C      DISTRIBUTION
```

```
DOUBLE PRECISION PARA(3), VCOV(6), X(N)
DOUBLE PRECISION A, ACCA, ACCG, ACCU, AI, AIGI, AN, D, DA, DAA,
* DAG, DELA, DELG, DELU, DG, DGG, DU, DUA, DUG, DUU, E, F, FOLD,
* G, GAI, GG, GI, GIPQ, GNORM, H, HALF, HE, HH, ONE, P, PA, PQ,
* PQG, PU, Q, QA, QU, R, RA, RATIO, RG, RU, SE, SH, SHE, SHH,
* SHHE, SMALL, SRF, STEPA, STEPG, STEPUP, SY, SYE, SYHE, SYYE,
* TEMP1, TEMP2, U, VLNEG, XMAX, XMIN, Y, YE, Z, ZERO
CHARACTER*8 ACTI1, ACTI2, ACTI3, ACTI4, ACTI5, ACTI6, ACTI7,
* ACTI8, ACTI9
DATA ACTI1/' NEWTON'/, ACTI2/' ST.ASC'/, ACTI3/' RESETK'/,
* ACTI4/' SR.INF'/, ACTI5/' SR.LIK'/, ACTI6/' MAX.SR'/,
* ACTI7/' MAX.EV'/, ACTI8/' MAX.IT'/, ACTI9/' CONVD' /
DATA ZERO /0.0D0/, HALF /0.5D0/, ONE/1.0D0/
```

```
C      ADDU,ACCA,ACCG ARE ACCURACY CRITERIA FOR TESTING CONVERGENCE
C      STEPUP,STEPSA,STEPG ARE MAXIMUM STEPLENGTHS FOR ITERATIONS
C      ACCU,ACCA,STEPUP,STEPSA ARE SCALED BY CURRENT VALUE OF A WHEN
C      USED IN PROGRAM
```

```
DATA ACCU, ACCA, ACCG /3 * 1D-5/, STEPUP, STEPSA, STEPG /
* 0.5D0, 0.25D0, 0.2D0/
```

```
C      MAXIT IS MAX. NO. OF ITERATIONS
C      MAXEV IS MAX. NO. OF EVALUATIONS OF LIKELIHOOD FUNCTION
C      SRF IS STEPLENGTH REDUCTION FACTOR
C      MAXSR IS MAX. NO. OF STEPLENGTH REDUCTIONS PERMITTED PER
C      ITERATION
```

```
DATA MAXIT /30/, MAXEV /50/, SRF /0.25D0/, MAXSR /30/
```

```
C      SMALL IS A SMALL NUMBER, USED TO ADJUST THE SHAPE PARAMETER TO
C      AVOID AN EXACT ZERO VALUE OR BORDERLINE INFEASIBILITY
C      ALNEG IS A LARGE NEGATIVE NUMBER, USED TO INITIALIZE
C      LOG-LIKELIHOOD
```

```
DATA SMALL /1.D-3/, VLNEG /-1.D37/
```

```
C      FIND MIN AND MAX DATA VALUE
```

```
DO 10 I = 1, 6
10  VCOV(I) = ZERO
    IFAULT = 1
    IF (N .LE. 2) GOTO 170
    XMIN = X(1)
    XMAX = X(1)
    DO 20 I = 2, N
        IF (X(I) .LT. XMIN) XMIN = X(I)
        IF (X(I) .GT. XMAX) XMAX = X(I)
```

```

20 CONTINUE
C
C     INITIALIZATION
C     U IS LOCATION PARAMETER
C     A IS SCALE PARAMETER
C     G IS SHAPE PARAMETER
C
IF (MONIT .GT. 0) WRITE (6, 6000)
IFAULT = 0
NITER = 0
NEVAL = 0
FOLD = VLNEG
U = PARA(1)
A = PARA(2)
G = PARA(3)
IF (ABS(G) .LT. SMALL) G = SMALL
IF (A .LE. ZERO) A = ONE
AN = DBLE(FLOAT(N))
C
C     CHECK WHETHER ALL DATA POINTS LIE WITHIN THE RANGE OF THE GEV
C     DISTRIBUTION WITH THE INITIAL PARAMETERS - IF NOT, ADJUST THE
C     SHAPE PARAMETER SO AS TO BRING ALL POINTS WITHIN RANGE
C
IF (G .GT. ZERO) GOTO 30
IF (XMIN .GE. U) GOTO 40
Z = A / (XMIN - U)
IF (G .GT. Z) GOTO 40
IF (MONIT .GT. 0) WRITE (6, 6010) NITER, NEVAL, U, A, G, ACTI3
G = Z + SMALL
IF (G .GE. ZERO) G = HALF * Z
GOTO 40
30 IF (XMAX .LE. U) GOTO 40
Z = A / (XMAX - U)
IF (G .LT. Z) GOTO 40
IF (MONIT .GT. 0) WRITE (6, 6010) NITER, NEVAL, U, A, G, ACTI3
G = Z - SMALL
IF (G .LE. ZERO) G = HALF * Z
C
C     START OF MAIN LOOP
C
40 DO 140 NITER = 1, MAXIT
C
NSR = 0
50 IF (NEVAL .GE. MAXEV) GOTO 150
NEVAL = NEVAL + 1
AI = ONE / A
GI = ONE / G
GAI = G * AI
AIGI = AI * GI
GG = ONE - G
C
C     ACCUMULATE SUMS OF QUANTITIES OCCURRING IN LIKELIHOOD
C     DERIVATIVES
C
C     IN PRESCOTT AND WALDEN'S NOTATION:
C     Z IS  $1 - K * (X(I) - U) / A$ 
C     Y IS THE REDUCED VARIATE -  $(1/K) * \text{LOG}(Z)$ 
C     E IS  $\text{EXP}(-Y)$ 
C     H IS  $\text{EXP}(K*Y)$ 
C
SY = ZERO

```

```

SE = ZERO
SYE = ZERO
SYYE = ZERO
SH = ZERO
SHE = ZERO
SYHE = ZERO
SHHE = ZERO
SHH = ZERO
DO 60 I = 1, N
  Z = ONE -GAI * (X(I) - U)
  Y = -GI * LOG(Z)
  E = EXP(-Y)
  H = ONE / Z
  YE = Y * E
  HE = H * E
  HH = H * H
  SY = SY + Y
  SE = SE + E
  SYE = SYE + YE
  SYYE = SYYE + Y * YE
  SH = SH + H
  SHE = SHE + HE
  SYHE = SYHE + Y * HE
  SHHE = SHHE + HH * E
  SHH = SHH + HH

```

60 CONTINUE

C  
C F IS CURRENT VALUE OF LIKELIHOOD FUNCTIONN  
C

```

F = -AN * LOG(A) - GG * SY - SE
IF (F .GT. FOLD) GOTO 90

```

C  
C LIKELIHOOD HAS NOT INCREASED - REDUCE STEPLENGTH AND TRY AGAIN  
C

```

IF (MONIT .GT. 0) WRITE(6, 6010) NITER, NEVAL, U, A, G, ACTI5, F
IF (NSR .EQ. MAXSR) GOTO 80

```

70 NSR = NSR + 1

```

U = U - DELU
A = A - DELA
G = G - DELG
DELU = SRF * DELU
DELA = SRF * DELA
DELG = SRF * DELG
U = U + DELU
A = A + DELA
G = G + DELG

```

IF (A .GT. G \* (XMIN - U) .AND. A .GT. G \* (XMAX - U) .AND. G .NE.  
\* ZERO) GO TO 50

```

IF (MONIT .GT. 0) WRITE (6, 6010) NITER, NEVAL, U, A, G, ACTI4
IF (NSR .LT. MAXSR) GOTO 70

```

C  
C MAX. NO. OF STEPLENGTH REDUCTIONS REACHED  
C IF CURRENT ITERATION IS NEWTON-RAPHSON, TRY STEEPEST ASCENT  
C INSTEAD. IF CURRENT ITERATION IS STEEPEST ASCENT, GIVE UP.  
C

80 U = U - DELU

```

A = A - DELA
G = G - DELG
IF (MONIT .GT. 0) WRITE(6, 6010) NITER, NEVAL, U, A, G, ACTI6
IF (ITYPE .EQ. 1) GOTO 100
IFFAULT = 4

```

```

      GOTO 160
C
C      P,Q,R, ARE AS DEFINED IN FLOOD STUDIES REPORT
C
90 FOLD = F
   P = AN - SE
   Q = SHE - GG * SH
   R = AN - SY + SYE
   PQ = P + Q
   GIPQ = GI * PQ
C
C      FIRST DERIVATIVES OF LOG-LIKELIHOOD
C
   DU = -AI * Q
   DA = -AIGI * PQ
   DG = -GI * (R - GIPQ)
   IF (MONIT .GT. 0) GNORM = SQRT(DU * DU + DA * DA + DG * DG)
C
C      DERIVATIVES OF P,Q,R
C
   PU = -AI * SHE
   PA = GI * PU + AIGI * SE
   QU = GG * AI * (SHHE + G * SHH)
   RU = AI * (SH - SHE + SYHE)
   RA = GI * RU - AIGI * (AN - SE + SYE)
   RG = GI * (SY - SYE + SYE - A * RA)
   QA = AI * Q + GI * (PU + QU)
   PQG = GIPQ + A * (RA - GI * (PA + QA))
C
C      MINUS SECOND DERIVATIVE OF LOG-LIKELIHOOD (HESSIAN MATRIX)
C
   DUU = AI * QU
   DUA = AIGI * (PU + QU)
   DAA = -AIGI * (AI * PQ - PA - QA)
   DUG = GI * (RU - GI * (PU + QU))
   DAG = -AIGI * (GIPQ - PQG)
   DGG = GI * (RG - GI * (PQG + R - GIPQ - GIPQ))
C
C      INVERT HESSIAN MATRIX
C
DO 95 KK = 1, 3
   IF (DUU .LE. ZERO) GO TO 100
   D = ONE / DUU
   TEMP1 = -DUA * D
   IF (KK .GT. 2) TEMP1 = -TEMP1
   TEMP2 = -DUG * D
   IF (KK .GT. 1) TEMP2 = -TEMP2
   DUU = DAA + TEMP1 * DUA
   DUA = DAG + TEMP1 * DUG
   DAA = DGG + TEMP2 * DUG
   DUG = TEMP1
   DAG = TEMP2
   DGG = D
95 CONTINUE
C
C      CALCULATE STEPLENGTHS
C
   ITYPE = 1
   IF (MONIT .GT. 0) WRITE(6, 6010) NITER, NEVAL, U, A, G, ACTI1, F,
*   GNORM
   DELU = DUU * DU + DUA * DA + DUG * DG

```

```

      DELA = DUA * DU + DAA * DA + DAG * DG
      DELG = DUG * DU + DAG * DA + DGG * DG
      RATIO = MAX(ABS(DELU) / (STEPU * A), ABS(DELA) / (STEPS * A),
*   ABS(DELG) / STEPG)
      IF (RATIO .LT. ONE) GOTO 110
      RATIO = ONE / RATIO
      DELU = DELU * RATIO
      DELA = DELA * RATIO
      DELG = DELG * RATIO
      GOTO 110

C
C       HESSIAN IS NOT POSITIVE DEFINITE - MAKE A LARGE STEP IN THE
C       DIRECTION OF STEEPEST ASCENT
C
100  ITYPE = 2
      IF (MONIT .GT. 0) WRITE(6, 6010) NITER, NEVAL, U, A, G, ACTI2, F,
*   GNORM
C----- NEXT 11 LINES ADDED, AUG.94
      D = ABS(VLNEG)
      TEMP1 = D
      IF (DU .NE. ZERO) TEMP1 = STEPDU / (ABS(DU) * A)
      TEMP2 = D
      IF (DA .NE. ZERO) TEMP2 = STEPA / (ABS(DA) * A)
      Z = D
      IF (DG .NE. ZERO) Z = STEPG / ABS(DG)
      RATIO = MIN(TEMP1, TEMP2, Z)
      DELU = RATIO * DU * A * A
      DELA = RATIO * DA * A * A
      DELG = RATIO * DG
C----- NEXT 11 LINES REMOVED, AUG.94
C       D = ABS(VLNEG)
C       TEMP1 = D
C       IF (DU .NE. ZERO) TEMP1 = STEPDU * A / ABS(DU)
C       TEMP2 = D
C       IF (DA .NE. ZERO) TEMP2 = STEPA * A / ABS(DA)
C       Z = D
C       IF (DG .NE. ZERO) Z = STEPG / ABS(DG)
C       RATIO = MIN(TEMP1, TEMP2, Z)
C       DELU = RATIO * DU
C       DELA = RATIO * DA
C       DELG = RATIO * DG
C----- END OF DELETED CODE
C
C       ADJUST PARAMETERS
C
110  U = U + DELU
      A = A + DELA
      G = G + DELG

C
C       TEST FOR FEASIBILITY
C
      IF (A .GT. G * (XMIN - U) .AND. A .GT. G * (XMAX - U) .AND. G .NE.
*   ZERO) GOTO 130
      DO 120 NSR = 1, MAXSR
      IF (MONIT .GT. 0) WRITE(6, 6010) NITER, NEVAL, U, A, G, ACTI4
      U = U - DELU
      A = A - DELA
      G = G - DELG
      DELU = SRF * DELU
      DELA = SRF * DELA
      DELG = SRF * DELG

```

```
      U = U + DELU
      A = A + DELA
      G = G + DELG
      IF (A .GT. G * (XMIN - U) .AND. A .GT. G * (XMAX - Y) .AND.
*       G .NE. ZERO) GOTO 140
120  CONTINUE
      GOTO 80
C
C       TEST FOR CONVERGENCE
C
130  IF (ABS(DELU) .GT. ACCU * A) GOTO 140
      IF (ABS(DELA) .GT. ACCA * A) GOTO 140
      IF (ABS(DELG) .GT. ACCG) GOTO 140
      IF (MONIT .GT. 0) WRITE(6, 6010) NITER, NEVAL, U, A, G, ACTI9
      VCOV(1) = DUU
      VCOV(2) = DUA
      VCOV(3) = DAA
      VCOV(4) = DUG
      VCOV(5) = DAG
      VCOV(6) = DGG
      GOTO 160
C
C       END OF MAIN LOOP
C
140  CONTINUE
C
C       ITERATIONS NOT CONVERGED - SET FAULT FLAG
C
      IFAULT = 2
      IF (MONIT .GT. 0) WRITE(6, 6010) MAXIT, NEVAL, U, A, G, ACTI8
      GOTO 160
150  IFAULT = 3
      IF (MONIT .GT. 0) WRITE(6, 6010) NITER, MAXEV, U, A, G, ACTI7
C
C       ITERATION FINISHED -COPY RESULTS INTO ARRAY PARA
C
160  IF (MONIT .GT. 0) WRITE(6, 6020)
      PARA(1) = U
      PARA(2) = A
      PARA(3) = G
      RETURN
C
170  DO 180 I = 1, 3
180  PARA(I) = ZERO
      RETURN
C
6000  FORMAT(/' MAXIMUM-LIKELIHOOD ESTIMATION OF GENERALIZED EXTREME',
* 1X, 'VALUE DISTRIBUTION'// ' ITER EVAL', 8X, 'XI', 5X, 'ALPHA',
* 9X, 'K ACTION', 6X, 'LOG-L', 7X, 'GNORM')
6010  FORMAT(1X, I4, I5, 3F10.4, 1X, A, F11.3, 1PD12.2)
6020  FORMAT(1H0)
      END
```

```

SUBROUTINE COMBIN(S, IS, R, IR, N, ODMAX, DIMAX, WORKSP, IFAULT)
C
C   ALGORITHM AS 216 APPL. STATIST. (1985) VOL.34, NO.3
C
C   COMBINES THE CHOLESKI FACTORISATIONS OF OBSERVATIONS WITH
C   POSITIVE WEIGHTS (S) AND NEGATIVE WEIGHTS (R) AND MAKES
C   GILL-MURRAY MODIFICATION. ALSO FINDS MAXIMUM DIAGONAL AND
C   OFF-DIAGONAL ELEMENTS OF HESSIAN.
C
REAL S(IS), R(IR), WORKSP(N), ODMAX, DIMAX
REAL ZERO, EPS, ELEM, BETA2, SII, RII, CMAX, SIINEW, EI, A, W
DATA ZERO /0.0/, EPS /1.0E-8/
C
C   CHECK FOR VALID PARAMETERS
C
IFAULT = 1
NNP1 = N * (N + 1) / 2
IF (N .LT. 2 .OR. IS .LT. NNP1 .OR. IR .LT. NNP1) RETURN
IFAULT = 0
NPARAM = N - 1
C
C   FIND MAXIMUM DIAG AND OFF-DIAG ELEMENTS
C
ODMAX = ZERO
DIMAX = ZERO
IJ = NNP1 - N
C
C   LOOP FOR I = N-1 DOWN TO 1
C
I = NPARAM
C
C   LOOP FOR J = I DOWN TO 1
C
10 J = I
JJ = IJ
20 IF (J .LE. 0) GOTO 50
IF (I .EQ. J) ELEM = S(JJ) - R(JJ)
IF (I .NE. J) ELEM = S(JJ) * S(IJ) - R(JJ) * R(IJ)
C
C   LOOP FOR K = 1 UP TO (J-1)
C
IF (J .EQ. 1) GOTO 40
KK = 0
IK = I * (I - 1) / 2
JMINUS = J - 1
JK = J * JMINUS / 2
DO 30 K = 1, JMINUS
KK = KK + K
IK = IK + 1
JK = JK + 1
30 ELEM = ELEM + S(IK) * S(JK) * S(KK) - R(IK) * R(JK) * R(KK)
C
40 CONTINUE
IF (I .EQ. J) DIMAX = AMAX1(DIMAX, ABS(ELEM))
IF (I .NE. J) ODMAX = AMAX1(ODMAX, ABS(ELEM))
IJ = IJ - 1
JJ = JJ - J
J = J - 1
GOTO 20
C
50 I = I - 1

```



```

      IF (I .GT. 0) GOTO 10
C
C      COMBINE POSITIVE DEFINITE AND NEGATIVE DEFINITE COMPONENTS
C
      BETA2 = AMAX1(DIMAX, ODMAX / FLOAT(NPARAM), EPS)
      II = 0
      DO 130 I = 1, N
C
C      ALTER ITH ROW OF CHOLESKI S      ....
C
      II = II + I
      SII = S(II)
      RII = R(II)
      IF (I .LT. N) GOTO 60
      S(II) = SII - RII
      RETURN
60 IF (RII .LE. ZERO) GOTO 130
      DO 70 J = 1, I
70 WORKSP(J) = ZERO
      IJ = II
      CMAX = ZERO
      IPLUS = I + 1
      DO 80 J = IPLUS, N
      IJ = IJ + J - 1
      WORKSP(J) = S(IJ)
      S(IJ) = S(IJ) * SII - R(IJ) * RII
      IF (J .LT. N .AND. ABS(S(IJ)) .GT. CMAX) CMAX = ABS(S(IJ))
80 CONTINUE
C
      SIINEW = AMAX1(CMAX * CMAX / BETA2, ABS(SII - RII), EPS)
      S(II) = SIINEW
C
C      .. IF GILL-MURRAY MODIFICATION IS NEEDED UPDATE REST OF S ..
C
      EI = SIINEW - SII * RII
      A = SII / (SII + EI)
      IJ = II
      DO 90 J = IPLUS, N
      IJ = IJ + J - 1
      R(IJ) = R(IJ) - A * WORKSP(J)
90 S(IJ) = S(IJ) / SIINEW
      IF (EI .LE. ZERO) GOTO 100
      IFAULT = -1
      W = EI * A
      CALL UPDATE(S, WORKSP, W, N, IS)
C
C      .... THEN UPDATE REST OF R
C
100 W = RII * (SII + EI) / SIINEW
      DO 110 J = 1, I
110 WORKSP(J) = ZERO
      IJ = II
      DO 120 J = IPLUS, N
      IJ = IJ + J - 1
120 WORKSP(J) = R(IJ)
      CALL UPDATE(R, WORKSP, W, N, IR)
130 CONTINUE
C
      END

      SUBROUTINE NUISNC(R, IR, NPARAM, DBDC, IDBDC, DC, DCDC, DIMAX,

```

```
* ODMAX, WORKSP, IFAULT)
C
C     ALGORITHM AS 216.1 APPL. STATIST. (1985) VOL.34, NO.3
C
C     INCORPORATES DERIVATIVES W.R.T A NUISANCE PARAMETER INTO THE
C     HESSIAN AND GRADIENT WHOSE CHOLESKI FACTORISATION IS IN R AND
C     MAKES GILL-MURRAY MODIFICATION TO GET POSITIVE-DEFINITE HESSIAN
C
REAL R(IR), DBDC(IDBDC), WORKSP(NPARAM), DC, DCDC, DIMAX, ODMAX
REAL ZERO, EPS, ONE, BETA2, W, A, TEMP, B
DATA ZERO /0.0/, EPS /1.0E-7/, ONE /1.0/
C
C     CHECK FOR VALID PARAMETERS
C
NPPLUS = NPARAM + 1
NPLESS = NPARAM - 1
L0 = NPARAM * NPPLUS / 2
IFault = 1
IF (NPARAM .LE. 1 .OR. L0 + NPPLUS .GT. IR .OR. IDBDC .LT. NPLESS)
* RETURN
IFault = 0
C
C     COPY DERIVATIVES INTO R AFTER ELEMENTS OF KDK' AND UPDATE
C     DIMAX AND ODMAX
C
LI = L0
DO 10 I = 1, NPLESS
LI = LI + 1
ODMAX = AMAX1(ODMAX, ABS(DBDC(I)))
10 R(LI) = -DBDC(I)
R(LI + 1) = DC
DIMAX = AMAX1(DIMAX, ABS(DCDC))
BETA2 = AMAX1(DIMAX, ODMAX / NPARAM, EPS)
C
C     REPLACE EACH DERIVATIVE BY THE APPROPRIATE ELEMENT FROM THE
C     REPRESENTATION OF MFM'
C
LI = L0
IJ = 0
DO 50 I = 1, NPARAM
LI = LI + 1
IF (I .EQ. 1) GOTO 30
IMINUS = I - 1
LJ = L0
DO 20 J = 1, IMINUS
LJ = LJ + 1
IJ = IJ + 1
20 R(LI) = R(LI) - R(IJ) * R(LJ)
30 IJ = IJ + 1
C
C     ADD TO DIAGONAL OF HESSIAN TO MAKE IT POSITIVE DEFINITE, IF
C     NECESSARY
C
IF (I .EQ. NPARAM) GOTO 50
W = AMAX1(R(LI) * R(LI) / BETA2, ABS(R(IJ)), EPS) - R(IJ)
IF (W .LE. ZERO) GOTO 50
IFault = -1
DO 40 J = 1, NPARAM
40 WORKSP(J) = ZERO
WORKSP(I) = ONE
```

```

      CALL UPDATE(R, WORKSP, W, NPARAM, L0)
50 CONTINUE
C
C      INTERCHANGE LAST TWO ROWS AND COLS OF MFM'
C
      A = -DCDC
      LI = L0
      KI = L0 - NPARAM
      II = 0
      DO 60 I = 1, NPLESS
      LI = LI + 1
      KI = KI + 1
      II = II + I
      TEMP = R(LI)
      R(LI) = R(KI)
      R(KI) = TEMP / R(II)
60 A = A - R(KI) * TEMP
C
      KI = KI + 1
      B = R(KI)
      IF (A .LT. EPS) IFAULT = -1
      R(KI) = AMAX1(ABS(A), EPS)
      LI = LI + 1
      TEMP = R(LI)
      R(LI) = TEMP / R(KI)
      R(LI + 1) = B - TEMP * R(LI)
C
      RETURN
      END

      SUBROUTINE STEP(R, IR, PARAMS, OLDDL, NPARAM, RIDGE, WORKSP, IW,
*   IFAULT)
C
C      ALGORITHM AS 216.2 APPL. STATIST. (1985) VOL.34, NO.3
C
C      TAKES A POSITIVE DEFINITE MODIFIED HESSIAN AND USES MARQUARDT'S
C      METHOD, INCREASING DIAGONAL UNTIL A LARGER LOG-LIKELIHOOD IS
C      FOUND
C
      REAL R(IR), PARAMS(NPARAM), WORKSP(IW), OLDDL, RIDGE
      REAL EPS, ZERO, ONE, C, ADDR, DIDIX, TEMP, W, ANEWLL
C
      DATA EPS /1.0E-7/, ZERO /0.0/, ONE /1.0/, C /10.0/
      DATA MAXIT /10/
C
      CHECK FOR VALID PARAMETERS
C
      IFAULT = 1
      NPPLUS = NPARAM + 1
      NRUSED = NPPLUS * (NPPLUS + 1) / 2
      IF (NPARAM .LE. 0 .OR. IR .LT. NRUSED .OR. IW .LT. NPPLUS) RETURN
      IFAULT = 0
C
      ITER = 1
      IF (RIDGE .LE. ZERO) GOTO 50
      IF (RIDGE .GE. EPS * C) RIDGE = RIDGE / C
      ADDR = RIDGE
C
      FIND DIAGONAL ELEMENTS OF HESSIAN ....
C

```

```
10 IJ = 0
   DO 40 I = 1, NPARAM
   DIDIX = ZERO
   JJ = 0
   DO 20 J = 1, I
   JJ = JJ + J
   IJ = IJ + 1
   TEMP = ONE
   IF (I .NE. J) TEMP = R(IJ)
20 DIDIX = DIDIX + TEMP * TEMP * R(JJ)
   IF (R(JJ) .LT. ZERO) GOTO 90
C
C     .... AND ADD TO THEM
C
   W = ADDR * DIDIX
   DO 30 J = 1, NPPLUS
30 WORKSP(J) = ZERO
   WORKSP(I) = ONE
   CALL UPDATE(R, WORKSP, W, NPPLUS, IR)
40 CONTINUE
C
C     IF LIKELIHOOD IS NOT INCREASED, ADD BIGGER RIDGE TO HESSIAN
C
50 CALL BSUB(R, IR, NPPLUS, WORKSP, IW, IFAIL)
   DO 60 I = 1, NPARAM
60 WORKSP(I) = WORKSP(I) + PARAMS(I)
   ANEWLL = ALLIKE(WORKSP, NPARAM)
   IF (ANEWLL .GE. OLDLL) GOTO 70
   ADDR = RIDGE * (C + ONE) / (ONE + RIDGE)
   IF (RIDGE .GE. ZERO) RIDGE = RIDGE * C
   ITER = ITER + 1
   IFAULT = -1
   IF (ITER .LE. MAXIT .AND. RIDGE .GT. ZERO) GOTO 10
C
C     TOO MANY ITERATIONS
C
   IFAULT = 2
   RETURN
C
C     RETURN IMPROVED PARAMETERS
C
70 OLDLL = ANEWLL
   DO 80 I = 1, NPARAM
80 PARAMS(I) = WORKSP(I)
   RETURN
C
C     HESSIAN NOT POSITIVE SEMI-DEFINITE ON INPUT
C
90 IFAULT = 3
   RETURN
   END
```

```
      SUBROUTINE DIPTST(X, N, DIP, XL, XU, IFAULT, GCM, LCM, MN, MJ)
C
C   ALGORITHM AS 217 APPL. STATIST. (1985) VOL.34, NO.3
C
C   Does the dip calculation for an ordered vector X using the
C   greatest convex minorant and the least concave majorant, skipping
C   through the data using the change points of these distributions.
C   It returns the dip statistic 'DIP' and the modal interval
C   (XL, XU).
C
      REAL X(N)
      INTEGER MN(N), MJ(N), LCM(N), GCM(N), HIGH
      REAL ZERO, HALF, ONE
      DATA ZERO/0.0/, HALF/0.5/, ONE/1.0/
C
      IFAULT = 1
      IF (N .LE. 0) RETURN
      IFAULT = 0
C
      Check if N = 1
C
      IF (N .EQ. 1) GO TO 4
C
      Check that X is sorted
C
      IFAULT = 2
      DO 3 K = 2, N
         IF (X(K) .LT. X(K-1)) RETURN
3     CONTINUE
      IFAULT = 0
C
      Check for all values of X identical,
      and for 1 < N < 4.
C
      IF (X(N) .GT. X(1) .AND. N .GE. 4) GO TO 5
4     XL = X(1)
      XU = X(N)
      DIP = ZERO
      RETURN
C
      LOW contains the index of the current estimate of the lower end
      of the modal interval, HIGH contains the index for the upper end.
C
5     FN = FLOAT(N)
      LOW = 1
      HIGH = N
      DIP = ONE / FN
      XL = X(LOW)
      XU = X(HIGH)
C
      Establish the indices over which combination is necessary for the
      convex minorant fit.
C
      MN(1) = 1
      DO 28 J = 2, N
         MN(J) = J - 1
25     MNJ = MN(J)
         MNMJ = MN(MNJ)
         A = FLOAT(MNJ - MNMJ)
         B = FLOAT(J - MNJ)
         IF (MNJ .EQ. 1 .OR. (X(J) - X(MNJ))*A .LT. (X(MNJ) - X(MNMNJ)))
```

```
+          *B) GO TO 28
      MN(J) = MNMNJ
      GO TO 25
28 CONTINUE
C
C      Establish the indices over which combination is necessary for the
C      concave majorant fit.
C
      MJ(N) = N
      NA = N - 1
      DO 34 JK = 1, NA
        K = N - JK
        MJ(K) = K + 1
32      MJK = MJ(K)
        MJMJK = MJ(MJK)
        A = FLOAT(MJK - MJMJK)
        B = FLOAT(K - MJK)
        IF (MJK .EQ. N .OR. (X(K) - X(MJK))*A .LT. (X(MJK) - X(MJMJK)))
+          *B) GO TO 34
        MJ(K) = MJMJK
        GO TO 32
34 CONTINUE
C
C      Start the cycling.
C      Collect the change points for the GCM from HIGH to LOW.
C
40 IC = 1
      GCM(1) = HIGH
42 IGCM1 = GCM(IC)
      IC = IC + 1
      GCM(IC) = MN(IGCM1)
      IF (GCM(IC) .GT. LOW) GO TO 42
      ICX = IC
C
C      Collect the change points for the LCM from LOW to HIGH.
C
      IC = 1
      LCM(1) = LOW
44 LCM1 = LCM(IC)
      IC = IC + 1
      LCM(IC) = MJ(LCM1)
      IF (LCM(IC) .LT. HIGH) GO TO 44
      ICV = IC
C
C      ICX, IX, IG are counters for the convex minorant,
C      ICV, IV, IH are counters for the concave majorant.
C
      IG = ICX
      IH = ICV
C
C      Find the largest distance greater than 'DIP' between the GCM and
C      the LCM from LOW to HIGH.
C
      IX = ICX - 1
      IV = 2
      D = ZERO
      IF (ICX .NE. 2 .OR. ICV .NE. 2) GO TO 50
      D = ONE / FN
      GO TO 65
50 IGCMX = GCM(IX)
      LCMIV = LCM(IV)
```

```

        IF (IGCMX .GT. LCMIV) GO TO 55
C
C   If the next point of either the GCM or LCM is from the LCM,
C   calculate the distance here.
C
        LCMIV1 = LCM(IV - 1)
        A = FLOAT(LCMIV - LCMIV1)
        B = FLOAT(IGCMX - LCMIV1 - 1)
        DX = (X(IGCMX) - X(LCMIV1)*A) / (FN*(X(LCMIV) - X(LCMIV1)))
+         - B / FN
        IX = IX - 1
        IF (DX .LT. D) GO TO 60
        D = DX
        IG = IX + 1
        IH = IV
        GO TO 60
C
C   If the next point of either the GCM or LCM is from the GCM,
C   calculate the distance here.
C
55 LCMIV = LCM(IV)
        IGCM = GCM(IX)
        IGCM1 = GCM(IX + 1)
        A = FLOAT(LCMIV - IGCM1 + 1)
        B = FLOAT(IGCM - IGCM1)
        DX = A / FN - ((X(LCMIV) - X(IGCM1))*B) / (FN * (X(IGCM)
+         - X(IGCM1)))
        IV = IV + 1
        IF (DX .LT. D) GO TO 60
        D = DX
        IG = IX + 1
        IH = IV - 1
60 IF (IX .LT. 1) IX = 1
        IF (IV .GT. ICV) IV = ICV
        IF (GCM(IX) .NE. LCM(IV)) GO TO 50
65 IF (D .LT. DIP) GO TO 100
C
C   Calculate the DIPS for the current LOW and HIGH.
C
C   The DIP for the convex minorant.
C
        DL = ZERO
        IF (IG .EQ. ICX) GO TO 80
        ICXA = ICX - 1
        DO 76 J = IG, ICXA
            TEMP = ONE / FN
            JB = GCM(J + 1)
            JE = GCM(J)
            IF (JE - JB .LE. 1) GO TO 74
            IF (X(JE) .EQ. X(JB)) GO TO 74
            A = FLOAT(JE - JB)
            CONST = A / (FN * (X(JE) - X(JB)))
            DO 72 JR = JB, JE
                B = FLOAT(JR - JB + 1)
                T = B / FN - (X(JR) - X(JB))*CONST
                IF (T .GT. TEMP) TEMP = T
72 CONTINUE
74 IF (DL .LT. TEMP) DL = TEMP
76 CONTINUE
C
C   The DIP for the concave majorant.

```

```
C
80 DU = ZERO
   IF (IH .EQ. ICV) GO TO 90
   ICVA = ICV - 1
   DO 88 K = IH, ICVA
     TEMP = ONE / FN
     KB = LCM(K)
     KE = LCM(K + 1)
     IF (KE - KB .LE. 1) GO TO 86
     IF (X(KE) .EQ. X(KB)) GO TO 86
     A = FLOAT(KE - KB)
     CONST = A / (FN * (X(KE) - X(KB)))
     DO 84 KR = KB, KE
       B = FLOAT(KR - KB - 1)
       T = (X(KR) - X(KB))*CONST - B / FN
       IF (T .GT. TEMP) TEMP = T
84   CONTINUE
86   IF (DU .LT. TEMP) DU = TEMP
88 CONTINUE
```

```
C
C   Determine the current maximum.
C
```

```
90 DIPNEW = DL
   IF (DU .GT. DL) DIPNEW = DU
   IF (DIP .LT. DIPNEW) DIP = DIPNEW
   LOW = GCM(IG)
   HIGH = LCM(IH)
```

```
C
C   Recycle
C
   GO TO 40
```

```
C
100 DIP = HALF * DIP
    XL = X(LOW)
    XU = X(HIGH)
```

```
C
   RETURN
   END
```



```
C This file contains:  
C 1. Single-precision version of AS 218 as supplied by the RSS Algorithms  
C Editor  
C 2. Double-precision version supplied by Luis Escobar (author)  
C 3. A demo program (double precision) supplied by the author  
C  
C
```

```
      SUBROUTINE SEVINP(ITYPE, ZL, ZR, F11, F12, F22, IFAULT)
```

```
      ALGORITHM AS218  APPL. STATIST. (1986) VOL. 35, NO. 1
```

```
      FISHER INFORMATION MATRIX ELEMENTS FOR TIME (TYPE I) OR  
      FAILURE (TYPE II) CENSORED SMALLEST EXTREME VALUE DATA
```

```
      REAL BG, DEN, ETA, F11, F12, F22, G, ONE, THET0L, THET0R, THET1L,  
*     THET1R, THET2L, THET2R, X, ZERO, ZL, ZMAX, ZMIN, ZR, ZU
```

```
      DATA ONE /1.0E0/, ZERO /0.0E0/, ZMAX /3.6E0/, ZMIN /-34.0E0/
```

```
      FUNCTION STATEMENTS - PDF (G(X)) AND CDF (BG(X)) FOR A  
      STANDARDIZED SMALLEST EXTREME VALUE RANDOM VARIABLE
```

```
      G(X) = EXP(X - EXP(X))  
      BG(X) = ONE - EXP(-EXP(X))
```

```
      CHECK FOR ILLEGAL ITYPE
```

```
      IF (ITYPE .LT. 1 .OR. ITYPE .GT. 4) GOTO 6
```

```
      IDENTIFY THE CENSORING TYPE  
      ITYPE = 1, 2, 3, 4 CORRESPOND TO COMPLETE, RIGHT,  
      LEFT, AND LEFT AND RIGHT CENSORED DATA, RESPECTIVELY
```

```
      GOTO (1, 2, 3, 4), ITYPE
```

```
      COMPLETE DATA - FISHER MATRIX ELEMENTS
```

```
1 CALL INTEGR(ZMAX, F11, F12, F22, IFAULT)  
   RETURN
```

```
      RIGHT CENSORED DATA - FISHER MATRIX ELEMENTS
```

```
2 CALL INTEGR(ZR, F11, F12, F22, IFAULT)  
   RETURN
```

```
      LEFT CENSORED DATA  
      SET THE RIGHT CENSORING BOUND (ZU) EQUAL TO ZMAX
```

```
3 ZU = ZMAX  
   GOTO 5
```

```
      LEFT AND RIGHT CENSORED DATA - CHECK THAT THE LEFT  
      CENSORING BOUND IS NOT GREATER THAN THE RIGHT BOUND
```

```
4 IF (ZL .GT. ZR) GOTO 7  
   ZU = ZR
```

```
      LEFT OR LEFT AND RIGHT CENSORED DATA - FISHER MATRIX ELEMENTS  
      ETA IS THE SECOND TERM IN THE EQUATION FOR F11
```

```
5 ETA = ZERO
```

```

DEN = ZERO
IF (ZL .GT. ZMIN .AND. ZL .LT. ZMAX) DEN = BG(ZL) * EXP(-EXP(ZL))
IF (DEN .GT. ZERO) ETA = G(ZL) ** 2 / DEN
CALL INTEGR(ZL, THET0L, THET1L, THET2L, IFAULT)
IF (IFAUULT .EQ. 1) RETURN
CALL INTEGR(ZU, THET0R, THET1R, THET2R, IFAULT)
IF (IFAUULT .EQ. 1) RETURN
F11 = THET0R - THET0L + ETA
F12 = THET1R - THET1L + ZL * ETA
F22 = THET2R - THET2L + ZL * ZL * ETA
RETURN

```

C  
C  
C

```

        SET IFAULT

```

```

6 IFAULT = 2

```

```

RETURN

```

```

7 IFAULT = 3

```

```

RETURN

```

```

END

```

C

```

SUBROUTINE INTEGR(Z, THETA0, THETA1, THETA2, IFAULT)

```

C

C COMPUTES THE INTEGRALS FROM (-INFINITY) TO Z OF THE FOLLOWING

C FUNCTIONS: G(X)=EXP(X-EXP(X)), G1(X)=(1+X)\*G(X), AND

C G2(X)=(1+X)\*G1(X). G(X) HAS A CLOSED FORM INTEGRAL.

C G1 AND G2 ARE INTEGRATED BY USING POWER SERIES EXPANSIONS

C WHEN Z.LE.1, AND BY POWER SERIES EXPANSIONS THROUGH Z=1

C PLUS A GAUSSIAN QUADRATURE FROM 1 TO Z WHEN Z.GT.1

C

```

REAL ASYMP1, ASYMP2, EZ, FACTOR, G1, G1XL, G1XR, G2XL, G2XR, HALF,
* ONE, S1, S2, THETA0, THETA1, THETA2, THET11, THET21, TOL, TWO,
* X, X1, X2, X3, X4, X5, Z, ZERO, ZMAX, ZMIN

```

C

```

REAL P(8), W(8)

```

C

C P AND W ARE CONSTANTS USED IN THE GAUSSIAN QUADRATURES

C

```

DATA P(1) /0.4947004674958250E0/, P(2) /0.4722875115366163E0/,
* P(3) /0.4328156011939159E0/, P(4) /0.3777022041775015E0/, P(5)
* /0.3089381222013219E0/, P(6) /0.2290083888286137E0/, P(7)
* /0.1408017753896295E0/, P(8) /0.4750625491881872E-1/
DATA W(1) /0.1357622970587705E-1/, W(2) /0.3112676196932395E-1/,
* W(3) /0.4757925584124639E-1/, W(4) /0.6231448562776694E-1/,
* W(5) /0.7479799440828837E-1/, W(6) /0.8457825969750127E-1/, W(7)
* /0.9130170752246179E-1/, W(8) /0.9472530522753425E-1/

```

C

C ASYMP1, ASYMP2, THET11, AND THET21 ARE THE INTEGRALS

C FOR G1 AND G2 WHEN Z=+INFINITY AND Z=1 ,RESPECTIVELY

C

```

DATA ASYMP1 /0.4227843350984671E0/, ASYMP2 /0.1823680660852879E1/,
* HALF /0.5E0/, JMAX /25/, ONE /1.0E0/, TOL /1.0E-11/, THET11 /
* 0.2720757938345342E0/, THET21 /0.1475933122158450E1/, TWO /
* 2.0E0/, ZERO /0.0E0/, ZMAX /3.6E0/, ZMIN /-34.0E0/

```

C

C FUNCTION REQUIRED IN THE GAUSSIAN QUADRATURE

C

```

G1(X) = (ONE + X) * EXP(X - EXP(X))

```

C

C CHECK FOR EXTREME VALUES

C

```

IFAUULT = 0

```

```

      IF (Z .GE. ZMAX) GOTO 5
      IF (Z .LE. ZMIN) GOTO 6
C
C      COMPUTATION OF THETA0 - INTEGRAL OF G(X)=EXP(X-EXP(X))
C
      EZ = EXP(Z)
      THETA0 = ONE - EXP(-EZ)
C
C      SELECT INTEGRATION BY POWER SERIES EXPANSIONS OR
C      BY POWER SERIES EXPANSIONS AND GAUSSIAN QUADRATURE
C
      IF (Z .GE. ONE) GOTO 3
C
C      Z IS LESS THAN 1 - INTEGRATION BY POWER SERIES EXPANSIONS
C
C      COMPUTATION OF THETA1 AND THETA2
C
      FACTOR = -ONE
      S1 = ZERO
      S2 = ZERO
      DO 1 J = 1, JMAX
C
C      TERMS TO EVALUATE THETA1(Z) - INTEGRAL OF G1(X)=(1+X)G(X)
C
      X5 = FLOAT(J)
      FACTOR = -FACTOR * EZ / X5
      X1 = Z - ONE / X5
      X3 = FACTOR * X1
      S1 = S1 + X3
C
C      TERMS TO EVALUATE THETA2(Z) - INTEGRAL OF G2(X)=(1+X)G1(X)
C
      X2 = X1 * X1 + ONE / (X5 * X5)
      X4 = FACTOR * X2
      S2 = S2 + X4
C
C      TESTS FOR CONVERGENCE OF THE SERIES - THE SUMMATIONS STOP WHEN
C      THE ABSOLUTE VALUE OF THE LAST ADDED TERM IS SMALLER THAN TOL
C      FOR BOTH SERIES - A FAULT IS DECLARED IF CONVERGENCE IS NOT
C      REACHED IN A MAXIMUM OF JMAX TERMS
C
      X5 = AMAX1(ABS(X3), ABS(X4))
      IF (X5 .LT. TOL) GOTO 2
1 CONTINUE
      IFAULT = 1
      RETURN
C
C      ADD TERMS TO OBTAIN INTEGRALS
C
2 THETA1 = THETA0 + S1
      THETA2 = TWO * THETA1 - THETA0 + S2
      RETURN
C
C      Z IS BETWEEN 1 AND 3.6.
C      THET11 AND THET12 CONTAIN THE INTEGRALS OF G1(X) AND G2(X)
C      OVER (-INFINITY,1) AND THEY ARE DEFINED IN THE DATA STATEMENTS
C
C      GAUSSIAN QUADRATURE TO INTEGRATE G1(X) AND G2(X) OVER (1,Z)
C
3 S1 = ZERO
      S2 = ZERO

```

```

X1 = HALF * (Z + ONE)
X2 = Z - ONE
DO 4 IQUAD = 1, 8
X3 = X1 - P(IQUAD) * X2
X4 = X1 + P(IQUAD) * X2
G1XL = G1(X3)
G1XR = G1(X4)
G2XL = (ONE + X3) * G1XL
G2XR = (ONE + X4) * G1XR
S1 = S1 + W(IQUAD) * (G1XL + G1XR)
S2 = S2 + W(IQUAD) * (G2XL + G2XR)
4 CONTINUE
S1 = S1 * X2
S2 = S2 * X2
C
C      ADD TERMS TO OBTAIN INTEGRALS
C
C      THETA1 = S1 + THET11
C      THETA2 = S2 + THET21
C      RETURN
C
C      ASYMPTOTIC VALUES.  Z IS GREATER THAN OR EQUAL TO 3.6
C
5 THETA0 = ONE
  THETA1 = ASYMP1
  THETA2 = ASYMP2
  RETURN
C
C      ASYMPTOTIC VALUES.  Z IS SMALLER THAN OR EQUAL TO -34
C
6 THETA0 = ZERO
  THETA1 = ZERO
  THETA2 = ZERO
  RETURN
END
C
C----- Double precision version -----
C
SUBROUTINE SEVINP(ITYPE,ZL,ZR,F11,F12,F22,IFAU)
C
C      ALGORITHM AS218  APPL. STATIST. (1986) VOL. 35, NO. 1
C
C      FISHER INFORMATION MATRIX ELEMENTS FOR TIME (TYPE I) OR
C      FAILURE (TYPE II) CENSORED SMALLEST EXTREME VALUE DATA
C
C      DOUBLE PRECISION BG, DEN, ETA, F11, F12, F22, G, ONE, THET0L,
* THET0R, THET1L, THET1R, THET2L, THET2R, X, ZERO,
* ZL, ZMAX, ZMIN, ZR, ZU
C
DATA ONE/1.0D0/, ZERO/0.0D0/, ZMAX/3.6D0/, ZMIN/-34.0D0/
C
C      FUNCTION STATEMENTS - PDF (G(X)) AND CDF (BG(X)) FOR A
C      STANDARDIZED SMALLEST EXTREME VALUE RANDOM VARIABLE
C
G(X) = EXP(X-EXP(X))
BG(X) = ONE-EXP(-EXP(X))
C
C      CHECK FOR ILLEGAL ITYPE
C
IF (ITYPE.LT.1 .OR. ITYPE.GT.4) GOTO 6
C

```

```
C      IDENTIFY THE CENSORING TYPE
C      ITYPE = 1, 2, 3, 4 CORRESPOND TO COMPLETE, RIGHT,
C      LEFT, AND LEFT AND RIGHT CENSORED DATA, RESPECTIVELY
C
C      GOTO (1,2,3,4), ITYPE
C
C      COMPLETE DATA - FISHER MATRIX ELEMENTS
C
1 CALL INTEGR(ZMAX,F11,F12,F22,IFAU)
RETURN
C
C      RIGHT CENSORED DATA - FISHER MATRIX ELEMENTS
C
2 CALL INTEGR(ZR,F11,F12,F22,IFAU)
RETURN
C
C      LEFT CENSORED DATA
C      SET THE RIGHT CENSORING BOUND (ZU) EQUAL TO ZMAX
C
3 ZU = ZMAX
GOTO 5
C
C      LEFT AND RIGHT CENSORED DATA - CHECK THAT THE LEFT
C      CENSORING BOUND IS NOT GREATER THAN THE RIGHT BOUND
C
4 IF (ZL.GT.ZR) GOTO 7
ZU = ZR
C
C      LEFT OR LEFT AND RIGHT CENSORED DATA - FISHER MATRIX ELEMENTS
C      ETA IS THE SECOND TERM IN THE EQUATION FOR F11
C
5 ETA = ZERO
DEN = ZERO
IF (ZL.GT.ZMIN.AND.ZL.LT.ZMAX) DEN = BG(ZL)*DEXP(-DEXP(ZL))
IF (DEN.GT.ZERO) ETA = G(ZL)**2/DEN
CALL INTEGR(ZL,THET0L,THET1L,THET2L,IFAU)
IF (IFAU.EQ.1) RETURN
CALL INTEGR(ZU,THET0R,THET1R,THET2R,IFAU)
IF (IFAU.EQ.1) RETURN
F11 = THET0R-THET0L+ETA
F12 = THET1R-THET1L+ZL*ETA
F22 = THET2R-THET2L+ZL*ZL*ETA
RETURN
C
C      SET IFAULT
C
6 IFAULT = 2
RETURN
7 IFAULT = 3
RETURN
END
C
SUBROUTINE INTEGR(Z,THETA0,THETA1,THETA2,IFAU)
C
C      COMPUTES THE INTEGRALS FROM (-INFINITY) TO Z OF THE FOLLOWING
C      FUNCTIONS: G(X) = EXP(X-EXP(X)), G1(X) = (1+X)*G(X), AND
C      G2(X) = (1+X)*G1(X). G(X) HAS A CLOSED FORM INTEGRAL.
C      G1 AND G2 ARE INTEGRATED BY USING POWER SERIES EXPANSIONS
C      WHEN Z.LE.1, AND BY POWER SERIES EXPANSIONS THROUGH Z = 1
C      PLUS A GAUSSIAN QUADRATURE FROM 1 TO Z WHEN Z.GT.1
C
```

```

DOUBLE PRECISION ASYMP1, ASYMP2, EZ, FACTOR, G1, G1XL, G1XR,
* G2XL, G2XR, HALF, ONE, S1, S2, THETA0, THETA1,
* THETA2, THET11, THET21, TOL, TWO, X, X1, X2, X3,
* X4, X5, Z, ZERO, ZMAX, ZMIN

```

C

```
DOUBLE PRECISION P(8), W(8)
```

C

C

C

```
P AND W ARE CONSTANTS USED IN THE GAUSSIAN QUADRATURES
```

```

DATA P(1)/0.4947004674958250D0 /, P(2)/0.4722875115366163D0 /,
* P(3)/0.4328156011939159D0 /, P(4)/0.3777022041775015D0 /,
* P(5)/0.3089381222013219D0 /, P(6)/0.2290083888286137D0 /,
* P(7)/0.1408017753896295D0 /, P(8)/0.4750625491881872D-1/
DATA W(1)/0.1357622970587705D-1/, W(2)/0.3112676196932395D-1/,
* W(3)/0.4757925584124639D-1/, W(4)/0.6231448562776694D-1/,
* W(5)/0.7479799440828837D-1/, W(6)/0.8457825969750127D-1/,
* W(7)/0.9130170752246179D-1/, W(8)/0.9472530522753425D-1/

```

C

C

C

C

```
ASYMP1, ASYMP2, THET11, AND THET21 ARE THE INTEGRALS
FOR G1 AND G2 WHEN Z = +INFINITY AND Z = 1 ,RESPECTIVELY
```

```

DATA ASYMP1/0.4227843350984671D0/, ASYMP2/0.1823680660852879D1/,
* HALF/0.5D0/, JMAX/25/, ONE/1.0D0/, TOL/1.0D-11/,
* THET11/0.2720757938345342D0/, THET21/0.1475933122158450D1/,
* TWO/2.0D0/, ZERO/0.0D0/, ZMAX/3.6D0/, ZMIN/-34.0D0/

```

C

C

C

```
FUNCTION REQUIRED IN THE GAUSSIAN QUADRATURE
```

```
G1(X) = (ONE+X)*EXP(X-EXP(X))
```

C

C

C

```
CHECK FOR EXTREME VALUES
```

```

IF(AULT = 0
IF(Z.GE.ZMAX) GOTO 5
IF(Z.LE.ZMIN) GOTO 6

```

C

C

C

```
COMPUTATION OF THETA0 - INTEGRAL OF G(X) = EXP(X-EXP(X))
```

```

EZ = DEXP(Z)
THETA0 = ONE-DEXP(-EZ)

```

C

C

C

C

```
SELECT INTEGRATION BY POWER SERIES EXPANSIONS OR
BY POWER SERIES EXPANSIONS AND GAUSSIAN QUADRATURE
```

```
IF(Z.GE.ONE) GOTO 3
```

C

C

C

```
Z IS LESS THAN 1 - INTEGRATION BY POWER SERIES EXPANSIONS
```

```
COMPUTATION OF THETA1 AND THETA2
```

```

FACTOR = -ONE
S1 = ZERO
S2 = ZERO
DO 1 J = 1, JMAX

```

C

C

C

```
TERMS TO EVALUATE THETA1(Z) - INTEGRAL OF G1(X) = (1+X)G(X)
```

```

X5 = FLOAT(J)
FACTOR = -FACTOR*EZ/X5
X1 = Z-ONE/X5
X3 = FACTOR*X1

```

```

S1 = S1+X3
C
C     TERMS TO EVALUATE THETA2(Z) - INTEGRAL OF G2(X) = (1+X)G1(X)
C
X2 = X1*X1+ONE/(X5*X5)
X4 = FACTOR*X2
S2 = S2+X4
C
C     TESTS FOR CONVERGENCE OF THE SERIES - THE SUMMATIONS STOP WHEN
C     THE ABSOLUTE VALUE OF THE LAST ADDED TERM IS SMALLER THAN TOL
C     FOR BOTH SERIES - A FAULT IS DECLARED IF CONVERGENCE IS NOT
C     REACHED IN A MAXIMUM OF JMAX TERMS
C
X5 = MAX1(ABS(X3),ABS(X4))
IF (X5.LT.TOL) GOTO 2
1 CONTINUE
IF AULT = 1
RETURN
C
C     ADD TERMS TO OBTAIN INTEGRALS
C
2 THETA1 = THETA0+S1
THETA2 = TWO*THETA1-THETA0+S2
RETURN
C
C     Z IS BETWEEN 1 AND 3.6.
C     THET11 AND THET12 CONTAIN THE INTEGRALS OF G1(X) AND G2(X)
C     OVER (-INFINITY,1) AND THEY ARE DEFINED IN THE DATA STATEMENTS
C
C     GAUSSIAN QUADRATURE TO INTEGRATE G1(X) AND G2(X) OVER (1,Z)
C
3 S1 = ZERO
S2 = ZERO
X1 = HALF*(Z+ONE)
X2 = Z-ONE
DO 4 IQUAD = 1,8
X3 = X1-P(IQUAD)*X2
X4 = X1+P(IQUAD)*X2
G1XL = G1(X3)
G1XR = G1(X4)
G2XL = (ONE+X3)*G1XL
G2XR = (ONE+X4)*G1XR
S1 = S1+W(IQUAD)*(G1XL+G1XR)
S2 = S2+W(IQUAD)*(G2XL+G2XR)
4 CONTINUE
S1 = S1*X2
S2 = S2*X2
C
C     ADD TERMS TO OBTAIN INTEGRALS
C
THETA1 = S1+THET11
THETA2 = S2+THET21
RETURN
C
C     ASYMPTOTIC VALUES. Z IS GREATER THAN OR EQUAL TO 3.6
C
5 THETA0 = ONE
THETA1 = ASYMP1
THETA2 = ASYMP2
RETURN
C

```

```

C      ASYMPTOTIC VALUES.  Z IS SMALLER THAN OR EQUAL TO -34
C
6 THETA0 = ZERO
  THETA1 = ZERO
  THETA2 = ZERO
  RETURN
  END
C
C----- Demo program (double precision) -----
C
C
C      DRIVER PROGRAM FOR SEVINP
C
C      PROGRAM DEM218
C      DOUBLE PRECISION
C      *      COV, DET, F11, F12, F22, ONE, Q1, Q2,
C      *      SEVEN, TENTH, VAR1, VAR2, ZERO, ZL, ZR
C
C      DATA ONE/1.0D0/, SEVEN/7.0D0/, TENTH/0.1D0/, ZERO/0.0D0/
C      DATA IUNIT0/10/, IUNIT1/15/
C
C      OPEN(IUNIT0, FILE='HARTER.OUT', STATUS='NEW')
C      OPEN(IUNIT1, FILE='MEEKER.OUT', STATUS='NEW')
C
1  FORMAT(1H1, 2X, 'Q1', 4X, 'Q2', 8X, 'VAR(U)', 8X, 'VAR(S)', 8X,
* 'COV(U,S)', 2X, 'IFAULT')
2  FORMAT(1H , 2F6.2, 3(3X, F11.6), I3)
3  FORMAT(1H1, ' ZETA', 4X, 'VAR(U)', 9X, 'VAR(S)', 9X,
* 'COV(U,S)', 2X, 'IFAULT')
4  FORMAT(1H , F5.2, 3(3X, F11.5), I3)
C
C      HERE WE REPRODUCE THE FIRST FIVE COLUMNS OF TABLE 1
C      IN HARTER AND MOORE JASA(1968), P. 889-901
C
C      WRITE(IUNIT0, 1)
C      DO 20 I = 1, 10
C          Q1 = TENTH*FLOAT(I-1)
C          IF (Q1.GT.ZERO) ZL = LOG(-LOG(ONE-Q1))
C          JMAX = 11 - I
C          DO 10 J = 1, JMAX
C              Q2 = TENTH*FLOAT(J-1)
C              ITYPE = 4
C              IF (Q1.GT.ZERO.AND.Q2.EQ.ZERO) ITYPE = 3
C              IF (Q1.EQ.ZERO.AND.Q2.GT.ZERO) ITYPE = 2
C              IF (Q1.EQ.ZERO.AND.Q2.EQ.ZERO) ITYPE = 1
C              IF (Q2.GT.ZERO) ZR = LOG(-LOG(Q2))
C              CALL SEVINP(ITYPE, ZL, ZR, F11, F12, F22, IFAULT)
C              DET = F11*F22 - F12*F12
C              VAR1 = F22/DET
C              VAR2 = F11/DET
C              COV = -F12/DET
C              WRITE(IUNIT0, 2) Q1, Q2, VAR1, VAR2, COV, IFAULT
10      CONTINUE
20      CONTINUE
C
C      HERE WE PARTIALLY REPRODUCE TABLE 1 IN MEEKER AND
C      NELSON, TECHNOMETRICS 1977, VOL. 19, NO. 4, 473-476
C
C      WRITE(IUNIT1, 3)
C      ITYPE = 2
C      DO 30 J = 1, 91

```



```
      ZR = -SEVEN + TENTH*FLOAT(J-1)
      CALL SEVINP(ITYPE, ZL, ZR, F11, F12, F22, IFAULT)
      DET = F11*F22 - F12*F12
      VAR1 = F22/DET
      VAR2 = F11/DET
      COV = -F12/DET
      WRITE(IUNIT1, 4) ZR, VAR1, VAR2, COV, IFAULT
30    CONTINUE
      STOP
      END
```

```

      SUBROUTINE BTREE(FIND, LOC, NODE, LLINK, RLINK, BF, MAXT, NTREE,
+         ROOT, LAST, IFAULT)
C
C   ALGORITHM AS219  APPL. STATIST. (1986) VOL. 35, NO. 2
C
C   BTREE returns the location (LOC) of an item (FIND) in a
C   height-balanced tree composed of NODE, LLINK, RLINK and BF.
C   The tree is rooted at ROOT and contains NTREE nodes.  LAST
C   points to the next available free location in the tree.
C
C***  N.B. The user is expected to provided a function ICOMP to replace
C      the example provided here. ***
C
      INTEGER LLINK(MAXT), RLINK(MAXT), BF(MAXT)
      INTEGER NTREE, T, S, PNTR, R, A, MAXT, K, ROOT, ICOMP
      REAL    NODE(MAXT), FIND
C
      IFAULT = 0
      IF (NTREE .GE. 1) GO TO 20
C
C   First item in tree
C
      LAST = LAST + 1
      IF (LAST .GT. MAXT) THEN
         IFAULT = 1
         RETURN
      END IF
      NODE(LAST) = FIND
      LLINK(LAST) = 0
      RLINK(LAST) = 0
      BF(LAST) = 0
      ROOT = LAST
      NTREE = 1
      LOC = LAST
      RETURN
C
C   Search through tree for current item.
C   If found, return.  PNTR moves through the tree.  S points to
C   the place from which re-balancing may be needed, and T points
C   to the parent of S.
C
20    T = 0
       S = ROOT
       PNTR = S
30    K = ICOMP(FIND, NODE(PNTR))
       IF (K .NE. 0) GO TO 40
       LOC = PNTR
       RETURN
40    IF (K .GT. 0) THEN
         LOC = RLINK(PNTR)
      ELSE IF (K .LT. 0) THEN
         LOC = LLINK(PNTR)
      END IF
       IF (LOC .NE. 0) GO TO 60
       NTREE = NTREE + 1
       LAST = LAST + 1
       IF (LAST .LE. MAXT) GO TO 50
       IFAULT = 1
       RETURN
C
50    LOC = LAST

```

```
        IF (K .GT. 0) THEN
            RLINK(PNTR) = LOC
        ELSE IF (K .LT. 0) THEN
            LLINK(PNTR) = LOC
        END IF
        GO TO 100
C
    60   IF (BF(LOC) .EQ. 0) GO TO 70
        T = PNTR
        S = LOC
    70   PNTR = LOC
        GO TO 30
C
C      Add new node to tree and adjust balance factors
C
    100  NODE(LOC) = FIND
        LLINK(LOC) = 0
        RLINK(LOC) = 0
        BF(LOC) = 0
        A = ICOMP(FIND, NODE(S))
        IF (A .GT. 0) THEN
            PNTR = RLINK(S)
        ELSE IF (A .LT. 0) THEN
            PNTR = LLINK(S)
        END IF
        R = PNTR
C
    110  IF (PNTR .EQ. LOC) GO TO 130
        K = ICOMP(FIND, NODE(PNTR))
        IF (K .GT. 0) GO TO 120
        BF(PNTR) = -1
        PNTR = LLINK(PNTR)
        GO TO 110
    120  BF(PNTR) = 1
        PNTR = RLINK(PNTR)
        GO TO 110
C
    130  IF (BF(S) .NE. 0) GO TO 140
        BF(S) = A
        RETURN
    140  IF (BF(S) .NE. -A) GO TO 150
        BF(S) = 0
        RETURN
    150  IF (BF(R) .NE. A) GO TO 190
C
C      Single rotation
C
        PNTR = R
        IF (A .NE. -1) GO TO 170
        LLINK(S) = RLINK(R)
        RLINK(R) = S
        GO TO 180
    170  RLINK(S) = LLINK(R)
        LLINK(R) = S
    180  BF(S) = 0
        BF(R) = 0
        GO TO 240
C
C      Double rotation
C
    190  IF (A .NE. -1) GO TO 200
```

```

        PNTR = RLINK(R)
        RLINK(R) = LLINK(PNTR)
        LLINK(PNTR) = R
        LLINK(S) = RLINK(PNTR)
        RLINK(PNTR) = S
200    GO TO 210
        PNTR = LLINK(R)
        LLINK(R) = RLINK(PNTR)
        RLINK(PNTR) = R
        RLINK(S) = LLINK(PNTR)
        LLINK(PNTR) = S
210    BF(S) = 0
        BF(R) = 0
        IF (BF(PNTR) .NE. A) GO TO 220
        BF(S) = -A
        GO TO 230
220    IF (BF(PNTR) .EQ. -A) BF(R) = A
230    BF(PNTR) = 0
240    IF (T .NE. 0) GO TO 250
        ROOT = PNTR
        RETURN
250    IF (S .NE. RLINK(T)) THEN
        LLINK(T) = PNTR
    ELSE
        RLINK(T) = PNTR
    END IF
C
    RETURN
    END
C
C
C
+    SUBROUTINE TREEP(PERM, LLINK, RLINK, MAXT, NTREE, ROOT, STACK,
        MAXSTA, IFAULT)
    INTEGER NTREE, PERM(NTREE), LLINK(MAXT), RLINK(MAXT)
    INTEGER PNTR, STACK(MAXSTA), SPTR, ROOT
C
C    Returns a permutation vector (PERM) to the tree contained in
C    NODE, LLINK, RLINK and rooted at ROOT
C
    IFAULT = 0
    IF (NTREE .LT. 1) RETURN
    SPTR = 0
    PNTR = ROOT
    I = 1
10    IF (PNTR .EQ. 0) GO TO 20
C
C    Traverse left subtree
C
    SPTR = SPTR + 1
    IF (SPTR .GT. MAXSTA) GO TO 900
    STACK(SPTR) = PNTR
    PNTR = LLINK(PNTR)
    GO TO 10
20    IF (SPTR .LT. 1) RETURN
C
C    Process NODE and traverse right subtree
C
    PNTR = STACK(SPTR)
    SPTR = SPTR - 1
    PERM(I) = PNTR

```

```
      I = I + 1
      PNTR = RLINK(PNTR)
      GO TO 10
C
900  IFAULT = 1
      RETURN
      END
C
C
C
+   INTEGER FUNCTION SEARCH(FIND, NODE, LLINK, RLINK, MAXT, NTREE,
      ROOT)
      INTEGER LLINK(MAXT), RLINK(MAXT)
      INTEGER NTREE, PNTR, MAXT, ROOT, ICOMP
      REAL    NODE(MAXT), FIND
C
C   Returns the location in the tree of the item FIND.
C   Returns 0 if FIND is not in the tree.
C
      SEARCH = 0
      IF (NTREE .LT. 0) RETURN
      PNTR = ROOT
10   K = ICOMP(FIND, NODE(PNTR))
      IF (K .EQ. 0) GO TO 20
      IF (K .LT. 0) THEN
          PNTR = LLINK(PNTR)
      ELSE
          PNTR = RLINK(PNTR)
      END IF
      IF (PNTR .NE. 0) GO TO 10
C
20   SEARCH = PNTR
      RETURN
      END
C
C
C
      INTEGER FUNCTION ICOMP(X, Y)
      REAL    X, Y, EPS, Z
C
C   The body of ICOMP will be supplied by the user.
C   ICOMP will return 0 if X and Y are equal to the accuracy
C   needed, and return -1 if X < Y, and +1 if X > Y.
C   The example given tests whether X and Y differ by more than
C   0.001 of the larger in magnitude.
C
      DATA ZERO, ONE, EPS /0.0, 1.0, 0.001/
C
C   Avoid comparison of very different X and Y
C
      IF (X .LT. ONE .OR. Y .GT. -ONE) GO TO 10
      ICOMP = 1
      RETURN
10   IF (X .GT. -ONE .OR. Y .LT. ONE) GO TO 20
      ICOMP = -1
      RETURN
C
20   Z = MAX(ABS(X), ABS(Y))
      ICOMP = 0
      IF (Z .EQ. ZERO) RETURN
      Z = (X - Y) / Z
```

```
IF (ABS(Z) .LT. EPS) RETURN
ICOMP = 1
IF (Z .GT. ZERO) RETURN
ICOMP = -1
RETURN
END
```

```

SUBROUTINE STEM(K, SDF, SDN, D, T, EPS, LG, ALGAMA, KW, WK, XPT,
* VAR, IFAULT)

```

```

C
C     ALGORITHM AS220  APPL. STATIST. (1986) VOL. 35, NO. 2
C

```

```

C     COMPUTES EXPECTATION AND VARIANCE OF STEIN AND
C     EFRON-MORRIS LIMITED TRANSLATION ESTIMATORS.
C

```

```

REAL SDF, SDN, D, T(K), XPT(K), VAR(K), ALGAMA(LG), WK(KW)
REAL EPS, EPS2, EPS3, HF, ONE, TWO, P, PM, RPM, DL, BD, C1, C2,
* C22, PNC, PP1, PP2
REAL SJJ, BJ, BJ2, R0, R1, R2, SLL, BV, BL, BL2, QSM, QSM2, XPG,
* TMP

```

```

REAL VC, DN, QTRM, EPS4, Q(101)

```

```

INTEGER THR

```

```

DATA ZERO, HF, ONE, TWO /0.0, 0.5, 1.0, 2.0/

```

```

DATA THR /3/

```

```

DATA EPS4 /1.0E-04/

```

```

DATA ITYPE /1/

```

```

LENQ = 101

```

```

IF (K .LT. THR .OR. D .LT. ZERO .OR. EPS .LE. ZERO .OR. (SDF .GT.
* ZERO .AND. SDN .LE. ZERO)) GOTO 21

```

```

IFault = 0

```

```

DL = D

```

```

P = K

```

```

PM = P - TWO

```

```

RPM = SQRT(PM)

```

```

IF (D .GT. RPM) DL = RPM

```

```

EPS2 = HF * HF * EPS

```

```

F1 = ONE

```

```

F2 = ONE

```

```

IF (SDF .LE. ZERO) GOTO 1

```

```

F1 = SDF / SDN

```

```

F2 = SDF * (TWO + SDF) / (SDN * SDN)

```

```

1 F3 = TWO * F1 + F2

```

```

BD = DL * DL / PM

```

```

C1 = F1 * TWO * RPM * DL

```

```

C22 = F2 * DL * DL

```

```

C2 = C22 * PM

```

```

PNC = ZERO

```

```

DO 2 J1 = 1, K

```

```

PNC = PNC + T(J1) * T(J1)

```

```

2 CONTINUE

```

```

PNC = HF * PNC

```

```

C
C     COMPUTE EXPECTATION OF THE NP-COMPONENT ESTIMATOR
C

```

```

DO 17 NP = 1, K

```

```

DO 3 J2 = 1, KW

```

```

WK(J2) = ZERO

```

```

3 CONTINUE

```

```

PP1 = HF * T(NP) * T(NP)

```

```

PP2 = PNC - PP1

```

```

EPS3 = EPS2

```

```

IF (T(NP) .LE. ONE) GOTO 4

```

```

EPS3 = EPS2 / (T(NP) * T(NP))

```

```

4 XPT(NP) = ZERO

```

```

VAR(NP) = ONE + T(NP) * T(NP)

```

```

C
C     CORRECTION FOR JAMES-STEIN-EFRON-MORRIS PARTS
C     SET UP INNER POISSON SUM
C

```

```

C
  JJ = 1
  WK(1) = EXP(-PP1)
  SJJ = WK(1)
  JXP = 0
  R0 = ONE
  R1 = ONE
5  JJ = JJ + 1
  IF (JJ .GT. KW) GOTO 19
  BJ = JJ - 1
  WK(JJ) = WK(JJ - 1) * PP1 / BJ
  SJJ = SJJ + WK(JJ)
  IF (SJJ .GT. ONE) SJJ = ONE
  R2 = R1
  R1 = R0
  R0 = (ONE - SJJ) + WK(JJ)
  IF (JXP .GT. 0) GOTO 6
  IF (R0 * T(NP) * (ONE + HF * C1) .LE. EPS3) JXP = JJ + 1
  IF (JXP .EQ. 0) GOTO 5
6  IF (R0 * C22 + R1 * (C1 * PP1 + F3) + TWO * F3 * PP1 * R2 .GT.
  * EPS2) GOTO 5
  LL = 1

C
C      SET UP OUTER POISSON SUM
C
  LP = JJ + 1
  IF (LP + 1 .GT. KW) GOTO 19
  LXP = 0
  WK(LP + 1) = EXP(-PP2)
  SLL = WK(LP + 1)
  BV = PP1 * (C1 + 2 * F3) + C22 + F3
7  LL = LL + 1
  IF (LP + LL .GT. KW) GOTO 19
  BL = LL - 1
  WK(LP + LL) = WK(LP + LL - 1) * PP2 / BL
  SLL = SLL + WK(LP + LL)
  IF (SLL .GT. ONE) SLL = ONE
  R0 = ONE - SLL
  IF (LXP .GT. 0) GOTO 8
  IF (R0 * T(NP) * (ONE + HF * C1) .LE. EPS3) LXP = LL + 1
  IF (LXP .EQ. 0) GOTO 7
8  IF (R0 * BV .GT. EPS2) GOTO 7
  KSTP = K + 2 * JXP + 2 * LXP - 3
  IF (KSTP .GT. LG) GOTO 18
  IF (2 * JXP + 2 .GT. LENQ) GOTO 20
  DO 12 L2P = 1, LXP
  L2 = L2P - 1
  BL2 = L2
  JDF = 2 * JXP
  LDF = K - 1 + 2 * L2
  DO 9 JX = 1, LENQ
  Q(JX) = ZERO
9  CONTINUE
  QSM = ZERO
  QSM2 = ZERO
  DO 10 J2P = 1, JXP
  J2 = J2P - 1
  BJ2 = J2
  JD1 = 2 * J2 + 3
  JD2 = 2 * J2 + 4
  JSB = K + 2 * J2 + 2 * L2

```



```

XPG = EXP(ALGAMA(JSB) - ALGAMA(JSB + 1) + ALGAMA(2 * J2 + 2)
* - ALGAMA(2 * J2 + 3))
Q(JD1) = -HF * DL * T(NP) * RPM * XPG * WK(J2 + 1) * WK(LP + L2 +
* 1)
Q(JD2) = T(NP) * WK(J2 + 1) * WK(LP + L2 + 1) * PM / (P +
* TWO * BL2 + TWO * BJ2)
QSM = QSM - Q(JD1)
QSM2 = QSM2 + Q(JD1) + Q(JD2)
10 CONTINUE
TMP = QSM2
IF (ABS(DL - RPM) .LE. EPS4) GOTO 11
TMP = BMIX(BD, JDF, LDF, Q, ITYPE, IFAULT)
IF (IFAILT .NE. 0) RETURN
11 XPT(NP) = XPT(NP) - QSM - TMP
12 CONTINUE
XPT(NP) = T(NP) + F1 * XPT(NP)
C
C      COMPUTE VARIANCE OF THE NP-COMPONENT ESTIMATOR
C
VC = ZERO
LLP = LL + 1
DO 16 L2P = 1, LLP
L2 = L2P - 1
BL2 = L2
JDF = 2 * JJ
LDF = K - 1 + 2 * L2
QSM = C2 * WK(1) * WK(LP + L2 + 1) / (PM + TWO * BL2)
DO 13 J2 = 1, LENQ
Q(J2) = ZERO
13 CONTINUE
Q(2) = -QSM
QSM2 = -QSM
DO 14 J2P = 1, JJ
J2 = J2P - 1
BJ2 = J2
JD1 = 2 * J2 + 3
JD2 = 2 * J2 + 4
JSB = K + 2 * J2 + 2 * L2
DN = JSB
QTRM = C2 * WK(J2 + 2) * WK(LP + L2 + 1) / DN
Q(JD2) = -QTRM + WK(J2 + 1) * WK(LP + L2 + 1) * PM * (TWO * BJ2 +
* ONE) / DN * (-TWO * F1 + PM * F2 / (DN - TWO))
XPG = EXP(ALGAMA(JSB) - ALGAMA(JSB + 1) + ALGAMA(2 * J2 + 2)
* - ALGAMA(2 * J2 + 1))
WK(LG + JD1) = C1 * WK(J2 + 1) * WK(LP + L2 + 1) * XPG
QSM = QSM + QTRM - WK(LG + JD1)
QSM2 = QSM2 + WK(LG + JD1) + WK(LG + JD2)
14 CONTINUE
TMP = QSM2
IF (ABS(DL - RPM) .LE. EPS4) GOTO 15
TMP = BMIX(BD, JDF, LDF, Q, ITYPE, IFAULT)
IF (IFAILT .NE. 0) RETURN
15 VC = VC + QSM + TMP
16 CONTINUE
VAR(NP) = VAR(NP) + VC - XPT(NP) * XPT(NP)
17 CONTINUE
RETURN
18 IFAULT = 6
RETURN
19 IFAULT = 7
RETURN

```

```
20 IFAULT = 8
   RETURN
21 IFAULT = 9
   RETURN
   END
```

C

```
   SUBROUTINE ALGAM(N, ALGAMA)
```

C

C

C

C

```
      COMPUTES ALOG(GAMMA(J/2)) FOR J = 1(1)N, N EVEN.
      PL2 IS HALF LOG(PI).
```

```
   DIMENSION ALGAMA(N)
```

```
   DATA ZERO, HF, PL2 /0.0, 0.5, 0.572364943/
```

```
   NHLF = N / 2
```

```
   ALGAMA(1) = PL2
```

```
   ALGAMA(2) = ZERO
```

```
   DO 1 J1 = 2, NHLF
```

```
   B1 = FLOAT(2 * J1 - 3)
```

```
   B2 = FLOAT(J1 - 1)
```

```
   ALGAMA(2 * J1) = ALGAMA(2 * J1 - 2) + ALOG(B2)
```

```
   ALGAMA(2 * J1 - 1) = ALGAMA(2 * J1 - 3) + ALOG(HF * B1)
```

```
1 CONTINUE
```

```
   RETURN
```

```
   END
```

```
      SUBROUTINE NPMLG(NI, NJ, ITER, ICYC, JN, DEPS, Y, S, R, P, DFL, X,  
*      W, M, V, AFI, LP, IFAULT)
```

```
      ALGORITHM AS221  APPL. STATIST. (1986) VOL. 35, NO. 3
```

```
      SUBROUTINE FOR CALCULATING THE NONPARAMETRIC MAXIMUM  
      LIKELIHOOD ESTIMATE OF THE MIXING DISTRIBUTION IN  
      A MIXTURE OF NORMALS
```

```
      N.B. The dimension of array R below has been changed in accordance  
      with the correction on page 176 of vol. 39 (1990) of Applied  
      Statistics.
```

```
      REAL R(0:NI), P(NI), Y(NI), S(NI), M(NI), V(NI), AFI(NI), X, W,  
*      DEPS, DFL, RMIN, RMAX, RCONS, A, Q, D, DENOM, PR, FL, DIFF,  
*      POLD, ROLD, PQ, RR, AI, ANB, TEMP, DFOLD, AN  
      INTEGER LP(ICYC), NI, NJ, ITER, ICYC, JN, IFAULT, JJ, IT, IC, IJ,  
*      JNN, NEXLAS, MORE  
      DATA DCONS /1.0E-6/, RCONS /1.0E-2/, DINF /1.0E-6/  
      DATA ZERO /0.0/, ONE /1.0/, TWO /2.0/, PI /6.2831853/
```

```
      CHECK INPUT VALUES FOR SAMPLING VARIANCES
```

```
      IFAULT = 0  
      DO 1 I = 1, NI  
      IF (S(I) .LE. ZERO) IFAULT = 2  
      IF (IFAULT .EQ. 2) GOTO 999
```

```
1 CONTINUE
```

```
      SET THE INITIAL ESTIMATE : UNIFORM DISTRIBUTION OVER  
      THE RANGE OF OBSERVED VALUES
```

```
      FNJ = FLOAT(NJ)  
      FNI = FLOAT(NI)  
      POLD = ONE / FNJ  
      RMIN = Y(1)  
      RMAX = Y(1)  
      DO 5 I = 2, NI  
      IF (RMIN .GT. Y(I)) RMIN = Y(I)  
      IF (RMAX .LT. Y(I)) RMAX = Y(I)
```

```
5 CONTINUE
```

```
      PQ = (RMAX - RMIN) / (FNJ - ONE)  
      DO 10 J = 1, NJ  
      FJ = FLOAT(J) - ONE  
      R(J) = RMIN + PQ * FJ  
      P(J) = POLD
```

```
10 CONTINUE
```

```
      CALCULATE GRID SIZE FOR EVALUATING CONVERGENCE  
      TO GLOBAL MAXIMUM
```

```
      CALL GRIDN(NI, Y, JN, RMIN, RMAX, RCONS, DEPS)
```

```
      START THE ITERATIONS
```

```
      DFOLD = DINF
```

```
      DFOLD REPRESENTS THE VALUE OF THE LOG LIKELIHOOD  
      FUNCTION FROM THE PREVIOUS ITERATION
```

```
      IT = 0
```

```
      IC = ICYC + 1
30  IT = IT + 1
C
C      'IT' COUNTS THE NUMBER OF EM CYCLES REQUIRED
C      TO REACH CONVERGENCE AT GLOBAL MAXIMUM
C
      DO 75 LPOUT = 1, ITER
      DFL = ZERO
      LP(IT) = LPOUT
      DO 40 I = 1, NI
      FL = ZERO
      DO 35 J = 1, NJ
      PR = (Y(I) - R(J)) * (Y(I) - R(J)) / (TWO * S(I))
      A = EXP(-PR) / SQRT(PI * S(I))
      FL = FL + P(J) * A
35  CONTINUE
C
C      A REPRESENTS THE SAMPLING DENSITY
C      FL REPRESENTS THE MARGINAL DENSITY
C      DFL REPERESENTS THE LOG LIKELIHOOD FUNCTION
C
      DFL = DFL + LOG(FL)
      AFI(I) = FL
40  CONTINUE
      DIFF = ABS((DFL - DFOLD) / DFOLD)
C
C      EVALUATE WHETHER THE RELATIVE CHANGE IN LOG
C      LIKELIHOOD IS LESS THAN DCONS
C
      IF (DIFF .LE. DCONS) GOTO 80
      DFOLD = DFL
C
C      CALCULATE THE NEW ESTIMATE
C
      DO 50 J = 1, NJ
      POLD = P(J)
      ROLD = R(J)
      R(J) = ZERO
      P(J) = ZERO
      DENOM = ZERO
      DO 45 I = 1, NI
      PR = (Y(I) - ROLD) * (Y(I) - ROLD) / (TWO * S(I))
      A = EXP(-PR) / SQRT(PI * S(I))
      Q = A / (S(I) * AFI(I))
      R(J) = R(J) + Y(I) * Q
      P(J) = P(J) + A / AFI(I)
      DENOM = DENOM + Q
45  CONTINUE
      R(J) = R(J) / DENOM
      P(J) = POLD * P(J) / FNI
50  CONTINUE
C
C      COLLAPSE THE NUMBER OF SUPPORT POINTS
C
      JJ = 1
      DO 70 J = 2, NJ
      DIFF = ABS(R(J) - R(JJ))
      IF (DIFF .LE. DEPS) GOTO 60
      JJ = JJ + 1
      R(JJ) = R(J)
      P(JJ) = P(J)
```

```
      GOTO 65
60 CONTINUE
   P(JJ) = P(JJ) + P(J)
65 CONTINUE
70 CONTINUE
   NJ = JJ
75 CONTINUE

C
C      END OF ITERATIONS
C
80 CONTINUE

C
C      CHECK IF THE ESTIMATE IS THE GLOBAL MAXIMUM
C
   IF (IT .EQ. IC) GOTO 169
   R(0) = RMIN
   IJ = 0
   JNN = 1
   FJN = FLOAT(JN)
   PQ = (RMAX - RMIN) / (FJN - ONE)
   DO 130 J = 1, JN
   FJ = FLOAT(J) - ONE
   RR = RMIN + PQ * FJ
   IF (RR .LT. R(IJ)) GOTO 130
   AI = ZERO
   DO 90 I = 1, NI
   PR = (Y(I) - RR) ** 2
   PR = PR / (TWO * S(I))
   A = EXP(-PR) / SQRT(PI * S(I))
   AI = AI + (A / AFI(I))
90 CONTINUE
   DIFF = AI - FNI

C
C      CHECK IF THE CRITERION OF GLOBAL MAXIMUM
C      HOLDS FOR ALL VALUES IN THE RANGE OF THE
C      OBSERVATIONS
C
   IF (DIFF .LE. DINF) GOTO 130
   DO 100 IJ = 1, JJ
   ANB = RR - R(IJ)
   AN = ABS(ANB)
   IF (AN .LE. DEPS) GOTO 130
   IF (ANB .LE. ZERO) GOTO 105
100 CONTINUE
105 CONTINUE

C
C      IF THE CRITERION OF GLOBAL MAXIMUM IS NOT MET,
C      NEW SUPPORT IS ADDED AT THE POINT OF FAILURE
C
   JNN = 0
   IF (NJ .GE. NI) GOTO 152
   NJ = NJ + 1
   FNJ = FLOAT(NJ)
   DO 110 I = 1, NJ
   P(I) = ONE / FNJ
110 CONTINUE
   R(NJ) = (R(IJ) + RR) / TWO
   IF (RR .GE. R(JJ)) R(NJ) = (RMAX + RR) / TWO
   IF (RR .GE. R(JJ)) GOTO 140
130 CONTINUE
140 CONTINUE
```

```
C
C      CHECK IF THE CRITERION OF GLOBAL MAXIMUM
C      HOLDS AT THE ESTIMATED POINTS OF SUPPORT
C
      DO 150 J = 1, JJ
      AI = ZERO
      DO 145 I = 1, NI
      PR = (Y(I) - R(J)) * (Y(I) - R(J)) / (TWO * S(I))
      A = EXP(-PR) / SQRT(PI * S(I))
      A = A / AFI(I)
      AI = AI + A
145 CONTINUE
      DIFF = ABS(AI - FNI)
      IF (DIFF .LE. DINF) GOTO 150
      IF (P(J) .LE. DINF) GOTO 150
      JNN = 0
150 CONTINUE
152 JJ = NJ
C
C      IF NO NEW SUPPORT IS ADDED, THEN CONVERGENCE TO
C      GLOBAL MAXIMUM IS ASSUMED
C
      IF (JNN .EQ. 1) GOTO 170
C
C      SORT THE POINTS OF SUPPORT IN AN ASCENDING ORDER
C
      NEXLAS = NJ - 1
      MORE = 0
155 IF (MORE .EQ. 1) GOTO 165
      MORE = 1
      DO 160 I = 1, NEXLAS
      J = I + 1
      IF (R(I) .LE. R(J)) GOTO 160
      TEMP = R(I)
      R(I) = R(J)
      R(J) = TEMP
      MORE = 0
160 CONTINUE
      GOTO 155
165 CONTINUE
C
C      IF THE GLOBAL MAXIMUM IS NOT REACHED AND IF THE
C      MAXIMUM ALLOWED NUMBER OF CYCLES IS NOT EXHAUSTED,
C      THEN A NEW CYCLE IS RESTARTED WITH THE NEW SUPPORT
C
      IF (IT .LE. ICYC) GOTO 30
C
C      IF THE GLOBAL MAXIMUM IS NOT REACHED AND IF THE
C      MAXIMUM ALLOWED NUMBER OF CYCLES IS EXHAUSTED,
C      THEN IFAULT IS SET TO 1
C
169 IFAULT = 1
170 CONTINUE
      ICYC = IT
      IF (IFAULT .EQ. 1) ICYC = ICYC - 1
      X = ZERO
      W = ZERO
C
C      CALCULATE THE PRIOR MEAN AND VARIANCE
C
      DO 175 J = 1, NJ
```

```
      X = X + P(J) * R(J)
175 CONTINUE
      DO 180 J = 1, NJ
      W = W + P(J) * ((R(J) - X) ** 2)
180 CONTINUE
C
C      CALCULATE THE POSTERIOR MEANS AND VARIANCES
C
      DO 195 I = 1, NI
      Q = ZERO
      D = ZERO
      DO 185 J = 1, NJ
      PR = (Y(I) - R(J)) * (Y(I) - R(J)) / (TWO * S(I))
      A = EXP(-PR) / SQRT(PI * S(I))
      A = A / AFI(I)
      Q = Q + P(J) * R(J) * A
185 CONTINUE
      DO 190 J = 1, NJ
      PR = (Y(I) - R(J)) * (Y(I) - R(J)) / (TWO * S(I))
      A = EXP(-PR) / SQRT(PI * S(I))
      A = A / AFI(I)
      D = D + P(J) * A * ((R(J) - Q) ** 2)
190 CONTINUE
      M(I) = Q
      V(I) = D
195 CONTINUE
999 CONTINUE
      RETURN
      END
C
      SUBROUTINE GRIDN(NI, Y, JN, RMIN, RMAX, RCONS, DEPS)
C
C      ALGORITHM AS221  APPL. STATIST. (1986) VOL. 35, NO. 3
C
C      AUXILIARY SUBROUTINE FOR CALCULATING THE GRID SIZE TO
C      BE USED IN EVALUATING CONVERGENCE TO THE GLOBAL MAXIMUM
C
      REAL Y(NI), RMIN, RMAX, RCONS, DEPS, SUM, AVE, VAR, SD
      INTEGER NI, JN
      DATA ZERO /0.0/
      SUM = ZERO
      VAR = ZERO
      DO 5 I = 1, NI
      SUM = SUM + Y(I)
5 CONTINUE
      FNI = FLOAT(NI)
      AVE = SUM / FNI
      DO 10 I = 1, NI
      VAR = VAR + (Y(I) - AVE) ** 2
10 CONTINUE
      VAR = VAR / (FNI - 1.0)
      SD = SQRT(VAR)
      DEPS = RCONS * SD
      JN = (RMAX - RMIN) / DEPS
      RETURN
      END
```

```
      SUBROUTINE RESSMO(X, Y, NIN, CUTOFF, XLO, XHI, BANDW, SMOOTH,  
+          NOUT, NEWCAL, IWK, W, WA, WB, WC, WK, IFAULT)  
C  
C      ALGORITHM AS222  APPL. STATIST. (1987) VOL. 36, NO. 1  
C      Modified by incorporating AS R73 (Appl. Statist. (1988) vol. 37  
C      (2), p.316)  
C  
C      Auxiliary routine required: FASTF = algorithm AS 83 as amended  
C      in Griffiths & Hill, 1985 (i.e. with extra final argument)  
C  
C      INTEGER    NIN, NOUT, IWK(NIN), NEWCAL, IFAULT  
C      REAL       X(NIN), Y(NIN), CUTOFF, XLO, XHI, BANDW, SMOOTH(NOUT),  
+          W(NIN), WA(NOUT), WB(NOUT), WC(NOUT), WK(6, NOUT)  
C  
C      Local variables  
C  
C      INTEGER NPOW, M, K, N2, JHI, JMAX, I, J, NC, ICAL  
C      REAL    ZERO, ONE, TWO, PI, BIG, RANGE, XSTEP, A, B, XLO1, TEMP,  
+          RES  
C      DATA ZERO, ONE, TWO, PI, BIG /0.0, 1.0, 2.0, 3.14159, 30.0/  
C  
C      RANGE = XHI - XLO  
C  
C      Check cutoff parameter  
C  
C      IF (CUTOFF .LE. ZERO) THEN  
C          IFAULT = 1  
C          RETURN  
C      END IF  
C  
C      Check if NOUT is a power of 2  
C  
C      NPOW = 8  
C      M = 16  
C      DO 2 K = 3, 11  
C          IF (NPOW .EQ. NOUT) GO TO 3  
C          M = M * 2  
C          NPOW = NPOW * 2  
2 CONTINUE  
C      IFAULT = 2  
C      RETURN  
C  
C      Check range  
C  
C      3 IF (RANGE .LE. ZERO) THEN  
C          IFAULT = 3  
C          RETURN  
C      END IF  
C  
C      Check bandwidth  
C  
C      IF (BANDW .LE. ZERO) THEN  
C          IFAULT = 4  
C          RETURN  
C      END IF  
C  
C      Check NEWCAL  
C  
C      IF (NEWCAL .LT. 0 .OR. NEWCAL .GT. 2) THEN  
C          IFAULT = 5  
C          RETURN
```



```
      END IF
C
XSTEP = RANGE / FLOAT(NOUT)
A = FLOAT(NOUT) / (RANGE * FLOAT(NIN))
N2 = NOUT / 2
B = TWO * (PI * BANDW / RANGE)**2
IF (NEWCAL .EQ. 2) GO TO 8
C
JHI = SQRT(BIG / B)
JMAX = MIN(N2-1, JHI)
XLO1 = XLO - XSTEP
IF (NEWCAL .EQ. 0) THEN
  DO 5 I = 1, NIN
    IWK(I) = (X(I) - XLO1) / XSTEP
    W(I) = ONE
5  CONTINUE
  END IF
C
C Refresh former results
C
IF (NEWCAL .EQ. 1) THEN
  DO 52 J = 1, NOUT
    WA(J) = WK(5, J)
    WB(J) = WK(6, J)
52 CONTINUE
  END IF
C
C Find numerator of Nadaraya-Watson estimate
C
CALL LINSMO(Y, IWK, NIN, SMOOTH, NOUT, NEWCAL, WA, WB, WC, N2,
+          JHI, JMAX, A, B, M)
C
C Transfer results to work area
C
DO 54 J = 1, NOUT
  WK(3, J) = WA(J)
  WK(4, J) = WB(J)
  WK(1, J) = SMOOTH(J)
54 CONTINUE
C
C Refresh former results
C
IF (NEWCAL .EQ. 1) THEN
  DO 55 J = 1, NOUT
    WA(J) = WK(5, J)
    WB(J) = WK(6, J)
55 CONTINUE
  END IF
C
C Find density estimate of marginal distribution of X.
C
CALL LINSMO(W, IWK, NIN, SMOOTH, NOUT, NEWCAL, WA, WB, WC, N2,
+          JHI, JMAX, A, B, M)
DO 65 J = 1, NOUT
  WK(5, J) = WA(J)
  WK(6, J) = WB(J)
65 CONTINUE
C
C Compute Nadaraya-Watson estimate
C
DO 7 J = 1, NOUT
```

```

        TEMP = ZERO
        IF (SMOOTH(J) .GT. ZERO) TEMP = WK(1, J) / SMOOTH(J)
        WK(1, J) = TEMP
7 CONTINUE
C
C      Compute Huber's PSI from the residuals
C
8 NC = 0
  DO 11 I = 1, NIN
    RES = Y(I) - WK(1, IWK(I))
    IF (RES .GT. -CUTOFF) GO TO 9
    NC = NC + 1
    W(I) = -CUTOFF
    GO TO 11
  9  IF (RES .LT. CUTOFF) GO TO 10
    NC = NC + 1
    W(I) = CUTOFF
    GO TO 11
10  W(I) = RES
11 CONTINUE
C
C      Compute non-linear correction
C
  IFAULT = -NC
  ICAL = 0
  CALL LINSMO(W, IWK, NIN, SMOOTH, NOUT, ICAL, WA, WB, WC, N2, JHI,
+           JMAX, A, B, M)
C
C      Store the results
C
  DO 111 J = 1, NOUT
111 WK(2, J) = SMOOTH(J)
C
C      Derivative of Huber's PSI from residuals
C
  DO 112 I = 1, NIN
    TEMP = ZERO
    IF (W(I) .LT. CUTOFF .AND. W(I) .GT. -CUTOFF) TEMP = ONE
    W(I) = TEMP
112 CONTINUE
C
C      Compute denominatot of non-linear correction
C
  CALL LINSMO(W, IWK, NIN, SMOOTH, NOUT, ICAL, WA, WB, WC, N2, JHI,
+           JMAX, A, B, M)
C
C      Compute the full estimator
C
  DO 13 J = 1, NOUT
    TEMP = WK(1, J)
    IF (SMOOTH(J) .GT. ZERO) TEMP = TEMP + WK(2, J) / SMOOTH(J)
    SMOOTH(J) = TEMP
13 CONTINUE
C
  RETURN
  END
C
C
C      SUBROUTINE LINSMO(Y, IWK, NIN, SMOOTH, NOUT, NEWCAL, WA, WB, WC,
+           N2, JHI, JMAX, A, B, M)

```

```
C
C      ALGORITHM AS222  APPL. STATIST. (1987) VOL. 36, NO. 1
C
C      INTEGER  NIN, IWK(NIN), NOUT, NEWCAL, N2, JHI, JMAX, M
C      REAL     Y(NIN), SMOOTH(NOUT), WA(NOUT), WB(NOUT),
+           WC(NOUT), A, B
C
C      Local variables
C
C      INTEGER M1, J, I, JI, ITYPE, J1, J2, JHI2, IFAULT
C      REAL ZERO, TEMP, C
C      DATA ZERO/0.0/
C
C      M1 = M / 2
C      IF (NEWCAL .NE. 0) GO TO 30
C
C      Transform
C
C      DO 10 J = 1, NOUT
C          WA(J) = ZERO
C          WB(J) = ZERO
10 CONTINUE
C
C      DO 20 I = 1, NIN
C          JI = IWK(I)
C          IF (JI .LT. 1 .OR. JI .GT. NOUT) GO TO 20
C          WA(JI) = WA(JI) + A*Y(I)
20 CONTINUE
C      ITYPE = 1
C
C      CALL FASTF(WA, WB, M1, ITYPE, IFAULT)
C
C      Filter Fourier transform
C
C      30 SMOOTH(1) = WA(1)
C      WC(1) = WB(1)
C      DO 40 J = 1, JMAX
C          C = EXP(-B * FLOAT(J*J))
C          J1 = J + 1
C          J2 = NOUT - J + 1
C          SMOOTH(J1) = C * WA(J1)
C          WC(J1) = C * WB(J1)
C          SMOOTH(J2) = C * WA(J2)
C          WC(J2) = C * WB(J2)
40 CONTINUE
C
C      Underflow correction
C
C      IF (JHI + 1 - N2 .GT. 0) THEN
C          TEMP = EXP(-B * FLOAT(N2*N2))
C          SMOOTH(N2 + 1) = TEMP * WA(N2 + 1)
C          WC(N2 + 1) = TEMP * WB(N2 + 1)
C      ELSE IF (JHI + 1 - N2 .LT. 0) THEN
C          JHI2 = JHI + 2
C          DO 61 J1 = JHI2, N2
C              J2 = NOUT - J1 + 2
C              SMOOTH(J1) = ZERO
C              WC(J1) = ZERO
C              SMOOTH(J2) = ZERO
C              WC(J2) = ZERO
61 CONTINUE
```

```
SMOOTH(N2 + 1) = ZERO  
WC(N2 + 1) = ZERO  
ELSE  
SMOOTH(N2 + 1) = ZERO  
WC(N2 + 1) = ZERO  
END IF
```

C

```
ITYPE = -1  
CALL FASTF(SMOOTH, WC, M1, ITYPE, IFAULT)
```

C

```
RETURN  
END
```

```
      SUBROUTINE ORPS1(ALPHA, LAMDA, DELTA, IP, SIGMA, KNEW, FM10, FM1K,  
*          FM20, FM2K, ITER, IFAULT)  
C  
C      ALGORITHM AS223  APPL. STATIST. (1987) VOL. 36, NO. 1  
C  
C      Calculates the optimum ridge parameter under the criterion of  
C      minimizing the mean squared error of parameter estimation.  
C  
      INTEGER FM20, IMAX, IP, ITER, IFAULT  
      REAL ALPHA(IP), LAMDA(IP), DELTA, K, KNEW, KOLD, DK, FM10, FM1K,  
*      FM2K, DFM1K, DDFM1K, S, SIGMA  
      REAL ZERO, TWO, THREE  
C  
      FM1(X, Y) = (Y * S**2 + (X * K)**2) / ((Y + K)**2 * S**2)  
      FM2(X, Y) = Y * FM1(X, Y)  
      DFM1(X, Y) = Y * (X**2 * K - S**2) / (Y + K)**3  
      DDFM1(X, Y) = Y * (Y * X**2 - TWO * X**2 * K + THREE * S**2) /  
*          (Y + K)**4  
      DATA ZERO/0.0/, TWO/2.0/, THREE/3.0/  
C  
      IFAULT = 1  
      IF (DELTA .LE. ZERO) RETURN  
      IFAULT = 2  
      IF (SIGMA .LE. ZERO) RETURN  
      IFAULT = 3  
      DO 10 J = 1, IP  
          IF (LAMDA(J) .LE. ZERO) RETURN  
10  CONTINUE  
      IFAULT = 0  
      K = ZERO  
      FM10 = ZERO  
      S = SIGMA  
      DO 20 J = 1, IP  
          FM10 = FM10 + FM1(ALPHA(J), LAMDA(J))  
20  CONTINUE  
      FM20 = IP  
      ITER = 0  
      IMAX = 20  
      KNEW = ZERO  
      DO 40 I = 1, IMAX  
          ITER = ITER + 1  
          FM1K = ZERO  
          FM2K = ZERO  
          DFM1K = ZERO  
          DDFM1K = ZERO  
          DO 30 J = 1, IP  
              FM1K = FM1K + FM1(ALPHA(J), LAMDA(J))  
              FM2K = FM2K + FM2(ALPHA(J), LAMDA(J))  
              DFM1K = DFM1K + DFM1(ALPHA(J), LAMDA(J))  
              DDFM1K = DDFM1K + DDFM1(ALPHA(J), LAMDA(J))  
30  CONTINUE  
          KOLD = KNEW  
          KNEW = KOLD - DFM1K / DDFM1K  
          K = KNEW  
          DK = ABS(KNEW - KOLD)  
          IF (DK .LE. DELTA) GO TO 50  
40  CONTINUE  
50  RETURN  
      END  
C  
C
```

```
C
SUBROUTINE ORPS2(ALPHA, LAMDA, DELTA, IP, SIGMA, KNEW, FM10, FM1K,
*           FM20, FM2K, ITER, IFAULT)
C
C   ALGORITHM AS223  APPL. STATIST. (1987) VOL. 36, NO. 1
C
C   Calculates the optimum ridge parameter under the criterion of
C   minimizing the mean squared error of prediction.
C
C   INTEGER FM20, IMAX, IP, ITER, IFAULT
C   REAL ALPHA(IP), LAMDA(IP), DELTA, K, KNEW, KOLD, DK, FM10, FM1K,
*   FM2K, DFM2K, DDFM2K, S, SIGMA
C   REAL ZERO, TWO, THREE
C
C   FM1(X, Y) = (Y * S**2 + (X * K)**2) / ((Y + K)**2 * S**2)
C   FM2(X, Y) = Y * FM1(X, Y)
C   DFM1(X, Y) = Y * (X**2 * K - S**2) / (Y + K)**3
C   DDFM1(X, Y) = Y * (Y * X**2 - TWO * X**2 * K + THREE * S**2) /
*           (Y + K)**4
C   DDFM2(X, Y) = Y * DDFM1(X, Y)
C   DATA ZERO/0.0/, TWO/2.0/, THREE/3.0/
C
C   IFAULT = 1
C   IF (DELTA .LE. ZERO) RETURN
C   IFAULT = 2
C   IF (SIGMA .LE. ZERO) RETURN
C   IFAULT = 3
C   DO 10 J = 1, IP
C       IF (LAMDA(J) .LE. ZERO) RETURN
10 CONTINUE
C   IFAULT = 0
C   K = ZERO
C   FM10 = ZERO
C   S = SIGMA
C   DO 20 J = 1, IP
C       FM10 = FM10 + FM1(ALPHA(J), LAMDA(J))
20 CONTINUE
C   FM20 = IP
C   ITER = 0
C   IMAX = 20
C   KNEW = ZERO
C   DO 40 I = 1, IMAX
C       ITER = ITER + 1
C       FM1K = ZERO
C       FM2K = ZERO
C       DFM2K = ZERO
C       DDFM2K = ZERO
C       DO 30 J = 1, IP
C           FM1K = FM1K + FM1(ALPHA(J), LAMDA(J))
C           FM2K = FM2K + FM2(ALPHA(J), LAMDA(J))
C           DFM2K = DFM2K + DFM2(ALPHA(J), LAMDA(J))
C           DDFM2K = DDFM2K + DDFM2(ALPHA(J), LAMDA(J))
30 CONTINUE
C       KOLD = KNEW
C       KNEW = KOLD - DFM2K / DDFM2K
C       K = KNEW
C       DK = ABS(KNEW - KOLD)
C       IF (DK .LE. DELTA) GO TO 50
40 CONTINUE
50 RETURN
END
```

```
      SUBROUTINE COMBDD(ND, NU, IV, NB, MAXNB, KBS, MAXKBS, NCOMP, IDES,
*   IFAULT)
C
C   ALGORITHM AS224 APPL. STATIST. (1987) VOL. 36, NO. 2
C
DIMENSION IB(5), NCOMP(5, 10, 36), KBS(5), IDES(72), NB(5)
DIMENSION ILIST(72), IR(72)
C
C   COMBINES ND COMPONENT DESIGNS TO FORM A DESIGN WITH
C   ND ORTHOGONAL BLOCKING FACTORS
C
C   NTH COMPONENT DESIGN STORED IN NCOMP(N,...)
C   .. .. .. HAS NB(N) BLOCKS OF SIZE KBS(N)
C
C   CHECK PARAMETERS
C
IFAULT = 1
IF (ND .LT. 2) RETURN
M = 1
DO 1 N = 1, ND
  IFAULT = 2
  L = NB(N) * KBS(N)
  IF (L .NE. NU) RETURN
  IFAULT = 3
  IF (NB(N) .GT. MAXNB) RETURN
  IFAULT = 4
  IF (KBS(N) .GT. MAXKBS) RETURN
  M = M * NB(N)
1 CONTINUE
IFAULT = 5
IF (M .NE. NU) RETURN
IFAULT = 6
C
C   INITIALISE ILIST AND IR
C   ILIST HOLDS TREATMENT LABELS AND IR THE REPLICATIONS
C
DO 2 I = 1, IV
  ILIST(I) = 0
  IR(I) = 0
2 CONTINUE
C
C   INITIALISE IDES.  IDES HOLDS COMBINED DESIGN
C
IL = 0
ID = 0
INB = NB(1)
K = KBS(1)
DO 5 I = 1, INB
  DO 5 J = 1, K
    ID = ID + 1
    IDES(ID) = -1
C
C   SET ITR EQUAL TO NEXT TREATMENT
C   IN FIRST COMPONENT DESIGN
C
ITR = NCOMP(1, I, J)
C
C   IF ITR IS ALREADY RECORDED IN ILIST, THEN
C   ADD ONE TO CORRESPONDING ELEMENT IN IR
C
```

```
      IF (IL .EQ. 0) GOTO 4
      DO 3 JL = 1, IL
      IF (ILIST(JL) .NE. ITR) GOTO 3
      IR(JL) = IR(JL) + 1
      GOTO 5
3 CONTINUE

C
C      RECORD ITR IN ILIST
C      SET CORRESPONDING ELEMENT IN IR EQUAL TO 1
C

4 IL = IL + 1
  IF (IL .GT. IV) RETURN
  ILIST(IL) = ITR
  IR(IL) = 1
5 CONTINUE
  IFAULT = 0

C
C      CHECK EVERY COMPONENT DESIGN CONTAINS SAME NUMBER
C      OF OCCURRENCES OF EVERY TREATMENT LABEL
C

DO 7 JL = 1, IV
  ITR = ILIST(JL)
  DO 7 JN = 2, ND
  KREP = 0
  INB = NB(JN)
  K = KBS(JN)
  DO 6 I = 1, INB
  DO 6 J = 1, K
  IF (NCOMP(JN, I, J) .NE. ITR) GOTO 6
  KREP = KREP + 1
6 CONTINUE
  IF (KREP .EQ. IR(JL)) GOTO 7
  IFAULT = 7
  RETURN
7 CONTINUE
  KREP = 0

C
C      SET ITR EQUAL TO FIRST TREATMENT TO BE FITTED
C
C
  IL = 1
  ITR = ILIST(IL)
  LSTFIT = 0

C
C      RETURN COMBINED DESIGN
C

8 IF (IL .EQ. IV .AND. KREP .EQ. IR(IL)) RETURN

C
C      INITIALISE IB.  IB(N) HOLDS NUMBER OF
C      CURRENT BLOCK IN NTH COMPONENT DESIGN
C

DO 9 N = 1, ND
9 IB(N) = 0
  N = 1

C
C      SET KREP EQUAL TO NEXT OCCURRENCE OF TREATMENT TO BE FITTED
C
C
  KREP = KREP + 1
  IF (KREP .LE. IR(IL)) GOTO 11

C
C      ALL OCCURRENCES OF PRESENT TREATMENT HAVE BEEN FITTED
C      FIND NEXT TREATMENT
```



```
C
  KREP = 1
  IL = IL + 1
  ITR = ILIST(IL)

C
C   INITIALISE THE MARKER LSTFIT
C   LSTFIT PREVENTS ANY TREATMENT BEING FITTED IN
C   AN EARLIER POSITION IN IDES
C
  LSTFIT = 0
  GOTO 11

C
C   MOVE TO PREVIOUS COMPONENT DESIGN
C
10  IB(N) = 0
  N = N - 1
  IF (N .EQ. 1) GOTO 18

C
C   MOVE TO NEXT BLOCK IN PRESENT COMPONENT DESIGN
C
11  IB(N) = IB(N) + 1
  IF (IB(N) .GT. NB(N)) GOTO 10

C
C   LOCATE IN PRESENT COMPONENT DESIGN
C   NEXT OCCURRENCE OF TREATMENT TO BE FITTED
C
12  IS = IB(N)
  INB = NB(N)
  IBS = KBS(N)
  DO 13 I = IS, INB
  DO 13 J = 1, IBS
  IF (NCOMP(N, I, J) .NE. ITR) GOTO 13
  IB(N) = I
  IF (N .EQ. ND) GOTO 14

C
C   MOVE TO NEXT COMPONENT DESIGN
C
  N = N + 1
  GOTO 11
13  CONTINUE
  GOTO 10

C
C   SEE IF CURRENT POSITION IN D-DIMENSIONAL DESIGN IS VACANT
C
14  ID = IB(1) - 1
  DO 15 N1 = 2, ND
15  ID = (ID * NB(N1)) + IB(N1) - 1
  ID = ID + 1
  IF (ID .LE. LSTFIT .OR. IDES(ID) .NE. -1) GOTO 11

C
C   FIT TREATMENT IN D-DIMENSIONAL DESIGN
C   SET LSTFIT EQUAL TO POSITION JUST FILLED
C
  IDES(ID) = ITR
  LSTFIT = ID

C
C   SET FITTED TREATMENT NEGATIVE IN COMPONENT DESIGNS
C
  DO 17 N = 1, ND
  I = IB(N)
  IBS = KBS(N)
```

```
      DO 16 J = 1, IBS
      IF (NCOMP(N, I, J) .NE. ITR) GOTO 16
      NCOMP(N, I, J) = -ITR
      IF (ITR .EQ. 0) NCOMP(N, I, J) = -9999
      GOTO 17
16 CONTINUE
17 CONTINUE
C
      GOTO 8
C
C      CURRENT OCCURRENCE OF TREATMENT CANNOT BE FITTED
C      DETERMINE PREVIOUSLY FITTED OCCURRENCE OF TREATMENT
C
18 KREP = KREP - 1
      IF (KREP .GE. 1) GOTO 20
      IL = IL - 1
      IF (IL .GT. 0) GOTO 19
C
C      DESIGNS CANNOT BE AMALGAMATED
C
      IFAULT = 8
      RETURN
C
C      DETERMINE LAST OCCURRENCE OF PREVIOUSLY FITTED TREATMENT
C
19 ITR = ILIST(IL)
      KREP = IR(IL)
C
C      REMOVE OCCURRENCE OF TREATMENT FROM ND-DIMENSIONAL DESIGN
C      SET LSTFIT EQUAL TO VACATED POSITION
C
20 DO 21 I = 1, NU
      ID = NU - I + 1
      IF (IDES(ID) .EQ. ITR) GOTO 22
21 CONTINUE
22 IDES(ID) = -1
      LSTFIT = ID
C
C      FIND LOCATION OF REMOVED TREATMENT IN COMPONENT DESIGNS
C
      ID = ID - 1
      DO 23 N = 1, ND
      I = ND - N + 1
      I1 = ID
      ID = ID / NB(I)
      IB(I) = I1 - (ID * NB(I)) + 1
23 CONTINUE
C
C      SET REMOVED TREATMENT POSITIVE IN COMPONENT DESIGNS
C
      DO 25 N = 1, ND
      I = IB(N)
      IBS = KBS(N)
      IF (ITR .EQ. 0) ITR = 9999
      DO 24 J = 1, IBS
      IF (NCOMP(N, I, J) .NE. -ITR) GOTO 24
      IF (ITR .EQ. 9999) ITR = 0
      NCOMP(N, I, J) = ITR
      GOTO 25
24 CONTINUE
25 CONTINUE
```

```
C
C      TRY TO REFIT REMOVED TREATMENT
C      OR REMOVE ANOTHER OCCURRENCE OF SAME TREATMENT
C
      IF (KREP .EQ. IR(IL)) GOTO 18
      N = ND
      GOTO 12
      END
```

```

SUBROUTINE LSTSQ(X, S, A, B, IFLAG, N, K, NWORK, ITMAX, EPS, EPS2,
* W, XHAT, XKT, ITER, SUPDIF, IFAULT)
DIMENSION X(N), S(N, N), A(K, N), B(K), IFLAG(K), W(NWORK),
* XHAT(N), XKT(K)

```

```

C
C     ALGORITHM AS225 APPL. STATIST. (1987) VOL. 36, NO. 2
C

```

```

C     COMPUTES THE LEAST-SQUARES PROJECTION OF X ONTO
C     THE INTERSECTION OF K SIMULTANEOUS AFFINE CONSTRAINTS,
C     USING THE MAHALANOBIS DISTANCE DETERMINED BY S.
C     THE ITH CONSTRAINT IS OF THE FORM
C     SUM OVER J OF A(I,J)*X(J) (.LE.,.EQ.) B(I)
C     --.LE. IF IFLAG(I) .EQ. 0
C     --.EQ. IF IFLAG(I) .EQ. 1
C

```

```

DATA ZERO, TWO /0.0E0, 2.0E0/

```

```

C
C     IFAULT = 0
C     NK = N * K
C     NK2 = NK + NK
C     NK2K = NK2 + K

```

```

C
C     CHECK INPUTS.
C

```

```

IF (N .LE. 0 .OR. K .LE. 0 .OR. ITMAX .LE. 0 .OR. EPS .LE.
* ZERO .OR. NWORK .LE. 0 .OR. EPS2 .LE. ZERO) GOTO 300
IF (NWORK .LT. NK2K + N) GOTO 320
DO 10 I = 1, K
IF (IFLAG(I) .EQ. 0 .OR. IFLAG(I) .EQ. 1) GOTO 10
GOTO 300

```

```

10 CONTINUE

```

```

C
C     INITIALIZE ARRAYS, AND COMPUTE
C     MATRIX PRODUCTS A*S AND DIAG(A*S*A').
C     WORKSPACE STRUCTURE IS AS FOLLOWS:
C     W(1)-W(N*K): ARRAY OF INCREMENT VECTORS. ITH INC VECTOR
C     IS (XKT(I)/2)*S*A(I,.).
C     W(NK+1)-W(N*K*2): MATRIX A*S.
C     W(NK2+1)-W(NK2+K): VECTOR DIAG(A*S*A').
C     W(NK2K+1)-W(NK2K+N): PREVIOUS XHAT VECTOR, TO CHECK FOR CONV.
C

```

```

DO 40 I = 1, K
DO 30 J = 1, N
INDEX = NK + (J - 1) * K + I
W(INDEX) = ZERO
DO 20 L = 1, N
20 W(INDEX) = W(INDEX) + A(I, L) * S(L, J)
30 CONTINUE
40 CONTINUE
DO 60 I = 1, K
INDEX = NK2 + I
W(INDEX) = ZERO
DO 50 J = 1, N
IND2 = NK + (J - 1) * K + I
W(INDEX) = W(INDEX) + A(I, J) * W(IND2)
50 CONTINUE
IF (ABS(W(INDEX)) .LE. EPS2) GOTO 310
60 CONTINUE
DO 80 J = 1, N
INDEX = NK2K + J
W(INDEX) = X(J)

```

```
XHAT(J) = X(J)
DO 70 I = 1, K
INDEX = (I - 1) * N + J
W(INDEX) = ZERO
70 CONTINUE
80 CONTINUE
ITER = 0

C
C     THE ITERATION LOOP:  LINES 100-200.
C
100 ITER = ITER + 1
    SUPDIF = ZERO
    DO 200 I = 1, K

C
C     REMOVE OLD INCREMENT VECTOR:
C
DO 110 J = 1, N
INDEX = (I - 1) * N + J
XHAT(J) = XHAT(J) + W(INDEX)
110 CONTINUE

C
C     EVALUATE ITH CONSTRAINT:
C
SUM = ZERO
DO 120 J = 1, N
120 SUM = SUM + A(I, J) * XHAT(J)
    SUM = SUM - B(I)
    IF (IFLAG(I) .EQ. 0 .AND. SUM .LE. ZERO) GOTO 140

C
C     COMPUTE NEW INCREMENT VECTOR THAT FORCES EQUALITY IN ITH CONST.
C
INDEX = NK2 + I
TEMP = SUM / W(INDEX)
DO 130 J = 1, N
IND1 = (I - 1) * N + J
IND2 = NK + (J - 1) * K + I
W(IND1) = W(IND2) * TEMP
XHAT(J) = XHAT(J) - W(IND1)
130 CONTINUE
GOTO 160

C
C     IF CONSTRAINT WAS SATISFIED, SET INCREMENT TO ZERO:
C
140 DO 150 J = 1, N
INDEX = (I - 1) * N + J
W(INDEX) = ZERO
150 CONTINUE

C
C     FIND LARGEST CHANGE, AND CHECK FOR CONVERGENCE:
C
160 DO 170 J = 1, N
INDEX = NK2K + J
ABDIF = ABS(XHAT(J) - W(INDEX))
IF (SUPDIF .LT. ABDIF) SUPDIF = ABDIF
170 CONTINUE
200 CONTINUE
IF (SUPDIF .LE. EPS) GOTO 400
DO 210 J = 1, N
INDEX = NK2K + J
W(INDEX) = XHAT(J)
210 CONTINUE
```

```
        IF (ITER .LT. ITMAX) GOTO 100
        IFAULT = 1
        RETURN
300    IFAULT = 2
        RETURN
310    IFAULT = 3
        RETURN
320    IFAULT = 4
        RETURN
C
C        COMPUTE KUHN-TUCKER COEFFICIENTS AND RETURN.
C
400    DO 430 I = 1, K
C
C        FIND A NON-ZERO DENOMINATOR:
C
        DO 410 J = 1, N
        INDEX = NK + (J - 1) * K + I
        IF (ABS(W(INDEX)) .GT. EPS2) GOTO 420
410    CONTINUE
420    IND2 = (I - 1) * N + J
        XKT(I) = TWO * W(IND2) / W(INDEX)
430    CONTINUE
        RETURN
        END
```

```

      REAL FUNCTION BETANC(X, A, B, LAMBDA, IFAULT)
C
C   ALGORITHM AS226 APPL. STATIST. (1987) VOL. 36, NO. 2
C   Incorporates modification AS R84 from AS vol. 39, pp311-2, 1990
C
C   Returns the cumulative probability of X for the non-central beta
C   distribution with parameters A, B and non-centrality LAMBDA
C
C   Auxiliary routines required: ALOGAM - log-gamma function (ACM
C   291 or AS 245), and BETAIN - incomplete-beta function (AS 63)
C
      REAL A, AX, B, BETA, C, ERRBD, ERRMAX, GX, HALF, LAMBDA, ONE, Q,
*      SUMQ, TEMP, X, XJ, ZERO
      REAL A0, X0, UALPHA
C
C   Change ERRMAX and ITRMAX if desired ...
C
      DATA ERRMAX, ITRMAX /1.0E-6, 100/, UALPHA /5.0/
C
      DATA ZERO, HALF, ONE /0.0, 0.5, 1.0/
C
      BETANC = X
C
      IFAULT = 2
      IF (LAMBDA .LT. ZERO .OR. A .LE. ZERO .OR. B .LE. ZERO) RETURN
      IFAULT = 3
      IF (X .LT. ZERO .OR. X .GT. ONE) RETURN
      IFAULT = 0
      IF (X .EQ. ZERO .OR. X .EQ. ONE) RETURN
C
      C = LAMBDA * HALF
C
C   Initialize the series ...
C
      X0 = INT(MAX(C - UALPHA*SQRT(C), ZERO))
      A0 = A + X0
      BETA = ALOGAM(A0, IFAULT) + ALOGAM(B, IFAULT) -
*      ALOGAM(A0+B, IFAULT)
      TEMP = BETAIN(X, A0, B, BETA, IFAULT)
      GX = EXP(A0 * LOG(X) + B * LOG(ONE - X) - BETA - LOG(A0))
      IF (A0 .GT. A) THEN
         Q = EXP(-C + X0*LOG(C) - ALOGAM(X0 + ONE, IFAULT))
      ELSE
         Q = EXP(-C)
      END IF
      XJ = ZERO
      AX = Q * TEMP
      SUMQ = ONE - Q
      BETANC = AX
C
C   Recur over subsequent terms until convergence is achieved...
C
      10 XJ = XJ + ONE
         TEMP = TEMP - GX
         GX = X * (A + B + XJ - ONE) * GX / (A + XJ)
         Q = Q * C / XJ
         SUMQ = SUMQ - Q
         AX = TEMP * Q
         BETANC = BETANC + AX
C
C   Check for convergence and act accordingly...

```

```
C
  ERRBD = (TEMP - GX) * SUMQ
  IF ((INT(XJ) .LT. ITRMAX) .AND. (ERRBD .GT. ERRMAX)) GO TO 10
  IF (ERRBD .GT. ERRMAX) IFAULT = 1
C
  RETURN
  END
```



```
      SUBROUTINE GCOUNT(N, APPLY, IFAULT)
C
C      ALGORITHM AS227  APPL. STATIST. (1987) VOL. 36, NO. 2
C
C      Generates all possible N-bit binary codes, and applies a users
C      procedure for each code generated.
C      N must be <= NMAX, which is set in the PARAMETER statement below.
C      IFAULT = 2 is returned otherwise.
C
C      Translated from Algol 60.
C
C      INTEGER N, IFAULT
C      EXTERNAL APPLY
C
C      Local variables
C
C      INTEGER NMAX
C      PARAMETER (NMAX = 100)
C      INTEGER CHANGE, I, TPOINT(NMAX)
C      LOGICAL STATUS(NMAX)
C
C      IF (N .LT. 1) THEN
C          IFAULT = 1
C          RETURN
C      END IF
C      IF (N .GT. NMAX) THEN
C          IFAULT = 2
C          RETURN
C      END IF
C      IFAULT = 0
C
C      Initialize and make first call to user's routine.
C
C      DO 10 I = 1, N
C          STATUS(I) = .FALSE.
C          TPOINT(I) = I + 1
10    CONTINUE
C      CALL APPLY(N, N, STATUS)
C
C      Generate a new code.  The user's routine is called twice each
C      cycle; the first time the bit which changes is bit 1.
C
20    IF (STATUS(1)) THEN
C          STATUS(1) = .FALSE.
C          CHANGE = TPOINT(2)
C      ELSE
C          STATUS(1) = .TRUE.
C          CHANGE = 2
C      END IF
C      CALL APPLY(N, 1, STATUS)
C
C      Check if count exhausted.
C
C      IF (CHANGE .GT. N) RETURN
C
C      IF (STATUS(CHANGE)) THEN
C          STATUS(CHANGE) = .FALSE.
C          TPOINT(CHANGE) = TPOINT(CHANGE + 1)
C      ELSE
C          STATUS(CHANGE) = .TRUE.
C          TPOINT(CHANGE) = CHANGE + 1
```

```
END IF  
CALL APPLY(N, CHANGE, STATUS)
```

C

```
GO TO 20  
END
```

```

SUBROUTINE IPROJ(R, C, B, L, K, EPS1, EPS2, ITMAX1, ITMAX2, NWORK,
* W, P, NIT, SUPDIF, DIV, IFAULT)

```

```

C
C     ALGORITHM AS228 APPL. STATIST. (1987) VOL. 36, NO. 3
C

```

```

DIMENSION R(L), P(L), C(L, K), B(K), W(NWORK)

```

```

C
C     COMPUTES THE I-PROJECTION OF THE VECTOR R
C     ONTO THE INTERSECTION OF K LINEAR INEQUALITY
C     CONSTRAINTS.  THE J-TH CONSTRAINT IS OF THE FORM
C     SUM OVER I OF C(I,J)*P(I) .LE. B(J)
C     THE DATA, R, IS A NON-NEGATIVE VECTOR.
C     THE I-PROJ IS RETURNED IN P, AS A VECTOR OF PROBABILITIES.
C

```

```

DATA ZERO, ZONE /0.0E0, 1.0E0/
NIT = 0
TOT = ZERO
IFAULT = 0
LK = L * K
LKL1 = LK + L
LKL2 = LKL1 + L
LKL3 = LKL2 + L
IF (NWORK .LT. LKL3 + K) GOTO 500

```

```

C
C     CHECK DATA FOR NEGATIVES, STANDARDIZE DATA (TO SUM TO 1),
C     INITIALIZE INCREMENT ARRAY AND DUAL ESTIMATE ARRAY.
C

```

```

DO 5 J = 1, K
INDEX = LKL3 + J
W(INDEX) = ZERO
5 CONTINUE
DO 20 I = 1, L
P(I) = R(I)
DO 10 J = 1, K
INDEX = (J - 1) * L + I
W(INDEX) = ZONE
10 CONTINUE
IF (P(I) .LT. ZERO) GOTO 300
TOT = TOT + P(I)
20 CONTINUE
IF (TOT .LE. ZERO) GOTO 300
DO 30 I = 1, L
30 P(I) = P(I) / TOT

```

```

C
C     CHECK DATA FOR NON-EXISTENCE OF A SOLUTION, AND LOCATE
C     AND INSERT FORCED ZEROS.
C

```

```

35 IFLAG = 0
DO 50 J = 1, K
SNEG = ZERO
SPOS = ZERO
SZERO = ZERO
DO 40 I = 1, L
CMB = C(I, J) - B(J)
IF (CMB .GT. ZERO) SPOS = SPOS + P(I)
IF (CMB .LT. ZERO) SNEG = SNEG + P(I)
IF (CMB .EQ. ZERO) SZERO = SZERO + P(I)
40 CONTINUE
IF (SNEG .GT. ZERO) GOTO 50
IF (SZERO .LE. ZERO) GOTO 400
IF (SPOS .LE. ZERO) GOTO 50

```

```

DO 45 I = 1, L
IF (C(I, J) - B(J) .GT. ZERO) P(I) = ZERO
P(I) = P(I) / SZERO
45 CONTINUE
IFLAG = 1
50 CONTINUE
IF (IFLAG .EQ. 1) GOTO 35
C
C     PERFORM AN ITERATION:  LINES 100 TO 200
C
100 SUPDIF = ZERO
DO 200 J = 1, K
SUM = ZERO
DO 110 I = 1, L
INDEX = LK + I
W(INDEX) = P(I)
INDEX = (J - 1) * L + I
P(I) = P(I) / W(INDEX)
INDEX = LKL1 + I
W(INDEX) = C(I, J) - B(J)
SUM = SUM + P(I)
110 CONTINUE
DO 115 I = 1, L
115 P(I) = P(I) / SUM
C
C     P PASSES DATA TO PROJ, AND RETURNS THE RESULT.
C     W(LK+I) STORES THE PREVIOUS RESULT, FOR COMPARISON.
C     W(LKL1+I) PASSES THE J-TH COLUMN OF THE CONSTRAINT
C     MATRIX TO PROJ.
C     W(LKL2+I) IS WORKSPACE FOR PROJ.
C     W(LKL3+J) IS THE PREVIOUS DUAL ESTIMATE.
C
INDEX = LKL3 + J
CALL PROJ(P, W, NWORK, L, LKL1, LKL2, J, W(INDEX), EPS2, ITMAX2,
* IFAULT)
IF (IFAULT .EQ. 2) RETURN
C
C     UPDATE THE INCREMENT ARRAY W(1)-W(LK) AND GET THE GREATEST
C     DIFFERENCE (TO TEST FOR CONVERGENCE).
C
DO 120 I = 1, L
IS = (J - 1) * L + I
INDEX = LK + I
IF (W(INDEX) .GT. ZERO) W(IS) = W(IS) * P(I) / W(INDEX)
DIFF = ABS(P(I) - W(INDEX))
IF (DIFF .GT. SUPDIF) SUPDIF = DIFF
120 CONTINUE
200 CONTINUE
C
C     COUNT ITERATIONS, AND CHECK FOR CONVERGENCE.
C
NIT = NIT + 1
IF (SUPDIF .GT. EPS1) GOTO 220
C
C     COMPUTE I-DIVERGENCE
C
DIV = ZERO
DO 210 I = 1, L
IF (P(I) .GT. ZERO) DIV = DIV + P(I) * ALOG(P(I) * TOT / R(I))
210 CONTINUE
RETURN

```

```
220 IF (NIT .LE. ITMAX1) GOTO 100
    IFAULT = 1
    RETURN
300 IFAULT = 3
    RETURN
400 IFAULT = 4
    RETURN
500 IFAULT = 5
    RETURN
    END

C
    SUBROUTINE PROJ(P, W, NWORK, L, LKL1, LKL2, J, ZLAST, EPS2,
*   ITMAX2, IFAULT)

C
    ALGORITHM AS228 APPL. STATIST. (1987) VOL. 36, NO. 3

C
    DIMENSION P(L), W(NWORK)
    DATA ZERO /0.0E0/

C
    THIS SUBROUTINE FINDS THE I-PROJ OF P SUBJECT TO THE LINEAR
C   CONSTRAINT IN W -- OF THE FORM
C   SUM OVER I OF W(LKL1+I)*P(I) .LE. ZERO.
C   THE FENCHEL DUAL SOLUTION IS OBTAINED BY NEWTON'S METHOD,
C   TO WITHIN EPS2, WHICH IS THEN USED TO CONSTRUCT THE I-PROJ.
C

    ITER = 0
    IFAULT = 0
    VAL = ZERO
    DERIV = ZERO
    DO 10 I = 1, L
        IND1 = LKL1 + I
        IND2 = LKL2 + I
        W(IND2) = P(I) * W(IND1)
        VAL = VAL + W(IND2)
        DERIV = DERIV - W(IND1) * W(IND2)
10 CONTINUE
    IF (VAL .GT. ZERO) GOTO 100

C
    IF VAL .LE. 0 THEN CONSTRAINT IS SATISFIED; RETURN.

C
    ZLAST = ZERO
    RETURN

C
    THE ITERATION BLOCK:  LINES 100 TO 110.

C
100 Z = ZLAST - VAL / DERIV
    IF (ABS(Z - ZLAST) .LE. EPS2) GOTO 200
    IF (ITER .GT. ITMAX2) GOTO 300
    ZLAST = Z
    VAL = ZERO
    DERIV = ZERO
    ITER = ITER + 1
    DO 110 I = 1, L
        IND1 = LKL1 + I
        IND2 = LKL2 + I
        TEMP = EXP(-Z * W(IND1))
        VAL = VAL + W(IND2) * TEMP
        DERIV = DERIV - W(IND1) * W(IND2) * TEMP
110 CONTINUE
    GOTO 100

C
```

```
C          GENERATE PROJECTION, STANDARDIZE AND RETURN.  
C  
200 SUM = ZERO  
    DO 210 I = 1, L  
      INDEX = LKL1 + I  
      P(I) = P(I) * EXP(-Z * W(INDEX))  
      SUM = SUM + P(I)  
210 CONTINUE  
    DO 220 I = 1, L  
220 P(I) = P(I) / SUM  
    RETURN  
300 IFAULT = 2  
    RETURN  
    END
```

```
subroutine rq(m,n,m5,n2,a,b,t,toler,ift,x,e,s,wa,wb,
1  nsol,sol,lsol)
implicit double precision (a-h,o-z)
c
c  Algorithm AS229 Appl. Statist. (1987) Vol. 36, No. 3
c
integer i,j,k,kl,kount,kr,l,lsol,m,m1,m2,m3,m4,m5,
1  ift
integer n,n1,n2,nsol,out,s(m)
logical stage,test,init,iend
double precision a1,aux,b1,big,d,dif,pivot,smax,t,t0,t1,tnt
double precision min,max,toler,zero,half,one,two,three,four,five
double precision b(m),sol(n2,nsol),a(m,n),x(n),wa(m5,n2),wb(m)
double precision sum,e(m)
double precision xx,y
data big /1.0d37/
data zero /0.0d0/
data half /0.5d0/
data one /1.0d0/
data two /2.0d0/
data three /3.0d0/
data four /4.0d0/
data five /5.0d0/
c
c  check dimension parameters
c
ift = 0
if (m5.ne.m + 5) ift = 3
if (n2.ne.n + 2) ift = 4
if (m.le.zero.or.n.le.zero) ift = 5
if (ift.gt.two) return
c
c  initialization
c
m1 = m + 1
n1 = n + 1
m2 = m + 2
m3 = m + 3
m4 = m + 4
do 2 i = 1,m
  wb(i) = b(i)
  do 1 j = 1,n
    wa(i,j) = a(i,j)
1  continue
2  continue
wa(m2,n1) = zero
dif = zero
iend = .true.
if (t.ge.zero.and.t.le.one) goto 3
t0 = one / float(m) - toler
t1 = one - t0
t = t0
iend = .false.
3  continue
init = .false.
lsol = 1
kount = 0
do 9 k = 1,n
  wa(m5,k) = zero
  do 8 i = 1,m
    wa(m5,k) = wa(m5,k) + wa(i,k)
```

```

8      continue
      wa(m5,k) = wa(m5,k) / float(m)
9      continue
      do 10 j = 1,n
        wa(m4,j) = j
        x(j) = zero
10     continue
      do 40 i = 1,m
        wa(i,n2) = n + i
        wa(i,n1) = wb(i)
        if (wb(i).ge.zero) goto 30
        do 20 j = 1,n2
          wa(i,j) = -wa(i,j)
20     continue
30     e(i) = zero
40     continue
      do 42 j = 1,n
        wa(m2,j) = zero
        wa(m3,j) = zero
        do 41 i = 1,m
          aux = sign(one,wa(m4,j)) * wa(i,j)
          wa(m2,j) = wa(m2,j) + aux * (one - sign(one,wa(i,n2)))
          wa(m3,j) = wa(m3,j) + aux * sign(one,wa(i,n2))
41     continue
        wa(m3,j) = two * wa(m3,j)
42     continue
      goto 48
43     continue
      lsol = lsol + 1
      do 44 i = 1,m
        s(i) = zero
44     continue
      do 45 j = 1,n
        x(j) = zero
45     continue
c
c     compute next t
c
      smax = two
      do 47 j = 1,n
        b1 = wa(m3,j)
        a1 = (-two - wa(m2,j)) / b1
        b1 = -wa(m2,j) / b1
        if (a1.lt.t) goto 46
        if (a1.ge.smax) goto 46
        smax = a1
        dif = (b1 - a1) / two
46     if (b1.le.t) goto 47
        if (b1.ge.smax) goto 47
        smax = b1
        dif = (b1 - a1) / two
47     continue
      tnt = smax + toler * (one + dabs(dif))
      if (tnt.ge.t1 + toler) iend = .true.
      t = tnt
      if (iend) t = t1
48     continue
c
c     compute new marginal costs
c
      do 49 j = 1,n

```



```
        wa(m1,j) = wa(m2,j) + wa(m3,j) * t
49  continue
    if (init) goto 265
c
c  stage 1
c
c  determine the vector to enter the basis
stage = .true.
kr = 1
kl = 1
70  max = -one
    do 80 j = kr,n
        if (abs(wa(m4,j)).gt.n) goto 80
        d = abs(wa(m1,j))
        if (d.le.max) goto 80
        max = d
        in = j
80  continue
    if (wa(m1,in).ge.zero) goto 100
    do 90 i = 1,m4
        wa(i,in) = -wa(i,in)
90  continue
c
c  determine the vector to leave the basis
c
100 k = 0
    do 110 i = kl,m
        d = wa(i,in)
        if (d.le.toler) goto 110
        k = k + 1
        wb(k) = wa(i,n1) / d
        s(k) = i
        test = .true.
110 continue
120 if (k.gt.0) goto 130
    test = .false.
    goto 150
130 min = big
    do 140 i = 1,k
        if (wb(i).ge.min) goto 140
        j = i
        min = wb(i)
        out = s(i)
140 continue
    wb(j) = wb(k)
    s(j) = s(k)
    k = k - 1
c
c  check for linear dependence in stage 1
c
150 if (test.or. .not.stage) goto 170
    do 160 i = 1,m4
        d = wa(i,kr)
        wa(i,kr) = wa(i,in)
        wa(i,in) = d
160 continue
    kr = kr + 1
    goto 260
170 if (test) goto 180
    wa(m2,n1) = two
    goto 390
```

```
180 pivot = wa(out,in)
    if (wa(m1,in) - pivot - pivot .le. toler) goto 200
    do 190 j = kr,n1
        d = wa(out,j)
        wa(m1,j) = wa(m1,j) - d - d
        wa(m2,j) = wa(m2,j) - d - d
        wa(out,j) = -d
190 continue
    wa(out,n2) = -wa(out,n2)
    goto 120
c
c     pivot on wa(out,in)
c
200 do 210 j = kr,n1
    if (j.eq.in) goto 210
    wa(out,j) = wa(out,j) / pivot
210 continue
    do 230 i = 1,m3
        if (i.eq.out) goto 230
        d = wa(i,in)
        do 220 j = kr,n1
            if (j.eq.in) goto 220
            wa(i,j) = wa(i,j) - d * wa(out,j)
220 continue
230 continue
    do 240 i = 1,m3
        if (i.eq.out) goto 240
        wa(i,in) = -wa(i,in) / pivot
240 continue
    wa(out,in) = one / pivot
    d = wa(out,n2)
    wa(out,n2) = wa(m4,in)
    wa(m4,in) = d
    kount = kount + 1
    if (.not.stage) goto 270
c
c     interchange rows in stage 1
c
    kl = kl + 1
    do 250 j = kr,n2
        d = wa(out,j)
        wa(out,j) = wa(kount,j)
        wa(kount,j) = d
250 continue
260 if (kount + kr.ne.n1) goto 70
c
c     stage 2
c
265 stage = .false.
c
c     determine the vector to enter the basis
c
270 max = -big
    do 290 j = kr,n
        d = wa(m1,j)
        if (d.ge.zero) goto 280
        if (d.gt. (-two)) goto 290
        d = -d - two
280 if (d.le.max) goto 290
    max = d
    in = j
```

```
290  continue
      if (max.le.toler) goto 310
      if (wa(m1,in) .gt.zero) goto 100
      do 300 i = 1,m4
          wa(i,in) = -wa(i,in)
300  continue
      wa(m1,in) = wa(m1,in) - two
      wa(m2,in) = wa(m2,in) - two
      goto 100

c
c      compute quantiles
310  continue
      do 320 i = 1,kl - 1
          k = wa(i,n2) * sign(one,wa(i,n2))
          x(k) = wa(i,n1) * sign(one,wa(i,n2))
320  continue
      sum = zero
      do 330 i = 1,n
          sum = sum + x(i) * wa(m5,i)
          sol(i + 2,lsol) = x(i)
330  continue
      sol(1,lsol) = t
      sol(2,lsol) = sum
      if (iend) goto 340
      init = .true.
      goto 43
340  continue
      if (lsol.le.2) goto 355
      do 350 i = 2,lsol
          sol(1,i-1) = sol(1,i)
350  continue
      lsol = lsol - 1
      sol(1,lsol) = one
355  continue
      l = kl - 1
      do 370 i = 1,l
          if (wa(i,n1).ge.zero) goto 370
          do 360 j = kr,n2
              wa(i,j) = -wa(i,j)
360  continue
370  continue
      wa(m2,n1) = zero
      if (kr.ne.1) goto 390
      do 380 j = 1,n
          d = abs(wa(m1,j))
          if (d.le.toler .or. two - d .le. toler) goto 390
380  continue
      wa(m2,n1) = one
390  do 400 i = kl,m
          k = wa(i,n2) * sign(one,wa(i,n2))
          d = wa(i,n1) * sign(one,wa(i,n2))
          k = k - n
          e(k) = d
400  continue
      wa(m2,n2) = kount
      wa(m1,n2) = n1 - kr
      sum = zero
      do 410 i = 1,m
          sum = sum + e(i) * (half + sign(one,e(i)) * (t - half))
410  continue
      wa(m1,n1) = sum
```

```
return  
end
```

```

SUBROUTINE QDISX(A, B, M, T, MAX, CZERO, MAX1, P0, P, Y, C0, C,
+           MEAN, SD, SUM, IFAULT)
C
C   ALGORITHM AS230  APPL. STATIST. (1986) VOL. 36, NO. 3
C
C   Tabulates approximate distribution of customers in multi-server
C   queues having random arrivals and Erlangian service times.
C   Hokstad's method is used.
C
REAL P(MAX), Y(MAX), C(MAX)
REAL A, B, C0, CZERO, FI, MEAN, ONE, PM1, PNNN, P0, R, R1, SD,
+     SUM, TERM, FT, TWO, ZERO, WT
INTEGER T
DATA ZERO/0.0/, ONE/1.0/, TWO/2.0/, PNNN/0.999/
C
IFault = 0
FT = FLOAT(T)
MAX0 = MAX
IF (MAX .GT. 4000) MAX0 = 4000
DO 5 I = 1, MAX0
  P(I) = ZERO
  Y(I) = ZERO
  C(I) = ZERO
5 CONTINUE
C
C   Calculate P0 to P(M-1)
C
R = A * B / FLOAT(M)
IF (R .GT. PNNN) GO TO 10
P0 = ONE - R
PM1 = P0
IF (M .EQ. 1) GO TO 15
P0 = ONE
TERM = ONE
M1 = M - 1
DO 20 I = 1, M1
  TERM = TERM * A * B / FLOAT(I)
  P0 = P0 + TERM
  P(I) = TERM
20 CONTINUE
TERM = TERM * A * B / ((ONE - R) * FLOAT(M))
P0 = ONE / (P0 + TERM)
DO 25 I = 1, M1
25 P(I) = P(I) * P0
PM1 = P(M1)
15 IF (T .GT. 100) GO TO 30
C
C   Calculate Y-values for Erlangian service
C
C0 = (ONE + R / FT) ** FT
P(M) = (C0 - ONE) * PM1
Y(1) = (ONE + R / FT) ** FT - R / (ONE + R / FT)
Y(2) = -(FT * (FT + ONE) / TWO) / (FT / R + ONE) ** 2
DO 35 I = 3, MAX0
35 Y(I) = ZERO
DO 40 I = 3, MAX0
  FI = FLOAT(I)
  IF (ABS(Y(I-1)) .LT. CZERO) GO TO 45
  Y(I) = (Y(I-1) * (FT + FI - ONE)) / (FI * (FT / R + ONE))
40 CONTINUE
GO TO 45

```

```
C
C      Calculate Y-values for constant service times
C
30 C0 = EXP(R)
   P(M) = (C0 - ONE) * PM1
   Y(1) = C0 - R
   Y(2) = -R * R / TWO
   DO 50 I = 3, MAX0
     Y(I) = ZERO
50 CONTINUE
   DO 55 I = 3, MAX0
     IF (ABS(Y(I-1)) .LT. CZERO) GO TO 45
     Y(I) = Y(I-1) * R / FLOAT(I)
55 CONTINUE

C
C      Calculate P(M+1) to P(MAX0)
C
45 R1 = ONE / (ONE - R)
   C(1) = C0 * Y(1)
   DO 60 I = 2, MAX0
     C(I) = ZERO
     I1 = I - 1
     DO 65 J = 1, I1
       C(I) = C(I) + C(I-J) * Y(J)
65 CONTINUE
     C(I) = C(I) + C0 * Y(I)
     IF (C(I) .GE. R1 .AND. C(I-1) .GE. R1) GO TO 95
60 CONTINUE
   I = MAX0
95 MAX1 = I
   M2 = MAX1 - M
   P(M+1) = (C(1) - C0) * PM1
   DO 70 I = 2, M2
70 P(M+I) = ZERO
   DO 75 I = 2, M2
     IF (ABS(P(M+I-1)) .LT. CZERO .AND. P(M+I-1) .LT. P(M+I-2))
+       GO TO 80
     P(M+I) = (C(I) - C(I-1)) * PM1
     IF (P(M+I) .GE. ZERO) GO TO 75
     P(M+I) = ZERO
     GO TO 80
75 CONTINUE

C
C      Calculate mean, standard deviation and sum of terms.
C      The algorithm for calculating the mean & standard deviation used
C      here is better than that in the journal.
C
80 SUM = P0
   MEAN = ZERO
   SD = ZERO
   DO 90 I = 1, MAX1
     FI = FLOAT(I)
     SUM = SUM + P(I)
     WT = P(I) / SUM
     TERM = FI - MEAN
     MEAN = MEAN + WT * TERM
     SD = SD + P(I) * TERM * (FI - MEAN)
90 CONTINUE
   SD = SQRT(SD / SUM)

C
   RETURN
```

C

```
10 IFAULT = -1  
   RETURN  
   END
```

```
FUNCTION chisqnc(idf: nonnegint; nc, arg, eps: real; VAR density: real;  
  VAR ifault: nonnegint): real;
```

```
{Algorithm AS 231 Appl. Statist. (1987) Vol.36, No.3}
```

```
{chisqnc evaluates the probability that a noncentral chi-squared  
  random variable is less than a given value, arg}
```

```
CONST tol = -50;  
  maxit = 500;  
  lnrtpi2 = 0.22579135264473;
```

```
VAR i, k: nonnegint;  
  m: 0 .. maxit;  
  ao, am, b1, eps2, hold, sum, dans, lans, pans, probability: real;  
  converged: Boolean;
```

```
PROCEDURE update(VAR j: nonnegint);  
  BEGIN  
  IF lans < tol THEN  
    BEGIN  
      lans := lans + ln(arg / j); dans := exp(lans)  
    END  
  ELSE dans := dans * arg / j;  
  pans := pans - dans; j := j + 2  
  END; {update}
```

```
BEGIN  
IF (nc < 0.0) OR (arg < 0.0) OR (eps <= 0.0) THEN  
  BEGIN  
    chisqnc := -1.0; density := -1.0;  
    ifault := 1  
  END  
ELSE IF (arg = 0.0) AND (idf > 0) THEN  
  BEGIN  
    chisqnc := 0.0; density := 0.0;  
    ifault := 0  
  END
```

```
ELSE  
  BEGIN  
  
    {Determine initial values}  
    k := idf; b1 := 0.5 * nc;  
    ao := exp(-b1); eps2 := eps / ao;  
    IF odd(k) THEN  
      BEGIN  
        i := 1; lans := -0.5 * (arg + ln(arg)) - lnrtpi2;  
        dans := exp(lans); pans := centnorm(sqrt(arg))  
      END  
    ELSE  
      BEGIN  
        i := 2; lans := -0.5 * arg;  
        dans := exp(lans); pans := 1.0 - dans  
      END  
  
    {Evaluate first term}  
    IF k = 0 THEN  
      BEGIN  
        m := 1; k := 2;  
        am := b1; sum := 1.0 / ao - 1.0 - am;  
        density := am * dans; probability := 1.0 + am * pans
```



```
        END
    ELSE
        BEGIN
            m := 0; k := k - 1;
            am := 1.0; sum := 1.0 / ao - 1.0;
            WHILE i < k DO update(i);
            k := k + 1;
            density := dans; probability := pans
            END;

        {Evaluate successive terms of the expansion}
        REPEAT
            m := m + 1; am := b1 * am / m;
            update(k); sum := sum - am;
            density := density + am * dans; hold := am * pans;
            probability := probability + hold;
            converged := (pans * sum < eps2) AND (hold < eps2)
        UNTIL (m = maxit) OR converged;

        IF converged THEN ifault := 0 ELSE ifault := 2;
        density := 0.5 * ao * density;
        chisqnc := ao * probability
        END
    END; {of chisqnc}
```

```

SUBROUTINE XCOVAR(K, P, Q, R, LMAX, KKRPl, PHI, THETA, SIGMA,
* GAMMA, PSI, C, W, Wl, IFAULT)
C
C     ALGORITHM AS232 APPL. STATIST. (1988) VOL. 37, NO. 1
C
C     INTEGER P, Q, R, S, ZROW, SMI, RP1, RML
C     LOGICAL POS, NEG, PZERO
C     DIMENSION PHI(K, K, 0:R), THETA(K, K, 0:R), PSI(K, K, 0:LMAX),
*     GAMMA(K, K, 0:LMAX), C(KKRPl, KKRPl), SIGMA(K, K), W(K, K),
*     Wl(K, K)
C
C     THE NEXT LINE IS THE STATEMENT FUNCTION GIVING THE MAPPING
C     USED FOR THE NUMBERING OF THE GAMMA(I,J,L) ELEMENTS IN THE
C     S.L.E. SYSTEM. C*Z=B (SEE EQUATIONS (1A) IN THE DESCRIPTION).
C     NOTE THAT IT TAKES THEM IN THE STORAGE ORDER FOR 3-D ARRAYS.
C
C     ZROW(I, J, L, K) = (L * K + J - 1) * K + I
C
C     IFAULT = 0
C     IF (R .EQ. MAX0(P, Q)) GOTO 10
C     IFAULT = -1
C     RETURN
10  RP1 = R + 1
C     IF (KKRPl .EQ. K * K * RP1) GOTO 20
C     IFAULT = -2
C     RETURN
20  PZERO = P .EQ. 0
C
C     ZEROISE PLANES OF PHI, THETA BEYOND THE INPUT PLANES (IF ANY).
C
C     IF (P .EQ. Q) GOTO 30
C
C     NONE IN THIS CASE.
C
C     IF (R .EQ. Q) CALL LINZER(PHI(1, 1, P + 1), K * K * (R - P))
C     IF (R .EQ. P) CALL LINZER(THETA(1, 1, Q + 1), K * K * (R - Q))
C
C     NEXT, FORM THE PSI-MATRICES, UP TO THE LMAX'TH.
C     NOTE THAT ONLY THE FIRST R OF THESE ARE NEEDED FOR THE CROSS-
C     CORRELATIONS.
C
30  CALL SCALAR(PSI(1, 1, 0), K, 1.0)
C
C     PSI(0) = IDENTITY
C
C     DO 50 S = 1, LMAX
C
C     FORM PSI(S)
C
C     IF (S .LE. R) CALL MATSUB(PSI(1, 1, S), PHI(1, 1, S), THETA(1, 1,
*     S), K, K)
C
C     IF (S .EQ. 1) GOTO 50
C
C     NO SUMMATION IN THIS CASE.
C
C     IF (S .GT. R) CALL LINZER(PSI(1, 1, S), K * K)
C
C     ZERO INITIAL TERM
C
C     IF (PZERO) GOTO 50

```

```

      IMAX = MIN0(P, S - 1)
C
C      BECAUSE PHI(I)=0 FOR I>P
C
      DO 40 I = 1, IMAX
      SMI = S - I
      CALL MATMUL(W, PHI(1, 1, I), PSI(1, 1, SMI), K, K, K, K)
      CALL MATADD(PSI(1, 1, S), PSI(1, 1, S), W, K, K)
40 CONTINUE
C
50 CONTINUE
C
      NEXT, FORM THE S.L.E. SYSTEM [EQNS. (1A)] FOR THE FIRST (1+R)
      GAMMA'S. THE RHS CONSTANTS ARE ASSEMBLED IN THE GAMMA ARRAY,
      BECAUSE THAT IS WHERE THE 'SOLVE' ROUTINE IS REQUIRED TO
      DEPOSIT THE SOLUTIONS. THE FORMULAE FOR THESE ARE:
C
      [B(L)](I,J) = [ SUM( PSI(S)*SIGMA*THETA'(S+L) )](I,J) ,
C
      WHERE THE SUM IS OVER S=0,1,...,R-L. NOTE THAT THE FIRST
      TERM (S=0) IN THE SUMMATION IS ALWAYS PSI(0)*SIGMA*THETA'(L),
      AND WE KNOW THAT PSI(0)=IDENTITY MATRIX.
C
      DO 70 LP1 = 1, RP1
C
      COMPUTE B(L)
C
      L = LP1 - 1
      CALL MULTRA(GAMMA(1, 1, L), SIGMA, THETA(1, 1, L), K, K, K, K)
      IF (L .EQ. R) GOTO 70
C
      ONLY ONE TERM IN THIS CASE
C
      RML = R - L
      DO 60 S = 1, RML
C
      FORM S'TH TERM AND ADD UP
C
      LPS = L + S
      CALL MULTRA(W, SIGMA, THETA(1, 1, LPS), K, K, K, K)
      CALL MATMUL(W1, PSI(1, 1, S), W, K, K, K, K)
      CALL MATADD(GAMMA(1, 1, L), GAMMA(1, 1, L), W1, K, K)
60 CONTINUE
70 CONTINUE
C
      NOW ASSEMBLE THE COEFFICIENT ARRAY C. THE MAPPING FUNCTION
      FOR THE LINEAR NUMBERING OF THE GAMMA(L)(I,J) ELEMENTS IS
      CHOSEN TO MATCH THE NATURAL STORE ORDERING; HENCE THE POINTER
      FUNCTION IS: ZROW(I,J,L,K)=L*K**2 + (J-1)*K + I
      HOWEVER, IF P=0 THEN GAMMA(L)=-B(L), AND NO SLE'S NEED BE
      SOLVED.
C
      IF (P .GT. 0) GOTO 80
      CALL NEGATE(GAMMA, KKR P1)
C
      LINEARISED VERSION
C
      GOTO 100
C
80 CALL LINZER(C, KKR P1 * KKR P1)
C

```

```
      DO 90 LP1 = 1, RP1
C
      L = LP1 - 1
C
      L'TH EQUATION OF SYSTEM (1A)
C
      LMR = L - R
C
      DO 90 I = 1, K
C
      I'TH ROW
C
      DO 90 J = 1, K
C
      J'TH COLUMN
C
      IROW = ZROW(I, J, L, K)
C
      DO 90 S = LMR, L
C
      OF S'TH TERM IN L-H SUMMATION
C
      MS = IABS(S)
      NEG = S .LT. 0
      POS = .NOT.NEG
      LMS = L - S
C
      DO 90 IA = 1, K
C
      S'TH TERM IS A MATRIX PRODUCT
C
      IF (POS) JCOL = ZROW(I, IA, S, K)
      IF (NEG) JCOL = ZROW(IA, I, MS, K)
C
      GAMMA(-S)=GAMMA'(S)
C
      C(IROW, JCOL) = PHI(J, IA, LMS)
90 CONTINUE
C
      PHI TRANSPOSED
C
      THIS COMPLETES THE ASSEMBLY OF SLE SYSTEM (1). NOW SOLVE THEM;
      THE SOLUTION IS OVERWRITTEN ON GAMMA.
C
      CALL SOLVE(KKRP1, .TRUE., C, GAMMA, DDET, GAMMA, IFAULT)
      IF (IFault .NE. 0) GOTO 130
C
      FINALLY, COMPUTE THE REMAINING GAMMA(L) FOR L=R+1,.....,LMAX
C
100 IF (LMAX .LE. R) GOTO 130
C
      CALL LINZER(GAMMA(1, 1, RP1), K * K * (LMAX - R))
C
      ZERO REMAINING
C
      IF (PZERO) GOTO 130
C
      DO 120 L = RP1, LMAX
      DO 110 S = 1, P
C
```

```
C      COMPUTE S'TH PRODUCT OF SUM
C
      LMS = L - S
      CALL MULTRA(W, GAMMA(1, 1, LMS), PHI(1, 1, S), K, K, K, K)
      CALL MATADD(GAMMA(1, 1, L), GAMMA(1, 1, L), W, K, K)
110 CONTINUE
120 CONTINUE
C
130 RETURN
      END

      SUBROUTINE CORREL(K, LMAX, G, RHO, W)
C
C      ALGORITHM AS232.1 APPL. STATIST. (1988) VOL. 37, NO. 1
C
      REAL WI, DENOM
      DIMENSION G(K, K, 0:LMAX), RHO(K, K, 0:LMAX), W(K)
C
      W IS A SCRATCH ARRAY; G(1:K,1:K,L) HOLDS THE GAMMA(L)
      MATRICES. FIRST SET UP THE VALUES SQR(G(I,I,0)) IN W(I)
C
      DO 10 I = 1, K
10 W(I) = SQR(G(I, I, 0))
C
      NOW DIVIDE THE G(I,J,L) BY THE W(I)*W(J)
C
      LM1 = LMAX + 1
      DO 20 I = 1, K
      WI = W(I)
      DO 20 J = 1, K
C
      DENOM = WI * W(J)
C
      DO 20 LP1 = 1, LM1
      L = LP1 - 1
      RHO(I, J, L) = G(I, J, L) / DENOM
20 CONTINUE
C
      RETURN
      END

      SUBROUTINE PARTLS(K, PSTAMX, KKLMAX, NOOPUT, GAMMA, PHISTA, C,
* IFAULT)
C
C      ALGORITHM AS232.2 APPL. STATIST. (1988) VOL. 37, NO. 1
C
      INTEGER PSTAR, PSTAMX
      DIMENSION GAMMA(K, K, 0:PSTAMX), PHISTA(K, K, 0:PSTAMX), C(KKLMAX,
* KKLMAX)
C
      TO COMPUTE THE PARTIAL CORRELATION MATRICES FOR
      PSTAR=1,2,...,PSTAMX. THESE ARE COMPUTED IN REVERSE ORDER SO
      THAT AT THE END THE 3-D ARRAY WILL KEEP THEM ALL IN ORDER
      (I.E. PHISTA( , ,L) CONTAINS THE L'TH).
C
      PSTAR = PSTAMX
10 KKPST = K * K * PSTAR
C
      ORDER OF SYSTEM (2) FOR THIS PSTAR
C
      CALL PUREAR(K, PSTAR, KKPST, GAMMA, PHISTA, C, IFAULT)
```

```
      IF (IFAUPT .NE. 0) RETURN
C
      PSTAR = PSTAR - 1
      IF (PSTAR .GE. 10) GOTO 10
C
      RETURN
      END

      SUBROUTINE PUREAR(K, PSTAR, KKPST, GAMMA, PHISTA, C, IFAULT)
C
C      ALGORITHM AS232.3 APPL. STATIST. (1988) VOL. 37, NO. 1
C
      INTEGER PSTAR, S, ZROW
      DIMENSION GAMMA(K, K, 0:PSTAR), PHISTA(K, K, 0:PSTAR), C(KKPST,
*   KKPST)
C
C      TO SOLVE FOR THE PHI* ARRAYS, GIVEN P*; KKPST=K*K*PSTAR
C      THE LINEAR MAPPING FUNCTION IS THE SAME AS IN S/R XCOVAR :
C
      ZROW(I, J, L, K) = ((L - 1) * K + J - 1) * K + I
C
C      NO ZERO PLANE HERE, THOUGH
C
      IFAULT = 0
      IF (KKPST .EQ. K * K * PSTAR) GOTO 10
      IFAULT = -1
      RETURN
10 CONTINUE
      CALL SCALAR(PHISTA(1, 1, 0), K, -1.0)
      CALL LINZER(C, KKPST ** 2)
C
      DO 20 L = 1, PSTAR
      DO 20 I = 1, K
      DO 20 J = 1, K
C
      IROW = ZROW(I, J, L, K)
C
      DO 20 S = 1, PSTAR
C
      LMS = L - S
      MLMS = IABS(LMS)
C
      DO 20 IA = 1, K
C
      JCOL = ZROW(J, IA, S, K)
C
      IF (LMS .GE. 0) G = GAMMA(I, IA, LMS)
      IF (LMS .LT. 0) G = GAMMA(IA, I, MLMS)
C
      GAMMA(-L)=GAMMA'(L)
C
      C(IROW, JCOL) = G
20 CONTINUE
C
C      THIS COMPLETES THE FORMATION OF THE COEFF MATRIX FOR SYSTEM (2)
C
      CALL SOLVE(KKPST, .TRUE., C, GAMMA(1, 1, 1), DDET,
* PHISTA(1, 1, 1), IFAULT)
      IF (IFAUPT .NE. 0) IFAULT = PSTAR
C
      RETURN
```

```
END
C
SUBROUTINE DETERM(K, LMAX, A, DETS, C)
C
C   ALGORITHM AS232.4 APPL. STATIST. (1988) VOL. 37, NO. 1
C
DIMENSION A(K, K, 0:LMAX), DETS(0:LMAX), C(K, K, 0:LMAX)
C
C   EVALUATE THE DETERMINANTS (BY LU FACTORISATION) OF EACH K-BY-K
C   MATRIX IN THE PLANES OF 'A'; STORE DET(A(,,L)) IN DETS(L).
C
KKLM1 = K * K * (LMAX + 1)
C
C   TOTAL NUMBER OF ELEMENTS
C
CALL LINCOP(C, A, KKLM1)
C
C   PRESERVE A
C
DO 1 L = 0, LMAX
1 CALL SOLVE(K, .FALSE., C(1, 1, L), DETS, DETS(L), DETS, IFAULT)
C
C   THE TWO ARGUMENTS 'DETS' ARE NOT ACCESSED BY S/R SOLVE, SINCE
C   THE 'RHS' PARAMETER HAS THE VALUE .FALSE.
C
RETURN
END
```

```
      SUBROUTINE BABSRT(N, M, L, NN, SI, X, AVAIL, NBRNCH, POINTR, LIST,
*   INDEX, VSORT, XIN, CSORT, C, CMAX, S, CRIT, BEST, NEVAL,
*   IFAULT)
C
C   ALGORITHM AS233  APPL. STATIST. (1988) VOL. 37, NO. 1
C
C   BRANCH AND BOUND ALGORITHM FOR FEATURE SUBSET SELECTION
C   USING SORTING TO IMPROVE EFFICIENCY
C
C   INTEGER N, M, MBAR, P, OMIT, NOMIT, PI, VJ, PP
C   INTEGER LIST(N), NBRNCH(N), POINTR(N), INDEX(N), VSORT(N),
*   NEVAL(N), BEST(N)
C   LOGICAL AVAIL(N)
C   REAL SI(N, N), X(N), XIN(N), CSORT(N), C(N), S(NN), CMAX(N),
*   ZERO, TWO
C
C   DATA ZERO, TWO /0.0, 2.0/
C
C   CHECK VALID VALUES OF L,M,N
C
C   IFAULT = 1
C   IF (M .LT. 2 .OR. M .GE. N .OR. L .LT. 0) RETURN
C   IFAULT = 0
C
C   COPY SI INTO START OF WORKSPACE ARRAY S. EVALUATE
C   CRITERION FUNCTION WITH ALL VARIABLES INCLUDED.
C   INITIALIZE WORKSPACE ARRAYS.
C
C   DOLD = ZERO
C   K = 0
C   DO 5 I = 1, N
C   DO 4 J = 1, I
C   K = K + 1
C   S(K) = SI(I, J)
C   DOLD = DOLD + TWO * S(K) * X(I) * X(J)
4 CONTINUE
C   DOLD = DOLD - S(K) * X(I) * X(I)
C   AVAIL(I) = .TRUE.
C   INDEX(I) = I
C   CMAX(I) = ZERO
C   NEVAL(I) = 0
5 CONTINUE
C
C   INITIALIZATION
C
C   NN6 = 6 * NN
C   MBAR = N - M + 1
C   P = M + 1
C   I = 2
C   POINTR(1) = 0
C
C   COPY INTO XIN VALUES OF X FOR VARIABLES INCLUDED AT LEVEL I-1
C
C   100 K = 0
C   DO 110 J = 1, N
C   IF (INDEX(J) .LT. 0) GOTO 110
C   K = K + 1
C   XIN(K) = X(J)
110 CONTINUE
C
C   EVALUATE CRITERION FUNCTION AFTER DROPPING EACH OF THE
```



```
C      VARIABLES WHICH ARE CURRENTLY AVAILABLE.  UPDATE
C      EVALUATION COUNTER.
C
MM = N - I + 2
II = (NN6 - MM * (MM + 1) * (MM + 12)) / 6
K = 0
DO 130 OMIT = 1, N
IF (.NOT.AVAIL(OMIT)) GOTO 130
NOMIT = INDEX(OMIT)
KK = II + (NOMIT * NOMIT + NOMIT) / 2
IK = KK - NOMIT
D = ZERO
DO 120 J = 1, MM
IK = IK + I
IF (J .GT. NOMIT) IK = IK + J - 2
D = D + S(IK) * XIN(J)
120 CONTINUE
K = K + 1
CSORT(K) = DOLD - D * D / S(KK)
VSORT(K) = OMIT
NEVAL(I - 1) = NEVAL(I - 1) + 1
130 CONTINUE
C
C      SORT SMALLEST P VALUES INTO INCREASING ORDER
C
PP = P
IF (K .EQ. P) PP = PP - 1
DO 150 IK = 1, PP
J1 = IK
K1 = IK + 1
DO 140 J = K1, K
IF (CSORT(J) .LT. CSORT(J1)) J1 = J
140 CONTINUE
IF (J1 .EQ. IK) GOTO 150
TEMP = CSORT(IK)
CSORT(IK) = CSORT(J1)
CSORT(J1) = TEMP
ITEMP = VSORT(IK)
VSORT(IK) = VSORT(J1)
VSORT(J1) = ITEMP
150 CONTINUE
C
C      STORE NUMBERS OF VARIABLES SELECTED IN LIST AND CRITERION
C      FUNCTION VALUES IN C. SIGNAL THAT THESE FEATURES ARE
C      NO LONGER AVAILABLE.
C
K = POINTR(I - 1)
DO 170 J = 1, P
K = K + 1
VJ = VSORT(J)
LIST(K) = VJ
C(K) = CSORT(J)
AVAIL(VJ) = .FALSE.
NBRNCH(K) = P - J + 1
170 CONTINUE
POINTR(I) = K + 1
C
C      BACKTRACK IF LIST AT LEVEL I IS EXHAUSTED OTHERWISE SELECT
C      NEXT VARIABLE TO THE LEFT ALONG LIST
C
200 IF (POINTR(I) .EQ. POINTR(I - 1) + 1) GOTO 400
```

```

        POINTR(I) = POINTR(I) - 1
C
C         ABANDON FURTHER SEARCH IF CRITERION FUNCTION IS LESS THAN
C         CURRENT MAXIMUM L LEVELS FURTHER DOWN TREE.
C
300 PI = POINTR(I)
    D = C(PI)
    IF (D .GT. CMAX(I)) CMAX(I) = D
    IL = I + L
    IF (IL .GT. MBAR) IL = MBAR
    IF (D .LT. CMAX(IL)) GOTO 600
C
C         IF AT LOWEST LEVEL OF TREE A NEW MAXIMUM HAS BEEN FOUND
C
    OMIT = LIST(PI)
    IF (I .EQ. MBAR) GOTO 500
C
C         UPDATE INVERSE MATRIX S READY FOR MOVE TO NEXT LEVEL DOWN
C
    NOMIT = INDEX(OMIT)
    MM = N - I + 2
    II = (NN6 - MM * (MM + 1) * (MM + 2)) / 6
    IJK = II + (MM * MM + MM) / 2
    KK = II + (NOMIT * NOMIT + NOMIT) / 2
    IK = KK - NOMIT
    IJ = II
    DO 316 J = 1, MM
    IK = IK + 1
    IF (J - NOMIT) 304, 302, 303
302 IJ = IJ + NOMIT
    GOTO 316
303 IK = IK + J - 2
304 JK = KK - NOMIT
    TEMP = S(IK) / S(KK)
    DO 310 K = 1, J
    IJ = IJ + 1
    JK = JK + 1
    IF (K - NOMIT) 307, 310, 306
306 JK = JK + K - 1
307 IJK = IJK + 1
    S(IJK) = S(IJ) - TEMP * S(JK)
310 CONTINUE
316 CONTINUE
C
C         UPDATE NUMBERING OF VARIABLES WITH RESPECT TO S
C         AND MOVE DOWN TO NEXT LEVEL
C
    INDEX(OMIT) = -N
    K = OMIT + 1
    DO 330 J = K, N
330 INDEX(J) = INDEX(J) - 1
    DOLD = D
    P = NBRNCH(PI)
    I = I + 1
    GOTO 100
C
C         IF AT LEVEL 2 THEN SEARCH IS COMPLETE. OTHERWISE BACKTRACK
C         ONE LEVEL
C
400 IF (I .EQ. 2) GOTO 999
    I = I - 1

```

```
    PI = POINTR(I)
    LPI = LIST(PI)
    AVAIL(LPI) = .TRUE.
    K = LPI + 1
    DO 410 J = K, N
410  INDEX(J) = INDEX(J) + 1
    INDEX(LPI) = 1
    J = LPI
420  J = J - 1
    IF (J .EQ. 0) GOTO 200
    IF (INDEX(J) .LT. 0) GO TO 420
    INDEX(LPI) = INDEX(J) + 1
    GOTO 200
C
C      STORE VARIABLE NUMBERS OF SUBSET WHICH HAS PRODUCED NEW MAX
C
500  K = 0
    DO 510 J = 1, N
    IF (INDEX(J) .LT. 0 .OR. J .EQ. OMIT) GOTO 510
    K = K + 1
    BEST(K) = J
510  CONTINUE
C
C      SIGNAL THAT VARIABLE AT CURRENT NODE AND ITS LEFT SIBLINGS
C      ARE AVAILABLE
C
600  LPI = LIST(PI)
    AVAIL(LPI) = .TRUE.
    PI = PI - 1
    IF (PI .GT. POINTR(I - 1)) GOTO 600
    GOTO 400
C
C      SEARCH COMPLETE - SET MAXIMUM AND RETURN
C
999  CRIT = CMAX(MBAR)
    RETURN
    END
```

```
      SUBROUTINE PPRANK(TA, UA, ET, SD, K3, K4, N, M, ISEL, IFAULT)
C
C      ALGORITHM AS234  APPL. STATIST. (1988) VOL. 37, NO. 2
C
C      Declaration formal parameters
C
      INTEGER N, M, ISEL, IFAULT
      REAL TA, UA, ET, SD, K3, K4
C
C      Auxiliary algorithm
C
      REAL SCORE
      EXTERNAL SCORE
C
C      Constants
C
      REAL ZERO, ONE, TWO, THREE, SIX, HALF, TWOHLF
      REAL CMT1, CMT2, CMT3, CTA1, CTA2, CTA3
      DATA ZERO, ONE, TWO, THREE /0.0E0, 1.0E0, 2.0E0, 3.0E0/
      DATA SIX, HALF, TWOHLF /6.0E0, 0.5E0, 2.5E0/
      DATA CMT1, CMT2, CMT3 /0.0833333E0, 2.3333333E0, 0.0125E0/
      DATA CTA1, CTA2, CTA3 /0.4166667E0, 0.0555555E0, 0.1666667E0/
C
C      Declaration internal variables
C
      INTEGER I
      REAL S1A, S2A, S3A, S4A, S1C, S2C, S3C, S4C, W, H1, H2, H3, H4,
*      MAXU
      DATA MAXU /1.0E+10/
C
C      Checking input
C
      IFAULT = 1
      IF ((ISEL .LE. 0) .OR. (ISEL .GT. 4)) RETURN
      IF (ISEL .EQ. 4) GOTO 400
      IFAULT = 2
      IF (N .LE. 3) RETURN
C
C      Initializing auxiliary variables
C
      H1 = N - THREE
      H2 = N - TWO
      H3 = N - ONE
      H4 = N + ONE
C
C      Compute S1a, S2A, S3a, S4a
C
      S1A = ZERO
      DO 10 I = 1, N
      S1A = S1A + SCORE(I / H4)
10 CONTINUE
      S1A = S1A / N
      S2A = ZERO
      S3A = ZERO
      S4A = ZERO
      DO 20 I = 1, N
      W = SCORE(I / H4) - S1A
      S2A = S2A + W ** 2
      S3A = S3A + W ** 3
      S4A = S4A + W ** 4
20 CONTINUE
```

```

        IFAULT = 3
        IF (S2A .LE. ZERO) RETURN
        S2A = S2A / H3
        S3A = S3A / H3
        S4A = S4A / H3
        GOTO (100, 200, 300), ISEL

```

```

C
C       Two-sample
C

```

```

100 IFAULT = 4
    IF (N .LT. 2 * M) RETURN
    S1C = (ONE * M) / N
    W = ONE - S1C
    S2C = (M * W ** 2 + (N - M) * S1C ** 2) / H3
    S3C = (M * W ** 3 + (N - M) * S1C ** 3) / H3
    S4C = (M * W ** 4 + (N - M) * S1C ** 4) / H3
    GOTO 500

```

```

C
C       Monotone trend
C

```

```

200 S1C = H4 * HALF
    S2C = H4 * N * CMT1
    S3C = ZERO
    S4C = (N * N - CMT2) * H4 * N * CMT3
    GOTO 500

```

```

C
C       Independence
C

```

```

300 S1C = S1A
    S2C = S2A
    S3C = S3A
    S4C = S4A
    GOTO 500

```

```

C
C       Compute ET, SD, K3, K4
C

```

```

500 W = (N / H3) * (H4 / H3)
    ET = N * S1A * S1C
    SD = SQRT(H3 * S2A * S2C)
    K3 = (N / H2) * (S3A / S2A) * (S3C / S2C) / SD
    K4 = (H3 / H1) * (W * S4A / (S2A ** 2) - THREE) * (W * S4C /
    * (S2C ** 2) - THREE) / (W * H2) - SIX / H4

```

```

C
C       Compute percentage point
C

```

```

400 IFAULT = 5
    IF (ABS(UA) .GT. MAXU) RETURN
    W = UA ** 2
    TA = (ONE + (W - THREE) * K4 * CTA1 - (W - TWOHLF) * (K3 ** 2)
    * * CTA2) * UA + (W - ONE) * K3 * CTA3
    TA = TA * SD + ET
    IFAULT = 0
    RETURN
END

```

```

      SUBROUTINE RTALLY(NEWVAL, EMAX, MVCODE, MMAX, N, VALUES, COUNT,
+         K, IFAULT)
C
C   ALGORITHM AS235  APPL. STATIST. (1988) VOL. 37, NO. 2
C
      INTEGER KCUT
      PARAMETER (K CUT = 25)
      INTEGER COUNT(*)
      INTEGER HI, I, J, K, KMAX, LO, M, N, IFAULT, MMAX
      REAL VALUES(*), NEWVAL, MVCODE(*)
C
C   Tallies (tabulates) input values NEWVAL with their frequencies.
C   The K distinct values are stored in array VALUES in ascending
C   order, and their frequencies are stored in COUNT.
C   N is the current number of observations.
C
      IFAULT = 0
      IF (MMAX .GT. 0) THEN
        DO 99 I = 1, MMAX
          IF (NEWVAL .EQ. MVCODE(I)) RETURN
99      CONTINUE
        END IF
        N = N + 1
C
C   Initialize
C
      IF (N .LE. 1) THEN
        N = 1
        K = 1
        J = 1
        GO TO 5
      END IF
      J = K + 1
      IF (NEWVAL .GT. VALUES(K)) GO TO 3
C
      IF (K .LT. KCUT) THEN
C
C   Simple searching of VALUES from first element, for small K
C
        DO 1 I = 1, K
          J = I
          IF (NEWVAL - VALUES(J)) 3, 6, 1
1      CONTINUE
        ELSE
C
C   Bisection search
C
          J = 1
          IF (NEWVAL .LT. VALUES(1)) GO TO 3
          LO = 0
          HI = K + 1
2      J = (HI + LO) / 2
          IF (NEWVAL .EQ. VALUES(J)) GO TO 6
C
C   J = LO means that NEWVAL is bracketed between VALUES(LO) and
C   VALUES(HI).  Insert NEWVAL at position HI and move the rest of
C   VALUES and COUNT up.
C
          IF (J .EQ. LO) THEN
            J = HI
            GO TO 3

```

```
        END IF
        IF (NEWVAL .LT. VALUES(J)) THEN
            HI = J
        ELSE
            LO = J
        END IF
        GO TO 2
    END IF
C
3  IF (K .EQ. KMAX) THEN
        IFAULT = 1
        N = N - 1
        RETURN
    END IF
    K = K + 1
    IF (K .GT. J) THEN
        DO 4 M = K, J+1, -1
            VALUES(M) = VALUES(M-1)
            COUNT(M) = COUNT(M-1)
        4  CONTINUE
    END IF
5  VALUES(J) = NEWVAL
    COUNT(J) = 1
    RETURN
C
6  COUNT(J) = COUNT(J) + 1
    RETURN
C
    END
```

```

{
    Algorithm AS236  Appl. Statist. (1988) Vol. 37, No. 2
}

{ To Enumerate all RxC tables having given row and column sums
  To Evaluate the conditional probability of each table under
  hypergeometric and multinomial models
  To Evaluate likelihood across all tables according to the multinomial
  model
}

{ ***** }

{
    DATA STRUCTURES
}

{ ***** }

CONST
maxtablesize=10;      { maximum dimensions of table }
maxN=300;             { maximum global total of table entries - the
                      values 10 and 300 may be changed, if desired }

TYPE
intvalues=0..maxN;   { permissible table entry type }
faultint=0..123;     { fault indicator type
                      0,100,20,3,120,103,23,123 }
dimension=1..maxtablesize; { table dimension type }
vector = ARRAY[1..maxtablesize] OF intvalues; { row and column vector type }
matrix = ARRAY[1..maxtablesize,1..maxtablesize] OF real; { matrix type }

return = ^returnlist; { pointer to function returns }
head = ^headlist;     { pointer to NODE information }
table = ^tablist;     { pointer to NODULE. All tables are stored in
                      in a single linked list of head and table records. }
tablist = RECORD      { Each table/nodule record contains the
                      value of the:- }
    entry:intvalues;  { current table entry }
    loghyper:real;    { current contribution to hypergeometric }
    multi:real;       { current contribution to multinomial }
    rest: head ;     { a pointer to the rest of the family of
                      tables built onto the current entry
                      ie to the next node }
    next:table        { a pointer to the next possible entry value
                      for the current position and associated
                      family of tables ie to the next nodule }

END;

headlist = RECORD
    number:integer;   { number of subtables emanating from the
                      current node }
    position:ARRAY[1..2] OF dimension; { current table position }
    first:table       { pointer to the first cell value and
                      associated tables ie to the first nodule }

END;

returnlist = RECORD
    tables:head;     { a function call returns a pointer to a }

```



```

value:real      { family of tables and the value of the
                  likelihood function evaluated across these }
END;

```

```

VAR
rowsum:vector;  { required row sums for tables }
colsum:vector;  { required column sums for tables }
rows,cols:dimension; { number of rows and columns in table }
pmatrx:matrix;  { proposed transition matrix }
result:return;  { variable to receive function return }
loghypercons,multicons:real; { constants for hypergeometric and
                               multinomial probabilities }
ifault:faultint; { fault indicator }

```

```

{ ***** }
{
      OUTPUT  PROCEDURES
}
{ ***** }

```

```
PROCEDURE Report(r:return;i:faultint);
```

```

TYPE
tabmatrix = ARRAY[1..maxtablesize,1..maxtablesize] OF intvalues;

```

```
PROCEDURE Printmat(tub:tabmatrix;prob1,prob2:real);
```

```

VAR
i,j:dimension;

BEGIN
                                     { write out probabilities and current
                                     table }

```

```

Writeln;
Writeln('Hypergeometric probability = ',prob1);
Writeln('Multinomial probability = ',prob2);
FOR i:=1 TO rows DO
  BEGIN
  Writeln;
  Write('row ',i:1,' * ');
  FOR j:=1 TO cols DO
    Write(tub[i,j],' ');
  END;

```

```

Writeln
END;

```

```
PROCEDURE Printtables(v:real;example:head);
```

```

CONST
assumedzero=1.0e-15;

```

```

VAR
tab:tabmatrix;
exam:table;
i,j:dimension;
hyperprob,multiprob:real;

```

```

BEGIN
WITH example^ DO
  BEGIN

```

```

    exam:=first;
    i:=position[1];
    j:=position[2]
    END;
REPEAT
    WITH exam^ DO
        BEGIN
            tab[i,j]:=entry;           { copy current table entry into
                                       matrix for output }
            IF (i=rows) AND (j=cols) THEN { if table complete print out }
                BEGIN
                    hyperprob:=Exp(loghyper+loghypercons);
                    IF v>assumedzero THEN multiprob:=multi/v
                    ELSE multiprob:=0.0;
                    Printmat(tab,hyperprob,multiprob)
                END
            ELSE Printtables(v,rest)    { assemble rest of table through
                                       a recursive call to Printtables }

            END;
        exam:=exam^.next;
    UNTIL exam=NIL
    END;

BEGIN { Report }
Writeln;
Writeln('IFAULT=',i:1);Writeln;
IF i=0 THEN                               { if evaluation successful print out
                                           all tables and probabilities }

    BEGIN
        Writeln('Number of Tables Generated = ',r^.tables^.number);
        Writeln('Multinomial likelihood = ',r^.value*multicons);
        Printtables(r^.value,r^.tables)
    END
END; { Report }

{ ***** }

{
    PRINCIPAL FUNCTION
}

{ ***** }

FUNCTION Enum(rows,cols:dimension; rowsum,colsum:vector;
    pmatrix:matrix; VAR ifault:faultint):return;

CONST
oneminus=0.99999;
oneplus=1.00001;

TYPE
dvector = ARRAY[0..maxN] OF real;    { real vector type }

VAR
logfact:dvector;
sfault,tfault:faultint;
i,j:dimension;
rowtotal,coltotal:intvalues;
total:real;

FUNCTION max(a,b:integer):integer;

```

```
BEGIN
IF a>b THEN max:=a ELSE max:=b
END; { max }

FUNCTION min(a,b:integer):integer;
BEGIN
IF a<b THEN min:=a ELSE min:=b
END; { min }

FUNCTION Eval(n:intvalues;x:real):real;
CONST assumedzero=1.0e-15;
BEGIN
IF n=0 THEN Eval:=1.0 ELSE
IF x<assumedzero THEN Eval:=0.0 ELSE
Eval:=Exp(n*Ln(x)-logfact[n])
END; { Eval }

PROCEDURE Evalconst(rowtotal:intvalues);
VAR
i:intvalues;
logprod1,logprod2:real;
BEGIN
logfact[0]:=0.0;
FOR i:=1 TO rowtotal DO
logfact[i]:=logfact[i-1]+Ln(i);
logprod1:=0.0;
FOR i:=1 TO rows DO
logprod1:=logprod1+logfact[rowsum[i]];
logprod2:=0.0;

FOR i:=1 TO cols DO
logprod2:=logprod2+logfact[colsum[i]];
loghypercons:=logprod1+logprod2-logfact[rowtotal];
multicons:=Exp(logprod1)
END; { Evalconst }

FUNCTION RxC(rno,cno:dimension;rt,ct:intvalues;hp,mp:real;
rowsum,colsum:vector):return;

VAR
count,val,upper,lower,newrt,newct:intvalues;
curloghyper,curmulti,newhp,newmp,total:real;
newrowsum:vector;
newcolsum:vector;
newhead:head;
result,newresult:return;
newtable,nexttable:table;

BEGIN { RxC }

New(newtable);
newrowsum:=rowsum;
newcolsum:=colsum;

IF (rno<rows) AND (cno<cols) THEN { current position rno,cno
in body of table }

BEGIN
nexttable:=newtable;
upper:=min(rowsum[rno],colsum[cno]);
lower:=max(0,rowsum[rno]+colsum[cno]-ct);
newct:= ct-colsum[cno];
```

```

count:=0;
total:=0.0;
FOR val:= lower TO upper DO      { step 2 - consider all possible values
                                  for the current position }

  BEGIN
  WITH nexttable^ DO
    BEGIN
    entry:=val;
                                  { evaluate contributions to likelihood }
    multi:=Eval(val,pmatrx[rno,cno]);
    loghyper:=-logfact[val];
    newrowsum[rno]:=rowsum[rno]-val;
    newcolsum[cno]:=colsum[cno]-val;
    newrt:=rt-val;
    newhp:=hp+loghyper;
    newmp:=mp*multi;
    New(result);
                                  { step 3 - obtain results for remainder
                                  of the table by recursive call to RxC }
    result:=RxC(rno,cno+1,newrt,newct,newhp,newmp,newrowsum,newcolsum);
    rest:=result^.tables;

    count:=count+rest^.number;
    total:=total+result^.value*multi;
    IF val<upper THEN
      BEGIN
      New(next);
      nexttable:=next
      END
    ELSE next:=NIL
    END
  END
END

ELSE
  BEGIN
  New (result);

  IF rno<rows THEN              { current position in right-hand
                                  margin }

    BEGIN
    val:=rowsum[rno];           { only one possible value }
    newrowsum[rno]:=0;
    newcolsum[cno]:=colsum[cno]-val;
    newrt:=rt-val;
    newct:=newct;
                                  { evaluate contributions to likelihood }
    curloghyper:=-logfact[val];
    curmulti:=Eval(val,pmatrx[rno,cno]);
    newhp:=hp+curloghyper;
    newmp:=mp*curmulti;
                                  { step 3 - obtain results for remainder
                                  of the table by recursive call to RxC }
    result:=RxC(rno+1,1,newrt,newct,newhp,newmp,newrowsum,newcolsum);
    count:=result^.tables^.number;
    total:=result^.value*curmulti
    END

  ELSE
    IF cno<cols THEN           { current position in last row }

```

```

    BEGIN
    val:=colsum[cno];           { only one possible value }
    newcolsum[cno]:=0;
    newrowsum[rno]:=rowsum[rno]-val;
    newrt:=rt-val;
    newct:=newrt;

                                { evaluate contributions to likelihood }
    curloghyper:=-logfact[val];
    curmulti:=Eval(val,pmatix[rno,cno]);
    newhp:=hp+curloghyper;
    newmp:=mp*curmulti;

                                { step 3 - obtain results for remainder
                                of the table by recursive call to RxC }
    result:=RxC(rno,cno+1,newrt,newct,newhp,newmp,newrowsum,newcolsum);
    count:=result^.tables^.number;

    total:=result^.value*curmulti
    END

ELSE                               { final cell }
    BEGIN
    val:=rt;                       { only one possible value }
    result^.tables:=NIL;           { table complete }
    count:=1;

                                { evaluate contributions to likelihood }
    curloghyper:=hp-logfact[val];
    curmulti:=Eval(val,pmatix[rno,cno]);
    total:=curmulti;
    curmulti:=curmulti*mp
    END;

WITH newtable^ DO
    BEGIN
    entry:=val;
    loghyper:=curloghyper;
    multi:=curmulti;
    rest:=result^.tables;
    next:=NIL
    END
END;

New(newhead);                       { assemble entries for current NODE }
WITH newhead^ DO
    BEGIN
    number:=count;
    position[1]:=rno;
    position[2]:=cno;
    first:=newtable
    END;
New(newresult);
WITH newresult^ DO
    BEGIN
    tables:=newhead;
    value:=total
    END;
RxC:=newresult
END; { RxC }

BEGIN { Enum }

                                { check validity of input values }
ifault:=0;

```

```
{ totals of row and column sums must be  
equal }
```

```
rowtotal:=0;  
coltotal:=0;  
FOR i:= 1 TO rows DO  
  rowtotal:=rowtotal+rowsum[i];  
FOR i:=1 TO cols DO  
  coltotal:=coltotal+colsum[i];  
  
IF rowtotal<>coltotal THEN ifault:=1;
```

```
{ pmatrix entries must be probabilities  
and rows must sum to one }
```

```
sfault:=0;  
tfault:=0;  
FOR i:=1 TO rows DO  
  BEGIN  
    total:=0.0;  
    FOR j:=1 TO cols DO  
      BEGIN  
        IF (pmatrix[i,j]<0.0) OR (pmatrix[i,j]>1.0) THEN sfault:=1;  
        total:=total+pmatrix[i,j]  
      END;  
      IF (total<oneminus) OR (total>oneplus) THEN tfault:=1  
    END;  
  ifault:=100*ifault+20*sfault+3*tfault;
```

```
{ if valid input, evaluate tables and  
probabilities }
```

```
IF ifault=0 THEN  
  BEGIN  
    Evalconst(rowtotal);  
    Enum:=RxC(1,1,rowtotal,coltotal,0.0,1.0,rowsum,colsum)  
  END  
ELSE  
  Enum:=NIL  
END; { Enum }
```

```

SUBROUTINE BGM(N, RHO, KMAX1, IWIND, TRUNC, TOLER, DELTA, TSTAT,
* CHSTAT, TSIGN, CHSIGN, MAXP, K, WKSP, LGTH, ISWCHI, ISWSGN,
* IFAULT)
C
C     ALGORITHM AS237  APPL. STATIST. (1988) VOL. 37, NO. 2
C
C     COMPUTES THE DELTA, T- AND CHI SQUARED-STATISTIC ARRAYS FOR THE
C     CORNER METHOD OF BEGUIN, GOURIEROUX AND MONFORT (IMPROVED)
C     SUBPROGRAMS : CEACMA, CALBGM, QFBGM, NORMAL(AS 2)
C
DIMENSION DELTA(MAXP, K), TSTAT(MAXP, K), CHSTAT(MAXP, K)
DIMENSION TSIGN(MAXP, K), CHSIGN(MAXP, K)
DIMENSION RHO(KMAX1), WKSP(LGTH)
C
REAL TRUNC, TOLER
REAL EPS, TENTH
C
DATA EPS, ETA, TENTH /1.0E-12, 1.0E-60, 0.1/
C
C     STORAGE MANAGEMENT AND ERROR DETECTION
C
K2 = K + 2
LCOVAR = (K + 1) * K / 2
LWRHO = KMAX1
LWLAM = 2 * KMAX1 - 1
IWKSP1 = 1
IWKSP2 = IWKSP1 + K2
IWKSP3 = IWKSP2 + K2
IWKSP4 = IWKSP3 + LCOVAR
IWKSP5 = IWKSP4 + LWRHO
IWKSP6 = IWKSP5 + LWLAM
IWKSP7 = IWKSP6 + K2 * K
IWKSP8 = IWKSP7 + K2 * K
LWKSP = LGTH - (IWKSP8 - 1)
IFAULT = 0
IF (MAXP .LT. K) IFAULT = 6
IF (ISWCHI .LT. (-1) .OR. ISWCHI .GT. 1) IFAULT = 7
IF (ISWSGN .NE. 0 .AND. ISWSGN .NE. 1) IFAULT = 7
IF (TOLER .GT. TENTH .OR. TOLER .LT. EPS) IFAULT = 8
IF (LWKSP .LT. 3 * K2) IFAULT = 9
IF (K .LE. 0) IFAULT = 1
IF (IFAULT .NE. 0) RETURN
C
C     PRELIMINARIES
C
CALL CEACMA(N, RHO, KMAX1, IWIND, TRUNC, WKSP(IWKSP4), LWRHO,
* WKSP(IWKSP5), LWLAM, WKSP(IWKSP3), LCOVAR, K, IFAULT)
IF (IFAULT .NE. 0) RETURN
C
C     CALL TO COMPUTING SUBROUTINE
C
CALL CALBGM(RHO, KMAX1, DELTA, TSTAT, CHSTAT, TSIGN, CHSIGN, MAXP,
* K, WKSP(IWKSP3), LCOVAR, WKSP(IWKSP1), WKSP(IWKSP2), K2,
* WKSP(IWKSP6), WKSP(IWKSP7), WKSP(IWKSP8), EPS, ETA, TOLER,
* ISWCHI, ISWSGN, IFAULT)
RETURN
END

SUBROUTINE CEACMA(N, RHO, KMAX1, IWIND, TRUNC, WRHO, LWRHO, WLAM,
* LWLAM, COVAR, LCOVAR, K, IFAULT)
C

```

```

C      ALGORITHM AS237.1  APPL. STATIST. (1988) VOL. 37, NO. 2
C
C      COMPUTATION OF A CONSISTENT ESTIMATOR OF THE ASYMPTOTIC
C      COVARIANCE MATRIX OF THE FIRST K AUTOCORRELATION ESTIMATORS
C
C      DIMENSION RHO(KMAX1), WRHO(LWRHO), WLAM(LWLAM), COVAR(LCOVAR)
C
C      REAL TRUNC
C      REAL ZERO, ONE, TWO, SIX, HALF
C
C      DATA ZERO, ONE, TWO, SIX, HALF /0.0, 1.0, 2.0, 6.0, 0.5/
C
C      FN = N
C      IF (K .LE. 0) IFAULT = 1
C      IF (IWIND .LT. 0 .OR. IWIND .GT. 2) IFAULT = 2
C      IF (KMAX1 .LE. K) IFAULT = 3
C      IF (TRUNC .LT. HALF .OR. TRUNC .GT. SIX) IFAULT = 4
C      IF (N .LE. K) IFAULT = 5
C      IF (LCOVAR .NE. (K + 1) * K / 2 .OR. LWRHO .NE. KMAX1 .OR.
*  LWLAM .NE. 2 * KMAX1 - 1) IFAULT = 20
C      IF (IFAILT .NE. 0) RETURN
C
C      COMPUTING WINDOWED AUTOCORRELATIONS WRHO
C
C      BN = INT(SQRT(FN) * TRUNC)
C      DO 100 MP1 = 1, LWRHO
C      FACT = ONE
C      IF (IWIND .EQ. 0) GOTO 90
C      X = FLOAT(MP1 - 1) / BN
C      FACT = ZERO
C      IF (IWIND .EQ. 2) GOTO 20
C      IF (X .LE. ONE) FACT = ONE - X
C      GOTO 90
20  IF (X .LE. HALF) FACT = ONE - SIX * X ** 2 * (ONE - X)
    IF (X .LE. ONE .AND. X .GT. HALF) FACT = TWO * (ONE - X) ** 3
90  WRHO(MP1) = RHO(MP1) * FACT
100 CONTINUE
C
C      COMPUTING WINDOWED LAMBDA
C
C      DO 250 MP1 = 1, LWLAM
C      WLAM(MP1) = ZERO
C      NTERM = LWLAM - MP1 + 1
C      DO 200 LP1 = 1, NTERM
C      LABS = IABS(LP1 - LWRHO) + 1
C      LPMABS = IABS(LP1 + MP1 - LWRHO - 1) + 1
C      WLAM(MP1) = WLAM(MP1) + WRHO(LABS) * WRHO(LPMABS)
200 CONTINUE
250 CONTINUE
C
C      EVALUATING THE ASYMPTOTIC COVARIANCE MATRIX OF THE
C      AUTOCORRELATIONS
C
C      IND = 0
C      K1 = K + 1
C      DO 300 M = 2, K1
C      DO 300 L = M, K1
C      LMM = L - M + 1
C      LPM = L + M - 1
C      IND = IND + 1
C      COVAR(IND) = (WLAM(LMM) + WLAM(LPM) - (WRHO(M) * WLAM(L) + WRHO(L)

```



```

* * WLAM(M) - WRHO(M) * WRHO(L) * WLAM(1)) * TWO) / FN
300 CONTINUE
RETURN
END

SUBROUTINE CALBGM(RHO, KMAX1, DELTA, TSTAT, CHSTAT, TSIGN, CHSIGN,
* MAXP, K, COVAR, LCOVAR, DELTA0, DELTA1, K2, DERIV0, DERIV1,
* WKSP, EPS, ETA, TOLER, ISWCHI, ISWSGN, IFAULT)
C
C     ALGORITHM AS237.2 APPL. STATIST. (1988) VOL. 37, NO. 2
C
DIMENSION RHO(KMAX1), WKSP(3, K2), COVAR(LCOVAR)
DIMENSION DELTA(MAXP, K), TSTAT(MAXP, K), CHSTAT(MAXP, K)
DIMENSION TSIGN(MAXP, K), CHSIGN(MAXP, K)
DIMENSION DELTA0(K2), DELTA1(K2)
DIMENSION DERIV0(K2, K), DERIV1(K2, K)
DIMENSION CHI(1), P(1), Q(1), Z(1)
C
LOGICAL ZDELTA
REAL TOLER
REAL EPS, ZERO, ONE, TWO, RT2PI
C
DATA ZERO, ONE, TWO, RT2PI /0.0, 1.0, 2.0, 2.5066282746/
C
C     INITIALIZATION OF TWO LINES OF THE DELTA AND DERIV ARRAYS
C
IFAIL1 = 0
IFAIL2 = 0
DO 440 IQ = 1, K2
DELTA1(IQ) = ONE
DO 420 M = 1, K
DERIV0(IQ, M) = ZERO
DERIV1(IQ, M) = ZERO
420 CONTINUE
440 CONTINUE
DO 460 I2 = 1, K2
IQ1 = IABS(I2 - 2) + 1
DELTA0(I2) = RHO(IQ1)
IF (I2 .NE. 2) DERIV0(I2, IQ1 - 1) = ONE
460 CONTINUE
C
C     LOOP ON P (THE AR ORDER)
C
DO 1000 IP = 1, K
K3MP = K - IP + 3
C
C     LOOP ON IQ (THE MA ORDER) FOR COMPUTING A LINE OF DELTA
C     AND DERIV
C
DO 900 I1 = 2, K3MP
ZDELTA = ABS(DELTA0(I1)) .LT. ETA
IF (IP .EQ. 1 .OR. ZDELTA) GOTO 600
TEMP = (DELTA1(I1) ** 2 - DELTA1(I1 - 1) * DELTA1(I1 + 1))
* / DELTA0(I1)
IF (ISWCHI .EQ. (-1)) GOTO 550
DO 500 M = 1, K
DERIV0(I1, M) = (TWO * DELTA1(I1) * DERIV1(I1, M) -
* DELTA1(I1 - 1) * DERIV1(I1 + 1, M) -
* DELTA1(I1 + 1) * DERIV1(I1 - 1, M) -
* TEMP * DERIV0(I1, M)) / DELTA0(I1)
500 CONTINUE

```

```

550 DELTA0(I1) = TEMP
C
C      EVALUATING THE ASYMPTOTIC VARIANCE OF AN ELEMENT OF DELTA
C      AND THE COVARIANCES WITH THREE OTHER DELTA ELEMENTS
C
600 IQ = I1 - 2
   IF (IQ .LT. 1) GOTO 900
   DELTA(IP, IQ) = DELTA0(I1)
   IF (ISWCHI .EQ. (-1)) GOTO 900
   TSTAT(IP, IQ) = ZERO
   IF (ISWSGN .EQ. 1) TSIGN(IP, IQ) = ONE
   IF (ZDELTA) GOTO 700
   VAR = ZERO
   IF (ISWCHI .EQ. 0) GOTO 610
   WKSP(2, IQ) = ZERO
   A31 = ZERO
   A32 = ZERO
610 INDM = 0
   KMAX = IP + IQ - 1
   DO 640 M = 1, KMAX
   FACTOR = ONE
   IND = INDM
   DO 630 L = M, KMAX
   IND = IND + 1
   VAR = VAR + FACTOR * DERIV0(I1, M) * COVAR(IND) * DERIV0(I1, L)
   FACTOR = TWO
   IF (ISWCHI .EQ. 0) GOTO 630
   TEMPM = COVAR(IND) * DERIV0(I1, M)
   WKSP(2, IQ) = WKSP(2, IQ) + TEMPM * DERIV0(I1 - 1, L)
   IF (IP .EQ. 1) GOTO 620
   A31 = A31 + TEMPM * DERIV1(I1, L)
   A32 = A32 + TEMPM * DERIV1(I1 + 1, L)
620 IF (L .EQ. M) GOTO 630
   TEMPL = COVAR(IND) * DERIV0(I1, L)
   WKSP(2, IQ) = WKSP(2, IQ) + TEMPL * DERIV0(I1 - 1, M)
   IF (IP .EQ. 1) GOTO 630
   A31 = A31 + TEMPL * DERIV1(I1, M)
   A32 = A32 + TEMPL * DERIV1(I1 + 1, M)
630 CONTINUE
   INDM = INDM + K - M + 1
640 CONTINUE
   IF (VAR .GT. ETA) GOTO 650
   IFAIL1 = 1
   GOTO 700
C
C      COMPUTING T-STATISTIC
C
650 TSTAT(IP, IQ) = DELTA0(I1) / SQRT(VAR)
C
C      COMPUTING T-PROBABILITY OF SIGNIFICANCE
C
   IF (ISWSGN .EQ. 0) GOTO 700
   CALL NORMAL(TSTAT(IP, IQ), 1, P, Q, Z, IFLT)
   PQ = P(1)
   IF (Q(1) .LT. PQ) PQ = Q(1)
   TSIGN(IP, IQ) = TWO * PQ
C
C      COMPUTING CHI2-STATISTIC
C
700 IF (ISWCHI .EQ. 0) GOTO 900
   CHSTAT(IP - 1, IQ) = ZERO

```



```
D11 = A11
IF (D11 .LT. ETA) GOTO 30
W1 = V1
S21 = A21 / D11
D22 = A22 - D11 * S21 ** 2
IF (D22 .LT. ETA) GOTO 20
T21 = -S21
W2 = T21 * V1 + V2
S31 = A31 / D11
S32 = (A32 - D11 * S21 * S31) / D22
D33 = A33 - D11 * S31 ** 2 - D22 * S32 ** 2
IF (D33 .LT. ABS(TOLER * A33)) GOTO 10
IF (D33 .LT. ETA) GOTO 10
T31 = -S31 - S32 * T21
T32 = -S32
W3 = T31 * V1 + T32 * V2 + V3
QFBGM = QFBGM + W3 ** 2 / D33
NDF = NDF + 1
10 IF (D22 .LT. ABS(TOLER * A22)) GOTO 20
QFBGM = QFBGM + W2 ** 2 / D22
NDF = NDF + 1
20 IF (D11 .LT. ABS(TOLER * A11)) GOTO 30
QFBGM = QFBGM + W1 ** 2 / D11
NDF = NDF + 1
30 CONTINUE
RETURN
END
```

```
SUBROUTINE CORNER(TABLE, MAXP, LAG, LAG1, CRIT, MINP, MDLP, MDLQ,
* NB, IFAULT)
```

```
C
C     ALGORITHM AS237.4  APPL. STATIST. (1988) VOL. 37, NO. 2
C
C     DETECTS ALL THE CORNERS IN TABLE
C     (THE ABSOLUTE VALUE OF THE ELEMENTS OF TABLE COMPARED TO CRIT)
C
C     DIMENSION TABLE(MAXP, LAG)
C     REAL ONE, CRIT
C     INTEGER MINP(LAG1), MDLP(LAG1), MDLQ(LAG1)
C
C     DATA ONE /1.0/
C
C     IFAULT = 0
C     IF (MAXP .LT. LAG .OR. LAG .LE. 0) IFAULT = 12
C     IF (LAG1 .NE. LAG + 1) IFAULT = 13
C     NB = 0
C     IF (IFAULT .NE. 0) RETURN
C
C     IQ = 0
C     DO 300 M = 1, LAG
C     IP = LAG + 1 - M
C     J = IQ + 1
C     DO 100 L = J, M
C     IQ = M + J - L
C
C     IF TABLE DOES NOT CONTAIN PROBABILITIES OF SIGNIFICANCE
C     BUT T OR CHI2 STATISTICS, REPLACE .LT. BY .GT. IN :
C
C     IF (ABS(TABLE(IP, IQ)) .LT. CRIT) GOTO 300
100 CONTINUE
200 IQ = J - 1
```

```
300 MINP(IP) = IQ
    MINP(LAG1) = 0
    IF (MINP(1) .EQ. 0) GOTO 500
    INDP = LAG1
    DO 400 M = 1, LAG1
    IF (MINP(M) .EQ. INDP) GOTO 400
    NB = NB + 1
    MDLP(NB) = M - 1
    MDLQ(NB) = MINP(M)
    INDP = MINP(M)
400 CONTINUE
500 RETURN
    END
```

```
PROCEDURE karstor(n:nonnegint;VAR x,y,d:realarray;VAR alpha,beta,sad:real;  
VAR ifault:nonnegint);
```

```
{Algorithm AS 238 Appl. Statist. (1988) Vol.37, No.3}
```

```
{Pascal translation of the original bubblesort variant of algorithm AS74  
for the L1 norm fitting of a straight line with real storage of integers  
Applied Statistics (1974),Vol 23,No 2}
```

```
CONST big=1000000;  
prec=0.000001;  
VAR a,b,i,j,it,p,q:nonnegint;  
sum,xa,ya,xi,yi:real;  
stop:boolean;  
t:ARRAY[nonnegint] of real; {pairwise slopes}
```

```
BEGIN  
i:=1;xa:=x[1];  
stop:=true;  
WHILE (i<n) AND stop DO  
  BEGIN  
    i:=i+1;stop:=abs(x[i]-xa)<prec  
  END;  
IF stop THEN ifault:=1  
ELSE  
  BEGIN  
    a:=1;b:=0;  
    it:=0;ifault:=2;  
    REPEAT  
      it:=it+1;  
  
      {calculate slopes}  
      sum:=0.0;  
      FOR i:=1 TO n DO  
        BEGIN  
          xa:=x[a];ya:=y[a];  
          xi:=x[i]-xa;yi:=y[i]-ya;  
          d[i]:=i;  
          IF abs(xi)<prec THEN t[i]:=big  
          ELSE t[i]:=yi/xi;  
          sum:=sum+abs(xi)  
        END;  
      sum:=0.5*sum;  
  
      {order slopes}  
      FOR j:=n-1 DOWNTO 1 DO  
        FOR i:=1 TO j DO  
          BEGIN  
            p:=trunc(d[i]+0.5);q:=trunc(d[i+1]+0.5);  
            IF t[p]>t[q] THEN  
              BEGIN  
                d[i]:=q;d[i+1]:=p  
              END  
          END;  
        END;  
  
      {select best line}  
      i:=0;xi:=0.0;  
      REPEAT  
        i:=i+1;p:=trunc(d[i]+0.5);  
        xi:=xi+abs(x[p]-xa);  
        IF xi>=sum THEN i:=n
```

```
UNTIL i=n;

IF p=b THEN
  BEGIN
    ifault:=0;it:=n
  END
ELSE
  BEGIN
    b:=a;a:=p
  END
UNTIL it=n;

{L1 estimates,norm and residuals}
beta:=t[p];alpha:=y[a]-beta*x[a];
sum:=0.0;
FOR i:= 1 TO n DO
  BEGIN
    yi:=y[i]-alpha-beta*x[i];d[i]:=yi;
    sum:=sum+abs(yi)
  END;
sad:=sum
END;
END;{of karstor}
```

```
PROCEDURE karst(n:nonnegint;VAR x,y,e:realarray;VAR alpha,beta,sad:real;
VAR ifault:nonnegint);
```

{Algorithm AS 238 Appl. Statist. (1988) Vol.37, No.3}

{partial insertionsort variant of algorithm AS74  
for the L1 norm fitting of a straight line with a boolean trap  
Applied Statistics (1974),Vol 23,No 2}

```
CONST big=10000000;
prec=0.000001;
VAR a,c,i,j,k:nonnegint;
hold,sum,sum2,xa,ya:real;
jump,stop:boolean;
d:ARRAY[nonnegint] of nonnegint; {permuted indices}
t:ARRAY[nonnegint] of real; {pairwise slopes}
old:ARRAY[nonnegint] of boolean; {previous values of a}
```

```
BEGIN
i:=1;xa:=x[1];
stop:=true;
WHILE (i<n) AND stop DO
  BEGIN
    i:=i+1;stop:=abs(x[i]-xa)<prec
  END;
IF stop THEN ifault:=1
ELSE
  BEGIN
    a:=1;stop:=false;
    ifault:=0;
    FOR i:=2 TO n DO old[i]:=false;

  REPEAT
```

```
    {calculate slopes}
    xa:=x[a];ya:=y[a];
```

```

old[a]:=true;sum:=0.0;
FOR i:=1 TO n DO
  BEGIN
  hold:=x[i]-xa;
  IF abs(hold)<prec
  THEN t[i]:=big
  ELSE t[i:=(y[i]-ya)/hold;
  sum:=sum+abs(hold)
  END;
sum2:=0.5*sum;

{locate weighted median}
k:=1;d[1]:=1;
sum:=abs(x[1]-xa);
FOR i:=2 TO n DO
  BEGIN k:=k+1;j:=k;
  sum:=sum+abs(x[i]-xa);hold:=t[i];
  REPEAT
    j:=j-1;c:=d[j];
    IF hold<t[c] THEN d[j+1]:=c
    ELSE
      BEGIN
        d[j+1]:=i;j:=0
      END
  UNTIL j<2;
  IF j=1 THEN d[1]:=i;

  jump:=false;
  REPEAT
    IF sum>sum2 THEN
      BEGIN
        hold:=sum-abs(x[d[k]]-xa);
        IF hold>sum2 THEN
          BEGIN
            sum:=hold;k:=k-1
          END
        ELSE jump:=true
        END
    ELSE jump:=true

  UNTIL jump
  END;

  c:=d[k];
  IF old[c] THEN stop:=true ELSE a:=c
UNTIL stop;

{L1 estimates,norm and residuals}
beta:=t[c];alpha:=y[a]-beta*x[a];
sum:=0.0;
FOR i:= 1 TO n DO
  BEGIN
  hold:=y[i]-alpha-beta*x[i];e[i]:=hold;
  sum:=sum+abs(hold)
  END;
sad:=sum
END
END;{of karst}

PROCEDURE simbarrob(n:nonnegint;VAR x,y,d:realarray;VAR alpha,beta,sad:real;

```



```
VAR ifault:nonnegint);

{Algorithm AS 238 Appl. Statist. (1988) Vol.37, No.3}

{Pascal translation of algorithm AS132
 for the L1 norm fitting of a straight line
 Applied Statistics (1978),Vol 27,No 3}

LABEL 160;
CONST big=10000000;
      acu=0.000001;
VAR a1,a2,aaa,aaaa,ahalf,aone,bbb,bbbb,ddd,det,hold,ratio,sum,t,test,
    tot1,tot2,y1,y2:real;
    i,j,ibas1,ibas2,iin,iout,isave,iter:nonnegint;
    rho,zzz:-2..2;
    flag,more,stop:boolean;
    inext:ARRAY[nonnegint] of posnegint;

FUNCTION isign(i:posnegint;k:posnegint):posnegint;
{Pascal implementation of Fortran isign function}
BEGIN
IF k>=0 THEN isign:=i ELSE isign:=-i
END;{of isign}

BEGIN

{determine initial basis}
a1:=x[1];y1:=y[1];
i:=1;stop:=true;
WHILE (i<n) AND stop DO
  BEGIN
    i:=i+1;stop:=abs(a1-x[i])<acu
  END;
IF stop THEN ifault:=1
ELSE
  BEGIN
    ifault:=0;iter:=0;
    ahalf:=0.5+acu;aone:=ahalf+ahalf;
    a2:=x[i];y2:=y[i];
    ibas1:=1;ibas2:=i;
    det:=1.0/(a2-a1);

    {initial values of a,b,d}
    aaaa:=(a2*y1-a1*y2)*det;bbbb:=(y2-y1)*det;
    FOR i:=2 TO n DO
      IF y[i]>=(aaaa+bbbb*x[i]) THEN d[i]:=1.0 ELSE d[i]:=-1.0;
      d[ibas1]:= 0.0;d[ibas2]:=-1.0;
      tot1:=1.0;tot2:=x[ibas2];
      FOR i:=2 TO n DO
        BEGIN
          tot1:=tot1+d[i];tot2:=tot2+d[i]*x[i];
        END;
      t:=(a2*tot1-tot2)*det;flag:=abs(t)>aone;

    {main iterative loop begins}
    REPEAT
      flag:= NOT flag;
    IF flag THEN
      BEGIN
        t:=(tot2-a1*tot1)*det;
        IF abs(t) < aone THEN GOTO 160;
```

```
    iout:=ibas2;x[iout]:=a1;
    aaa:=a1;bbb:=a2;
    END
ELSE
    BEGIN
    IF iter=0 THEN det:=-det
    ELSE
        BEGIN
        t:=(tot2-a2*tot1)*det;
        IF abs(t) < aone THEN GOTO 160;
        END;
        aaa:=a2;bbb:=a1;
        iout:=ibas1;
        END;{not flag}
    IF t>0.0 THEN rho:=1
    ELSE
        BEGIN
        rho:=-1;t:=-t;
        det:=-det
        END;
    t:=0.5*t;

    {perform partial sort of ratios}
    ratio:=big;sum:=ahalf;
    inext[ibas1]:=ibas2;
    FOR i:=1 TO n DO
    BEGIN
        ddd:=(x[i]-aaa)*det;
        IF ddd*d[i]>acu THEN
            BEGIN
                test:=(y[i]-(aaaa+bbbb*x[i]))/ddd;
                IF test<ratio THEN
                    BEGIN
                        j:=ibas1;sum:=sum+abs(ddd);
                        more:=true;stop:=false;
                        REPEAT
                            isave:=abs(inext[j]);
                            IF test >= d[isave] THEN
                                BEGIN
                                    more:=false;stop:=true
                                END
                            ELSE
                                BEGIN
                                    IF sum<t THEN stop:=true
                                ELSE
                                    BEGIN
                                        hold:=sum-abs((x[isave]-aaa)*det);
                                        IF hold<t THEN stop:=true
                                    ELSE
                                        BEGIN
                                            d[isave]:=isign(1,inext[j]);sum:=hold;
                                            inext[j]:=inext[isave]
                                        END{hold>=t}
                                    END{sum>=t}
                                END;{test<d[isave]}
                            UNTIL stop;
                        IF more THEN
                            REPEAT
                                j:=isave;isave:=abs(inext[j]);
                                UNTIL test>=d[isave];
```

```

        inext[i]:=inext[j];
        IF d[i]>=0.0 THEN inext[j]:=i ELSE inext[j]:=-i;
        d[i]:=test;
        IF sum>=t THEN
            BEGIN
                iin:=abs(inext[ibas1]);ratio:=d[iin]
            END
        END;{test<ratio}
    END;{ddd*d[i]>acu}
END;{i loop}

{update basis indicaTOrs}
iin:=abs(inext[ibas1]);j:=iin;
stop:=false;
REPEAT
    isave:=abs(inext[j]);
    IF isave=ibas2 THEN stop:=true
    ELSE
        BEGIN
            zzz:=isign(1,inext[j]);d[isave]:=-zzz;
            zzz:=zzz+zzz;j:=isave;
            tot1:=tot1-zzz;tot2:=tot2-zzz*x[isave]
        END;
    UNTIL stop;

zzz:=isign(1,inext[ibas1]);d[iout]:=-rho;
tot1:=tot1-rho-zzz;tot2:=tot2-rho*bbb-zzz*x[iin];
iter:=iter+1;
IF flag THEN
    BEGIN
        x[ibas2]:=a2;ibas2:=iin;
        a2:=x[iin];y2:=y[iin];
        det:=1.0/(a1-a2);d[ibas2]:=-1.0;
        aaaa:=(a1*y2-a2*y1)*det;bbbb:=(y1-y2)*det
    END
ELSE
    BEGIN
        ibas1:=iin;ibas1:=iin;
        a1:=x[iin];y1:=y[iin];
        det:=1.0/(a2-a1);d[ibas1]:=0.0;
        aaaa:=(a2*y1-a1*y2)*det;bbbb:=(y2-y1)*det
    END;
UNTIL false;

{calculate estimates,deviations,sad}
160:sum:=0.0;
FOR i:=1 TO n DO
    BEGIN
        ddd:=y[i]-(aaaa+bbbb*x[i]);d[i]:=ddd;
        sum:=sum+abs(ddd)
    END;
alpha:=aaaa;beta :=bbbb;
sad:=sum;

END
END;{of simbarrob}

```

```

      DOUBLE PRECISION FUNCTION GAMMAD(X, P, IFAULT)
C
C      ALGORITHM AS239  APPL. STATIST. (1988) VOL. 37, NO. 3
C
C      Computation of the Incomplete Gamma Integral
C
C      Auxiliary functions required: ALOGAM = logarithm of the gamma
C      function, and ALNORM = algorithm AS66
C
      INTEGER IFAULT
      DOUBLE PRECISION PN1, PN2, PN3, PN4, PN5, PN6, X, TOL, OFLO,
*          XBIG, ARG, C, RN, P, A, B, ONE, ZERO, ALOGAM,
*          AN, TWO, ELIMIT, PLIMIT, ALNORM, THREE, NINE
      PARAMETER (ZERO = 0.D0, ONE = 1.D0, TWO = 2.D0, OFLO = 1.D+37,
*          THREE = 3.D0, NINE = 9.D0, TOL = 1.D-14, XBIG = 1.D+8,
*          PLIMIT = 1000.D0, ELIMIT = -88.D0)
      EXTERNAL ALOGAM, ALNORM
C
      GAMMAD = ZERO
C
C      Check that we have valid values for X and P
C
      IF (P .LE. ZERO .OR. X .LT. ZERO) THEN
          IFAULT = 1
          RETURN
      END IF
      IFAULT = 0
      IF (X .EQ. ZERO) RETURN
C
C      Use a normal approximation if P > PLIMIT
C
      IF (P .GT. PLIMIT) THEN
          PN1 = THREE * SQRT(P) * ((X / P) ** (ONE / THREE) + ONE /
*          (NINE * P) - ONE)
          GAMMAD = ALNORM(PN1, .FALSE.)
          RETURN
      END IF
C
C      If X is extremely large compared to P then set GAMMAD = 1
C
      IF (X .GT. XBIG) THEN
          GAMMAD = ONE
          RETURN
      END IF
C
      IF (X .LE. ONE .OR. X .LT. P) THEN
C
C      Use Pearson's series expansion.
C      (Note that P is not large enough to force overflow in ALOGAM).
C      No need to test IFAULT on exit since P > 0.
C
          ARG = P * LOG(X) - X - ALOGAM(P + ONE, IFAULT)
          C = ONE
          GAMMAD = ONE
          A = P
40          A = A + ONE
          C = C * X / A
          GAMMAD = GAMMAD + C
          IF (C .GT. TOL) GO TO 40
          ARG = ARG + LOG(GAMMAD)
          GAMMAD = ZERO

```

```
        IF (ARG .GE. ELIMIT) GAMMAD = EXP(ARG)
C
    ELSE
C
C    Use a continued fraction expansion
C
        ARG = P * LOG(X) - X - ALOGAM(P, IFAULT)
        A = ONE - P
        B = A + X + ONE
        C = ZERO
        PN1 = ONE
        PN2 = X
        PN3 = X + ONE
        PN4 = X * B
        GAMMAD = PN3 / PN4
60      A = A + ONE
        B = B + TWO
        C = C + ONE
        AN = A * C
        PN5 = B * PN3 - AN * PN1
        PN6 = B * PN4 - AN * PN2
        IF (ABS(PN6) .GT. ZERO) THEN
            RN = PN5 / PN6
            IF (ABS(GAMMAD - RN) .LE. MIN(TOL, TOL * RN)) GO TO 80
            GAMMAD = RN
        END IF
C
        PN1 = PN3
        PN2 = PN4
        PN3 = PN5
        PN4 = PN6
        IF (ABS(PN5) .GE. OFLO) THEN
C
C    Re-scale terms in continued fraction if terms are large
C
            PN1 = PN1 / OFLO
            PN2 = PN2 / OFLO
            PN3 = PN3 / OFLO
            PN4 = PN4 / OFLO
        END IF
        GO TO 60
80      ARG = ARG + LOG(GAMMAD)
        GAMMAD = ONE
        IF (ARG .GE. ELIMIT) GAMMAD = ONE - EXP(ARG)
    END IF
C
    RETURN
    END
```

```

SUBROUTINE SSPINV(X, XM, XSSPI, E, WT, SUMWT, NP, NPP, IFAULT)
C
C   ALGORITHM AS240  APPL. STATIST. (1988) VOL. 37, NO. 3
C
C   THIS SUBROUTINE UPDATES THE MEAN VECTOR XM, AND THE INVERSE
C   MATRIX OF CORRECTED SUMS OF SQUARES AND PRODUCTS XSSPI.
C   A DATA VECTOR X WITH WEIGHT WT .GT. 0 IS INCLUDED,
C   OR EXCLUDED WHEN WT .LT. 0.
C   IFAULT = 2, IF UPDATED SUMWT .LE. 0,
C           = 1, IF MANIPULATED MATRIX XSSPI DOESN'T EXIST,
C           = 0, OTHERWISE.
C
REAL X(NP), XM(NP), E(NP), XSSPI(NPP), WT, SUMWT, ZERO, ONE, EPS,
*  A, B, C, ZABS
C
DATA ZERO, ONE, EPS /0.0, 1.0, 1.0E-5/
C
ZABS(A) = ABS(A)
C
IFAUULT = 2
SUMWT = SUMWT + WT
IF (SUMWT .LE. ZERO) RETURN
IFAUULT = 1
C
C   UPDATE MEANS AND INVERSE MATRIX OF SUMS OF SQUARES AND
C   PRODUCTS.
C
B = WT / SUMWT
C = WT - B * WT
DO 10 I = 1, NP
X(I) = X(I) - XM(I)
10 XM(I) = XM(I) + B * X(I)
C
DO 30 I = 1, NP - 1
E(I) = ZERO
K = I * (I - 1) / 2
DO 20 J = 1, I
K = K + 1
20 E(I) = E(I) + XSSPI(K) * X(J)
DO 25 J = I + 1, NP
K = K + J - 1
25 E(I) = E(I) + XSSPI(K) * X(J)
30 CONTINUE
E(NP) = ZERO
K = NP * (NP - 1) / 2
DO 35 J = 1, NP
K = K + 1
35 E(NP) = E(NP) + XSSPI(K) * X(J)
C
A = ZERO
DO 40 I = 1, NP
40 A = A + X(I) * E(I)
A = A + ONE / C
IF (ZABS(A) .LE. EPS) RETURN
IFAUULT = 0
C
K = 0
DO 70 I = 1, NP
DO 70 J = 1, I
K = K + 1
XSSPI(K) = XSSPI(K) - E(I) * E(J) / A

```

70 CONTINUE  
RETURN  
END

```

REAL FUNCTION PPND7 (P, IFAULT)
C
C   ALGORITHM AS241  APPL. STATIST. (1988) VOL. 37, NO. 3, 477-
C   484.
C
C   Produces the normal deviate Z corresponding to a given lower
C   tail area of P; Z is accurate to about 1 part in 10**7.
C
C   The hash sums below are the sums of the mantissas of the
C   coefficients.  They are included for use in checking
C   transcription.
C
REAL ZERO, ONE, HALF, SPLIT1, SPLIT2, CONST1, CONST2, A0, A1,
*   A2, A3, B1, B2, B3, C0, C1, C2, C3, D1, D2, E0, E1, E2,
*   E3, F1, F2, P, Q, R
PARAMETER (ZERO = 0.0, ONE = 1.0, HALF = 0.5,
*   SPLIT1 = 0.425, SPLIT2 = 5.0,
*   CONST1 = 0.180625, CONST2 = 1.6)
C
C   Coefficients for P close to 0.5
C
PARAMETER (A0 = 3.38713 27179E+00, A1 = 5.04342 71938E+01,
*   A2 = 1.59291 13202E+02, A3 = 5.91093 74720E+01,
*   B1 = 1.78951 69469E+01, B2 = 7.87577 57664E+01,
*   B3 = 6.71875 63600E+01)
C   HASH SUM AB    32.31845 77772
C
C   Coefficients for P not close to 0, 0.5 or 1.
C
PARAMETER (C0 = 1.42343 72777E+00, C1 = 2.75681 53900E+00,
*   C2 = 1.30672 84816E+00, C3 = 1.70238 21103E-01,
*   D1 = 7.37001 64250E-01, D2 = 1.20211 32975E-01)
C   HASH SUM CD    15.76149 29821
C
C   Coefficients for P near 0 or 1.
C
PARAMETER (E0 = 6.65790 51150E+00, E1 = 3.08122 63860E+00,
*   E2 = 4.28682 94337E-01, E3 = 1.73372 03997E-02,
*   F1 = 2.41978 94225E-01, F2 = 1.22582 02635E-02)
C   HASH SUM EF    19.40529 10204
C
C
IFAULT = 0
Q = P - HALF
IF (ABS(Q) .LE. SPLIT1) THEN
  R = CONST1 - Q * Q
  PPND7 = Q * (((A3 * R + A2) * R + A1) * R + A0) /
*   (((B3 * R + B2) * R + B1) * R + ONE)
  RETURN
ELSE
  IF (Q .LT. ZERO) THEN
    R = P
  ELSE
    R = ONE - P
  END IF
  IF (R .LE. ZERO) THEN
    IFAULT = 1
    PPND7 = ZERO
    RETURN
  END IF
  R = SQRT(-LOG(R))
  IF (R .LE. SPLIT2) THEN

```



```

      R = R - CONST2
      PPND7 = (((C3 * R + C2) * R + C1) * R + C0) /
*           ((D2 * R + D1) * R + ONE)
      ELSE
      R = R - SPLIT2
      PPND7 = (((E3 * R + E2) * R + E1) * R + E0) /
*           ((F2 * R + F1) * R + ONE)
      END IF
      IF (Q .LT. ZERO) PPND7 = - PPND7
      RETURN
    END IF
  END

```

```

C
C
C   DOUBLE PRECISION FUNCTION PPND16 (P, IFAULT)
C
C   ALGORITHM AS241  APPL. STATIST. (1988) VOL. 37, NO. 3
C
C   Produces the normal deviate Z corresponding to a given lower
C   tail area of P; Z is accurate to about 1 part in 10**16.
C
C   The hash sums below are the sums of the mantissas of the
C   coefficients.  They are included for use in checking
C   transcription.
C

```

```

    DOUBLE PRECISION ZERO, ONE, HALF, SPLIT1, SPLIT2, CONST1,
*           CONST2, A0, A1, A2, A3, A4, A5, A6, A7, B1, B2, B3,
*           B4, B5, B6, B7,
*           C0, C1, C2, C3, C4, C5, C6, C7, D1, D2, D3, D4, D5,
*           D6, D7, E0, E1, E2, E3, E4, E5, E6, E7, F1, F2, F3,
*           F4, F5, F6, F7, P, Q, R
    PARAMETER (ZERO = 0.D0, ONE = 1.D0, HALF = 0.5D0,
*           SPLIT1 = 0.425D0, SPLIT2 = 5.D0,
*           CONST1 = 0.180625D0, CONST2 = 1.6D0)

```

```

C
C   Coefficients for P close to 0.5
C

```

```

    PARAMETER (A0 = 3.38713 28727 96366 6080D0,
*           A1 = 1.33141 66789 17843 7745D+2,
*           A2 = 1.97159 09503 06551 4427D+3,
*           A3 = 1.37316 93765 50946 1125D+4,
*           A4 = 4.59219 53931 54987 1457D+4,
*           A5 = 6.72657 70927 00870 0853D+4,
*           A6 = 3.34305 75583 58812 8105D+4,
*           A7 = 2.50908 09287 30122 6727D+3,
*           B1 = 4.23133 30701 60091 1252D+1,
*           B2 = 6.87187 00749 20579 0830D+2,
*           B3 = 5.39419 60214 24751 1077D+3,
*           B4 = 2.12137 94301 58659 5867D+4,
*           B5 = 3.93078 95800 09271 0610D+4,
*           B6 = 2.87290 85735 72194 2674D+4,
*           B7 = 5.22649 52788 52854 5610D+3)

```

```

C   HASH SUM AB    55.88319 28806 14901 4439
C

```

```

C   Coefficients for P not close to 0, 0.5 or 1.
C

```

```

    PARAMETER (C0 = 1.42343 71107 49683 57734D0,
*           C1 = 4.63033 78461 56545 29590D0,
*           C2 = 5.76949 72214 60691 40550D0,
*           C3 = 3.64784 83247 63204 60504D0,
*           C4 = 1.27045 82524 52368 38258D0,

```

```

*          C5 = 2.41780 72517 74506 11770D-1,
*          C6 = 2.27238 44989 26918 45833D-2,
*          C7 = 7.74545 01427 83414 07640D-4,
*          D1 = 2.05319 16266 37758 82187D0,
*          D2 = 1.67638 48301 83803 84940D0,
*          D3 = 6.89767 33498 51000 04550D-1,
*          D4 = 1.48103 97642 74800 74590D-1,
*          D5 = 1.51986 66563 61645 71966D-2,
*          D6 = 5.47593 80849 95344 94600D-4,
*          D7 = 1.05075 00716 44416 84324D-9)
C          HASH SUM CD      49.33206 50330 16102 89036
C
C          Coefficients for P near 0 or 1.
C
C          PARAMETER (E0 = 6.65790 46435 01103 77720D0,
*          E1 = 5.46378 49111 64114 36990D0,
*          E2 = 1.78482 65399 17291 33580D0,
*          E3 = 2.96560 57182 85048 91230D-1,
*          E4 = 2.65321 89526 57612 30930D-2,
*          E5 = 1.24266 09473 88078 43860D-3,
*          E6 = 2.71155 55687 43487 57815D-5,
*          E7 = 2.01033 43992 92288 13265D-7,
*          F1 = 5.99832 20655 58879 37690D-1,
*          F2 = 1.36929 88092 27358 05310D-1,
*          F3 = 1.48753 61290 85061 48525D-2,
*          F4 = 7.86869 13114 56132 59100D-4,
*          F5 = 1.84631 83175 10054 68180D-5,
*          F6 = 1.42151 17583 16445 88870D-7,
*          F7 = 2.04426 31033 89939 78564D-15)
C          HASH SUM EF      47.52583 31754 92896 71629
C
C          IFAULT = 0
C          Q = P - HALF
C          IF (ABS(Q) .LE. SPLIT1) THEN
C              R = CONST1 - Q * Q
C              PPND16 = Q * (((((((A7 * R + A6) * R + A5) * R + A4) * R + A3)
*                  * R + A2) * R + A1) * R + A0) /
C                  (((((((B7 * R + B6) * R + B5) * R + B4) * R + B3)
*                  * R + B2) * R + B1) * R + ONE)
C              RETURN
C          ELSE
C              IF (Q .LT. ZERO) THEN
C                  R = P
C              ELSE
C                  R = ONE - P
C              END IF
C              IF (R .LE. ZERO) THEN
C                  IFAULT = 1
C                  PPND16 = ZERO
C                  RETURN
C              END IF
C              R = SQRT(-LOG(R))
C              IF (R .LE. SPLIT2) THEN
C                  R = R - CONST2
C                  PPND16 = (((((((C7 * R + C6) * R + C5) * R + C4) * R + C3)
*                  * R + C2) * R + C1) * R + C0) /
C                  (((((((D7 * R + D6) * R + D5) * R + D4) * R + D3)
*                  * R + D2) * R + D1) * R + ONE)
C              ELSE
C                  R = R - SPLIT2
C                  PPND16 = (((((((E7 * R + E6) * R + E5) * R + E4) * R + E3)

```

```
*          * R + E2) * R + E1) * R + E0) /
*          ((((((F7 * R + F6) * R + F5) * R + F4) * R + F3)
*          * R + F2) * R + F1) * R + ONE)
      END IF
      IF (Q .LT. ZERO) PPND16 = - PPND16
      RETURN
    END IF
  END
```

```

SUBROUTINE MARMA(K, N, P, Q, W, IK, PHI, THETA, MEAN, MEANS,
*          QQ, XTOL, RLOGL, V, WORK, LWORK, IWORK, LIWORK,
*          IFAULT)
C
C   ALGORITHM AS 242.1  APPL. STATIST. (1989), VOL.38, NO. 1
C
C   Auxiliary routines required: DECOMP & SOLVE from CACM algorithm 423
C
C   INTEGER          P, Q, R, K, N, LWORK, IFAULT, KR, KMAT, KC, LW1,
*                   LW2, LW3, LW4, LW5, LW6, LW7, LW8, LW9, LW10,
*                   LW11, LW12, LW13, IK, I, J, LIWORK, IWORK(LIWORK)
C   LOGICAL          MEAN
C   REAL             MEANS(K), PHI(IK,P*K+1), QQ(IK,K), REAL,
*                   V(IK,N), W(IK,N), WORK(LWORK), THETA(IK,Q*K+1),
*                   TWO, LOG2PI, CONST, RLOGL, XTOL, TSIG
C   PARAMETER        (TWO = 2.0, LOG2PI = 1.8378771)
C   INTRINSIC        MAX, REAL
C   EXTERNAL         VARMA, CHOL
C
C   test for errors in the input data
C
C   IFAULT = 0
C   IF(K .LT. 1) IFAULT = 1
C   IF(IFAULT .EQ. 1) RETURN
C   IF(N .LT. 1) IFAULT = 2
C   IF(IFAULT .EQ. 2) RETURN
C   IF(P .LT. 0) IFAULT = 3
C   IF(IFAULT .EQ. 3) RETURN
C   IF(Q .LT. 0) IFAULT = 4
C   IF(IFAULT .EQ. 4) RETURN
C   IF(P .EQ. 0 .AND. Q .EQ. 0) IFAULT = 5
C   IF(IFAULT .EQ. 5) RETURN
C   IF(IK .LT. K) IFAULT = 6
C   IF(IFAULT .EQ. 6) RETURN
C
C   check that workspace arrays are big enough
C
C   R = MAX(P,Q)
C   KR = K * R
C   KMAT = K * MAX(R, K * (P + 1))
C   CONST = (REAL(N * K) / TWO) * LOG2PI
C
C   KC = K * K
C   LW1 = 1
C   LW2 = K * KR + LW1
C   LW3 = K * KR + LW2
C   LW4 = K * KR + LW3
C   LW5 = KC + LW4
C   LW6 = KC + LW5
C   LW7 = KC + LW6
C   LW8 = KC + LW7
C   LW9 = KC + LW8
C   LW10 = KC + LW9
C   LW11 = KC * (P + 1) + LW10
C   LW12 = KC * (R + 1) + LW11
C   LW13 = KMAT * KMAT + LW12
C
C   I = MAX(IK * K, LW13 + KC - 1)
C   IF(LWORK .LT. I) IFAULT = 7
C   IF(IFAULT .EQ. 7) RETURN
C   IF(LIWORK .LT. KMAT) IFAULT = 8

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      IF(IFAULT .EQ. 8) RETURN
C
C   set upper triangle of QQ to lower triangle of QQ
C
      DO 30 I = 2, K
          DO 31 J = 1, I - 1
              QQ(J,I) = QQ(I,J)
31      CONTINUE
30      CONTINUE
C
C   check whether QQ is positive-definite and evaluate its determinant
C   (storing it in TSIG)
C
      CALL CHOL(QQ, IK, K, WORK, IFAULT)
      IF(IFAULT .GT. 0) THEN
          IFAULT = 9
          RETURN
      ELSE
          TSIG = WORK(1)
          DO 20 I = 2, K
              TSIG = TSIG * WORK((I - 1) * IK + I)
20      CONTINUE
          TSIG = TSIG * TSIG
      ENDIF
C
C   now call VARMA to calculate the log likelihood function
C
      CALL VARMA(K, N, P, Q, R, W, IK, PHI, THETA, MEAN, MEANS, QQ,
*           TSIG, CONST, V, XTOL, RLOGL, KR, KMAT, WORK(LW1),
*           WORK(LW2), WORK(LW3), WORK(LW4), WORK(LW5),
*           WORK(LW6), WORK(LW7), WORK(LW8), WORK(LW9),
*           WORK(LW10), WORK(LW11), WORK(LW12), WORK(LW13),
*           IWORK, IFAULT)
C
      END
      SUBROUTINE VARMA(K, N, P, Q, R, W, IK, PHI, THETA, MEAN, MEANS,
*           QQ, TSIG, CONST, V, XTOL, RLOGL, KR, KMAT,
*           GAMMA, TEMP, TEMPK, TEMPL, F, INV, TEMPM, A,
*           MT, B, Z, MAT, WA, IWORK, IFAULT)
C
C   ALGORITHM AS 242.2 APPL. STATIST. (1989), VOL.38, NO. 1
C
      INTEGER          IFAULT, K, KMAT, KR, N, P, Q, R, IK, I, J,
*           J7, K1, K2, L, L8, M, T, IWORK(KMAT)
      LOGICAL          MEAN, ANOTT, DELTA, PEARL
      REAL             CONST, RLOGL, TSIG, XTOL, ZERO, ONE, TWO,
*           A(K,K), B(K*K*(P+1)), F(K,K), GAMMA(K,KR),
*           INV(K,K), MAT(KMAT,KMAT), MEANS(K), MT(K,K),
*           PHI(IK,P*K+1), QQ(IK,K), TEMP(K,KR),
*           TEMPL(K,K), TEMPM(K,K), THETA(IK,Q*K+1),
*           W(IK,N), Z(K*K*(R+1)), WA(K,K), TEMPK(K,KR),
*           DETP, SIG, SM, SSQ, SUM, REAL, V(IK,N)
      PARAMETER       (ZERO = 0.0, ONE = 1.0, TWO = 2.0)
      INTRINSIC       LOG, REAL, ABS, MAX
      EXTERNAL        COVAR, CHOL, BKSB
C
C   This subroutine computes the log likelihood function of a vector
C   ARMA model
C
      ANOTT = .FALSE.
      IF(P .GT. Q) ANOTT = .TRUE.

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C
C   call COVARs to calculate the autocovariances of W(t) and the
C   cross-covariances between W(t) and E(t)
C
CALL COVARs(K, P, Q, R, IK, PHI, THETA, QQ, GAMMA, Z, KMAT,
*           MAT, B, IWORK, IFAULT)
C
IF(IFAULT .GT. 0) IFAULT = 10
IF(IFAULT .EQ. 10) RETURN
C
calculate the first k columns of P(1/0) and store as TEMPK
C
DO 140 K1 = 1, R
  DO 120 I = 1, K
    DO 100 J = 1, K
      SUM = ZERO
      DO 40 K2 = 1, K
        DO 20 M = K1, P
          SUM = SUM + PHI(I, (M - 1) * K + K2) *
*           Z((M - K1 + 1) * K * K + (K2 - 1) * K + J)
20          CONTINUE
40          CONTINUE
          DO 80 M = K1, Q
            DO 60 K2 = 1, K
              SUM = SUM - THETA(I, (M - 1) * K + K2) *
*             GAMMA(J, (M - K1) * K + K2)
60            CONTINUE
80            CONTINUE
C
          TEMPK(I, (K1 - 1) * K + J) = SUM
100          CONTINUE
120          CONTINUE
140 CONTINUE
C
initialize A(1/0), V(1), SSQ, F(1) and DETP
C
DO 160 I = 1, KR
  Z(I) = ZERO
160 CONTINUE
C
DO 200 I = 1, K
  DO 180 J = 1, K
    F(I,J) = TEMPK(I,J) + QQ(I,J)
180 CONTINUE
    V(I,1) = W(I,1)
    IF(MEAN) V(I,1) = V(I,1) - MEANS(I)
    B(I) = V(I,1)
200 CONTINUE
C
factorise F(1) as LL' and store L as A
C
CALL CHOL(F, K, K, A, IFAULT)
IF(IFAULT .NE. 0) THEN
  IFAULT = 11
  RETURN
ENDIF
C
calculate determinant (DETP) of F(1)
C
DETP = A(1,1)
DO 220 I = 2, K

```

```

        DETP = DETP * A(I,I)
220 CONTINUE
        DETP = DETP * DETP
C
C      set MT = F(1) inverse
C
        DO 260 I = 1, K
            DO 240 J = 1, K
                MT(I,J) = ZERO
240         CONTINUE
            MT(I,I) = ONE
260 CONTINUE
C
C      note that BKSB cannot fail
C
        CALL BKSB(A, K, K, K, .FALSE., MT, IFAULT)
C
C      set upper triangle of INVF to A'
C
        DO 300 J = 1, K
            DO 280 I = 1, J
                INVF(I,J) = A(J,I)
280         CONTINUE
300 CONTINUE
        CALL BKSB(INVF, K, K, K, .TRUE., MT, IFAULT)
C
        CALL BKSB(A, K, K, 1, .FALSE., B, IFAULT)
        SSQ = ZERO
        DO 320 I = 1, K
            SSQ = SSQ + B(I) * B(I)
320 CONTINUE
C
        DETP = LOG(DETP)
C
C      calculate L(1) and K(1)
C
        DO 360 I = 1, K
            DO 340 J = 1, KR
                MAT(I,J) = ZERO
                GAMMA(I,J) = ZERO
340         CONTINUE
360 CONTINUE
C
        DO 480 L = 1, R
            DO 460 I = 1, K
                DO 440 J = 1, K
                    SUM = ZERO
                    IF(L .LE. P) THEN
                        DO 380 K2 = 1, K
                            SUM = SUM + PHI(I, (L - 1) * K + K2) *
*                               TEMPK(K2,J)
380                 CONTINUE
                    ENDIF
                    IF(L .LT. R) SUM = SUM + TEMPK(I, L * K + J)
                    DO 420 K2 = 1, K
                        SM = ZERO
                        IF(L .LE. P) SM = PHI(I, (L - 1) * K + K2)
                        IF(L .LE. Q) SM = SM - THETA(I, (L - 1) * K + K2)
                        SUM = SUM + SM * QQ(K2,J)
420                 CONTINUE
                    MAT(I, (L - 1) * K + J) = SUM

```

```
C
  440      CONTINUE
  460      CONTINUE
  480      CONTINUE
C
      IF(ANOTT) THEN
C
          DO 580 L = 1, R
              DO 560 I = 1, K
                  DO 540 J = 1, K
                      SUM = ZERO
                      IF(L .LE. Q) THEN
                          DO 500 K2 = 1, K
                              SUM = SUM + THETA(I, (L - 1) * K + K2) *
*
                              TEMPK(K2,J)
  500                      CONTINUE
                          ENDIF
                          IF(L .LT. R) SUM = SUM + TEMPK(I, L * K + J)
                          GAMMA(I, (L - 1) * K + J) = SUM
  540                      CONTINUE
  560                      CONTINUE
  580                      CONTINUE
C
          ELSE
C
              DO 640 L = 1, R
                  DO 620 I = 1, K
                      DO 600 J = 1, K
                          GAMMA(I, (L - 1) * K + J) = MAT(I, (L - 1) * K + J)
  600                      CONTINUE
  620                      CONTINUE
  640                      CONTINUE
C
          ENDIF
C
      start the recursions
C
      DELTA = .FALSE.
      PEARL = .FALSE.
      J7 = N
C
      DO 2240 T = 2, N
C
          IF(ANOTT .AND. T .GT. P - Q) PEARL = .TRUE.
C
          calculate TEMPK
C
          IF(.NOT.DELTA) THEN
C
              find L' (inverse) and store as INVF
C
              DO 680 J = 1, K
                  DO 660 I = 1, K
                      TEMPK(I,J) = A(J,I)
                      INVF(I,J) = ZERO
  660                  CONTINUE
                      INVF(J,J) = ONE
  680                  CONTINUE
                  CALL BKSB(TEMPK, K, K, K, .TRUE., INVF, IFAULT)
C
              DO 760 L = 1, R
```



```

        DO 740 I = 1, K
            DO 720 J = 1, K
                SUM = ZERO
                DO 700 K2 = 1, K
                    SUM = SUM + GAMMA(I, (L - 1) * K + K2) *
*
                    INVF(K2,J)
700                CONTINUE
                    TEMPK(I, (L - 1) * K + J) = SUM
720                CONTINUE
740                CONTINUE
760                CONTINUE
C
C            calculate TEMP
C
        ENDIF
        DO 800 L = 1, KR
            TEMP(1,L) = ZERO
800        CONTINUE
C
        IF(ANOTT) GOTO 900
C
C        TEMP = T * A(t-1/t-2)
C
        IF(T .EQ. 2) GOTO 1080
        DO 880 L = 1, R
            DO 860 I = 1, K
                SUM = ZERO
                IF(L .LE. P) THEN
                    DO 820 K2 = 1, K
                        SUM = SUM + PHI(I, (L - 1) * K + K2) * Z(K2)
820                    CONTINUE
                ENDIF
                IF(L .LT. R) SUM = SUM + Z(L * K + I)
                TEMP(1, (L - 1) * K + I) = SUM
860            CONTINUE
880        CONTINUE
        GOTO 1080
900        IF(T .GT. 2) THEN
C
C            TEMP = A * A(t-1/t-2) + R * W(t-1)
C
            DO 980 L = 1, R
                DO 960 I = 1, K
                    SUM = ZERO
                    IF(L .LE. Q) THEN
                        DO 920 K2 = 1, K
                            SUM = SUM + THETA(I, (L - 1) * K + K2) * Z(K2)
920                        CONTINUE
                    ENDIF
                    IF(L .LT. R) SUM = SUM + Z(L * K + I)
                    TEMP(1, (L - 1) * K + I) = SUM
960                CONTINUE
980            CONTINUE
C
        ENDIF
        DO 1060 L = 1, R
            DO 1040 I = 1, K
                SUM = ZERO
                DO 1020 K2 = 1, K
                    SM = ZERO
                    IF(L .LE. P) SM = PHI(I, (L - 1) * K + K2)

```

```

                IF(L .LE. Q) SM = SM - THETA(I, (L - 1) * K + K2)
                IF(MEAN) THEN
                    SUM = SUM + SM * (W(K2,T - 1) - MEANS(K2))
                ELSE
                    SUM = SUM + SM * W(K2,T - 1)
                ENDIF
1020            CONTINUE
                TEMP(1, (L - 1) * K + I) = TEMP(1, (L - 1) * K + I)
*                + SUM
1040            CONTINUE
1060            CONTINUE
C
C            A(t/t-1) = TEMP + TEMPK * V(t-1)
C
1080            DO 1160 L = 1, R
                DO 1140 L8 = 1, K
                    SUM = TEMP(1, (L - 1) * K + L8)
                    IF((.NOT.DELTA) .OR. (.NOT.ANOTT)) THEN
                        DO 1100 K2 = 1, K
                            SUM = SUM + TEMPK(L8, (L - 1) * K + K2) * B(K2)
1100                        CONTINUE
                    ENDIF
                    Z((L - 1) * K + L8) = SUM
1140                CONTINUE
1160            CONTINUE
C
                IF(DELTA) GOTO 2180
C
C            calculate TEMPL
C
                DO 1200 I = 1, K
                    DO 1180 J = 1, K
                        TEMPL(I,J) = MAT(I,J)
1180                CONTINUE
1200            CONTINUE
C
C            recalculate TEMP
C
                IF(.NOT.ANOTT) THEN
C
C                TEMP = T * L(t-1)
C
                DO 1300 L = 1, R
                    DO 1280 I = 1, K
                        DO 1260 J = 1, K
                            SUM = ZERO
                            IF(L .LE. P) THEN
                                DO 1220 K2 = 1, K
                                    SUM = SUM + PHI(I, (L - 1) * K + K2) *
*                                    MAT(K2,J)
1220                                CONTINUE
                            ENDIF
                            IF(L .LT. R) SUM = SUM + MAT(I, L * K + J)
                            TEMP(I, (L - 1) * K + J) = SUM
C
1260                        CONTINUE
1280                    CONTINUE
1300                CONTINUE
C
                ELSE
C

```

```

C          TEMP = A * L(t-1)
C
          DO 1420 L = 1, R
            DO 1400 I = 1, K
              DO 1380 J = 1, K
                SUM = ZERO
                IF(L .LE. Q) THEN
                  DO 1340 K2 = 1, K
                    SUM = SUM + THETA(I, (L - 1) * K + K2) *
*
1340                      MAT(K2,J)
                  CONTINUE
                ENDIF
                IF(L .LT. R) SUM = SUM + MAT(I, L * K + J)
                TEMP(I, (L - 1) * K + J) = SUM
C
1380          CONTINUE
1400          CONTINUE
1420          CONTINUE
ENDIF
C
C          calculate TEMPM = M(t-1) * (h'L(t-1))'
C
C          calculate choleski factorization of MT and store as INVF
C
          CALL CHOL(MT, K, K, INVF, IFAULT)
C
C          compute h'L(t-1) * INVF
C
          DO 1500 I = 1, K
            DO 1480 J = 1, K
              SUM = ZERO
              DO 1460 K2 = J, K
                SUM = SUM + TEMPL(I,K2) * INVF(K2,J)
1460          CONTINUE
              WA(I,J) = SUM
1480          CONTINUE
1500          CONTINUE
C
C          compute INVF * WA'
C
          DO 1560 I = 1, K
            DO 1540 J = 1, K
              SUM = ZERO
              DO 1520 K2 = 1, I
                SUM = SUM + INVF(I,K2) * WA(J,K2)
1520          CONTINUE
              TEMPM(I,J) = SUM
1540          CONTINUE
1560          CONTINUE
C
C          update K(t)
C
          DO 1640 L = 1, R
            DO 1620 I = 1, K
              DO 1600 J = 1, K
                SUM = ZERO
                IF(PEARL .AND. L .GE. Q + 1) GAMMA(I, (L - 1) * K + J)
*
= SUM
                IF((.NOT.PEARL) .OR. L .LT. Q + 1) THEN
                  DO 1580 K2 = 1, K
                    SUM = SUM - TEMP(I, (L - 1) * K + K2) *

```

```

*
1580          TEMPM(K2,J)
          CONTINUE
          GAMMA(I, (L - 1) * K + J) = GAMMA(I, (L - 1) * K
*
          + J) + SUM
          ENDIF
1600          CONTINUE
1620          CONTINUE
1640          CONTINUE
C
C      update F(t)
C
      DO 1700 I = 1, K
          DO 1680 J = I, K
              SUM = F(I,J)
              DO 1660 K2 = 1, K
                  SUM = SUM - WA(I,K2) * WA(J,K2)
1660          CONTINUE
              F(I,J) = SUM
              F(J,I) = SUM
1680          CONTINUE
1700          CONTINUE
C
C      test for convergence of F(t)'s
C
      SUM = ZERO
      DO 1720 I = 1, K
          IF(QQ(I,I) .GT. ZERO) THEN
              SUM = MAX(SUM, ABS(F(I,I) - QQ(I,I)) / QQ(I,I))
          ELSE
              SUM = MAX(SUM, ABS(F(I,I) - QQ(I,I)))
          ENDIF
1720          CONTINUE
      IF(SUM .LT. XTOL) DELTA = .TRUE.
C
      IF(.NOT. DELTA) GOTO 1920
C
      set TEMPK = R * L'
C
      J7 = T
      DO 1780 I = 1, K
          DO 1760 J = 1, K
              DO 1740 L = 1, R
                  SUM = ZERO
                  IF(L .LE. P) SUM = PHI(I, (L - 1) * K + J)
                  IF(L .LE. Q) SUM = SUM - THETA(I, (L - 1) * K + J)
                  TEMPK(I, (L - 1) * K + J) = SUM
1740          CONTINUE
1760          CONTINUE
1780          CONTINUE
C
      DO 1900 L = 1, R
          DO 1840 I = 1, K
              DO 1820 J = 1, K
                  SUM = ZERO
                  DO 1800 K2 = J, K
                      SUM = SUM + TEMPK(I, (L - 1) * K + K2) * A(K2,J)
1800          CONTINUE
                  WA(I,J) = SUM
1820          CONTINUE
1840          CONTINUE
          DO 1880 I = 1, K

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```

                DO 1860 J = 1, K
                    TEMPK(I, (L - 1) * K + J) = WA(I,J)
1860             CONTINUE
1880             CONTINUE
1900             CONTINUE
C
C             calculate choleski decomposition of F(t) and det(F(t))
C
C             copy old A onto WA
C
1920             DO 1960 I = 1, K
                    DO 1940 J = 1, K
                        WA(I,J) = A(I,J)
1940             CONTINUE
1960             CONTINUE
                CALL CHOL(F, K, K, A, IFAULT)
                IF(IFAULT .NE. 0) THEN
                    IFAULT = 11
                    RETURN
                ENDIF
                SIG = A(1,1)
                DO 1980 I = 2, K
                    SIG = SIG * A(I,I)
1980             CONTINUE
                SIG = SIG * SIG
C
                IF(DELTA) GOTO 2180
C
C             update M(t)
C
C             transpose TEMPM
C
                DO 2020 I = 1, K
                    DO 2000 J = 1, I
                        SUM = TEMPM(I,J)
                        TEMPM(I,J) = TEMPM(J,I)
                        TEMPM(J,I) = SUM
2000             CONTINUE
2020             CONTINUE
                CALL BKSB(A, K, K, K, .FALSE., TEMPM, IFAULT)
                DO 2080 I = 1, K
                    DO 2060 J = I, K
                        SUM = MT(I,J)
                        DO 2040 K2 = 1, K
                            SUM = SUM + TEMPM(K2,I) * TEMPM(K2,J)
2040             CONTINUE
                        MT(I,J) = SUM
                        MT(J,I) = SUM
2060             CONTINUE
2080             CONTINUE
C
C             update L(t)
C
                CALL BKSB(WA, K, K, K, .FALSE., TEMPL, IFAULT)
                DO 2160 L = 1, R
                    DO 2140 I = 1, K
                        DO 2120 J = 1, K
                            SUM = ZERO
                            IF(PEARL .AND. L .GE. Q + 1) MAT(I, (L - 1) * K + J)
*                               = SUM
                            IF((.NOT.PEARL) .OR. L .LT. Q + 1) THEN

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```

                DO 2100 K2 = 1, K
                    SUM = SUM + TEMPK(I, (L - 1) * K + K2)
*                    * TEMPL(K2,J)
2100                CONTINUE
                    MAT(I, (L - 1) * K + J) = TEMP(I, (L - 1) * K + J)
*                    - SUM
                ENDIF
2120                CONTINUE
2140                CONTINUE
2160                CONTINUE
C
2180                DO 2200 I = 1, K
                    V(I,T) = W(I,T) - Z(I)
                    IF(MEAN) V(I,T) = V(I,T) - MEANS(I)
                    B(I) = V(I,T)
2200                CONTINUE
C
                CALL BKSB(A, K, K, 1, .FALSE., B, IFAULT)
                DO 2220 I = 1, K
                    SSQ = SSQ + B(I) * B(I)
2220                CONTINUE
                    IF((.NOT.DELTA) .OR. T .LE. J7) DETP = DETP + LOG(SIG)
C
2240                CONTINUE
C
                RLOGL = - CONST - (SSQ + DETP + REAL(N - J7) * LOG(TSIG)) / TWO
C
                END
C
                SUBROUTINE COVARS(K, P, Q, R, IK, PHI, THETA, QQ, GAMMA,
*                    Z, KMAT, MAT, B, IWORK, IFAULT)
C
C                ALGORITHM AS242.3  APPL. STATIST. (1989), VOL.38, NO. 1
C
                INTEGER          P, Q, R, K, KMAT, IFAULT, M, I, J, I2, K2, J2,
*                    KW, L, L4, IK, IWORK(KMAT)
                REAL             QQ(IK,K), PHI(IK,P*K+1), THETA(IK,Q*K+1),
*                    GAMMA(K,K*R), Z(K*K*(R+1)), MAT(KMAT,KMAT),
*                    B(K*K*(P+1)), SUM, ZERO, ONE
                PARAMETER        (ZERO = 0.0, ONE = 1.0)
                EXTERNAL         DECOMP, SOLVE
C
C                This auxiliary routine calculates the theoretical cross
C                covariances between the W(t)'s and between the W(t)'s and the
C                E(t)'s
C
                IFAULT = 0
C
C                generate the q gamma's
C
                DO 140 M = 1, Q
                    DO 120 I = 1, K
                        DO 100 J = 1, K
                            SUM = ZERO
                            DO 20 I2 = 1, K
                                SUM = SUM - THETA(I, (M - 1) * K + I2) * QQ(I2,J)
20                            CONTINUE
                                DO 60 K2 = 1, P
                                    DO 40 J2 = 1, K
                                        IF(M .GT. K2) SUM = SUM + PHI(I, (K2 - 1) * K + J2)
*                                        * GAMMA(J2, (M - K2 - 1) * K + J)

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```

                IF(M .EQ. K2) SUM = SUM + PHI(I, (K2 - 1) * K + J2)
*                * QQ(J2,J)
40          CONTINUE
60          CONTINUE
          GAMMA(I, (M - 1) * K + J) = SUM
100         CONTINUE
120        CONTINUE
140       CONTINUE
C
C      calculate the first p c(j)'s
C
C      first initialise MAT and Z to zero
C
      KW = K * K * (P + 1)
      DO 180 J = 1, KW
        DO 160 I = 1, KW
          MAT(I,J) = ZERO
160       CONTINUE
          Z(J) = ZERO
180      CONTINUE
C
      DO 360 M = 0, P
        DO 340 I = 1, K
          DO 320 J = 1, K
            L = M * K * K + (I - 1) * K + J
C
C      first calculate right-hand side vector Z
C
          IF(M .EQ. 0) Z(L) = QQ(I,J)
          IF(M .GT. 0 .AND. M .LE. Q) THEN
            DO 200 I2 = 1, K
              Z(L) = Z(L) - QQ(I,I2) * THETA(J, (M - 1) * K + I2)
200         CONTINUE
            ENDIF
            DO 260 L4 = M + 1, Q
              DO 240 I2 = 1, K
                Z(L) = Z(L) - GAMMA(I, (L4 - M - 1) * K + I2) *
*                THETA(J, (L4 - 1) * K + I2)
240         CONTINUE
260       CONTINUE
C
C      now set up MAT array
C
          MAT(L,L) = ONE
          DO 300 I2 = 1, P
            DO 280 K2 = 1, K
              IF(M .GE. I2) L4 = (M - I2) * K * K + (I - 1) * K
*              + K2
              IF(M .LT. I2) L4 = (I2 - M) * K * K + (K2 - 1)
*              * K + I
              MAT(L,L4) = MAT(L,L4) - PHI(J, (I2 - 1) * K + K2)
280         CONTINUE
300       CONTINUE
C
320      CONTINUE
340     CONTINUE
360    CONTINUE
C
      IF(P .GT. 0) THEN
        CALL DECOMP(KW, KMAT, MAT, IWORK)
        IF(IWORK(KW) .EQ. 0) THEN

```

```

        IFAULT = 1
        RETURN
    ELSE
        CALL SOLVE(KW, KMAT, MAT, Z, IWORK)
    ENDIF
ENDIF
C
C calculate C(j)'s for j = p + 1, ..., r (if needed)
C
DO 540 M = P + 1, R
    DO 520 I = 1, K
        DO 500 J = 1, K
            SUM = ZERO
            DO 400 L4 = 1, P
                DO 380 I2 = 1, K
                    SUM = SUM + Z((M - L4) * K * K + (I - 1) * K + I2)
                    * PHI(J, (L4 - 1) * K + I2)
                CONTINUE
            CONTINUE
        CONTINUE
        IF(M .LE. Q) THEN
            DO 420 I2 = 1, K
                SUM = SUM - QQ(I, I2) * THETA(J, (M - 1) * K + I2)
            CONTINUE
            DO 460 I2 = M + 1, Q
                DO 440 L4 = 1, K
                    SUM = SUM - GAMMA(I, (I2 - M - 1) * K + L4)
                    * THETA(J, (I2 - 1) * K + L4)
                CONTINUE
            CONTINUE
        ENDIF
        Z(M * K * K + (I - 1) * K + J) = SUM
    CONTINUE
CONTINUE
520 CONTINUE
540 CONTINUE
C
END
C
SUBROUTINE CHOL(A, IK, K, L, IFAULT)
C
C ALGORITHM AS 242.4 APPL. STATIST. (1989), VOL.38, NO. 1
C
INTEGER          IK, K, I, J, IFAULT, K2
REAL             A(IK,K), L(IK,K), SUM, ZERO
PARAMETER       (ZERO = 0.0)
INTRINSIC       Sqrt
C
    IFAULT = 0
    DO 180 J = 1, K
        SUM = A(J,J)
        DO 60 K2 = 1, J - 1
            SUM = SUM - L(J,K2) * L(J,K2)
        CONTINUE
        IF(SUM .LE. ZERO) THEN
            IFAULT = 1
            RETURN
        ELSE
            L(J,J) = Sqrt(SUM)
        ENDIF
        DO 160 I = J + 1, K
            SUM = A(I,J)

```



```
        DO 120 K2 = 1, J - 1
            SUM = SUM - L(I,K2) * L(J,K2)
120     CONTINUE
        L(I,J) = SUM / L(J,J)
        L(J,I) = ZERO
160     CONTINUE
180 CONTINUE
C
    END
C
    SUBROUTINE BKSB(L, IK, K, M, UPPER, B, IFAULT)
C
C    ALGORITHM AS 242.5 APPL. STATIST. (1989), VOL.38, NO. 1
C
    INTEGER          IK, K, IFAULT, I, J, M, J2
    REAL             L(IK,K), B(IK,M), SUM, ZERO
    LOGICAL          UPPER
    PARAMETER        (ZERO = 0.0)
C
    IFAULT = 0
    IF(UPPER) THEN
        DO 21 J2 = 1, M
            DO 40 I = K, 1, -1
                SUM = B(I,J2)
                DO 20 J = I + 1, K
                    SUM = SUM - L(I,J) * B(J,J2)
20             CONTINUE
                IF(L(I,I) .NE. ZERO) THEN
                    B(I,J2) = SUM / L(I,I)
                ELSE
                    IFAULT = 1
                    RETURN
                ENDIF
40             CONTINUE
21             CONTINUE
        ELSE
            DO 22 J2 = 1, M
                DO 80 I = 1, K
                    SUM = B(I,J2)
                    DO 60 J = 1, I - 1
                        SUM = SUM - L(I,J) * B(J,J2)
60             CONTINUE
                    IF(L(I,I) .NE. ZERO) THEN
                        B(I,J2) = SUM / L(I,I)
                    ELSE
                        IFAULT = 1
                        RETURN
                    ENDIF
80             CONTINUE
22             CONTINUE
            ENDIF
C
    END
C
    SUBROUTINE DECOMP(N, NDIM, A, IP)
    INTEGER          N, NDIM, K, KP1, M, I, J, IP(NDIM)
    REAL             A(NDIM,NDIM), T
    INTRINSIC        ABS
C
C    matrix triangularization by Gaussian elimination.
C    INPUT..
```

```

C      N = order of matrix.
C      NDIM = declared dimension of array A.
C      A = matrix to be triangularized.
C      OUTPUT..
C      A(I,J), I .LE. J = upper triangular factor, U.
C      A(I,J), I .GT. J = multipliers = lower triangular
C                          factor, I - L.
C      IP(K), K .LT. N = index of k-th pivot row.
C      IP(N) = (-1) ** (number of interchanges) or 0.
C      use 'SOLVE' to obtain solution of linear system.
C      determ(A) = IP(N) * A(1,1) * A(2,2) * ... * A(N,N).
C      if IP(N) = 0, A is singular, 'SOLVE' will divide by zero.
C      interchanges finished in U, only partly in L.

```

```

C
C      IP(N) = 1
C      DO 6 K = 1, N
C          IF(K .EQ. N) GOTO 5
C          KP1 = K + 1
C          M = K
C          DO 1 I = KP1, N
C              IF(ABS(A(I,K)) .GT. ABS(A(M,K))) M = I
1      CONTINUE
C          IP(K) = M
C          IF(M .NE. K) IP(N) = - IP(N)
C          T = A(M,K)
C          A(M,K) = A(K,K)
C          A(K,K) = T
C          IF(T .EQ. 0.0) GOTO 5
C          DO 2 I = KP1, N
2      A(I,K) = - A(I,K) / T
C          DO 4 J = KP1, N
C              T = A(M,J)
C              A(M,J) = A(K,J)
C              A(K,J) = T
C              IF(T .EQ. 0.0) GOTO 4
C              DO 3 I = KP1, N
3      A(I,J) = A(I,J) + A(I,K) * T
C          CONTINUE
C          IF(A(K,K) .EQ. 0.0) IP(N) = 0
C      CONTINUE
C      RETURN
C      END

```

```

C
C      SUBROUTINE SOLVE(N, NDIM, A, B, IP)
C      INTEGER          I, N, NDIM, IP(NDIM), NM1, K, KP1, M, KM1, KB
C      REAL             A(NDIM,NDIM), B(NDIM), T

```

```

C
C      solution of linear system, A * x = b.
C      INPUT..
C      N = order of matrix.
C      NDIM = declared dimension of array A.
C      A = triangularized matrix obtained from 'DECOMP'.
C      B = right-hand side vector.
C      IP = pivot vector obtained from 'DECOMP'.
C      DO NOT USE if 'DECOMP' has set IP(N) = 0.
C      OUTPUT..
C      B = solution vector, X.

```

```

C
C      IF(N .EQ. 1) GOTO 9
C      NM1 = N - 1
C      DO 7 K = 1, NM1

```

```
      KP1 = K + 1
      M = IP(K)
      T = B(M)
      B(M) = B(K)
      B(K) = T
      DO 7 I = KP1, N
7 B(I) = B(I) + A(I,K) * T
      DO 8 KB = 1, NM1
      KM1 = N - KB
      K = KM1 + 1
      B(K) = B(K) / A(K,K)
      T = - B(K)
      DO 8 I = 1, KM1
8 B(I) = B(I) + A(I,K) * T
9 B(1) = B(1) / A(1,1)
      RETURN
      END
```

```

REAL FUNCTION TNC(T, DF, DELTA, IFAULT)
C
C   ALGORITHM AS 243  APPL. STATIST. (1989), VOL.38, NO. 1
C
C   Cumulative probability at T of the non-central t-distribution
C   with DF degrees of freedom (may be fractional) and non-centrality
C   parameter DELTA.
C
C   Note - requires the following auxiliary routines
C   ALOGAM (X)                - ACM 291 or AS 245
C   BETAIN (X, A, B, ALBETA, IFAULT) - AS 63 (updated in ASR 19)
C   ALNORM (X, UPPER)         - AS 66
C
REAL A, ALBETA, ALNRPI, B, DEL, DELTA, DF, EN, ERRBD, ERRMAX,
* GEVEN, GODD, HALF, ITRMAX, LAMBDA, ONE, P, Q, R2PI, RXB, S, T,
* TT, TWO, X, XEVEN, XODD, ZERO
LOGICAL NEGDEL
C
C   Note - ITRMAX and ERRMAX may be changed to suit one's needs.
C
DATA ITRMAX/100.1/, ERRMAX/1.E-06/
C
C   Constants - R2PI = 1/ {GAMMA(1.5) * SQRT(2)} = SQRT(2 / PI)
C               ALNRPI = LN(SQRT(PI))
C
DATA ZERO/0.0/, HALF/0.5/, ONE/1.0/, TWO/2.0/,
* R2PI/0.79788 45608 02865 35588/,
* ALNRPI/0.57236 49429 24700 08707/
C
TNC = ZERO
IFAULT = 2
IF (DF .LE. ZERO) RETURN
IFAULT = 0
C
TT = T
DEL = DELTA
NEGDEL = .FALSE.
IF (T .GE. ZERO) GO TO 1
NEGDEL = .TRUE.
TT = -TT
DEL = -DEL
1 CONTINUE
C
C   Initialize twin series (Guenther, J. Statist. Computn. Simuln.
C   vol.6, 199, 1978).
C
EN = ONE
X = T * T / (T* T + DF)
IF (X .LE. ZERO) GO TO 20
LAMBDA = DEL * DEL
P = HALF * EXP(-HALF * LAMBDA)
Q = R2PI * P * DEL
S = HALF - P
A = HALF
B = HALF * DF
RXB = (ONE - X) ** B
ALBETA = ALNRPI + ALOGAM(B, IFAULT) - ALOGAM(A + B, IFAULT)
XODD = BETAIN(X, A, B, ALBETA, IFAULT)
GODD = TWO * RXB * EXP(A * LOG(X) - ALBETA)
XEVEN = ONE - RXB
GEVEN = B * X * RXB

```

```
TNC = P * XODD + Q * XEVEN
C
C Repeat until convergence
C
10 A = A + ONE
XODD = XODD - GODD
XEVEN = XEVEN - GEVEN
GODD = GODD * X * (A + B - ONE) / A
GEVEN = GEVEN * X * (A + B - HALF) / (A + HALF)
P = P * LAMBDA / (TWO * EN)
Q = Q * LAMBDA / (TWO * EN + ONE)
S = S - P
EN = EN + ONE
TNC = TNC + P * XODD + Q * XEVEN
ERRBD = TWO * S * (XODD - GODD)
IF (ERRBD .GT. ERRMAX .AND. EN .LE. ITRMAX) GO TO 10
C
20 IFAULT = 1
IF (EN .GT. ITRMAX) RETURN
IFAILT = 0
TNC = TNC + ALNORM(DEL, .TRUE.)
IF (NEGDEL) TNC = ONE - TNC
C
RETURN
END
```

```
{
    Algorithm AS244 Appl. Statist. (1989) Vol. 38, No. 1 }

{ The procedure HiModel can be used to
  (1) Check decomposability for a hierarchical loglinear model;
  (2) Obtain the sets of variables onto which the model is collapsible;
  (3) Find the factor formula of MLEs for the model;
  (4) Find the reduced formula of the likelihood ratio test statistic. }
```

```
{ ***** }
```

DATA STRUCTURES

```
***** }
```

```
CONST MaxVar=50;
      MaxGenerator=50;
      MaxSubGeClass=20;
      MaxInt=51;
```

```
TYPE IntSet = SET OF 1..MaxVar;
     SetArr = ARRAY[1..MaxGenerator] OF IntSet;
     SetArr2 = ARRAY[1..MaxSubGeClass,1..MaxGenerator] OF IntSet;
     IntArr = ARRAY [1..MaxSubGeClass] OF 1..MaxGenerator;
     IntGC = 0..MaxGenerator;
     IntSubGC = 0..MaxSubGeClass;
     NonnegInt= 0..MaxInt;
```

```
{ ***** }
```

PRINCIPAL PROCEDURE

```
***** }
```

```
PROCEDURE HiModel(NumModels: NonnegInt;
                  M1SizeGeClass, M2SizeGeClass: IntGC;
                  M1GeClass, M2GeClass: SetArr;
                  VAR M1NumNumer, M2NumNumer, M1NumDenom, M2NumDenom,
                      LRNumNumer, LRNumDenom: IntGC;
                  VAR M1NumSubGC, M2NumSubGC, LRNumGCNumer, LRNumGCDenom: IntSubGC;
                  VAR Fault: NonnegInt;
                  VAR M1Numerator, M2Numerator, M1Denominator,
                      M2Denominator, LRNumerator, LRDenominator: SetArr;
                  VAR M1SubGeClass, M2SubGeClass, LRGCNumer, LRGCDenom: SetArr2;
                  VAR M1SizeSubGC, M2SizeSubGC, LRSizeNumerGC, LRSizeDenomGC: IntArr;
                  VAR VariableSet: IntSet);
```

```
VAR i,j,k,m,n: NonnegInt; VarSetModel: IntSet;
```

```
PROCEDURE Error(VAR Size: IntGC; MaxSize: IntGC; ErrorNumber: NonnegInt;
                AnotherError: Boolean);
```

```
BEGIN IF (Size>MaxSize) OR AnotherError THEN
      BEGIN Fault:=ErrorNumber; Size:=MaxSize
      END
END; { of Error }
```

```
{ Reduce the fraction: NumeratorSet/DenominatorSet. }
```

```
PROCEDURE Reduce(VAR NumNumerSet,NumDenomSet: IntGC;
                 VAR NumeratorSet, DenominatorSet: SetArr);
```

```
VAR i,j,k,m: IntGC;
BEGIN k:=0;
FOR i:=1 TO NumNumerSet DO
  BEGIN j:=1;
  WHILE (NumeratorSet[i]<>DenominatorSet[j]) AND
    (j<=NumDenomSet) DO j:=j+1;
  IF j>NumDenomSet THEN
    BEGIN k:=k+1; NumeratorSet[k]:=NumeratorSet[i]
    END
  ELSE
    BEGIN
    FOR m:=j+1 TO NumDenomSet DO
      DenominatorSet[m-1]:=DenominatorSet[m];
      NumDenomSet:=NumDenomSet-1
    END
    END;
  NumNumerSet:=k
END; { of Reduce }

{ Check collapsibility and decomposability. }
PROCEDURE CollDeco (SizeGeClass: IntGC; GeClass: SetArr; VAR NumNumer,
  NumDenom: IntGC; VAR NumSubGC: IntSubGC; VAR Numerator,Denominator:
  SetArr; VAR SubGeClass: SetArr2; VAR SizeSubGC: IntArr);
VAR i: IntGC;

{ Check whether the generating class is decomposable or not. }
PROCEDURE Deco(VAR SizeGeClass: IntGC; VAR GeClass: SetArr);
VAR i,j: IntGC; OneClass: IntSet;
  GeClassUnchange,GeneratorUnchange,NoSubGenerator: Boolean;
BEGIN
  REPEAT GeClassUnchange:=true;
  { Delete variables which exist in only a single generator. }
  REPEAT GeneratorUnchange:=true;
  FOR i:=1 TO SizeGeClass DO
    BEGIN OneClass:=GeClass[i];
    FOR j:=1 TO SizeGeClass DO
      IF i<>j THEN OneClass:=OneClass-GeClass[j];
    IF OneClass<>[] THEN
      BEGIN
        NumNumer:=NumNumer+1; Error(NumNumer,MaxGenerator,3,false);
        Numerator[NumNumer]:=GeClass[i];
        IF GeClass[i]-OneClass<>[] THEN
          BEGIN NumDenom:=NumDenom+1;
            Error(NumDenom,MaxGenerator,4,false);
            Denominator[NumDenom]:=GeClass[i]-OneClass
          END;
          GeClass[i]:=GeClass[i]-OneClass; GeneratorUnchange:=false
        END
      END
    UNTIL GeneratorUnchange;
  { Delete generators which are contained in others. }
  REPEAT NoSubGenerator:=true;
  FOR i:=1 TO SizeGeClass DO
    FOR j:=1 TO SizeGeClass DO
      IF (i<>j) AND (GeClass[i]<=GeClass[j]) AND (GeClass[i]<>[]) THEN
        BEGIN GeClass[i]:=[];
          NoSubGenerator:=false; GeClassUnchange:=false
        END;
  { Delete the null generators. }
  j:=0;
  FOR i:=1 TO SizeGeClass DO
```

```

    IF GeClass[i]<>[] THEN
        BEGIN j:=j+1; GeClass[j]:=GeClass[i]
        END;
    SizeGeClass:=j
    UNTIL NoSubGenerator OR (SizeGeClass=0)
    UNTIL GeClassUnchange OR (SizeGeClass=0)
END; { of Deco }

{ Decompose generating class. }
PROCEDURE DecompGC(VAR SizeGeClass: IntGC; VAR GeClass: SetArr);
VAR i,j,k,InAGeneratorsNum,InBGeneratorsNum: IntGC; GeClassA: SetArr;
    BoundaryOfAB,VarInA,VarInB: IntSet;
    Researched: ARRAY [1..MaxGenerator] OF Boolean;
    DecomposedOrCannotDecompose,NoVarAddedInA: Boolean;
BEGIN
    Deco(SizeGeClass,GeClass);
    IF SizeGeClass<>0 THEN
        BEGIN i:=0; DecomposedOrCannotDecompose:=false;
        { Find variables in A. }
        REPEAT
            IF i=0 THEN BoundaryOfAB:=[] ELSE BoundaryOfAB:=GeClass[i];
            InAGeneratorsNum:=1;
            IF i<>1 THEN k:=1 ELSE k:=2;
            GeClassA[1]:=GeClass[k]; Researched[k]:=true; VarInA:=GeClassA[1];
            FOR j:=1 TO SizeGeClass DO IF j<>k THEN Researched[j]:=false;
            REPEAT NoVarAddedInA:=true;
                FOR j:=1 TO SizeGeClass DO
                    IF (i<>j) AND NOT Researched[j] AND
                        (VarInA*GeClass[j]-BoundaryOfAB<>[]) THEN
                        BEGIN NoVarAddedInA:=false; InAGeneratorsNum:=InAGeneratorsNum+1;
                            GeClassA[InAGeneratorsNum]:=GeClass[j]; Researched[j]:=true;
                            VarInA:=VarInA+GeClass[j]
                        END
                    UNTIL NoVarAddedInA;
                IF i<>0 THEN InBGeneratorsNum:=SizeGeClass-InAGeneratorsNum-1
                    ELSE InBGeneratorsNum:=SizeGeClass-InAGeneratorsNum;
                VarInB:=[];
                IF InBGeneratorsNum<>0 THEN
                    { The generating class can be decomposed by GeClass[i]. }
                    BEGIN j:=0; DecomposedOrCannotDecompose:=true;
                    { Find variables in B. }
                    FOR k:=1 TO SizeGeClass DO
                        IF (k<>i) AND NOT Researched[k] THEN
                            BEGIN j:=j+1; VarInB:=VarInB+GeClass[k]; GeClass[j]:=GeClass[k]
                            END;
                        IF i<>0 THEN
                            BEGIN InAGeneratorsNum:=InAGeneratorsNum+1;
                                GeClassA[InAGeneratorsNum]:=BoundaryOfAB;
                                InBGeneratorsNum:=InBGeneratorsNum+1;
                                GeClass[InBGeneratorsNum]:=BoundaryOfAB*VarInB;
                                NumDenom:=NumDenom+1; Error(NumDenom,MaxGenerator,4,false);
                                Denominator[NumDenom]:=GeClass[InBGeneratorsNum]
                            END;
                        { Decompose recursively A and B. }
                            DecompGC(InAGeneratorsNum,GeClassA);
                            DecompGC(InBGeneratorsNum,GeClass)
                        END
                    ELSE
                    { The generating class cannot be decomposed by GeClass[i]. }
                    IF i=SizeGeClass THEN
                        { The generating class cannot be decomposed by any generator. }

```



```

    BEGIN DecomposedOrCannotDecompose:=true; NumSubGC:=NumSubGC+1;
    IF NumSubGC>MaxSubGeClass THEN
        BEGIN Fault:=5; NumSubGC:=MaxSubGeClass
        END;
    SizeSubGC[NumSubGC]:=SizeGeClass;
    FOR k:=1 TO SizeGeClass DO SubGeClass[NumSubGC,k]:=GeClass[k]
    END
    ELSE i:=i+1
    UNTIL DecomposedOrCannotDecompose
    END
END; { of DecompGC }

BEGIN { of CollDeco }
Error(SizeGeClass,MaxGenerator,1,SizeGeClass<1); VarSetModel:=[];
IF Fault=0 THEN
    FOR i:=1 TO SizeGeClass DO
        BEGIN
            IF NOT([1..MaxVar]>=GeClass[i]) OR (GeClass[i]=[]) THEN Fault:=2;
            VarSetModel:=VarSetModel+GeClass[i]
            END;
        NumNumer:=0; NumDenom:=0; NumSubGC:=0;
        IF Fault=0 THEN
            BEGIN
                DecompGC(SizeGeClass,GeClass);
                Reduce(NumNumer,NumDenom,Numerator,Denominator)
            END
        END; { of CollDeco }

{ Check whether the sub-generating classes in models 1 and 2 are same. }
FUNCTION ClassesNotSame: Boolean;
VAR k: IntGC; m: NonnegInt; NotSame: Boolean;
BEGIN k:=0; NotSame:=M1SizeSubGC[i]<>LRSizeDenomGC[j];
    WHILE NOT NotSame AND (k<M1SizeSubGC[i]) DO
        BEGIN k:=k+1; m:=1;
            WHILE (m<=LRSizeDenomGC[j]) AND
                (M1SubGeClass[i,k]<>LRGCDenom[j,m]) DO m:=m+1;
            NotSame:=NotSame OR (m>LRSizeDenomGC[j])
            END;
        ClassesNotSame:=NotSame
    END; { of ClassesNotSame }

BEGIN { of HiModel }
M1NumNumer:=0; M1NumDenom:=0; M1NumSubGC:=0; VariableSet:=[];
M2NumNumer:=0; M2NumDenom:=0; M2NumSubGC:=0; Fault:=0;
LRNumNumer:=0; LRNumDenom:=0; LRNumGCNumber:=0; LRNumGCDenom:=0;
IF (NumModels<1) OR (NumModels>2) THEN Fault:=6
ELSE
    BEGIN
        CollDeco(M1SizeGeClass,M1GeClass,M1NumNumer,M1NumDenom,M1NumSubGC,
            M1Numerator,M1Denominator,M1SubGeClass,M1SizeSubGC);
        VariableSet:=VarSetModel;
        IF NumModels>1 THEN
            BEGIN
                CollDeco(M2SizeGeClass,M2GeClass,M2NumNumer,M2NumDenom,M2NumSubGC,
                    M2Numerator,M2Denominator,M2SubGeClass,M2SizeSubGC);
                IF VariableSet<>VarSetModel THEN Fault:=9;
            { Find the likelihood ratio: M1/M2. }
            LRNumNumer:=M1NumNumer+M2NumDenom;
            Error(LRNumNumer,MaxGenerator,7,false);
            FOR i:=1 TO LRNumNumer DO
                IF i<=M1NumNumer THEN LRNumerator[i]:=M1Numerator[i]

```

```
    ELSE LRNumDenom:=M2Denominator[i-M1NumNumer];
    LRNumDenom:=M2NumNumer+M1NumDenom;
    Error(LRNumDenom,MaxGenerator,8,false);
    FOR i:=1 TO LRNumDenom DO
      IF i<=M1NumDenom THEN LRDenominator[i]:=M1Denominator[i]
      ELSE LRDenominator[i]:=M2Numerator[i-M1NumDenom];
    Reduce(LRNumNumer,LRNumDenom,LRNumerator,LRDenominator);
  { Reduce sub-generating classes of M1 and M2. }
  LRNumGCDenom:=M2NumSubGC;
  FOR m:=1 TO LRNumGCDenom DO
    BEGIN LRSizeDenomGC[m]:=M2SizeSubGC[m];
    FOR n:=1 TO LRSizeDenomGC[m] DO LRGCDenom[m,n]:=M2SubGeClass[m,n]
    END;
  k:=0;
  FOR i:=1 TO M1NumSubGC DO
    BEGIN j:=1;
    WHILE (j<=LRNumGCDenom) AND ClassesNotSame DO j:=j+1;
    IF j>LRNumGCDenom THEN
      BEGIN k:=k+1; LRSizeNumerGC[k]:=M1SizeSubGC[i];
      FOR m:=1 TO LRSizeNumerGC[k] DO
        LRGCNumer[k,m]:=M1SubGeClass[i,m]
      END
    ELSE
      BEGIN
        FOR m:=j+1 TO LRNumGCDenom DO
          BEGIN LRSizeDenomGC[m-1]:=LRSizeDenomGC[m];
          FOR n:=1 TO LRSizeDenomGC[m-1] DO
            LRGCDenom[m-1,n]:=LRGCDenom[m,n]
          END;
          LRNumGCDenom:=LRNumGCDenom-1
        END
      END;
    LRNumGCNumer:=k
  END
END
END; { of HiModel }
```

c This file contains two algorithms for the logarithm of the gamma function.  
c Algorithm AS 245 is the faster (but longer) and gives an accuracy of about  
c 10-12 significant decimal digits except for small regions around  $X = 1$  and  
c  $X = 2$ , where the function goes to zero.  
c The second algorithm is not part of the AS algorithms. It is slower but  
c gives 14 or more significant decimal digits accuracy, except around  $X = 1$   
c and  $X = 2$ . The Lanczos series from which this algorithm is derived is  
c interesting in that it is a convergent series approximation for the gamma  
c function, whereas the familiar series due to De Moivre (and usually wrongly  
c called Stirling's approximation) is only an asymptotic approximation, as  
c is the true and preferable approximation due to Stirling.

c  
c  
c

DOUBLE PRECISION FUNCTION ALNGAM(XVALUE, IFAULT)

C  
C  
C  
C  
C

ALGORITHM AS245 APPL. STATIST. (1989) VOL. 38, NO. 2

Calculation of the logarithm of the gamma function

INTEGER IFAULT

DOUBLE PRECISION ALR2PI, FOUR, HALF, ONE, ONEP5, R1(9), R2(9),  
+ R3(9), R4(5), TWELVE, X, X1, X2, XLGE, XLGST, XVALUE,  
+ Y, ZERO

C  
C  
C

Coefficients of rational functions

DATA R1/-2.66685 51149 5D0, -2.44387 53423 7D1,  
+ -2.19698 95892 8D1, 1.11667 54126 2D1,  
+ 3.13060 54762 3D0, 6.07771 38777 1D-1,  
+ 1.19400 90572 1D1, 3.14690 11574 9D1,  
+ 1.52346 87407 0D1/  
DATA R2/-7.83359 29944 9D1, -1.42046 29668 8D2,  
+ 1.37519 41641 6D2, 7.86994 92415 4D1,  
+ 4.16438 92222 8D0, 4.70668 76606 0D1,  
+ 3.13399 21589 4D2, 2.63505 07472 1D2,  
+ 4.33400 02251 4D1/  
DATA R3/-2.12159 57232 3D5, 2.30661 51061 6D5,  
+ 2.74647 64470 5D4, -4.02621 11997 5D4,  
+ -2.29660 72978 0D3, -1.16328 49500 4D5,  
+ -1.46025 93751 1D5, -2.42357 40962 9D4,  
+ -5.70691 00932 4D2/  
DATA R4/ 2.79195 31791 8525D-1, 4.91731 76105 05968D-1,  
+ 6.92910 59929 1889D-2, 3.35034 38150 22304D0,  
+ 6.01245 92597 64103D0/

C  
C  
C

Fixed constants

DATA ALR2PI/9.18938 53320 4673D-1/, FOUR/4.D0/, HALF/0.5D0/,  
+ ONE/1.D0/, ONEP5/1.5D0/, TWELVE/12.D0/, ZERO/0.D0/

C  
C  
C  
C  
C  
C

Machine-dependant constants.

A table of values is given at the top of page 399 of the paper.  
These values are for the IEEE double-precision format for which  
 $B = 2$ ,  $t = 53$  and  $U = 1023$  in the notation of the paper.

DATA XLGE/5.10D6/, XLGST/1.D+305/

C  
C  
C

X = XVALUE  
ALNGAM = ZERO

```

C      Test for valid function argument
C
      IFAULT = 2
      IF (X .GE. XLGST) RETURN
      IFAULT = 1
      IF (X .LE. ZERO) RETURN
      IFAULT = 0

C
C      Calculation for 0 < X < 0.5 and 0.5 <= X < 1.5 combined
C
      IF (X .LT. ONEP5) THEN
        IF (X .LT. HALF) THEN
          ALNGAM = -LOG(X)
          Y = X + ONE

C
C      Test whether X < machine epsilon
C
          IF (Y .EQ. ONE) RETURN
          ELSE
            ALNGAM = ZERO
            Y = X
            X = (X - HALF) - HALF
          END IF
          ALNGAM = ALNGAM + X * (((R1(5)*Y + R1(4))*Y + R1(3))*Y
+
          + R1(2))*Y + R1(1)) / (((Y + R1(9))*Y + R1(8))*Y
+
          + R1(7))*Y + R1(6))
          RETURN
        END IF

C
C      Calculation for 1.5 <= X < 4.0
C
      IF (X .LT. FOUR) THEN
        Y = (X - ONE) - ONE
        ALNGAM = Y * (((R2(5)*X + R2(4))*X + R2(3))*X + R2(2))*X
+
        + R2(1)) / (((X + R2(9))*X + R2(8))*X + R2(7))*X
+
        + R2(6))
        RETURN
      END IF

C
C      Calculation for 4.0 <= X < 12.0
C
      IF (X .LT. TWELVE) THEN
        ALNGAM = (((R3(5)*X + R3(4))*X + R3(3))*X + R3(2))*X + R3(1)) /
+
        (((X + R3(9))*X + R3(8))*X + R3(7))*X + R3(6))
        RETURN
      END IF

C
C      Calculation for X >= 12.0
C
      Y = LOG(X)
      ALNGAM = X * (Y - ONE) - HALF * Y + ALR2PI
      IF (X .GT. XLGE) RETURN
      X1 = ONE / X
      X2 = X1 * X1
      ALNGAM = ALNGAM + X1 * ((R4(3)*X2 + R4(2))*X2 + R4(1)) /
+
      ((X2 + R4(5))*X2 + R4(4))
      RETURN
    END

```

```

C
C
C

```

```
c
      double precision function lngamma(z, ier)
c
c      Uses Lanczos-type approximation to ln(gamma) for z > 0.
c      Reference:
c          Lanczos, C. 'A precision approximation of the gamma
c              function', J. SIAM Numer. Anal., B, 1, 86-96, 1964.
c      Accuracy: About 14 significant digits except for small regions
c              in the vicinity of 1 and 2.
c
c      Programmer: Alan Miller
c                  CSIRO Division of Mathematics & Statistics
c
c      N.B. It is assumed that the Fortran compiler supports long
c            variable names, including the underline character.  Some
c            compilers will not accept the 'implicit none' statement
c            below.
c
c      Latest revision - 17 April 1988
c
      implicit none
      double precision a(9), z, lnsqrt2pi, tmp
      integer ier, j
      data a/0.999999999995183d0, 676.5203681218835d0,
+          -1259.139216722289d0, 771.3234287757674d0,
+          -176.6150291498386d0, 12.50734324009056d0,
+          -0.1385710331296526d0, 0.9934937113930748d-05,
+          0.1659470187408462d-06/
c
      data lnsqrt2pi/0.91893 85332 04672 7d0/
c
      if (z .le. 0.d0) then
          ier = 1
          return
      end if
      ier = 0
c
      lngamma = 0.d0
      tmp = z + 7.d0
      do 10 j = 9, 2, -1
          lngamma = lngamma + a(j)/tmp
          tmp = tmp - 1.d0
10      continue
      lngamma = lngamma + a(1)
      lngamma = log(lngamma) + lnsqrt2pi - (z+6.5d0) +
+          (z-0.5d0)*log(z+6.5d0)
      end
```

```

C---- SUBROUTINE ARAVSS -----
C
C Computes sufficient statistics for analysis of variance table when
C the errors follow AR(1) normal process, given the design matrix X(N,P),
C observation matrix Y(N,T) and assuming that XXINV(P,P) contains
C the inverse matrix of Xtranspose*X.
C-----
      SUBROUTINE ARAVSS(Y,N,T,P,QS,XD1,XD2,YBAR,X,XXINV,IFAU)
C
C ALGORITHM AS 246.1 APPL. STATIST. (1989), VOL.38, NO. 2
C
      INTEGER T,P
      REAL Y(N,T),X(N,P),DLIN(2),DQUAD(3),YBAR(T)
      REAL XD1(P),XD2(P),XXINV(P,P),QS(14),ZERO,PROD
      DATA ZERO/0.0/
C
      Computes admissibility of parameters
C
      IFAU=0
      IF(P.LT.1) IFAU=1
      IF(T.LT.3) IFAU=IFAU+2
      IF(N.LT.P) IFAU=IFAU+4
      J=0
      DO 10 I=1,N
10      IF(X(I,1).NE.1.0) J=1
      IF(J.NE.0) IFAU=IFAU+8
      IF(IFAU.GT.0) RETURN
C
      Sets initial values to zero
C
      DO 20 I=1,14
20      QS(I)=ZERO
      DO 30 I=1,P
          XD1(I)=ZERO
          XD2(I)=ZERO
30      CONTINUE
C
      For each individual time series, sufficient
      statistics are computed and accumulated
C
      DO 60 I=1,N
          DO 40 J=1,T
40          YBAR(J)=Y(I,J)
          CALL ARSUFF(YBAR,T,1,DLIN,DQUAD,IFAU)
          QS(1)=QS(1)+DQUAD(1)
          QS(2)=QS(2)+DQUAD(2)
          QS(3)=QS(3)+DQUAD(3)
          QS(4)=QS(4)+DLIN(1)**2
          QS(5)=QS(5)+DLIN(1)*DLIN(2)
          QS(6)=QS(6)+DLIN(2)**2
          DO 50 J=1,P
              XD1(J)=XD1(J)+X(I,J)*DLIN(1)
              XD2(J)=XD2(J)+X(I,J)*DLIN(2)
50          CONTINUE
60      CONTINUE
C
      Computes d(i)'X(X'X)**(-1)X'd(j) for i,j=1,2
C
      QS(7)=PROD(XD1,XXINV,XD1,P)
      QS(8)=PROD(XD1,XXINV,XD2,P)

```

```

      QS(9)=PROD(XD2,XXINV,XD2,P)
C
C      Computing column means and their sufficient statistics
C
      DO 80 J=1,T
        YBAR(J)=ZERO
        DO 70 I=1,N
70          YBAR(J)=YBAR(J)+Y(I,J)
        YBAR(J)=YBAR(J)/N
80      CONTINUE
      CALL ARSUFF(YBAR,T,1,DLIN,DQUAD,IFAU)
      QS(10)=DQUAD(1)
      QS(11)=DQUAD(2)
      QS(12)=DQUAD(3)
      QS(13)=DLIN(1)
      QS(14)=DLIN(2)
      RETURN
      END

C----- SUBROUTINE ARAVLK -----
C
C Computes the log-likelihood and the components of the analysis of
C variance table supposing that the errors follow an AR(1) stationary
C normal process, and that the autoregressive parameter is equal to
C alpha. The sufficient statistics must have been previously computed
C using SUBROUTINE ARAVSS.
C-----
      SUBROUTINE ARAVLK(ALPHA,N,T,P,QS,XD1,XD2,XXINV,LOGLIK,GM,
+          BETA,SE,SIGMA2,PSI,SS,DF,RANDOM,TIME,IFAU)
C
C ALGORITHM AS 246.2 APPL. STATIST. (1989), VOL.38, NO. 2
C
      INTEGER T,P,DF(6),DFR
      REAL LOGLIK,SS(6),BETA(P),SE(P)
      REAL XD1(P),XD2(P),XXINV(P,P),QS(14),DELTA,RSS,DA,HA,BA
      LOGICAL RANDOM,TIME
      DELTA(B11,B12,B22)=B11-2.0*ALPHA*B12+ALPHA*ALPHA*B22
C
C Checks whether alpha is between -1 and 1
C
      IF(ALPHA**2.LT.1.0) THEN
        IFAU=0
      ELSE
        IFAU=1
        RETURN
      ENDIF
C
      FN=FLOAT(N)
      TAU=T-(T-2)*ALPHA
      CTAU=(1.0-ALPHA)/TAU
C
C Computes D(alpha), H(alpha), B(alpha)
C
      DA=DELTA(QS(1),QS(2),QS(3))
      HA=DELTA(QS(4),QS(5),QS(6))
      BA=DELTA(QS(7),QS(8),QS(9))
      RSS=DA
      DFR=N*T
C

```

```
C      Subtracts required sum of squares from RSS
C      and computes profile log-likelihood
C
GM=(QS(13)-ALPHA*QS(14))/TAU
SS(1)=CTAU*FN*(GM*TAU)**2
DF(1)=1
SS(6)=DA
DF(6)=N*T
DO 10 I=2,5
  SS(I)=0.0
  DF(I)=0
10  CONTINUE
IF(P.GT.1) THEN
  SS(2)=CTAU*BA-SS(1)
  DF(2)=P-1
ENDIF

C
C      Branch for time effect
C
IF(TIME) THEN
  SS(4)=FN*DELTA(QS(10),QS(11),QS(12))-SS(1)
  DF(4)=T-1
  RSS=RSS-SS(4)
  DFR=DFR-DF(4)
ENDIF

IF(RANDOM) THEN

C
C      Random effect model
C
  SS(3)=(HA-BA)*CTAU
  DF(3)=N-P
  PSI=SS(3)/FN
  RSS=RSS-CTAU*HA
  DFR=DFR-N
  SIGMA2=RSS/((T-1)*FN)
  IF(PSI.LT.SIGMA2) THEN
    SIGMA2=(RSS+CTAU*(HA-BA))/(FN*T)
    PSI=SIGMA2
  ENDIF
  LOGLIK=(T-1)*ALOG(SIGMA2)+ALOG(PSI)-ALOG(1.0-ALPHA**2)
ELSE

C
C      Fixed effect model
C
  RSS=RSS-BA*CTAU
  DFR=DFR-P
  SIGMA2=RSS/(N*T)
  PSI=SIGMA2
  LOGLIK=T*ALOG(SIGMA2)-ALOG(1.0-ALPHA**2)
ENDIF

SS(5)=RSS
DF(5)=DFR
LOGLIK=-0.5*FN*LOGLIK

C
C      Computes estimates of BETA()
C
DO 20 I=1,P
  BETA(I)=0.0
  SE(I)=(XD1(I)-ALPHA*XD2(I))/TAU
```



```
20    CONTINUE
      DO 40 I=1,P
        DO 30 J=1,P
30      BETA(I)=BETA(I)+XXINV(I,J)*SE(J)
40    CONTINUE
C
C      Computes standard errors for BETA()
C
      U=PSI/((1.0-ALPHA)*TAU)
      DO 50 I=1,P
50    SE(I)=SQRT(U*XXINV(I,I))
      RETURN
      END
```

```
C---- SUBROUTINE ARSUFF -----
C
C  Computes sufficient statistics for stationary autoregressive
C  normal process Y(1),...,Y(T) of order ORDER.
C  The output values are stored in vector DLIN (linear terms) and
C  DQUAD (quadratic terms, packed upper triangular).
C  A. Azzalini (Dipart. di Statistica, Universita` di Padova) Feb.1982
C-----
```

```
      SUBROUTINE ARSUFF(Y,T,ORDER,DLIN,DQUAD,IFAU)
C
C  ALGORITHM AS 246.3  APPL. STATIST. (1989), VOL.38, NO. 2
C
      INTEGER T,ORDER,R,S,SMR
      REAL Y(T),DLIN(ORDER+1),DQUAD((ORDER+1)*(ORDER+2)/2)
      IFAU=0
      IF(ORDER.LT.0) IFAU=1
      IF(T.LE.2*ORDER) IFAU=IFAU+2
      IF(IFAU.GT.0) RETURN
      M=ORDER+1
      N=M*(ORDER+2)/2
      SUM1=0.
      SUM2=0.
      DO 10 J=M,T-ORDER
        YJ=Y(J)
        SUM1=SUM1+YJ
        SUM2=SUM2+YJ*YJ
10    CONTINUE
      DLIN(M)=SUM1
      DQUAD(N)=SUM2
      DO 20 K=1,ORDER
        R=ORDER-K+1
        YJ=Y(R)
        SUM1=SUM1+YJ
        SUM2=SUM2+YJ*YJ
        YJ=Y(T-R+1)
        SUM1=SUM1+YJ
        SUM2=SUM2+YJ*YJ
        DLIN(R)=SUM1
        DQUAD(R*(R+1)/2)=SUM2
20    CONTINUE
      DO 50 SMR=1,ORDER
        SUM2=0.
        DO 30 J=M,T-ORDER+SMR
          SUM2=SUM2+Y(J)*Y(J-SMR)
30    CONTINUE
        DQUAD(N-SMR)=SUM2
```

```
      DO 40 R=ORDER-SMR,1,-1
        S=R+SMR
        SUM2=SUM2+Y(R)*Y(S)+Y(T-R+1)*Y(T-S+1)
        DQUAD(S*(S-1)/2+R)=SUM2
40     CONTINUE
50     CONTINUE
      RETURN
      END
```

C-----

C

```
      FUNCTION PROD(XD1,XX,XD2,M)
      REAL A,ZERO,XD1(M),XD2(M),XX(M,M)
      DATA ZERO/0.0/
      PROD=ZERO
      DO 20 I=1,M
        A=ZERO
        DO 10 J=1,M
10         A=A+XX(I,J)*XD2(J)
20        PROD=PROD+XD1(I)*A
      RETURN
      END
```

```
FUNCTION EdgeOperation(VAR Graph : GraphType; m, n : NodeType;  
                      NodeSet : CliqueType; Add : boolean) : integer;
```

```
{Algorithm AS 247.1 Appl. Statist. (1989) Vol.38, No.2}
```

```
VAR
```

```
    exist      : boolean;  
    error      : integer;  
    i          : integer;
```

```
BEGIN
```

```
exist := false;
```

```
WITH Graph DO
```

```
    FOR i := 1 TO NoOfCliques DO
```

```
        IF ([m,n] <= cliques[i]) THEN
```

```
            exist := true;
```

```
error := 0;
```

```
{ Check for invalid inputs.}
```

```
IF NOT (m IN NodeSet) OR NOT (n IN NodeSet) THEN
```

```
    m := n;
```

```
IF m = n THEN
```

```
    error := 1
```

```
ELSE
```

```
    IF exist AND Add THEN
```

```
        error := 2
```

```
    ELSE
```

```
        IF NOT exist AND NOT Add THEN
```

```
            error := 3
```

```
        ELSE
```

```
            {If input ok then perform operation.}
```

```
            IF Add THEN
```

```
                AddEdge(Graph,m,n)
```

```
            ELSE
```

```
                DeleteEdge(Graph,m,n);
```

```
EdgeOperation := error;
```

```
END; { of EdgeOperation }
```

```
PROCEDURE AddEdge (VAR Graph : GraphType;  
                  m, n : NodeType);
```

```
{Algorithm AS 247.2 Appl. Statist. (1989) Vol.38, No.2}
```

```
{ This procedure replaces the cliques of the current graph held in the  
  structure cliques of type GraphType by the cliques of the graph  
  obtained by adding edge m-n.}
```

```
VAR
```

```
    mSubgraph, nSubgraph, mnSubgraph : GraphType;
```

```
    ThisClique, mClique, nClique, mnClique : CliqueType;
```

```
    i, j, k, NoOfCliques : CliqueIndex;
```

```
    mCliqueOK, nCliqueOK, mnCliqueOK : ARRAY[1..Cliquemax] OF Boolean;
```

```
BEGIN
```

```
NoOfCliques := Graph.NoOfCliques;
```

```
Graph.NoOfCliques := 0;
```

```
mSubgraph.NoOfCliques := 0;
```

```
nSubgraph.NoOfCliques := 0;
```

```
mnSubgraph.NoOfCliques := 0;
```

```
{ 1. Scan through the cliques of the current graph in Graph. if a clique contains neither node of the edge, copy it as a clique of the new graph back to Graph. If it contains one of the nodes copy it as one of the temporary cliques to mSubgraph or nSubgraph setting the associated flag true.}
```

```
FOR i := 1 TO NoOfCliques DO  
  BEGIN  
    ThisClique := Graph.Cliques[i];  
    IF m IN ThisClique THEN  
      WITH mSubgraph DO  
        BEGIN  
          NoOfCliques := NoOfCliques + 1;  
          Cliques[NoOfCliques] := ThisClique;  
          mCliqueOK[NoOfCliques] := true  
        END  
      ELSE IF n IN ThisClique THEN  
        WITH nSubgraph DO  
          BEGIN  
            NoOfCliques := NoOfCliques + 1;  
            Cliques[NoOfCliques] := ThisClique;  
            nCliqueOK[NoOfCliques] := true  
          END  
        ELSE  
          WITH Graph DO  
            BEGIN  
              NoOfCliques := NoOfCliques + 1;  
              Cliques[NoOfCliques] := ThisClique  
            END  
          END;  
END;
```

```
{ 2. Compare each clique from mSubgraph with each clique from nSubgraph in turn, generate the clique created from the intersection of the pair combined with the nodes m and n (It will, most often, be simply the edge m-n) and put it into mnSubgraph, setting the associated flag true. Compare both of the creating cliques with the created one and if either is a subset of it, set the associated flag false. Compare the created one with all previous created ones; if it is a subset of any of them remove it; if any of them is a subset of it set their associated flags false. }
```

```
FOR i := 1 TO mSubgraph.NoOfCliques DO  
  BEGIN  
    mClique := mSubgraph.Cliques[i];  
    FOR j := 1 TO nSubgraph.NoOfCliques DO  
      BEGIN  
        nClique := nSubgraph.Cliques[j];  
        WITH mnSubgraph DO  
          BEGIN  
            mnClique := mClique * nClique + [m, n];  
            IF mClique <= mnClique THEN  
              mCliqueOK[i] := false;  
            IF nClique <= mnClique THEN  
              nCliqueOK[j] := false;  
            NoOfCliques := NoOfCliques + 1;  
            Cliques[NoOfCliques] := mnClique;  
            mnCliqueOK[NoOfCliques] := true;  
            k := 1;  
            WHILE NOT (mnClique <= Cliques[k]) DO  
              BEGIN
```

```
        IF mnClique >= Cliques[k] THEN
            mnCliqueOK[k] := false;
            k := k + 1
        END;
    IF k <> NoOfCliques THEN
        NoOfCliques := NoOfCliques - 1
    END
END
END;
```

{ 3. Scan mnSubgraph, mSubgraph and nSubgraph in turn, copying to Graph each clique whose associated flag is still set true.}

```
WITH Graph DO
BEGIN
    FOR i := 1 TO mnSubgraph.NoOfCliques DO
        IF mnCliqueOK[i] THEN
            BEGIN
                NoOfCliques := NoOfCliques + 1;
                Cliques[NoOfCliques] := mnSubgraph.Cliques[i]
            END;
        FOR i := 1 TO mSubgraph.NoOfCliques DO
            IF mCliqueOK[i] THEN
                BEGIN
                    NoOfCliques := NoOfCliques + 1;
                    Cliques[NoOfCliques] := mSubgraph.Cliques[i]
                END;
            FOR i := 1 TO nSubgraph.NoOfCliques DO
                IF nCliqueOK[i] THEN
                    BEGIN
                        NoOfCliques := NoOfCliques + 1;
                        Cliques[NoOfCliques] := nSubgraph.Cliques[i]
                    END
                END
            END
        END
    END;{of AddEdge }
```

```
PROCEDURE DeleteEdge (VAR Graph : GraphType;
    m, n : NodeType);
```

{Algorithm AS 247.3 Appl. Statist. (1989) Vol.38, No.2}

{ This procedure replaces the cliques of the current graph held in the structure cliques of type GraphType by the cliques of the graph obtained by deleting edge m-n. }

```
VAR
    Subgraph : GraphType;
    ThisClique : CliqueType;
    i, j, NoOfCliques, buffer : CliqueIndex;
```

```
BEGIN
    NoOfCliques := Graph.NoOfCliques;
    Graph.NoOfCliques := 0;
    Subgraph.NoOfCliques := 0;
```

{ 1. Scan through the cliques of the current graph held in Graph. For each clique containing the edge m-n, store in Subgraph the two (possibly redundant) cliques obtained by deleting each node of the edge. Copy each clique not containing the edge back to Graph as a clique of the new graph. }

```
FOR i := 1 TO NoOfCliques DO
  BEGIN
    ThisClique := Graph.Cliques[i];
    IF [m, n] <= ThisClique THEN
      WITH Subgraph DO
        BEGIN
          NoOfCliques := NoOfCliques + 2;
          Cliques[NoOfCliques - 1] := ThisClique - [m];
          Cliques[NoOfCliques] := ThisClique - [n];
        END
      ELSE
        WITH Graph DO
          BEGIN
            NoOfCliques := NoOfCliques + 1;
            Cliques[NoOfCliques] := ThisClique
          END
        END;

```

{ 2. Compare each clique in Subgraph with those directly placed in Graph. If it is a subset of any clique in Graph it is ignored, otherwise it is added to Graph. The searching process uses a variation of the technique of adding the item as a sentinel at the end of the sequence being searched to simplify the loop termination. Here, since Graph is being extended but the searching takes place only over its initial part, a buffer is left at the interface to be filled in just before exit. }

```
WITH Graph DO
  BEGIN
    NoOfCliques := NoOfCliques + 1;
    buffer := NoOfCliques;
    FOR i := 1 TO Subgraph.NoOfCliques DO
      BEGIN
        ThisClique := Subgraph.Cliques[i];
        Cliques[buffer] := ThisClique;
        j := 1;
        WHILE NOT (ThisClique <= Cliques[j]) DO
          j := j + 1;
        IF j = buffer THEN
          BEGIN
            NoOfCliques := NoOfCliques + 1;
            Cliques[NoOfCliques] := ThisClique
          END
        END;
        Cliques[buffer] := Cliques[NoOfCliques];
        NoOfCliques := NoOfCliques - 1
      END
    END;{of DeleteEdge }

```

```

SUBROUTINE EDFGOF(X, N, ITEST, Z, XBAR, S2, D, V, W2, W2P, U2,
+ U2P, A2, A2P, IFAULT)

```

```

C
C ALGORITHM AS 248.1 APPL. STATIST. (1989), VOL.38, NO. 3
C

```

```

C Tests a sample for uniformity, normality or exponentiality
C using goodness-of-fit statistics based on the empirical
C distribution function
C

```

```

C Auxiliary routines called: ALNORM from AS 66
C

```

```

INTEGER I, IFAULT, ITEST, J, N
REAL X(N), Z(N), XBAR, S2, D, V, W2, W2P, U2, U2P, A2, A2P, RN,
+ ROOTN, RN2, S, ZERO, PT01, PT05, PT1, PT11, PT12, PT155,
+ PT16, PT2, PT24, PT26, PT3, PT35, PT4, PT5, PT6, PT75, PT8,
+ PT82, PT85, ONE, TWOP25, WCUT2(3), WCOEF2(4, 3), WCUT3(3),
+ WCOEF3(4, 3), UCUT2(3), UCOEF2(4, 3), UCUT3(3),
+ UCOEF3(4, 3), ACUT2(3), ACOEF2(4, 3), ACUT3(3), ACOEF3(4, 3)
REAL ALNORM, PVALUE
DATA ZERO, PT01, PT05, PT1, PT11, PT12, PT155, PT16, PT2, PT24
+ /0.0, 0.01, 0.05, 0.1, 0.11, 0.12, 0.155, 0.16, 0.2, 0.24/
DATA PT26, PT3, PT35, PT4, PT5, PT6, PT75, PT8, PT82, PT85, ONE
+ /0.26, 0.3, 0.35, 0.4, 0.5, 0.6, 0.75, 0.8, 0.82, 0.85, 1.0/
DATA TWOP25 /2.25/
DATA WCUT2, WCUT3, UCUT2, UCUT3, ACUT2, ACUT3 /0.0275, 0.051,
+ 0.092, 0.035, 0.074, 0.160, 0.0262, 0.048, 0.094, 0.029,
+ 0.062, 0.120, 0.200, 0.340, 0.600, 0.260, 0.510, 0.950/
DATA ((WCOEF2(I,J), J=1,3), I=1,4) / -13.953, 775.5, -12542.61,
+ -5.903, 179.546, -1515.29, 0.886, -31.62, 10.897, 1.111,
+ -34.242, 12.832/
DATA ((WCOEF3(I,J), J=1,3), I=1,4) / -11.334, 459.098, -5652.1,
+ -5.779, 132.89, -866.58, 0.586, -17.87, 7.417, 0.447,
+ -16.592, 4.849/
DATA ((UCOEF2(I,J), J=1,3), I=1,4) / -13.642, 766.31, -12432.74,
+ -6.3328, 214.57, -2022.28, 0.8510, -32.006, -3.45, 1.325,
+ -38.918, 16.45/
DATA ((UCOEF3(I,J), J=1,3), I=1,4) / -11.703, 542.5, -7574.59,
+ -6.3288, 178.1, -1399.49, 0.8071, -25.166, 8.44, 0.7663,
+ -24.359, 4.539/
DATA ((ACOE2(I,J), J=1,3), I=1,4) / -13.436, 101.14, -223.73,
+ -8.318, 42.796, -59.938, 0.9177, -4.279, -1.38, 1.2937,
+ -5.709, 0.0186/
DATA ((ACOE3(I,J), J=1,3), I=1,4) / -12.2204, 67.459, -110.3,
+ -6.1327, 20.218, -18.663, 0.9209, -3.353, 0.3, 0.731, -3.009,
+ 0.15/

```

```

C
C IFAULT = 1
C IF (ITEST .LT. 1 .OR. ITEST .GT. 3) RETURN
C IFAULT = 2
C IF (N .LT. 2 .OR. (ITEST .EQ. 2 .AND. N .EQ. 2)) RETURN
C IFAULT = 3
C DO 10 I = 2, N
C IF (X(I) .LT. X(I-1)) RETURN
10 CONTINUE
C RN = N
C ROOTN = SQRT(RN)
C RN2 = RN * RN
C IF (ITEST .EQ. 1) THEN

```

```

C
C Test for uniformity (F(x) is completely specified)
C

```

```

        IFAULT = 0
        CALL STATS(X, N, D, V, W2, U2, A2, IFAULT)
        IF (IFAULT .NE. 0) RETURN
C
C   Modifications when F(x) is completely specified
C
        D = D * (ROOTN + PT12 + PT11 / ROOTN)
        V = V * (ROOTN + PT155 + PT24 / ROOTN)
        W2 = (W2 - PT4 / RN + PT6 / RN2) * (ONE + ONE / RN)
        U2 = (U2 - PT1 / RN + PT1 / RN2) * (ONE + PT8 / RN)
        RETURN
    ELSE
C
C   Estimate the mean XBAR
C
        XBAR = ZERO
        DO 20 I = 1, N
            XBAR = XBAR + X(I)
20    CONTINUE
        XBAR = XBAR / RN
        IF (ITEST .EQ. 2) THEN
C
C   Test for normality (MU and SIGMA**2 unspecified).
C   First estimate the variance S**2
C
        IFAULT = 5
        S2 = ZERO
        DO 30 I = 1, N
            S2 = S2 + (X(I) - XBAR)**2
30    CONTINUE
        S2 = S2 / (RN - ONE)
        IF (S2 .LE. ZERO) RETURN
C
C   Compute Z(I) = F(XI - XBAR)/S
C
        S = SQRT(S2)
        DO 40 I = 1, N
            Z(I) = ALNORM((X(I) - XBAR)/S, .FALSE.)
40    CONTINUE
        CALL STATS(Z, N, D, V, W2, U2, A2, IFAULT)
        IF (IFAULT .NE. 0) RETURN
C
C   Modifications when F(x) is the normal distribution
C
        D = D * (ROOTN - PT01 + PT85 / ROOTN)
        V = V * (ROOTN + PT05 + PT82 / ROOTN)
        W2 = W2 * (ONE + PT5 / RN)
        W2P = PVALUE(W2, WCUT2, WCOEF2)
        U2 = U2 * (ONE + PT5 / RN)
        U2P = PVALUE(U2, UCUT2, UCOEF2)
        A2 = A2 * (ONE + PT75 / RN + TWOP25 / RN2)
        A2P = PVALUE(A2, ACUT2, ACOEF2)
        RETURN
    ELSE
C
C   Test for exponentiality (scale parameter unspecified)
C
        IFAULT = 6
        IF (XBAR .LE. ZERO) RETURN
        DO 50 I = 1, N
            Z(I) = ONE - EXP(-X(I) / XBAR)

```



```

50      CONTINUE
        CALL STATS(Z, N, D, V, W2, U2, A2, IFAULT)
        IF (IFAULT .NE. 0) RETURN
C
C      Modifications when F(x) is the exponential distribution
C
        D = (D - PT2 / RN) * (ROOTN + PT26 + PT5 / ROOTN)
        V = (V - PT2 / RN) * (ROOTN + PT24 + PT35 / ROOTN)
        W2 = W2 * (ONE + PT16 / RN)
        W2P = PVALUE(W2, WCUT3, WCOEF3)
        U2 = U2 * (ONE + PT16 / RN)
        U2P = PVALUE(U2, UCUT3, UCOEF3)
        A2 = A2 * (ONE + PT3 / RN)
        A2P = PVALUE(A2, ACUT3, ACOEF3)
        RETURN
      END IF
    END IF
  END
C
C      SUBROUTINE STATS(Z, N, D, V, W2, U2, A2, IFAULT)
C
C      ALGORITHM AS 248.2 APPL. STATIST. (1989), VOL.38, NO. 3
C
C      Computes the goodness-of-fit statistics D, V, W**2, U**2 and
C      A**2 from the transformed Z values
C
      INTEGER I, IFAULT, N, NI
      REAL Z(N), D, V, W2, U2, A2, RI, RN, DPLUS, DMINUS, D1, D2, SUMZ,
+      TWON, ZM1, A2SUM, ZERO, SMALL, HALF, ONE, TWO, TWELVE
C
C      Initialize constants
C
      DATA ZERO/0.0/, SMALL/1.E-37/, HALF/0.5/, ONE/1.0/,
+      TWO/2.0/, TWELVE/12.0/
C
      RN = N
      TWON = TWO * RN
C
C      Calculating the Kolmogorov statistics DPLUS, DMINUS, D and
C      the Kuiper statistic V.
C
      DPLUS = ZERO
      DMINUS = ZERO
      IFAULT = 4
      DO 10 I = 1, N
        IF (Z(I) .LE. ZERO .OR. Z(I) .GE. ONE) RETURN
        RI = I
        D1 = RI / RN - Z(I)
        IF (D1 .GT. DPLUS) DPLUS = D1
        D2 = Z(I) - (RI - ONE) / RN
        IF (D2 .GT. DMINUS) DMINUS = D2
10    CONTINUE
      IFAULT = 0
      D = DPLUS
      IF (DMINUS .GT. DPLUS) D = DMINUS
      V = DPLUS + DMINUS
C
C      Calculating the Cramer-von Mises statistic W2 and the Watson
C      statistic U2
C

```

```
      W2 = ONE / (TWELVE * RN)
      SUMZ = ZERO
      DO 20 I = 1, N
        W2 = W2 + (Z(I) - (TWO * I - ONE) / TWON)**2
        SUMZ = SUMZ + Z(I)
20 CONTINUE
      U2 = W2 - RN * (SUMZ / RN - HALF)**2
C
C   Calculating the Anderson-Darling statistic A2
C
      A2SUM = ZERO
      NI = N
      DO 30 I = 1, N
        IF (Z(I) .LT. SMALL) Z(I) = SMALL
        ZM1 = ONE - Z(NI)
        IF (ZM1 .LT. SMALL) ZM1 = SMALL
        A2SUM = A2SUM + (TWO * I - ONE) * LOG(Z(I) * ZM1)
        NI = NI - 1
30 CONTINUE
      A2 = -A2SUM / RN - RN
C
      RETURN
      END
C
C   REAL FUNCTION PVALUE(T, CUT, COEF)
C
C   ALGORITHM AS 248.3 APPL. STATIST. (1989), VOL.38, NO. 3
C
C   Computes the approximate significance level for W**2, U**2 or
C   A**2 when testing for normality or exponentiality
C
      INTEGER I, J
      REAL T, CUT(3), COEF(4, 3), ONE
      DATA ONE /1.0/
C
      I = 4
      DO 10 J = 1, 3
        IF (T .LT. CUT(J)) I = I - 1
10 CONTINUE
      PVALUE = EXP(COEF(I, 1) + T * (COEF(I, 2) + T * COEF(I, 3)))
      IF (I .LT. 3) PVALUE = ONE - PVALUE
C
      RETURN
      END
```

c This file contains algorithm AS 249 for the evaluation of the mean and  
c covariance of the truncated multinormal distribution, followed by code  
c by the same authors for the numerical estimation of the observed  
c information matrix (= maximum likelihood covariance estimates). As  
c the latter is not in the published algorithm, a test program is included  
c showing its use. For further details, contact Phil Leppard, Statistics  
c Department, University of Adelaide. E-mail: PLEPPARD@f.ua.oz

c  
c  
c  
c subroutine mvntrc(n,bounds,u,v,ndim,eps,tmean,tvar,ifault)

c ALGORITHM AS 249 APPL. STATIST. (1989) VOL. 38, NO. 3 (?)

c Auxiliary routines required: MULNOR and MATINV from AS 195.  
c MATINV calls LINRG from the IMSL Stat/Library, but AS 7 can  
c be substituted.

c dimension bounds(ndim),u(ndim),v(ndim,ndim),tmean(ndim,1),  
+ tvar(ndim,ndim,1),r(5,5),rinv(5,5),rq(5,5),rqr(5,5),  
+ ind(5),iord(5),sd(5),a(5),aq(5),aqr(5),  
+ phiu(5),phib(5,5),phin1(5),ephin1(5),phin2(5,5),ephin2(5,5),  
+ alpha(3),sum(3),w(10),ww(5,5)  
c data zero,one,two/0.0, 1.0, 2.0/  
c data twopi/6.283185308/  
c data rtwopi/2.506628275/  
c data alphas/1.e-3/  
c data ind/5\*0/

c ifault=0  
c if(n.gt.5) go to 100

c Calculate normalised truncation points and correlation  
c matrix R

c do 1 i=1,n  
c iord(i)=i  
c if(v(i,i).le.zero) go to 200  
1 sd(i)=sqrt(v(i,i))  
c do 2 i=1,n  
c a(i)=(bounds(i)-u(i))/sd(i)  
c do 2 j=1,n  
2 r(i,j)=v(i,j)/(sd(i)\*sd(j))

c Order variates by decreasing size of range of integration  
c to increase the speed of MULNOR at highest level  
c (Smallest standardised boundary = largest range, etc)

c  
c if(n.gt.2) then  
c do 3 i=1,n-1  
c do 3 j=i+1,n  
c if(a(i).gt.a(j)) then  
c aa=a(i)  
c a(i)=a(j)  
c a(j)=aa  
c k=iord(i)  
c iord(i)=iord(j)  
c iord(j)=k  
c do 4 k=1,n  
c aa=r(i,k)  
c r(i,k)=r(j,k)

```
4      r(j,k)=aa
      do 5 k=1,n
        aa=r(k,i)
        r(k,i)=r(k,j)
5      r(k,j)=aa
      end if
3     continue
end if

c
c
c     Evaluate n dimensional integral alpha = Phi(a:R) and error bound
c
c     alpha(1)=alpha+error   alpha(2)=alpha   alpha(3)=alpha-error
c
c     l=0
do 6 i=1,n
  do 6 j=1,i-1
    l=l+1
6  w(l)=r(i,j)
  call mulnor(w,a,w,eps,n,ind,alpha(2),error,i)
  alpha(1)=alpha(2)+error
  alpha(3)=alpha(2)-error
  if(i.ne.0.or.alpha(2).le.alphas) go to 400

c
c
c     Evaluate univariate and bivariate normal densities
c     Initialise multinormals of dimension n-1 and n-2
c
c
do 7 i=1,n
  phiu(i)=exp(-a(i)*a(i)/two)/rtwopi
  phin1(i)=one
  ephin1(i)=zero
  do 7 j=i+1,n
    phib(i,j)=(a(i)*a(i)-two*r(i,j)*a(i)*a(j)+a(j)*a(j))/
+    (two*(1-r(i,j)*r(i,j)))
    phib(i,j)=exp(-phib(i,j))/(twopi*sqrt(one-r(i,j)*r(i,j)))
    phib(j,i)=phib(i,j)
    phin2(i,j)=one
    phin2(j,i)=one
    ephin2(i,j)=zero
7  ephin2(j,i)=zero

c
c
c     Calculation of n-1 dimensional integrals Phi(Aq:Rq)
c
c
c     if(n.gt.1) then
do 8 i=1,n
  do 8 j=1,n
8  rinv(i,j)=r(i,j)
  call matinv(rinv,5,n,ifault)
  if(ifault.gt.0) go to 300
  do 9 iq=1,n
    m1=0

c
c     Determine bounds of integration,vector Aq
c
c
do 10 i=1,n
  if(i.ne.iq) then
    m1=m1+1
```

```

aq(m1)=(a(i)-r(i,iq)*a(iq))/sqrt(one-r(i,iq)*r(i,iq))
m2=0
do 11 j=1,n
  if(j.ne.iq) then
    m2=m2+1
    ww(m1,m2)=rinv(i,j)
  end if
11  continue
end if
10  continue
c
c  Determine n-1 x n-1 correlation matrix Rq
c
  call matinv(ww,5,n-1,ifault)
  if(ifault.gt.0) go to 300
  do 13 i=1,m1
    do 13 j=1,m1
13   rq(i,j)=ww(i,j)/sqrt(ww(i,i)*ww(j,j))
c
c  Evaluate n-1 dimensional integral Phi(Aq:Rq) and error bound
c
  l=0
  do 14 i=1,m1
    do 14 j=1,i-1
      l=l+1
14   w(l)=rq(i,j)
    call mulnor(w,aq,w,eps,n-1,ind,phin1(iq),ephin1(iq),i)
9   if(i.ne.0) go to 500
end if
c
c  Calculation of n-2 dimensional integrals Phi(Aqr:Rqr)
c
  if(n.gt.2) then
do 15 iq=1,n
  do 15 ir=iq+1,n
c
c  Determine n-2 x n-2 correlation matrix Rqr
c
  m1=0
  do 16 i=1,n
    if(i.ne.iq.and.i.ne.ir) then
      m1=m1+1
      m2=0
      do 17 j=1,n
        if(j.ne.iq.and.j.ne.ir) then
          m2=m2+1
          ww(m1,m2)=rinv(i,j)
        end if
17   continue
      end if
16  continue
      call matinv(ww,5,n-2,ifault)
      if(ifault.gt.0) go to 300
      do 19 i=1,m1
        do 19 j=1,m1
19   rqr(i,j)=ww(i,j)/sqrt(ww(i,i)*ww(j,j))
c
c  Determine bounds of integration,vector Aqr
c
  m2=0
  do 20 i=1,n

```

```

        if(i.ne.iq.and.i.ne.ir) then
        m2=m2+1
        bsqr=(r(iq,i)-r(iq,ir)*r(ir,i))/(one-r(iq,ir)*r(iq,ir))
        bsrq=(r(ir,i)-r(iq,ir)*r(iq,i))/(one-r(iq,ir)*r(iq,ir))
        rsrq=(one-r(i,iq)*r(i,iq))*(one-r(ir,iq)*r(ir,iq))
        rsrq=(r(i,ir)-r(i,iq)*r(iq,ir))/sqrt(rsrq)
        aqr(m2)=a(i)-bsqr*a(iq)-bsrq*a(ir)
        aqr(m2)=aqr(m2)/sqrt((one-r(i,iq)*r(i,iq))*(one-rsrq*rsrq))
        end if
20      continue
c
c      Evaluate n-2 dimensional integral Phi(Aqr:Rqr) and error bound
c
        l=0
        do 21 i=1,m2
          do 21 j=1,i-1
            l=l+1
21      w(l)=rqr(i,j)
            call mulnor(w,aqr,w,eps,n-2,ind,phin2(iq,ir),ephin2(iq,ir),i)
            if(i.ne.0) go to 600
            phin2(ir,iq)=phin2(iq,ir)
15      ephin2(ir,iq)=ephin2(iq,ir)
            end if
c
c      Calculation of E(Xi) ,with upper and lower bounds
c      Tallis(1961) , equation (3).
c
        do 22 i=1,n
          do 23 j=1,3
23      sum(j)=zero
          do 24 j=1,n
            aa=r(i,j)*phiu(j)
            do 25 k=1,3
25      w(k)=aa*(phin1(j)+(k-2)*ephin1(j))
            if(w(1).gt.w(3)) then
              aa=w(1)
              w(1)=w(3)
              w(3)=aa
            end if
            do 24 k=1,3
24      sum(k)=sum(k)+w(k)
            k=iord(i)
            do 22 j=1,3
22      tmean(k,j)=sum(j)/alpha(j)
c
c      Calculation of E(Xi,Xj), with upper and lower bounds
c      Tallis(1961), equation (4).
c
        do 26 i=1,n
          do 26 j=i,n
            do 27 k=1,3
27      sum(k)=zero
            do 28 k=1,n
              aa=r(k,i)*r(k,j)*a(k)*phiu(k)
              do 29 m1=1,3
29      w(m1)=aa*(phin1(k)+(m1-2)*ephin1(k))
              if(w(1).gt.w(3)) then
                aa=w(1)
                w(1)=w(3)
                w(3)=aa
              end if

```

```

do 30 m1=1,3
sum(m1)=sum(m1)+w(m1)
do 28 l=1,n
  if(l.ne.k) then
    aa=(r(l,j)-r(k,l)*r(k,j))*r(k,i)*phib(k,l)
do 31 m1=1,3
w(m1)=aa*(phin2(k,l)+(m1-2)*ephin2(k,l))
if(w(1).gt.w(3)) then
  aa=w(1)
  w(1)=w(3)
  w(3)=aa
end if
do 32 m1=1,3
sum(m1)=sum(m1)+w(m1)
end if
28 continue
m1=iord(i)
m2=iord(j)
do 26 m3=1,3
  tvar(m1,m2,m3)=r(i,j)+sum(m3)/alpha(m3)
26 tvar(m2,m1,m3)=tvar(m1,m2,m3)
c
c Calculate truncated covariance matrix, with upper and
c lower bounds. Original scale restored.
c
do 33 i=1,n
  do 33 j=i,n
    tvar(i,j,2)=(tvar(i,j,2)-tmean(i,2)*tmean(j,2))*sd(i)*sd(j)
    l=0
    do 34 m1=1,3,2
      do 34 m2=1,3,2
        do 34 m3=1,3,2
          l=l+1
34 w(l)=(tvar(i,j,m1)-tmean(i,m2)*tmean(j,m3))*sd(i)*sd(j)
tvar(i,j,1)=min(w(1),w(2),w(3),w(4),w(5),w(6),w(7),w(8))
tvar(i,j,3)=max(w(1),w(2),w(3),w(4),w(5),w(6),w(7),w(8))
do 33 k=1,3
33 tvar(j,i,k)=tvar(i,j,k)
c
c Original location and scale restored to truncated mean
c
do 35 i=1,n
  do 35 j=1,3
35 tmean(i,j)=u(i)+sd(i)*tmean(i,j)
c
c Normal termination of subroutine
c
return
c
c Error conditions
c
c
100 ifault=100
c Dimension n greater than 5
return
c
200 ifault=200+i
c i-th variance less than or equal to zero
return
c
300 ifault=300+i

```

```
c      Error in inversion of i x i matrix
      return
c
c      ifault=400+i
c      Error in Phi(n)...MULNOR error number i
c          or
c      truncated region, ie alpha, "too small" (then ifault=400)
c
      return
c
c      ifault=500+i
c      Error in Phi(n-1)...MULNOR error number i
      return
c
c      ifault=600+i
c      Error in Phi(n-2)...MULNOR error number i
      return
c
      end
c
c      **      End of AS 249
c
c-----
c
      program covtest
      implicit double precision (a-h,o-z)
      dimension cov(5,5),a(5),b(5),x(5)
      common r(1000),nn,y(1000,3)
      external fnorm,fmult
      data a,b/10*777.d0/

C      TEST RUN FROM N(0,4)

      nn=100
      x(1)=0.
      x(2)=0.
      do 1 i=1,nn
          r(i)=dnorin((i-.5)/nn)*2
          x(1)=x(1)+r(i)/nn
1      x(2)=x(2)+r(i)*r(i)
          x(2)=(x(2)-nn*x(1)*x(1))/nn
          print 5,x(1),x(2)
5      format(/5x'Mle = ',5f10.3)
          call mlecov(fnorm,x,2,a,b,cov,5,10,1.d-06,1,ifault)
          print 3,ifault
3      format(/5x'Final estimate   ifault='i4)
          do 4 i=1,2
4      print 2,(cov(i,j),j=1,2)
2      format(5x,3f10.5)
          do 20 i=1,2
20     cov(i,i)=sqrt(cov(i,i))
          cov(1,2)=cov(1,2)/(cov(1,1)*cov(2,2))
          cov(2,1)=cov(1,2)
          print 26
26     format(40x'Standard errors and correlations')
          do 21 i=1,2
21     print 22,(cov(i,j),j=1,2)
22     format(40x,3f10.5)

C      TEST RUN FROM MULTINOMIAL P=(.5,.2,.2,.1)
```



```
      nn=4
      r(1)=500
      r(2)=200
      r(3)=200
      r(4)=100
      x(1)=.5
      x(2)=.2
      x(3)=.2
      x(4)=.1
      print 5,(x(i),i=1,3)
      call mlecov(fmult,x,3,a,b,cov,5,20,1.d-10,1,ifault)
      print 3,ifault
      do 8 i=1,3
8      print 2,(cov(i,j),j=1,3)
      do 23 i=1,3
23     cov(i,i)=sqrt(cov(i,i))
      do 25 i=1,3
      do 25 j=1,3
25     if(i.ne.j) cov(i,j)=cov(i,j)/(cov(i,i)*cov(j,j))
      print 26
      do 24 i=1,3
24     print 22,(cov(i,j),j=1,3)
      end
c
c
c
      subroutine matinv(cov,nd,n,ifault)
      implicit double precision (a-h,o-z)
      dimension cov(nd,1)
c
      call dlinrg(n,cov,nd,cov,nd)
      ifault=0
      return
      end
c
c
c
      double precision function fnorm(x)
      implicit double precision (a-h,o-z)
      common r(1000),nn
      dimension x(1)
c
      fnorm=0.
      do 73 i=1,nn
73     fnorm=fnorm-(r(i)-x(1))*(r(i)-x(1))
      fnorm=fnorm/(2*x(2))-nn*log(x(2))/2
      return
      end
c
c
c
      double precision function fmult(x)
      implicit double precision (a-h,o-z)
      dimension x(1),p(5)
      common r(1000),nn
c
      fmult=0.
      p(nn)=1.
      do 1 i=1,nn-1
      p(i)=x(i)
1     p(nn)=p(nn)-p(i)
```

```

      do 2 i=1,nn
2      fmult=fmult+r(i)*log(p(i))
      return
      end

c
c
c  **   End of test program and functions
c-----
c
      subroutine mlecov(f,theta,n,a,b,cov,nd,maxh,eps,iprint,ifault)
      implicit double precision (a-h,o-z)
      dimension cov(nd,1),theta(*),a(*),b(*),x(5),h(5),store(5,5)
      external f
      data zero,small,two,hun/0.d0, .001d0, 2.d0, 100.d0/

c
      ifault=0
      if(n.gt.5.or.n.gt.nd) go to 100

c
c      Determine initial values for h(i), i=1,..n
c
      do 1 i=1,n
          h(i)=small
          h(i)=max(h(i),abs(theta(i))/hun)
          if(a(i).eq.b(i)) go to 1
          if(theta(i).lt.a(i).or.theta(i).gt.b(i)) go to 200
          h(i)=min(h(i),abs(a(i)-theta(i)),abs(b(i)-theta(i)))
1      continue
      f00=f(theta)
      ncy=0
2      ncy=ncy+1
      if(ncy.gt.maxh) go to 300

c
c      Evaluation of diagonal elements of -I(theta)
c
      do 3 i=1,n
          cov(i,i)=-two*f00
          do 4 j=1,n
4          x(j)=theta(j)
          x(i)=x(i)-h(i)
          do 3 j=1,2
              cov(i,i)=cov(i,i)+f(x)
3          x(i)=x(i)+two*h(i)

c
c      Evaluation of off-diagonal elements of -I(theta)
c
      do 5 i=1,n
          jj=i+1
          if(jj.gt.n) go to 5
          do 7 j=jj,n
              cov(i,j)=cov(i,i)+cov(j,j)+two*f00
              do 6 k=1,n
6              x(k)=theta(k)
              x(i)=x(i)-h(i)
              x(j)=x(j)-h(j)
              do 8 k=1,2
                  cov(i,j)=cov(i,j)-f(x)
                  x(i)=x(i)+two*h(i)
8              x(j)=x(j)+two*h(j)
                  cov(i,j)=cov(i,j)/(two*h(i)*h(j))
7              cov(j,i)=cov(i,j)
5              cov(i,i)=-cov(i,i)/(h(i)*h(i))

```

```
c
c      In-place inversion of COV
c
c      call matinv(cov,nd,n,ifault)
c      if(ifault.ne.0) go to 400
c
c      Check for convergence
c
c      s=zero
c      if(ncy.eq.1) go to 9
c      do 10 i=1,n
c          do 10 j=i,n
10      s=max(s,abs(cov(i,j)-store(i,j)))
c
c      Display option if requested
c
c      if(iprint.eq.0) go to 11
c      print 12,ncy-1,s
12      format(//5x'Covariance estimate at halving ',i3/
+ 5x'Maximum absolute difference from previous estimate = ',e14.7)
c      do 13 i=1,n
c          print 14,(cov(i,j),j=1,n)
14      format(5x,5(e14.7,2x))
c
c      Vector h halved and process repeated
c
c      if(s.le.eps.and.ncy.gt.1) return
c      do 15 i=1,n
c          h(i)=h(i)/two
c          do 15 j=i,n
15      store(i,j)=cov(i,j)
c          go to 2
c
c      Error conditions
c
c      ifault=100
c      Dimension or problem size misspecified
c      return
c      ifault=200+i
c      Maximum likelihood estimate for i-th parameter outside bounds
c      return
c      ifault=300
c      Convergence not achieved in maxh iterations
c      return
c      ifault=400+ncy
c      Matrix inversion difficulties at iteration ncy
c      return
c      end
```

```

SUBROUTINE DMAT(KSET, NP, ND, NM, NG, X, XSIGMA, MDF, CHI, DETMUL,
*           W2, IFAULT)
C
C           ALGORITHM AS 250 APPL. STATIST. (1989), VOL. 38, NO. 3
C
C           Test of equality of dispersion matrices using
C           Sen & Puri's non-parametric and Anderson's parametric methods.
C
C           Auxiliary routine required: CHOL from AS 6
C
C           INTEGER IA, IB, IC, ID, IE
C           PARAMETER (IA=9, IB=10, IC=IA * (IA + 1)/2, ID=1000,
*           IE=IC * (IC + 1)/2)
C
C           Arguments
C           INTEGER NG( * ), IFAULT, KSET, MDF, ND, NM, NP
C           REAL X(IA, * ), XSIGMA(IC, * ), CHI, DETMUL, W2
C
C           Local variables
C           INTEGER I, I1, II, IM, J, J1, JJ, K, L, M, MP, MR, MS, N, NPT, NT,
*           NULLTY
C           REAL XMEAN(IA, IB), XMALL(IA), DET(IB), XSALL(IC), Y(ID), VRS(IE),
*           W(IE), DE, DETALL, F48, F6, HALF, ONE, R1, R2, RHO, S12,
*           TEMP, TWO
C           DATA HALF, ONE, TWO, F6, S12, F48 / 0.5, 1.0, 2.0, 6.0,
*           3.4641016151377, 48.0 /
C
C           NT = 0
C           DO 10 K = 1, KSET
C               NT = NT + NG(K)
10 CONTINUE
C           MP = NP * (NP + 1) / 2
C           MDF = 0
C           CHI = 0.0
C           W2 = 0.0
C           DETMUL = 0.0
C
C           Check input data for failure.
C
C           IFAULT = 0
C           IF (KSET .LT. 1 .OR. NP .LT. 1 .OR.
*           (ND .NE. 1 .AND. ND .NE. 2) .OR.
*           (NM .NE. 1 .AND. NM .NE. 2)) IFAULT = 1
C           IF (ND .EQ. 2 .AND. NM .NE. 2) IFAULT = 2
C           DO 20 K = 1, KSET
C               IF (NG(K) .LT. 1) IFAULT = 3
20 CONTINUE
C
C           Partial check on dimensions.
C
C           IF (IA .LT. NP .OR. IB .LT. KSET .OR. ID .LT. NT) IFAULT = 4
C           IF (IFAULT .NE. 0) RETURN
C
C           Check the `type' of data input
C
C           IF (ND .EQ. 2) GO TO 290
C
C           Manipulate raw data according to flag given by NM and
C           calculate MEAN and SIGMA. Note that `raw' data is `ordered'
C           if Sen & Puri's method(NM=1) is used.
C

```

```
C      Rank order the raw data if NM=1 and load it in X(L,N).
C      Ordered data for each variable are temporarily stored in Y(N).
C      Map the ranked data into its general score such that variate
C      means = 0 and variate std = 1 across all samples.
C
      IF (NM .EQ. 1) THEN
        DO 70 L = 1, NP
          DO 30 N = 1, NT
            Y(N) = ONE
30          CONTINUE
          DO 50 I = 1, NT
            DO 40 N = 1, I - 1
C
              IF (X(L, I) .LT. X(L, N)) THEN
                Y(N) = Y(N) + ONE
              ELSE IF (X(L, I) .EQ. X(L, N)) THEN
                Y(N) = Y(N) + HALF
                Y(I) = Y(I) + HALF
              ELSE
                Y(I) = Y(I) + ONE
              END IF
C
            40          CONTINUE
            50          CONTINUE
C
              DO 60 N = 1, NT
                X(L, N) = S12 * (AINT(Y(N)) / (NT + 1) - HALF)
60              CONTINUE
70              CONTINUE
            END IF
C
      The `raw' or `ordered' data are now in X(L,N).  Compute mean
      of each variate for each sample and store in XMEAN(L,K).
C
      Compute mean of each variate over all samples, store in
      XMALL(L).  Note that when NM=1, this step is known and is
      equal to zero since the ranks are scaled.  When NM=2, XMALL(L)
      is not needed.
C
      DO 100 L = 1, NP
        NPT = 0
        XMALL(L) = 0.0
        DO 90 K = 1, KSET
          XMEAN(L, K) = 0.0
          DO 80 N = 1, NG(K)
            NPT = NPT + 1
            XMEAN(L, K) = XMEAN(L, K) + X(L, NPT)
80          CONTINUE
          XMEAN(L, K) = XMEAN(L, K) / NG(K)
          90          CONTINUE
        100 CONTINUE
C
      Compute sigma matrix for each sample XSIGMA(M,K) where M takes
      values 1 through NP*(NP+1)/2.  Compute sigma of all samples
      XSALL(M).  Calculation of these matrices is controlled by NM.
C
      M = 0
      DO 140 I = 1, NP
        DO 130 J = 1, NP
          M = M + 1
          NPT = 0
```

```

        XSALL(M) = 0.0
        DO 120 K = 1, KSET
            XSIGMA(M, K) = 0.0
            DO 110 N = 1, NG(K)
                NPT = NPT + 1
                XSIGMA(M, K) = XSIGMA(M, K) +
*                               (X(I, NPT) - XMEAN(I, K)) *
*                               (X(J, NPT) - XMEAN(J, K))
110          CONTINUE
C
        IF (NM .EQ. 1) THEN
            XSALL(M) = XSALL(M) + XSIGMA(M, K) +
*                               XMEAN(I, K) * XMEAN(J, K) * NG(K)
            XSIGMA(M, K) = XSIGMA(M, K) / (NG(K) - 1)
        ELSE
            XSALL(M) = XSALL(M) + XSIGMA(M, K)
        END IF
C
120          CONTINUE
            IF (NM .EQ. 1) XSALL(M) = XSALL(M) / (NT - 1)
130          CONTINUE
140          CONTINUE
C
C          Check the method chosen: Sen and Puri (NM=1) or Anderson (NM=2)
C
C          IF (NM .EQ. 2) GO TO 330
C
C          Sen and Puri's method
C
C          Compute the lower triangle of 4th moment matrix VRS of order
C          (MP,MP), where MP=MP*(NP+1)/2, in the one dimensional array
C          VRS.
C
L = 0
MR = 0
DO 200 I = 1, NP
    DO 190 J = I, NP
        MR = MR + 1
        MS = 0
        DO 180 I1 = 1, I
            DO 170 J1 = I1, NP
                MS = MS + 1
                IF (MR .GE. MS) THEN
                    L = L + 1
                    NPT = 0
                    VRS(L) = 0.0
                    DO 160 K = 1, KSET
                        DO 150 N = 1, NG(K)
                            NPT = NPT + 1
                            VRS(L) = VRS(L) + X(I, NPT) * X(J, NPT) *
*                               X(I1, NPT) * X(J1, NPT)
150                          CONTINUE
160                          CONTINUE
                                VRS(L) = VRS(L) / NT - XSALL(MR) * XSALL(MS)
                            END IF
170                          CONTINUE
180                          CONTINUE
190                          CONTINUE
200                        CONTINUE
C
C          Compute XSIGMA (M,K)-XSALL(M) for all M,K. Sotre the results

```

```

C      in XSIGMA(M,K).
C
      DO 220 K = 1, KSET
        DO 210 M = 1, MP
          XSIGMA(M, K) = XSIGMA(M, K) - XSALL(M)
210      CONTINUE
220      CONTINUE
C
C      Compute the quadratic form:
C      CHI = (XSIGMA transpose * VRS inverse * XSIGMA)
C      by first getting the square root W of VRS (see sub. CHOL), then
C      finding W inverse * XSIGMA, and finally CHI.
C
      CALL CHOL(VRS, MP, MP * (MP + 1) / 2, W, NULLTY, IFAULT)
C
C      Invert root of VRS (=W). Note that W is an upper diagonal
C      matrix and is inverted `in place'.
C
      IF (NULLTY .GT. 0 .OR. IFAULT .GT. 0) THEN
        IFAULT = 5
        RETURN
      END IF
      DO 250 J = MP, 1, -1
        JJ = J * (J + 1) / 2
        W(JJ) = 1.0 / W(JJ)
        DO 240 I = J - 1, 1, -1
          II = I * (I + 1) / 2
          IM = II
          TEMP = 0.0
          DO 230 M = I + 1, J
            IM = IM + M - 1
            TEMP = TEMP + W(IM) * W(JJ + M - J)
230          CONTINUE
          W(IM) = -TEMP / W(II)
240          CONTINUE
250          CONTINUE
C
C      Compute CHI
C
      CHI = 0.0
      DO 280 K = 1, KSET
        DO 270 I = 1, MP
          N = I * (I - 1) / 2
          TEMP = 0.0
          DO 260 J = 1, I
            TEMP = TEMP + W(N + J) * XSIGMA(J, K)
260          CONTINUE
          CHI = CHI + TEMP ** 2
270          CONTINUE
280          CONTINUE
        MDF = (KSET - 1) * MP
C
      RETURN
C
C      Anderson's method, XSIGMA input
C
C      Calculate the total matrix for all samples and store it in
C      XSALL(M).
C
290      CONTINUE
      DO 300 M = 1, MP

```

```

        XSALL(M) = 0.0
300 CONTINUE
        DO 320 K = 1, KSET
            DO 310 M = 1, MP
                XSALL(M) = XSALL(M) + XSIGMA(M, K)
310     CONTINUE
320 CONTINUE
C
C     Anderson's method, raw data or XSIGMA input.
C     From the diagonal XSIGMA matrix and XSALL generate the lower
C     triangle of respective covariance matrices. Store these lower
C     triangles in the one dimensional array VRS. Get the
C     log(determinant) for each matrix by calling subroutine `CHOL'.
C     store results in DET(K) and DETALL.
C
330 DO 370 K = 1, KSET
        M = 0
        DO 350 I = 1, NP
            N = I * (I - 1) / 2 + 1
            DO 340 J = I, NP
                M = M + 1
                N = N + J - 1
                VRS(N) = XSIGMA(M, K) / (NG(K) - 1)
340     CONTINUE
350 CONTINUE
        CALL CHOL(VRS, NP, NP * (NP + 1) / 2, W, NULLTY, IFAULT)
        IF (NULLTY .GT. 0 .OR. IFAULT .GT. 0) THEN
            IFAULT = 5
            RETURN
        END IF
        DE = 1.0
        N = 0
        DO 360 I = 1, NP
            N = N + I
            DE = DE * W(N)
360     CONTINUE
        DET(K) = TWO * LOG(DE)
370 CONTINUE
C
        M = 0
        DO 390 I = 1, NP
            N = I * (I - 1) / 2 + 1
            DO 380 J = I, NP
                M = M + 1
                N = N + J - 1
                VRS(N) = XSALL(M) / (NT - KSET)
380     CONTINUE
390 CONTINUE
        CALL CHOL(VRS, NP, NP * (NP + 1) / 2, W, NULLTY, IFAULT)
        IF (NULLTY .GT. 0 .OR. IFAULT .GT. 0) THEN
            IFAULT = 5
            RETURN
        END IF
        DE = 1.0
        N = 0
        DO 400 I = 1, NP
            N = N + I
            DE = DE * W(N)
400 CONTINUE
        DETALL = TWO * LOG(DE)
C

```



```
C      Compute log(V), store in DETMUL.  Compute CHI.
C
      DETMUL = 0.0
      DO 410 K = 1, KSET
          DETMUL = DETMUL + (DET(K) - DETALL) * (NG(K) - 1) / TWO
410 CONTINUE
C
C      Calculate RHO and W2
C
      M = NT - KSET
      R1 = 0.0
      R2 = 0.0
      DO 420 K = 1, KSET
          R1 = R1 + ONE / (NG(K) - 1)
          R2 = R2 + ONE / (NG(K) - 1) ** 2
420 CONTINUE
      RHO = ONE - (R1 - ONE / M) * (2 * (NP ** 2) + 3 * NP - 1) /
*      (F6 * (NP + 1) * (KSET - 1))
      W2 = NP * (NP + 1) * ((NP - 1) * (NP + 2) * (R2 - ONE / M ** 2) -
*      F6 * (KSET - 1) * (1 - RHO) * * 2) / (F48 * RHO ** 2)
C
      MDF = (KSET - 1) * MP
      CHI = -TWO * RHO * DETMUL
      RETURN
      END
```

This file contains:

1. A Readme file provided by Charles Dunnett, the author of AS 251.
2. The published algorithm AS 251 together with the two other AS algorithms which it calls (AS 66 and AS 241).
3. A driver program (MVTIN) for either multivariate normal or t.
4. MVSTUD for calculating multivariate t probabilities.

\*\*\*\*\*

Date: Mon, 10 Apr 1995 16:49:10 +0059 (EDT)  
From: "Charles W. Dunnett" <dunnett@mcmail.cis.mcmaster.ca>  
Subject: Readme for AS251 (extended version incl. multivariate t)

MVTIN is a driver program for computing multivariate normal or t probability integrals over arbitrary rectangular regions. The correlation structure is assumed to be of product form,  $\rho_{ij} = b_i \times b_j$ , where  $-1 < b_i < +1$ .

It requires the following:-

1. MVNPRD (published as algorithm AS 251 in Applied Statistics (1989), 38: 564-579; see also the correction note in Applied Statistics (1993), 42: 709),
2. ALNORM and PPND7 (published as algorithms AS 66 and AS 241, respectively, in Applied Statistics, and
3. MVSTUD (which Studentizes MVNPRD).

Special cases of correlations which are of product form include the following:-

- a) Equal correlations,  $\rho \geq 0$ . Then  $b_i = \sqrt{\rho}$ , all  $i$ .
- b) Multiple comparisons between treatments and a specified treatment. Then  $b_i = 1 / \sqrt{1 + n_0/n_i}$ , where  $n_0$  and  $n_i$  are the sample sizes for the specified treatment and  $i$ -th treatment, respectively.

MVTIN computes

$$\text{PROB} = P\{ B(I) < T_I < A(I), \text{ for } I = 1, \dots, N \}$$

where  $(T_1, \dots, T_N)$  is a multivariate normal or t random variable with product correlation structure. The  $B(I)$  may be  $-\infty$  or finite and the  $A(I)$  may be finite or  $+\infty$ .

The program can be used on any mainframe computer (such as a VAX) which has a Fortran compiler. A PC can also be used, but the execution times will be much longer, especially for multivariate t integrals (unless your PC uses a 486 or faster chip). Typical computing times for a multivariate t p-value range from about three minutes on an IBM/XT with math co-processor to 2.4 seconds on a 486DX2/66 PC.

The first time you use the program, it is recommended that you specify  $\text{NDF} = 0$  (which denotes the multivariate normal case), since computing times are shorter than for multivariate t.

The accuracy is determined by the value of the parameter  $\text{EPS}$ , which has been pre-set to  $\text{EPS} = 0.0001$ . For increased accuracy, you may change the value of  $\text{EPS}$  in the  $\text{DATA}$  statement of  $\text{MVTIN}$  to

EPS = 0.00001 (Smaller values than this are not recommended).

EXAMPLES:-

(1) Suppose the problem is to determine  $g^*$  such that

$$\begin{aligned} & P\{\min(Z_1, \dots, Z_k) > g^*\} \\ &= P\{Z_1 > g^*, \dots, Z_k > g^*\} = \alpha \end{aligned}$$

where  $Z_1, \dots, Z_k$  are  $N(0,1)$  with equal correlations,  $\rho_{ij} = 0.5$ . The first prompt you receive is for N and NDF. You enter the value of k for N, and 0 for NDF (indicating d.f.= infinity). (At the end of each problem, the program returns to this prompt for the next problem. If there is no further problem, enter 0 0 to exit from the program.)

The next prompt is to specify the correlation structure. You are given three choices: 1) equal correlations, 2) correlations defined from sample sizes as in b) above, and 3) unequal correlations of the form  $\rho_{ij} = b_i \times b_j$ . For this example, enter 1, followed by 0.50 when you receive a prompt for rho.

Next you are asked whether you want equal or unequal limits. Since all your limits are to be  $g^*$  to +infinity, you specify equal limits. You are also asked whether you want the central or non-central case: if the latter, you are asked to enter the value(s) of the non-centrality parameters.

Then you are prompted to enter the values of INF and the limit(s). You enter 0 (to indicate upper 1-sided) followed by a trial value for  $g^*$ .

After computing PROB, you have the option of entering new limits to obtain a new value of PROB, or returning to the beginning for a new problem.

For example, for  $k = 5$  and  $\rho = 0.50$ , I found that  $g^* = 0.564$  achieved the value  $\alpha = 0.05$ .

(2) For the next example, consider a mc/control problem with sample sizes 11 for the control and 10, 10, 12, 10 and 9 for the treatment groups. Here,  $k = 5$  and d.f. = 56. Suppose the largest of the t-statistics comparing treatments with the control has the value 2.50. You want to determine its two-sided p-value, which is given by

$$p = 1 - P\{ |T_1| < 2.5, \dots, |T_5| < 2.5 \}.$$

At the prompt for N and NDF, enter: 5 56.

At the prompt for correlation structure: enter 2 to denote it is to be determined from the sample sizes, followed by the sample sizes at the next prompt.

At the prompt for equal or unequal limits, enter: 1.

Enter 0 for the central case.

Then for the value of INF and the limits, enter: 2 -2.50 2.50

You should obtain the value  $PROB = .9375$ . This is the probability for  $-2.50 < T_i < 2.50$  (all  $i$ ); then  $p\text{-value} = 1 - .9375 = .0625$ .

Let me know if you encounter problems. Also, please let me know if it does not meet your needs in some way, or if you think of any improvements.

Good luck!

With best wishes, Charles Dunnett.

```

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* * * * *

```

```

SUBROUTINE MVNPRD(A, B, BPD, EPS, N, INF, IERC, HINC, PROB, BOUND,
* IFAULT)
C
C   ALGORITHM AS 251.1  APPL.STATIST. (1989), VOL.38, NO.3
C
C   FOR A MULTIVARIATE NORMAL VECTOR WITH CORRELATION STRUCTURE
C   DEFINED BY  $\rho(I,J) = BPD(I) * BPD(J)$ , COMPUTES THE PROBABILITY
C   THAT THE VECTOR FALLS IN A RECTANGLE IN N-SPACE WITH ERROR
C   LESS THAN EPS.
C
C   INTEGER NN
C   PARAMETER (NN = 50)
C   REAL A(*), B(*), BPD(*), ESTT(22), FV(5), FD(5), F1T(22),
* F2T(22), F3T(22), G1T(22), G3T(22), PSUM(22), H(NN), HL(NN),
* BB(NN)
C   INTEGER INF(*), INFT(NN), LDIR(22)
C   REAL ZERO, HALF, ONE, TWO, FOUR, SIX, PT1, PT24, ONEP5,
* X2880, SMALL, DXMIN, SQRT2, PROB, ERRL, BI, START,
* Z, HINC, ADDN, EPS2, EPS1, EPS, ZU, Z2, Z3, Z4, Z5, ZZ,
* ERFAC, EL, EL1, BOUND, PART0, PART2, PART3, FUNC0, FUNC2,
* FUNCN, WT, CONTRB, DLG, DX, DA, ESTL, ESTR, SUM, EXCESS, ERROR,
* PROB1, SAFE
C   INTEGER N, IERC, IFAULT, I, NTM, NMAX, LVL, NR, NDIM
C   REAL ALNORM, PPND7
C   EXTERNAL ALNORM, PPND7
C   DATA ZERO, HALF, ONE, TWO, FOUR, SIX /0.0, 0.5, 1.0, 2.0,
* 4.0, 6.0/
C   DATA PT1, PT24, ONEP5, X2880 /0.1, 0.24, 1.5, 2880.0/
C   DATA SMALL, DXMIN, SQRT2 /1.0E-10, 0.0000001, 1.41421356237310/
C
C   CHECK FOR INPUT VALUES OUT OF RANGE.
C
C   PROB = ZERO
C   BOUND = ZERO
C   IFAULT = 1
C   IF (N .LT. 1 .OR. N .GT. NN) RETURN

```

```

DO 10 I = 1, N
  BI = ABS(BPD(I))
  IFAULT = 2
  IF (BI .GE. ONE) RETURN
  IFAULT = 3
  IF (INF(I) .LT. 0 .OR. INF(I) .GT. 2) RETURN
  IFAULT = 4
  IF (INF(I) .EQ. 2 .AND. A(I) .LE. B(I)) RETURN
10 CONTINUE
  IFAULT = 0
  PROB = ONE

C
C      CHECK WHETHER ANY BPD(I) = 0.
C

NDIM = 0
DO 20 I = 1, N
  IF (BPD(I) .NE. ZERO) THEN
    NDIM = NDIM + 1
    H(NDIM) = A(I)
    HL(NDIM) = B(I)
    BB(NDIM) = BPD(I)
    INFT(NDIM) = INF(I)
  ELSE

C
C      IF ANY BPD(I) = 0, THE CONTRIBUTION TO PROB FOR THAT
C      VARIABLE IS COMPUTED FROM A UNIVARIATE NORMAL.
C
    IF (INF(I) .LT. 1) THEN
      PROB = PROB * (ONE - ALNORM(B(I), .FALSE.))
    ELSE IF (INF(I) .EQ. 1) THEN
      PROB = PROB * ALNORM(A(I), .FALSE.)
    ELSE
      PROB = PROB * (ALNORM(A(I), .FALSE.) -
*          ALNORM(B(I), .FALSE.))
    END IF
    IF (PROB .LE. SMALL) PROB = ZERO
  END IF
20 CONTINUE
  IF (NDIM .EQ. 0 .OR. PROB .EQ. ZERO) RETURN

C
C      IF NOT ALL BPD(I) = 0, PROB IS COMPUTED BY SIMPSON'S RULE.
C      BUT FIRST, INITIALIZE THE VARIABLES.
C

  Z = ZERO
  IF (HINC .LE. ZERO) HINC = PT24
  ADDN = -ONE
  DO 30 I = 1, NDIM
    IF (INFT(I) .EQ. 2 .OR.
*      (INFT(I) .NE. INFT(1) .AND. BB(I) * BB(1) .GT. ZERO) .OR.
*      (INFT(I) .EQ. INFT(1) .AND. BB(I) * BB(1) .LT. ZERO))
*        ADDN = ZERO
30 CONTINUE

C
C      THE VALUE OF ADDN IS TO BE ADDED TO THE PRODUCT EXPRESSIONS IN
C      THE INTEGRAND TO INSURE THAT THE LIMITING VALUE IS ZERO.
C

  PROB1 = ZERO
  NTM = 0
  NMAX = 400
  IF (IERC .EQ. 0) NMAX = NMAX * 2
  CALL PFUNC (Z, H, HL, BB, NDIM, INFT, ADDN, SAFE, FUNC0, NTM,

```

```
*   IERC, PART0)
EPS2 = EPS * PT1 * HALF
C
C       SET UPPER BOUND ON Z AND APPORTION EPS.
C
ZU = -PPND7(EPS2, IFAULT) / SQRT2
IF (IFAULT .NE. 0) THEN
    IFAULT = 6
    RETURN
END IF
NR = IFIX(ZU / HINC) + 1
ERFAC = ONE
IF (IERC .NE. 0) ERFAC = X2880 / HINC ** 5
EL = (EPS - EPS2) / FLOAT(NR) * ERFAC
EL1 = EL
C
C       START COMPUTATIONS FOR THE INTERVAL (Z, Z + HINC).
C
40 ERROR = ZERO
LVL = 0
FV(1) = PART0
FD(1) = SAFE
START = Z
DA = HINC
Z3 = START + HALF * DA
CALL PFUNC(Z3, H, HL, BB, NDIM, INFT, ADDN, FD(3), FUNCN, NTM,
*   IERC, FV(3))
Z5 = START + DA
CALL PFUNC(Z5, H, HL, BB, NDIM, INFT, ADDN, FD(5), FUNC2, NTM,
*   IERC, FV(5))
PART2 = FV(5)
SAFE = FD(5)
WT = DA / SIX
CONTRB = WT * (FV(1) + FOUR * FV(3) + FV(5))
DLG = ZERO
IF (IERC .NE. 0) THEN
    CALL WMAX(FD(1), FD(3), FD(5), DLG)
    IF (DLG .LE. EL) GO TO 90
    DX = DA
    GO TO 60
END IF
LVL = 1
LDIR(LVL) = 2
PSUM(LVL) = ZERO
C
C       BISECT INTERVAL.  IF IERC = 1, COMPUTE ESTIMATE ON LEFT
C       HALF; IF IERC = 0, ON BOTH HALVES.
C
50 DX = HALF * DA
WT = DX / SIX
Z2 = START + HALF * DX
CALL PFUNC(Z2, H, HL, BB, NDIM, INFT, ADDN, FD(2), FUNCN, NTM,
*   IERC, FV(2))
ESTL = WT * (FV(1) + FOUR * FV(2) + FV(3))
IF (IERC .EQ. 0) THEN
    Z4 = START + ONEP5 * DX
    CALL PFUNC(Z4, H, HL, BB, NDIM, INFT, ADDN, FD(4), FUNCN,
*       NTM, IERC, FV(4))
    ESTR = WT * (FV(3) + FOUR * FV(4) + FV(5))
    SUM = ESTL + ESTR
    DLG = ABS(CONTRB - SUM)
```

```
        EPS1 = EL / TWO ** (LVL - 1)
        ERRL = DLG
ELSE
        FV(3) = FV(2)
        FD(3) = FD(2)
        CALL WMAX(FD(1), FD(3), FD(5), DLG)
        ERRL = DLG / TWO ** (5 * LVL)
        SUM = ESTL
        EPS1 = EL * (TWO ** LVL) ** 4
END IF

C
C        STOP SUBDIVIDING INTERVAL WHEN ACCURACY IS SUFFICIENT,
C        OR IF INTERVAL TOO NARROW OR SUBDIVIDED TOO OFTEN.
C

IF (DLG .LE. EPS1 .OR. DLG .LT. SMALL) GO TO 70
IF (IFAUULT .EQ. 0 .AND. NTM .GE. NMAX) IFAUULT = 5
IF (ABS(DX) .LE. DXMIN .OR. LVL .GT. 21) IFAUULT = 7
IF (IFAUULT .NE. 0) GO TO 70

C
C        RAISE LEVEL.  STORE INFORMATION FOR RIGHT HALF AND APPLY
C        SIMPSON'S RULE TO LEFT HALF.
C

60 LVL = LVL + 1
   LDIR(LVL) = 1
   F1T(LVL) = FV(3)
   F3T(LVL) = FV(5)
   DA = DX
   FV(5) = FV(3)
   IF (IERC .EQ. 0) THEN
       F2T(LVL) = FV(4)
       ESTT(LVL) = ESTR
       CONTRB = ESTL
       FV(3) = FV(2)
   ELSE
       G1T(LVL) = FD(3)
       G3T(LVL) = FD(5)
       FD(5) = FD(3)
   END IF
   GO TO 50

C
C        ACCEPT APPROXIMATE VALUE FOR INTERVAL.
C        RESTORE SAVED INFORMATION TO PROCESS
C        RIGHT HALF INTERVAL.
C

70 ERROR = ERROR + ERRL
80 IF (LDIR(LVL) .EQ. 1) THEN
    PSUM(LVL) = SUM
    LDIR(LVL) = 2
    IF (IERC .EQ. 0) DX = DX * TWO
    START = START + DX
    DA = HINC / TWO ** (LVL - 1)
    FV(1) = F1T(LVL)
    IF (IERC .EQ. 0) THEN
        FV(3) = F2T(LVL)
        CONTRB = ESTT(LVL)
    ELSE
        FV(3) = F3T(LVL)
        FD(1) = G1T(LVL)
        FD(5) = G3T(LVL)
    END IF
    FV(5) = F3T(LVL)
```

```

        GO TO 50
    END IF
    SUM = SUM + PSUM(LVL)
    LVL = LVL - 1
    IF (LVL .GT. 0) GO TO 80
    CONTRB = SUM
    LVL = 1
    DLG = ERROR
90  PROB1 = PROB1 + CONTRB
    BOUND = BOUND + DLG
    EXCESS = EL - DLG
    EL = EL1
    IF (EXCESS .GT. ZERO) EL = EL1 + EXCESS
    IF ((FUNC0 .GT. ZERO .AND. FUNC2 .LE. FUNC0) .OR.
*   (FUNC0 .LT. ZERO .AND. FUNC2 .GE. FUNC0)) THEN
        ZZ = -SQRT2 * Z5
        PART3 = ABS(FUNC2) * ALNORM(ZZ, .FALSE.) + BOUND / ERFAC
        IF (PART3 .LE. EPS .OR. NTM .GE. NMAX .OR. Z5 .GE. ZU) GOTO 100
    END IF
    Z = Z5
    PART0 = PART2
    FUNC0 = FUNC2
    IF (Z .LT. ZU .AND. NTM .LT. NMAX) GO TO 40
100  PROB = (PROB1 - ADDN * HALF) * PROB
    BOUND = PART3
    IF (NTM .GE. NMAX .AND. IFAULT .EQ. 0) IFAULT = 5
    IF (BOUND .GT. EPS .AND. IFAULT .EQ. 0) IFAULT = 8
    RETURN
    END
    SUBROUTINE PFUNC(Z, A, B, BPD, N, INF, ADDN, DERIV, FUNCN, NTM,
*   IERC, RESULT)

```

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C
C   ALGORITHM AS 251.2  APPL.STATIST. (1989), VOL.38, NO.3
C

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C   COMPUTE FUNCTION IN INTEGRAND AND ITS 4TH DERIVATIVE.
C

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```

    INTEGER NN
    PARAMETER (NN = 50)
    REAL A(*), B(*), BPD(*), FOU(NN), FOU1(4, NN), TMP(4), GOU(NN),
*   GOU1(4, NN), FF(4), GF(4), TERM(4), GERM(4)
    INTEGER INF(*)
    REAL ZERO, ONE, TWO, THREE, FOUR, SIX, EIGHT, TWELVE, SIXTN,
*   SMALL, Z, U, U1, U2, BI, HI, HLI, BP, ADDN, DERIV, FUNCN,
*   RESULT, RSLT1, RSLT2, DEN, SQRT2, SQRTPI, PHI, PHI1, PHI2,
*   PHI3, PHI4, FRM, GRM
    INTEGER N, NTM, IERC, INFI, I, J, K, M, L, IK
    REAL ALNORM
    EXTERNAL ALNORM
    DATA ZERO, ONE, TWO, THREE, FOUR, SIX, EIGHT, TWELVE, SIXTN,
*   SMALL /0.0, 1.0, 2.0, 3.0, 4.0, 6.0, 8.0, 12.0, 16.0, 0.1E-12/
    DATA SQRT2, SQRTPI /1.41421356237310, 1.77245385090552/
    DERIV = ZERO
    NTM = NTM + 1
    RSLT1 = ONE
    RSLT2 = ONE
    BI = ONE
    HI = A(1) + ONE
    HLI = B(1) + ONE
    INFI = -1
    DO 60 I = 1, N

```



```

      IF (BPD(I) .EQ. BI .AND. A(I) .EQ. HI .AND. B(I) .EQ. HLI .AND.
*      INF(I) .EQ. INFI) THEN
      FOU(I) = FOU(I - 1)
      GOU(I) = GOU(I - 1)
      DO 10 IK = 1, 4
          FOU1(IK, I) = FOU1(IK, I - 1)
          GOU1(IK, I) = GOU1(IK, I - 1)
10     CONTINUE
      ELSE
      BI = BPD(I)
      HI = A(I)
      HLI = B(I)
      INFI = INF(I)
      IF (BI .EQ. ZERO) THEN
      IF (INFI .LT. 1) THEN
          FOU(I) = ONE - ALNORM(HLI, .FALSE.)
      ELSE IF (INFI .EQ. 1) THEN
          FOU(I) = ALNORM(HI, .FALSE.)
      ELSE
          FOU(I) = ALNORM(HI, .FALSE.) - ALNORM(HLI, .FALSE.)
      END IF
      GOU(I) = FOU(I)
      DO 20 IK = 1, 4
          FOU1(IK, I) = ZERO
          GOU1(IK, I) = ZERO
20     CONTINUE
      ELSE
      DEN = SQRT(ONE - BI * BI)
      BP = BI * SQRT2 / DEN
      IF (INFI .LT. 1) THEN
          U = -HLI / DEN + Z * BP
          FOU(I) = ALNORM(U, .FALSE.)
          CALL ASSIGN (U, BP, FOU1(1, I))
          BP = -BP
          U = -HLI / DEN + Z * BP
          GOU(I) = ALNORM(U, .FALSE.)
          CALL ASSIGN (U, BP, GOU1(1, I))
      ELSE IF (INFI .EQ. 1) THEN
          U = HI / DEN + Z * BP
          GOU(I) = ALNORM(U, .FALSE.)
          CALL ASSIGN (U, BP, GOU1(1, I))
          BP = -BP
          U = HI / DEN + Z * BP
          FOU(I) = ALNORM(U, .FALSE.)
          CALL ASSIGN (U, BP, FOU1(1, I))
      ELSE
          U2 = -HLI / DEN + Z * BP
          CALL ASSIGN (U2, BP, FOU1(1, I))
          BP = -BP
          U1 = HI / DEN + Z * BP
          CALL ASSIGN (U1, BP, TMP(1))
          FOU(I) = ALNORM(U1, .FALSE.) + ALNORM(U2, .FALSE.) - ONE
          DO 30 IK = 1, 4
              FOU1(IK, I) = FOU1(IK, I) + TMP(IK)
30     CONTINUE
          IF (-HLI .EQ. HI) THEN
              GOU(I) = FOU(I)
              DO 40 IK = 1, 4
                  GOU1(IK, I) = FOU1(IK, I)
40     CONTINUE
          ELSE

```

```

        U2 = -HLI / DEN + Z * BP
        CALL ASSIGN (U2, BP, GOU1(1, I))
        BP = -BP
        U1 = HI / DEN + Z * BP
        GOU(I) = ALNORM(U1, .FALSE.) + ALNORM(U2, .FALSE.)-ONE
        CALL ASSIGN (U1, BP, TMP(1))
        DO 50 IK = 1, 4
            GOU1(IK, I) = GOU1(IK, I) + TMP(IK)
50      CONTINUE
        END IF
    END IF
END IF
RSLT1 = RSLT1 * FOU(I)
RSLT2 = RSLT2 * GOU(I)
IF (RSLT1 .LE. SMALL) RSLT1 = ZERO
IF (RSLT2 .LE. SMALL) RSLT2 = ZERO
60 CONTINUE
FUNCN = RSLT1 + RSLT2 + ADDN
RESULT = FUNCN * EXP(-Z * Z) / SQRTPI
C
C     IF 4TH DERIVATIVE IS NOT WANTED, STOP HERE.
C     OTHERWISE, PROCEED TO COMPUTE 4TH DERIVATIVE.
C
IF (IERC .EQ. 0) RETURN
DO 70 IK = 1, 4
    FF(IK) = ZERO
    GF(IK) = ZERO
70 CONTINUE
DO 100 I = 1, N
    FRM = ONE
    GRM = ONE
    DO 80 J = 1, N
        IF (J .EQ. 1) GO TO 80
        FRM = FRM * FOU(J)
        GRM = GRM * GOU(J)
        IF (FRM .LE. SMALL) FRM = ZERO
        IF (GRM .LE. SMALL) GRM = ZERO
80    CONTINUE
    DO 90 IK = 1, 4
        FF(IK) = FF(IK) + FRM * FOU1(IK, I)
        GF(IK) = GF(IK) + GRM * GOU1(IK, I)
90    CONTINUE
100 CONTINUE
IF (N .LE. 2) GO TO 230
DO 130 I = 1, N
    DO 120 J = I + 1, N
        TERM(2) = FOU1(1, I) * FOU1(1, J)
        GERM(2) = GOU1(1, I) * GOU1(1, J)
        TERM(3) = FOU1(2, I) * FOU1(1, J)
        GERM(3) = GOU1(2, I) * GOU1(1, J)
        TERM(4) = FOU1(3, I) * FOU1(1, J)
        GERM(4) = GOU1(3, I) * GOU1(1, J)
        TERM(1) = FOU1(2, I) * FOU1(2, J)
        GERM(1) = GOU1(2, I) * GOU1(2, J)
    DO 110 K = 1, N
        IF (K .EQ. I .OR. K .EQ. J) GO TO 110
        CALL TOOSML (1, TERM, FOU(K))
        CALL TOOSML (1, GERM, GOU(K))
110    CONTINUE
        FF(2) = FF(2) + TWO * TERM(2)

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      FF(3) = FF(3) + TWO * TERM(3) * THREE
      FF(4) = FF(4) + TWO * (TERM(4) * FOUR + TERM(1) * THREE)
      GF(2) = GF(2) + TWO * GERM(2)
      GF(3) = GF(3) + TWO * GERM(3) * THREE
      GF(4) = GF(4) + TWO * (GERM(4) * FOUR + GERM(1) * THREE)
120   CONTINUE
130   CONTINUE
      DO 170 I = 1, N
          DO 160 J = I + 1, N
              DO 150 K = J + 1, N
                  TERM(3) = FOU1(1, I) * FOU1(1, J) * FOU1(1, K)
                  TERM(4) = FOU1(2, I) * FOU1(1, J) * FOU1(1, K)
                  GERM(3) = GOU1(1, I) * GOU1(1, J) * GOU1(1, K)
                  GERM(4) = GOU1(2, I) * GOU1(1, J) * GOU1(1, K)
                  IF (N .GT. 3) THEN
                      DO 140 M = 1, N
                          IF (M .EQ. I .OR. M .EQ. J .OR. M .EQ. K) GO TO 140
                          CALL TOOSML (3, TERM, FOU(M))
                          CALL TOOSML (3, GERM, GOU(M))
140   CONTINUE
                      END IF
                      FF(3) = FF(3) + SIX * TERM(3)
                      FF(4) = FF(4) + SIX * TERM(4) * SIX
                      GF(3) = GF(3) + SIX * GERM(3)
                      GF(4) = GF(4) + SIX * GERM(4) * SIX
150   CONTINUE
160   CONTINUE
170   CONTINUE
          IF (N .LE. 3) GO TO 230
          DO 220 I = 1, N
              DO 210 J = I + 1, N
                  DO 200 K = J + 1, N
                      DO 190 M = K + 1, N
                          TERM(4) = FOU1(1, I) * FOU1(1, J) * FOU1(1, K) * FOU1(1, M)
                          GERM(4) = GOU1(1, I) * GOU1(1, J) * GOU1(1, K) * GOU1(1, M)
                          IF (N .GT. 4) THEN
                              DO 180 L = 1, N
                                  IF (L .EQ. I .OR. L .EQ. J .OR. L .EQ. K .OR. L .EQ. M) GOTO 180
                                  CALL TOOSML (4, TERM, FOU(L))
                                  CALL TOOSML (4, GERM, GOU(L))
180   CONTINUE
                              END IF
                              FF(4) = FF(4) + FOUR * SIX * TERM(4)
                              GF(4) = GF(4) + FOUR * SIX * GERM(4)
190   CONTINUE
200   CONTINUE
210   CONTINUE
220   CONTINUE
C
230   CONTINUE
      PHI = EXP(-Z * Z) / SQRTPI
      PHI1 = -TWO * Z * PHI
      PHI2 = (FOUR * Z ** 2 - TWO) * PHI
      PHI3 = (-EIGHT * Z ** 3 + TWELVE * Z) * PHI
      PHI4 = (SIXTN * Z ** 2 * (Z ** 2 - THREE) + TWELVE) * PHI
      DERIV = PHI * (FF(4) + GF(4)) + FOUR * PHI1 * (FF(3) + GF(3))
* + SIX * PHI2 * (FF(2) + GF(2)) + FOUR * PHI3 * (FF(1) + GF(1))
* + PHI4 * FUNCN
      RETURN
      END
      SUBROUTINE ASSIGN (U, BP, FF)

```

```
C
C      ALGORITHM AS 251.3  APPL.STATIST. (1989), VOL.38, NO.3
C
C      COMPUTE DERIVATIVES OF NORMAL CDF'S.
C
REAL FF(4)
REAL U, U2, BP, HALF, ONE, THREE, SQ2PI, T1, T2, T3
INTEGER I
DATA HALF, ONE, THREE, SQ2PI /0.5, 1.0, 3.0, 2.50662827463100/
DATA ZERO, UMAX, SMALL /0.0, 8.0, 0.1E-07/
IF (ABS(U) .GT. UMAX) THEN
  DO 10 I = 1, 4
    FF(I) = ZERO
10  CONTINUE
ELSE
  U2 = U * U
  T1 = BP * EXP(-HALF * U2) / SQ2PI
  T2 = BP * T1
  T3 = BP * T2
  FF(1) = T1
  FF(2) = -U * T2
  FF(3) = (U2 - ONE) * T3
  FF(4) = (THREE - U2) * U * BP * T3
  DO 20 I = 1, 4
    IF(ABS(FF(I)) .LT. SMALL) FF(I) = ZERO
20  CONTINUE
END IF
RETURN
END
SUBROUTINE WMAX(W1, W2, W3, DLG)
```

```
C
C      ALGORITHM AS 251.4  APPL.STATIST. (1989), VOL.38, NO.3
C
C      LARGEST ABSOLUTE VALUE OF QUADRATIC FUNCTION FITTED
C      TO THREE POINTS.
C
REAL W1, W2, W3, DLG, QUAD, QLIM, QMIN, ONE, TWO, B2C
DATA ONE, TWO, QMIN /1.0, 2.0, 0.00001/
DLG = MAX( ABS(W1), ABS(W3) )
QUAD = W1 - W2 * TWO + W3
QLIM = MAX( ABS(W1 - W3) / TWO , QMIN)
IF (ABS(QUAD) .LE. QLIM) RETURN
B2C = (W1 - W3) / QUAD / TWO
IF (ABS(B2C) .GE. ONE) RETURN
DLG = MAX( DLG, ABS(W2 - B2C * QUAD * B2C / TWO) )
RETURN
END
SUBROUTINE TOOSML (N, FF, F)
```

```
C
C      ALGORITHM AS 251.5  APPL.STATIST. (1989), VOL.38, NO.3
C
C      MULTIPLY FF(I) BY F FOR I = N TO 4.  SET TO ZERO IF TOO SMALL.
C
REAL FF(4), F, ZERO, SMALL
INTEGER N, I
DATA ZERO, SMALL /0.0, 0.1E-12/
DO 10 I = N, 4
  FF(I) = FF(I) * F
```

```

        IF (ABS(FF(I)) .LE. SMALL) FF(I) = ZERO
10 CONTINUE
    RETURN
    END
    REAL FUNCTION ALNORM(X, UPPER)
C
C     ALGORITHM AS 66  APPL. STATIST. (1973) VOL.22, P.424
C
C     EVALUATES THE TAIL AREA OF THE STANDARDIZED NORMAL CURVE
C     FROM X TO INFINITY IF UPPER IS .TRUE. OR
C     FROM MINUS INFINITY TO X IF UPPER IS .FALSE.
C
    REAL LTONE, UTZERO, ZERO, HALF, ONE, CON, A1, A2, A3,
$   A4, A5, A6, A7, B1, B2, B3, B4, B5, B6, B7, B8, B9,
$   B10, B11, B12, X, Y, Z, ZEXP
    LOGICAL UPPER, UP
C
C     LTONE AND UTZERO MUST BE SET TO SUIT THE PARTICULAR COMPUTER
C     (SEE INTRODUCTORY TEXT)
C
    DATA LTONE, UTZERO /7.0, 18.66/
    DATA ZERO, HALF, ONE, CON /0.0, 0.5, 1.0, 1.28/
    DATA
$   A1,           A2,           A3,
$   A4,           A5,           A6,
$   A7
$   /0.398942280444, 0.399903438504, 5.75885480458,
$   29.8213557808, 2.62433121679, 48.6959930692,
$   5.92885724438/
    DATA
$   B1,           B2,           B3,
$   B4,           B5,           B6,
$   B7,           B8,           B9,
$   B10,          B11,          B12
$   /0.398942280385, 3.8052E-8, 1.00000615302,
$   3.98064794E-4, 1.98615381364, 0.151679116635,
$   5.29330324926, 4.8385912808, 15.1508972451,
$   0.742380924027, 30.789933034, 3.99019417011/
C
    ZEXP(Z) = EXP(Z)
C
    UP = UPPER
    Z = X
    IF (Z .GE. ZERO) GOTO 10
    UP = .NOT. UP
    Z = -Z
10 IF (Z .LE. LTONE .OR. UP .AND. Z .LE. UTZERO) GOTO 20
    ALNORM = ZERO
    GOTO 40
20 Y = HALF * Z * Z
    IF (Z .GT. CON) GOTO 30
C
    ALNORM = HALF - Z * (A1 - A2 * Y / (Y + A3 - A4 / (Y + A5 +
$   A6 / (Y + A7))))
    GOTO 40
C
30 ALNORM = B1 * ZEXP(-Y) / (Z - B2 + B3 / (Z + B4 + B5 / (Z -
$   B6 + B7 / (Z + B8 - B9 / (Z + B10 + B11 / (Z + B12))))))
C
40 IF (.NOT. UP) ALNORM = ONE - ALNORM
    RETURN
    END
    REAL FUNCTION PPND7 (P, IFAULT)

```

```

C
C      ALGORITHM AS241  APPL. STATIST. (1988) VOL. 37, NO. 3
C
C      PRODUCES THE NORMAL DEVIATE Z CORRESPONDING TO A GIVEN LOWER
C      TAIL AREA OF P; Z IS ACCURATE TO ABOUT 1 PART IN 10**7.
C
C      THE HASH SUMS BELOW ARE THE SUMS OF THE MANTISSAS OF THE
C      COEFFICIENTS. THEY ARE INCLUDED FOR USE IN CHECKING
C      TRANSCRIPTION.
C
      INTEGER IFAULT
      REAL ZERO, ONE, HALF, SPLIT1, SPLIT2, CONST1, CONST2,
*      A0, A1, A2, A3, B1, B2, B3, C0, C1, C2, C3, D1, D2,
*      E0, E1, E2, E3, F1, F2, P, Q, R
      PARAMETER (ZERO = 0.0E0, ONE = 1.0E0, HALF = 0.5E0,
*      SPLIT1 = 0.425E0, SPLIT2 = 5.0E0,
*      CONST1 = 0.180625E0, CONST2 = 1.6E0)
C
C      COEFFICIENTS FOR P CLOSE TO 1/2
      PARAMETER (A0 = 3.38713 27179E0,
*      A1 = 5.04342 71938E1,
*      A2 = 1.59291 13202E2,
*      A3 = 5.91093 74720E1,
*      B1 = 1.78951 69469E1,
*      B2 = 7.87577 57664E1,
*      B3 = 6.71875 63600E1)
C      HASH SUM AB      32.31845 77772
C
C      COEFFICIENTS FOR P NEITHER CLOSE TO 1/2 NOR 0 OR 1
      PARAMETER (C0 = 1.42343 72777E0,
*      C1 = 2.75681 53900E0,
*      C2 = 1.30672 84816E0,
*      C3 = 1.70238 21103E-1,
*      D1 = 7.37001 64250E-1,
*      D2 = 1.20211 32975E-1)
C      HASH SUM CD      15.76149 29821
C
C      COEFFICIENTS FOR P NEAR 0 OR 1
      PARAMETER (E0 = 6.65790 51150E0,
*      E1 = 3.08122 63860E0,
*      E2 = 4.28682 94337E-1,
*      E3 = 1.73372 03997E-2,
*      F1 = 2.41978 94225E-1,
*      F2 = 1.22582 02635E-2)
C      HASH SUM EF      19.40529 10204
C
      IFAULT = 0
      Q = P - HALF
      IF (ABS(Q) .LE. SPLIT1) THEN
        R = CONST1 - Q * Q
        PPND7 = Q * (((A3 * R + A2) * R + A1) * R + A0) /
*          (((B3 * R + B2) * R + B1) * R + ONE)
        RETURN
      ELSE
        IF (Q .LT. 0) THEN
          R = P
        ELSE
          R = ONE - P
        ENDIF
        IF (R .LE. ZERO) THEN
          IFAULT = 1
        ENDIF
      ENDIF

```

```

        PPND7 = ZERO
        RETURN
    ENDIF
    R = SQRT(-LOG(R))
    IF (R .LE. SPLIT2) THEN
        R = R - CONST2
        PPND7 = (((C3 * R + C2) * R + C1) * R + C0) /
*           ((D2 * R + D1) * R + ONE)
    ELSE
        R = R - SPLIT2
        PPND7 = (((E3 * R + E2) * R + E1) * R + E0) /
*           ((F2 * R + F1) * R + ONE)
    ENDIF
    IF (Q .LT. 0) PPND7 = -PPND7
    RETURN
ENDIF
END
PROGRAM MVTIN
C
C     COMPUTE PROBABILITY INTEGRAL FOR A MULTIVARIATE
C     NORMAL OR A MULTIVARIATE T WITH PRODUCT CORRELATION
C     STRUCTURE USING MVSTUD AND MVNPRD.
C
    DIMENSION A(50),B(50),BPD(50),INF(50),D(50),TMP(2)
    DATA ZERO, ONE, EPS / 0.0, 1.0, 0.0001 /
    IERC = 0
    HNC = ZERO
C
C     START A NEW PROBLEM:-
C     ENTER N = NO. DIMENSIONS, AND NDF = DEG. OF FREEDOM
C     (FOR INFINITE D.F., ENTER NDF = 0)
C
    10 WRITE (*, 200)
    READ (*, *) N, NDF
    IF (N .LE. 0 .OR. NDF .LT. 0) STOP
    IF (N .GT. 50) THEN
        WRITE (*, 300)
        STOP
    ELSE
        XN = FLOAT(N)
    ENDIF
C
C     SPECIFY THE CORRELATION STRUCTURE:-
C     ENTER IX = 1 IF THERE IS A FIXED RHO
C     OR IX = 2 IF RHO IS DETERMINED FROM SAMPLE SIZES
C     OR IX = 3 IF RHO(I,J) = BPD(I)*BPD(J)
C     OR IX = 4 IF RHO(I,J) = 1 / (1 + SQRT(N))
C
    20 WRITE (*, 210)
    READ (*,*) IX
    IF (IX .LT. 1 .OR. IX .GT. 4) GO TO 10
    IF (IX .EQ. 1 .OR. IX .EQ. 4) THEN
        IF (IX .EQ. 4) THEN
            RHO = ONE / (ONE + SQRT(XN))
        ELSE
    30     WRITE (*, 220)
            READ (*, *) RHO
            IF (RHO .LT. ZERO .OR. RHO .GE. ONE) GO TO 30
        ENDIF
        SQTRHO = ZERO
        IF (RHO .GT. ZERO) SQTRHO = SQRT(RHO)

```

```
        DO 40 I = 1, N
          BPD(I) = SQTRHO
40      CONTINUE
      ELSE
        IF (IX .EQ. 2) THEN
          WRITE (*, 310)
          READ (*, *) X0, (BPD(I), I = 1, N)
          DO 50 I = 1, N
            BPD(I) = ONE / SQRT(ONE + X0 / BPD(I))
50      CONTINUE
        ELSE
          WRITE (*, 230) N
          READ (*, *) (BPD(I), I = 1, N)
        ENDIF
      ENDIF
C
C      SPECIFY MEANS
C
80    WRITE (*, 205)
      READ (*, *) IDEL
      IF (IDEL .EQ. 0) THEN
        DO 90 I = 1, N
          D(I) = ZERO
90    CONTINUE
      ELSE
        NCM = 1
        IF (IDEL .NE. 1) NCM = N
        WRITE (*, 270) NCM
        READ (*, *) (D(I), I = 1, NCM)
        IF (NCM .EQ. N) GO TO 120
        DO 110 I = 1, N
          D(I) = D(1)
110   CONTINUE
      ENDIF
120  CONTINUE
      WRITE (*, 240)
      READ (*, *) NCM
      IF (NCM .NE. 1) NCM = N
      NSTRT = 1
125  CONTINUE
C
C      SPECIFY THE VALUES FOR THE ENDPOINTS
C
      WRITE (*, 245)
      DO 130 I = NSTRT, NCM
132  IF (NCM .EQ. 1) THEN
          WRITE (*, 250)
        ELSE
          WRITE (*, 260) I
        END IF
        READ (*, *) INF1, TMP(1), (TMP(J), J = 2, INF1)
        IF (INF1 .LT. 0 .OR. INF1 .GT. 2) GO TO 132
        INF(I) = INF1
        IF (INF1 .EQ. 0) THEN
          B(I) = TMP(1)
          A(I) = ZERO
        ELSE
          IF (INF1 .EQ. 1) THEN
            B(I) = ZERO
            A(I) = TMP(1)
          ELSE
```



```

                B(I) = TMP(1)
                A(I) = TMP(2)
            ENDIF
        ENDIF
        IF (NCM .EQ. 1) GO TO 131
130     CONTINUE
131     IF (NCM .EQ. 1) THEN
            DO 140 I = 2, N
                A(I) = A(1)
                B(I) = B(1)
                INF(I) = INF(1)
140     CONTINUE
            ELSE
                CONTINUE
            ENDIF
        NX = N
        IF (N .GT. 4) NX = 4
        WRITE (*, 180) NX
        DO 150 I = 1, NX
            WRITE (*, 190) I, B(I), A(I), INF(I), BPD(I), D(I)
150     CONTINUE
C
C         COMPUTE PROB
C
        WRITE (*, 290) N, NDF
        CALL MVSTUD(NDF,A,B,BPD,EPS,N,INF,D,IERC,HNC,PROB,BND,IFLT)
        WRITE (*, 280) PROB, BND, IFLT
160     WRITE (*, 170)
        READ (*, *) NSTRT
        IF (NSTRT .GT. N) GO TO 160
        IF (NSTRT .GE. 1) GO TO 125
        GO TO 10
170     FORMAT(1X,'Enter 1 to repeat with new values for limits',
*           /1X,' or J for new values for J-th to N-th limits, incl.',
*           /1X ' or 0 for new problem')
180     FORMAT(1X,'First',I2,' parameter sets:-',
*           /,1X,' i      L_i      U_i      Type      b_i      \mu_i')
190     FORMAT(1X, I2, 2F9.3, I6, 2F9.3)
200     FORMAT(1X, 'Enter No. Dimensions, and D.o.F. (0 for MVN)',
*           /8X, '(or enter 0, 0 to terminate)')
205     FORMAT(1X, 'Enter 0 for central case, '/'
*           1X, ' or 1 for vector (D,...,D), '/'
*           1X, ' or 2 for vector (D_1,...,D_N)')
210     FORMAT(1X, 'Enter 1 for equal-rho case, '/'
*           1X, ' or 2 to compute \rho_ij from sample sizes, '/'
*           1X, ' or 3 if \rho_ij = b_i*b_j, '/'
*           1X, ' or 4 for \rho = 1 / (1+sqrt(N))')
220     FORMAT(1X, 'Enter common \rho')
230     FORMAT(1X, 'Enter b_i, i = 1, ',I3)
240     FORMAT(1X, 'Enter 1 for a common set of limits or 0 if not')
245     FORMAT(1X,'For each variable enter type of interval and limits,/'
*           1X,'Type = 0 iff [a,\infty], = 1 iff [-\infty,b]',
*           ', = 2 iff [a,b]')
250     FORMAT(1X, 'Enter common values of TYPE and limit(s)')
260     FORMAT(1X, 'Enter TYPE and limit(s) for I =',I3)
270     FORMAT(1X, 'Enter',I3,' mean value(s)')
280     FORMAT(1X, 'PROB =',F10.6,/,1X,'BOUND =',F10.6,/,1X,
*           'FAULT =', I10, /)
290     FORMAT(/,1X,'Computed results for N =',I3,', NDF =',I4,':-')
300     FORMAT(1X, 'DIMENSION LIMITS EXCEEDED',/)
310     FORMAT(1X, 'Enter sample sizes (control first)',/)

```

```

      END
      SUBROUTINE MVSTUD(NDF,A,B,BPD,ERRB,N,INF,D,IERC,HNC,PROB,
*      BND,IFLT)
C
C      COMPUTE MULTIVARIATE STUDENT INTEGRAL,
C      USING MVNPRD (DUNNETT, APPL. STAT., 1989)
C      IF RHO(I,J) = BPD(I)*BPD(J).
C
C      IF RHO(I,J) HAS GENERAL STRUCTURE, USE
C      MULNOR (SCHERVISH, APPL. STAT., 1984) AND REPLACE
C      CALL MVNPRD(A,B,BPD,EPS,N,INF,IERC,HNC,PROB,BND,IFLT)
C      BY CALL MULNOR(A,B,SIG,EPS,N,INF,PROB,BND,IFLT).
C
C      AUTHOR: C.W. DUNNETT, MCMASTER UNVERSITY
C
C      BASED ON ADAPTIVE SIMPSON'S RULE ALGORITHM
C      DESCRIBED IN SHAMPINE & ALLEN: "NUMERICAL
C      COMPUTING", (1974), PAGE 240.
C
C      PARAMETERS ARE SAME AS IN ALGORITHM AS 251
C      IN APPL. STAT. (1989), VOL. 38: 564-579
C      WITH THE FOLLOWING ADDITIONS:
C          NDF    INTEGER        INPUT  DEGREES OF FREEDOM
C          D      REAL ARRAY     INPUT  NON-CENTRALITY VECTOR
C          (PUT NDF = 0 FOR INFINITE D.F.)
C
      INTEGER NN
      PARAMETER (NN=50)
      DIMENSION A(*),B(*),BPD(*),INF(*),D(*),F(3),AA(NN),BB(NN)
      DATA ZERO,HALF,TWO,THREE,FOUR / 0.0, 0.5, 2.0, 3.0, 4.0 /
      DO 10 I = 1, N
          AA(I) = A(I) - D(I)
          BB(I) = B(I) - D(I)
10  CONTINUE
      IF (NDF .LE. 0) THEN
          CALL MVNPRD(AA,BB,BPD,ERRB,N,INF,IERC,HNC,PROB,BND,IFLT)
          RETURN
      ENDIF
      BND = ZERO
      IFLT = 0
      MAXDF = 150
      ERB2 = ERB
C
C      CHECK IF D.F. EXCEED MAXDF; IF YES, THEN PROB
C      IS COMPUTED BY QUADRATIC INTERPOLATION ON 1./D.F.
C
      IF (NDF .LE. MAXDF) GO TO 20
      CALL MVNPRD(AA,BB,BPD,ERB2,N,INF,IERC,HNC,F(1),BND,IFLT)
      NF = MAXDF / 2
      CALL SIMPSN(NF,A,B,BPD,ERB2,N,INF,D,IERC,HNC,F(3),BND,IFLT)
      NF = NF * 2
      CALL SIMPSN(NF,A,B,BPD,ERB2,N,INF,D,IERC,HNC,F(2),BND,IFLT)
      XX = FLOAT(NF) / FLOAT(NDF)
      AX = F(3) - F(2)*TWO + F(1)
      BX = F(2)*FOUR - F(3) - F(1)*THREE
      PROB = F(1) + XX * (AX * XX + BX) * HALF
      RETURN
20  CALL SIMPSN (NDF,A,B,BPD,ERB2,N,INF,D,IERC,HNC,PROB,BND,IFLT)
      RETURN
      END
      SUBROUTINE SIMPSN (NDF,A,B,BPD,ERRB,N,INF,D,IERC,HNC,PROB,

```

```

*   BND , IFLT)
C
C   STUDENTIZES A MULTIVARIATE INTEGRAL USING SIMPSON'S RULE.
C
  DIMENSION A(*),B(*),BPD(*),INF(*),D(*),
*   FV(5),F1T(30),F2T(30),F3T(30),
*   LDIR(30),PSUM(30),ESTT(30),ERRR(30),GV(5),G1T(30),G2T(30),
*   G3T(30),GSUM(30)
  DATA ZERO,HALF,ONE,ONEP5,TWO,FOUR,SIX,DXMIN /0.0,0.5,1.0,1.5,
*   2.0,4.0,6.0,0.000004/
  PROB      = ZERO
  BOUNDA    = ZERO
  BOUNDG    = ZERO
  IFLAG     = 0
  IER       = 0
  START     = -ONE
  DAX       = ONE
  ERB2      = ERB * HALF
  EPS1      = ERB2 * HALF
  CALL FUN (ZERO,NDF,A,B,BPD,ERB2,N,INF,D,F0,G0,IERC,HNC,IER)
10 FV(1)    = ZERO
   GV(1)    = ZERO
   ERROR    = ZERO
   DA       = DAX
   LVL      = 1
   Z3       = START + HALF*DA
   CALL FUN (Z3,NDF,A,B,BPD,ERB2,N,INF,D,FV(3),GV(3),IERC,HNC,IER)
   FV(5)    = F0
   GV(5)    = G0
   WT       = ABS(DA) / SIX
   CONTRB   = WT * (FV(1) + FOUR * FV(3) + FV(5))
   CONTRG   = WT * (GV(1) + FOUR * GV(3) + GV(5))
   LDIR(LVL) = 2
   PSUM(LVL) = ZERO
   GSUM(LVL) = ZERO
C
C   BISECT INTERVAL; COMPUTE ESTIMATES FOR EACH HALF.
C
20 DX      = HALF * DA
   WT      = ABS(DX) / SIX
   Z2      = START + HALF * DX
   CALL FUN (Z2,NDF,A,B,BPD,ERB2,N,INF,D,FV(2),GV(2),IERC,HNC,IER)
   Z4      = START + ONEP5 * DX
   CALL FUN (Z4,NDF,A,B,BPD,ERB2,N,INF,D,FV(4),GV(4),IERC,HNC,IER)
   ESTL    = WT * (FV(1) + FOUR * FV(2) + FV(3))
   ESTR    = WT * (FV(3) + FOUR * FV(4) + FV(5))
   ESTGL   = WT * (GV(1) + FOUR * GV(2) + GV(3))
   ESTGR   = WT * (GV(3) + FOUR * GV(4) + GV(5))
   SUM     = ESTL + ESTR
   SUMG    = ESTGL + ESTGR
   DLG     = ABS(CONTRB - SUM)
   ERRL    = DLG
C
C   STOP BISECTING WHEN ACCURACY SUFFICIENT, OR IF
C   INTERVAL TOO NARROW OR BIASECTED TOO OFTEN.
C
30 IF (DLG .LE. EPS1) GO TO 50
   IF (ABS(DX) .LE. DXMIN .OR. LVL .GE. 30) GO TO 40
C
C   RAISE LEVEL.  STORE INFORMATION FOR RIGHT HALF
C   AND APPLY SIMPSON'S RULE TO LEFT HALF.

```

C

```

LVL      = LVL + 1
LDIR(LVL) = 1
F1T(LVL) = FV(3)
F2T(LVL) = FV(4)
F3T(LVL) = FV(5)
G1T(LVL) = GV(3)
G2T(LVL) = GV(4)
G3T(LVL) = GV(5)
DA       = DX
FV(5)    = FV(3)
FV(3)    = FV(2)
GV(5)    = GV(3)
GV(3)    = GV(2)
ESTT(LVL) = ESTR
CONTRB   = ESTL
CONTRG   = ESTGL
EPS1     = EPS1 * HALF
ERRR(LVL) = EPS1
GO TO 20

```

C

C

C

```

ACCEPT APPROXIMATE VALUE FOR INTERVAL.

```

```

40 IFLAG   = 11
50 ERROR   = ERROR + ERRL
60 IF (LDIR(LVL) .EQ. 1) GO TO 70
SUM        = SUM + PSUM(LVL)
SUMG       = SUMG + GSUM(LVL)
LVL        = LVL - 1
IF (LVL .GT. 0) GO TO 60
CONTRB     = SUM
CONTRG     = SUMG
LVL        = 1
DLG        = ERROR
GO TO 80

```

C

C

C

```

RESTORE SAVED INFORMATION TO PROCESS RIGHT HALF.

```

```

70 PSUM(LVL) = SUM
   GSUM(LVL) = SUMG
   LDIR(LVL) = 2
   DA        = DAX / TWO**(LVL-1)
   START     = START + DX * TWO
   FV(1)     = F1T(LVL)
   FV(3)     = F2T(LVL)
   FV(5)     = F3T(LVL)
   GV(1)     = G1T(LVL)
   GV(3)     = G2T(LVL)
   GV(5)     = G3T(LVL)
   CONTRB    = ESTT(LVL)
   EXCESS    = EPS1 - DLG
   EPS1      = ERRR(LVL)
   IF (EXCESS .GT. ZERO) EPS1 = EPS1 + EXCESS
   GO TO 20
80 PROB      = PROB + CONTRB
   BOUNDG    = BOUNDG + CONTRG
   BOUNDA    = BOUNDA + DLG
   IF (Z4 .LE. ZERO) GO TO 90
   IF (IFLT .EQ. 0) IFLT = IER
   IF (IFLT .EQ. 0) IFLT = IFLAG
   BOUNDA    = BOUNDA + BOUNDG

```

```

        IF (BND .LT. BOUNDA) BND = BOUNDA
        RETURN
90 EPS1      =   ERB2 * HALF
    EXCESS   =   EPS1 - BND
    IF (EXCESS .GT. ZERO) EPS1 = EPS1 + EXCESS
    START    =   ONE
    DAX      =  -ONE
    GO TO 10
    END
    FUNCTION SDIST(Y,N)
C
C      COMPUTE Y**(N/2 - 1) EXP(-Y) / GAMMA(N/2)
C
C      (Revised: 1994-01-19)
C
DATA ZERO, HALF, ONE, X23 / 0.0, 0.5, 1.0, -23.0 /
DATA SQRTPI / 1.77245385090552 /
SDIST      =   ZERO
IF (Y .LE. ZERO) RETURN
JJ         =   N/2 - 1
JK         =   2 * JJ - N + 2
JKP        =   JJ - JK
SDIST      =   ONE
IF (JK .LT. 0) SDIST = SDIST / SQRT(Y) / SQRTPI
IF (JKP .EQ. 0) GO TO 20
XN         =   FLOAT(N) * HALF
TEST       =   ALOG(Y) - Y / FLOAT(JKP)
IF ( TEST .LT. X23 ) THEN
    SDIST = ZERO
    RETURN
ENDIF
SDIST = ALOG ( SDIST )
DO 10 J = 1, JKP
    XN    =   XN - ONE
    SDIST =   SDIST + TEST - ALOG(XN)
10 CONTINUE
IF ( SDIST .LT. X23 ) THEN
    SDIST = ZERO
ELSE
    SDIST = EXP( SDIST )
ENDIF
RETURN
20 SDIST      =   SDIST * EXP(-Y)
    RETURN
    END
SUBROUTINE FUN ( Z, NDF, H, HL, BPD, ERB2, N, INF, D, F0, G0, IERC
*      , HNC, IER)
    INTEGER NN
    PARAMETER (NN=50)
    DIMENSION A(NN), B(NN), H(*), HL(*), BPD(*), INF(*), D(*)
    DATA ZERO, ONE, TWO, SMALL / 0.0, 1.0, 2.0, 1.0E-08 /
    F0    =   ZERO
    G0    =   ZERO
    IF (Z .LE. -ONE .OR. Z .GE. ONE) RETURN
    DF    =   FLOAT(NDF)
    ARG   =   (ONE + Z) / (ONE - Z)
    TERM = ARG * DF * TWO / (ONE-Z)**2 * SDIST(DF/TWO*ARG*ARG, NDF)
    IF (TERM .LE. SMALL) RETURN
    DO 10 I = 1, N
        A(I) = ARG * H(I)    - D(I)
        B(I) = ARG * HL(I)   - D(I)

```

```
10 CONTINUE
   CALL MVNPRD (A,B,BPD,ERB2,N,INF,IERC,HNC,PROB,BND,IFLT)
   IF (IER .EQ. 0) IER = IFLT
   G0 = TERM * BND
   F0 = TERM * PROB
   RETURN
   END
```

```
C * * * * *
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C Dept. of Mathematics and Statistics
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C Hamilton, Ontario L8S 4K1
C Canada
C E-mail: dunnett@mcmaster.ca
C Tel.: (905) 525-9140 (Ext. 27104)
C * * * * *
```

```

SUBROUTINE GESAT(NVAR, NP, ISET, NUM, SATMOD, IFAULT)
C
C   ALGORITHM AS 252.1  APPL.STATIST. (1990), VOL.39, NO.1
C
C   Obtains the description of all interactions
C   in the saturated model
C
C   Auxiliary routine required: COMBO from AS 160 (included here)
C
C   INTEGER NVAR, NP, IFAULT, ISET(NVAR), NUM(NVAR), SATMOD(NVAR, NP)
C   INTEGER NVMAX, I, J, K, M, N
C   LOGICAL LAST
C   DATA NVMAX / 15 /
C
C   IFAULT = 1
C   IF (NVAR .LT. 1 .OR. NVAR .GT. NVMAX) RETURN
C   IFAULT = 2
C   I = 2 ** NVAR - 1
C   IF (NP .LT. I) RETURN
C   IFAULT = 0
C   DO 20 I = 1, NVAR
C     DO 10 J = 1, NP
C       SATMOD(I, J) = 0
10    CONTINUE
20  CONTINUE
C   M = 0
C   N = 0
C   DO 50 K = 1, NVAR
C     I = NVAR - K + 1
C     LAST = .TRUE.
30    CALL COMBO(ISET, NVAR, I, LAST)
C     IF ( .NOT. LAST) THEN
C       N = N + 1
C       DO 40 J = 1, I
C         SATMOD(J, N) = ISET(J)
40    CONTINUE
C       GO TO 30
C     END IF
C     M = M + 1
C     NUM(M) = N
50  CONTINUE
C   RETURN
C   END
C
C
C   SUBROUTINE CLAGEN(NVAR, NP, NUM, SATMOD, IPAR, DES, NG, INTG,
*                   IGEN, ISET, JSET, IDES, JDES, NCON, CONFIG,
*                   IFAULT)
C
C   ALGORITHM AS 252.2  APPL.STATIST. (1990), VOL.39, NO.1
C
C   Obtains the generating class or dual generating class
C   of the model defined in terms of interactions which
C   must be present/absent or which must be added/omitted
C   to/from given model
C
C   INTEGER NVAR, NP, IPAR, NG, IGEN, NCON, IFAULT, NUM(NVAR),
*   SATMOD(NVAR, NP), ISET(NVAR), JSET(NVAR), INTG(NVAR, NG),
*   CONFIG(NVAR, NP)
C   LOGICAL DES(NP), IDES(NP), JDES(NP)
C   INTEGER I, IP, J, J1, J2, K, KZ, LF, M, M1, M2, M3, M4, N, NI,

```

```
*          NR, NR1, NR2, NST, NVMAX
LOGICAL IND, LG, LW, STER
EXTERNAL INSET
LOGICAL INSET
C
C          NVMAX:  Set to 15 for 16 bit integers - see text.
C
DATA NVMAX / 15 /
C
C          Check input parameters
C
IFAULT = 1
IF (NVAR .LT. 1 .OR. NVAR .GT. NVMAX) RETURN
IFAULT = 2
I = 2 ** NVAR - 1
IF (NP .LT. I) RETURN
IFAULT = 3
IF (IPAR .LT. 1 .OR. IPAR .GT. 4) RETURN
STER = IPAR .EQ. 1 .OR. IPAR .EQ. 3
IFAULT = 4
IF (NG .LT. 1) RETURN
IFAULT = 5
DO 20 I = 1, NG
  DO 10 J = 1, NVAR
    K = INTG(J, I)
    IF (K .LT. 0 .OR. K .GT. NVAR) RETURN
10  CONTINUE
20  CONTINUE
IFAULT = 6
IF (IGEN .NE. 1 .AND. IGEN .NE. 2) RETURN
IFAULT = 0
C
C          Initialize workspaces and variables
C
LG = IPAR .EQ. 3 .OR. IPAR .EQ. 4
IF ( .NOT. LG) THEN
  DO 30 I = 1, NP
    DES(I) = .NOT. STER
30  CONTINUE
END IF
DO 40 I = 1, NP
  LW = DES(I)
  IDES(I) = LW
  JDES(I) = LW
40  CONTINUE
IF (STER) THEN
  K = -1
  KZ = 1
ELSE
  K = 1
  KZ = NVAR
END IF
C
C          Find full description of the model
C
DO 140 NI = 1, NG
  DO 50 I = 1, NVAR
    JSET(I) = 0
50  CONTINUE
NR = 0
DO 60 I = 1, NVAR
```



```

        J = INTG(I, NI)
        IF (J .EQ. 0) GO TO 70
        NR = NR + 1
        JSET(NR) = J
60    CONTINUE
70    N = NR
        IF (N .EQ. 0) THEN
            IF (STER) GO TO 140
            DO 80 I = 1, NP
                IDES(I) = .FALSE.
80    CONTINUE
        GO TO 150
    END IF
90    IF (N .EQ. NVAR) THEN
        M3 = 1
        M4 = 1
    ELSE
        J = NVAR - N
        M3 = NUM(J) + 1
        M4 = NUM(J + 1)
    END IF
    DO 120 I = M3, M4
        IDES(I) = STER
        IF (JDES(I) .NEQV. STER) THEN
            IP = 0
            DO 100 J = 1, NVAR
                IF (SATMOD(J, I) .EQ. 0) GO TO 110
                IP = IP + 1
                ISET(IP) = SATMOD(J, I)
100    CONTINUE
110    IF (STER) THEN
                IND = INSET(NR, JSET, IP, ISET)
            ELSE
                IND = INSET(IP, ISET, NR, JSET)
            END IF
            IDES(I) = JDES(I)
            IF (IND) IDES(I) = STER
        END IF
120    CONTINUE
        N = N + K
        IF (STER) THEN
            IF (N .GE. KZ) GO TO 90
        ELSE
            IF (N .LE. KZ) GO TO 90
        END IF
        DO 130 J = 1, NP
            JDES(J) = IDES(J)
130    CONTINUE
140 CONTINUE
150 IF (LG) GO TO 170
C
C    If the model is defined by interactions which must be
C    present/absent, store its full description in DES
C
        DO 160 I = 1, NP
            DES(I) = IDES(I)
160 CONTINUE
C
C    Find the (dual) generating class if the model is saturated
C
170 STER = IGEN .EQ. 1

```

```

        NCON = 1
        LW = IDES(1)
        LG = LW .EQV. STER
        DO 180 I = 1, NVAR
            K = 0
            IF (LG) K = I
            CONFIG(I, 1) = K
180 CONTINUE
        IF (LW) RETURN
C
C         Find the (dual) generating class if the model is unsaturated
C
        LW = .TRUE.
        NCON = 0
        NR1 = NVAR - 1
        IF (STER) THEN
            NR2 = NR1
            NR1 = 1
            NST = 1
        ELSE
            NR2 = 1
            NST = -1
        END IF
        DO 240 M = NR1, NR2, NST
            I = NVAR - M
            LF = 0
            M1 = NUM(M) + 1
            M2 = NUM(M + 1)
            DO 230 J = M1, M2
                IF (STER .EQV. IDES(J)) THEN
                    IF ( .NOT. LW) THEN
                        DO 190 J1 = 1, I
                            ISET(J1) = SATMOD(J1, J)
190 CONTINUE
                            IF (I .NE. NR2) THEN
                                M3 = NUM(M - NST) + 1
                                M4 = NUM(M - NST + 1)
                                DO 210 J1 = M3, M4
                                    IF (IDES(J1) .EQV. STER) THEN
                                        IP = I + NST
                                        DO 200 J2 = 1, IP
                                            JSET(J2) = SATMOD(J2, J1)
200 CONTINUE
                                            IF ( .NOT. STER) THEN
                                                LG = INSET(I, ISET, IP, JSET)
                                            ELSE
                                                LG = INSET(IP, JSET, I, ISET)
                                            END IF
                                        IF (LG) GO TO 230
                                    END IF
                                END IF
                            CONTINUE
                        END IF
                    END IF
                    NCON = NCON + 1
                    DO 220 J1 = 1, NVAR
                        CONFIG(J1, NCON) = SATMOD(J1, J)
220 CONTINUE
                    ELSE
                        LF = LF + 1
                    END IF
                230 CONTINUE
            END IF
        END IF
    
```

```
        IF (LF .EQ. 0) RETURN
        J = M2 - M1 + 1
        LW = LF .EQ. J
240 CONTINUE
        IF (NCON .EQ. 0) NCON = 1
        RETURN
        END
C
C
        LOGICAL FUNCTION INSET(N, ISET, M, JSET)
C
C        ALGORITHM AS 252.3  APPL.STATIST. (1990), VOL.39, NO.1
C
        INTEGER N, M, ISET(N), JSET(M)
        INTEGER I, J
C
        INSET = .FALSE.
        DO 20 I = 1, M
            DO 10 J = 1, N
                IF (JSET(I) .EQ. ISET(J)) GO TO 20
10         CONTINUE
            RETURN
20        CONTINUE
        INSET = .TRUE.
        RETURN
        END
C
C
        SUBROUTINE COMBO(ISET, N, M, LAST)
C
C        ALGORITHM AS 160.2  APPL. STATIST. (1981) VOL.30, NO.1
C
C        Subroutine to generate all possible combinations of M of the
C        integers from 1 to N in a stepwise fashion.  Prior to the first
C        call, LAST should be set to .FALSE.  Thereafter, as long as LAST
C        is returned .FALSE., a new valid combination has been generated.
C        When LAST goes .TRUE., there are no more combinations.
C
        LOGICAL LAST
        INTEGER N, M, ISET(M)
C
        IF (LAST) GO TO 110
C
C        Get next element to increment
C
        K = M
100     L = ISET(K) + 1
        IF (L + M - K .LE. N) GO TO 150
        K = K - 1
C
C        See if we are done
C
        IF (K .LE. 0) GO TO 130
        GO TO 100
C
C        Initialize first combination
C
110     DO 120 I = 1, M
120     ISET(I) = I
130     LAST = .NOT. LAST
        RETURN
```

```
C
C      Fill in remainder of combination.
C
150   DO 160 I = K, M
      ISET(I) = L
      L = L + 1
160   CONTINUE
C
      RETURN
      END
```

```

      SUBROUTINE RCM(TAB, FIT, FF, L, LR, LC, MU, NU, PHI, DETAIL, TOL,
*           RWT, CWT, WRK, WRK2, ITER, NTAB, NR, NC, NM, NW,
*           NW2, MAXIT, IFAULT)
C
C       ALGORITHM AS 253.1  APPL. STATIST. (1990) VOL.39, NO. 1
C
C       Maximum likelihood estimation of the RC(M) association model
C
      INTEGER FF(NTAB), ITER, NTAB, NR, NC, NM, NW, NW2, MAXIT, IFAULT
      REAL TAB(NTAB), FIT(NTAB), L, LR(NR), LC(NC), MU( * ), NU( * ),
*       PHI( * ), DETAIL(MAXIT), TOL, RWT(NR), CWT(NC), WRK(NW),
*       WRK2(NW2)
      INTEGER IPT(8), I, ICON, II, J, MNRC, JOB
      REAL SALE, TOT, ZERO
      DATA ZERO / 0.0 /
C
C       Check for errors
C
      IFAULT = 0
      IF (NM .GT. (NR - 1) .OR. NM .GT. (NC - 1)) IFAULT = 1
      IF (NM .LT. 0) IFAULT = 1
      IF (TOL .LE. ZERO) IFAULT = 2
      IF (NR .LT. 2 .OR. NC .LT. 2) IFAULT = 3
      DO 10 J = 1, NTAB
         IF (TAB(J) .LT. ZERO) IFAULT = 4
10  CONTINUE
      IF (NTAB .LT. (NR * NC)) IFAULT = 6
      IF (NW .LT. (2 * (NR + NC) + (NR * NC))) IFAULT = 7
      IF (NW2 .LT. ((MAX(NR, NC)) + (NC + 1) + (NC ** 2) + NR +
*       NC)) IFAULT = 7
      DO 20 I = 1, NTAB
         IF (FF(I) .NE. 1 .AND. FF(I) .NE. 0) IFAULT = 8
20  CONTINUE
      IF (IFAULT .NE. 0) RETURN
C
C       Set pointers to locations in work space
C
      MNRC = MAX(NR, NC)
C
      IPT(1) = NR + 1
      IPT(2) = NR + NC + 1
      IPT(3) = 2 * NR + NC + 1
      IPT(4) = 2 * (NR + NC) + 1
      IPT(5) = MNRC * NC + 1
      IPT(6) = (MNRC * NC) + NC + 2
      IPT(7) = (MNRC * NC) + (NC * NC) + NC + 2
      IPT(8) = (MNRC * NC) + (NC * NC) + NR + NC + 2
C
C       Get the marginal totals for the observed table
C
      CALL MARGIN(TAB, WRK(1), WRK(IPT(1)), TOT, NR, NC)
C
C       Compute intial parameter estimates
C
      JOB = 21
      CALL START(TAB, L, LR, LC, MU, NU, PHI, RWT, CWT, WRK2(1),
*       WRK2(IPT(5)), WRK2(IPT(6)), WRK2(IPT(7)), WRK2(IPT(8)),
*       WRK(IPT(4)), WRK(IPT(2)), WRK(IPT(3)), NR, NC, NM,
*       MNRC, JOB, IFAULT)
      IF (IFAULT .NE. 0) THEN
         IFAULT = 5

```

```

      RETURN
    END IF
C
C      ***** Iterations *****
C
      ITER = MAXIT
      DO 30 II = 1, MAXIT
C
C      Update the LAMBDAs
C
      CALL LAMFIT(1, TAB, FIT, FF, L, LR, LC, MU, NU, PHI, WRK(1),
*              WRK(IPT(1)), WRK(IPT(2)), WRK(IPT(3)), TOT, NR, NC,
*              NR, NC, NM)
      CALL LAMFIT(2, TAB, FIT, FF, L, LC, LR, NU, MU, PHI, WRK(1),
*              WRK(IPT(1)), WRK(IPT(2)), WRK(IPT(3)), TOT, NR, NC,
*              NC, NR, NM)
C
      IF (NM .GT. 0) THEN
C
C      Update the MU's and NU's
C
      CALL SCRFIT(1, TAB, FIT, FF, L, LR, LC, MU, NU, PHI, NR, NC,
*              NM, NR, NC)
      CALL SCRFIT(2, TAB, FIT, FF, L, LC, LR, NU, MU, PHI, NR, NC,
*              NM, NC, NR)
C
C      Update the PHI's
C
      CALL PHIFIT(TAB, FIT, FF, L, LR, LC, MU, NU, PHI, NR, NC,
*              NM)
C
C      Centre the MU's and NU's about zero
C
      CALL CENTRE(L, LR, LC, MU, NU, PHI, RWT, CWT, NR, NC, NM)
C
      END IF
C
C      Check for convergence
C
      CALL CONV(TAB, FIT, FF, WRK, L, LR, LC, MU, NU, PHI, IPT, TOT,
*             TOL, SALE, NR, NC, NM, NW, ICON)
C
      DETAIL(II) = SALE
      IF (ICON .EQ. 1 .AND. NM .GT. 0) THEN
C
C      Rescale the MU's and NU's so that they satisfy the
C      identifying restrictions
C
      CALL SCALE(MU, NU, PHI, RWT, CWT, WRK2(1), WRK2(IPT(5)),
*             WRK2(IPT(6)), WRK2(IPT(7)), WRK2(IPT(8)), NR, NC,
*             NM, MNRC, JOB, IFAULT)
      IF (IFAULT .NE. 0) IFAULT = 5
C
      ITER = II
      RETURN
      ELSE IF (ICON .EQ. 1) THEN
      ITER = II
      RETURN
      END IF
      30 CONTINUE
C

```

```

        IFAULT = 9
        RETURN
        END
        SUBROUTINE MARGIN(T, R, C, N, NR, NC)
C
C     ALGORITHM AS 253.2  APPL. STATIST. (1990) VOL.39, NO. 1
C
C     Compute total sample size, and row and column marginal totals
C
        INTEGER NR, NC
        REAL T(NR, NC), R(NR), C(NC), N
        INTEGER I, J
        REAL ZERO
        DATA ZERO / 0.0 /
C
        DO 10 I = 1, NR
            R(I) = ZERO
10    CONTINUE
        DO 20 J = 1, NC
            C(J) = ZERO
20    CONTINUE
        N = ZERO
C
        DO 40 J = 1, NC
            DO 30 I = 1, NR
                R(I) = R(I) + T(I, J)
                C(J) = C(J) + T(I, J)
                N = N + T(I, J)
30    CONTINUE
40    CONTINUE
C
        RETURN
        END
        SUBROUTINE EXPTAB(TAB, FIT, FF, LAMBDA, LR, LC, MU, NU, PHI, NR,
*           NC, NM)
C
C     ALGORITHM AS 253.3  APPL. STATIST. (1990) VOL.39, NO. 1
C
C     Compute expected frequencies
C
        INTEGER FF(NR, NC), NR, NC, NM
        REAL TAB(NR, NC), FIT(NR, NC), LAMBDA, LR(NR), LC(NC), MU(NR, * ),
*           NU(NC, * ), PHI( * )
        INTEGER I, J, L
        REAL ONE, X, ZERO
        DATA ZERO / 0.0 / ONE / 1.0 /
C
        DO 30 J = 1, NC
            DO 20 I = 1, NR
                X = ZERO
                IF (NM .GT. 0) THEN
                    DO 10 L = 1, NM
                        X = X + MU(I, L) * NU(J, L) * PHI(L)
10                CONTINUE
                END IF
                FIT(I, J) = (EXP(LAMBDA + LR(I) + LC(J) + X) * FF(I, J)) +
*                   ((ONE - FF(I, J)) * TAB(I, J))
20            CONTINUE
30        CONTINUE
C
        RETURN

```

```

      END
      SUBROUTINE START(TAB, LAMBDA, LR, LC, M, N, P, RWT, CWT, A, W, V,
*          WORK, E, LTAB, LRM, LCM, NR, NC, NM, MNRC, JOB,
*          IFAULT)
C
C      ALGORITHM AS 253.4  APPL. STATIST. (1990) VOL.39, NO. 1
C
C      Compute initial parameter estimates
C
      INTEGER NR, NC, NM, MNRC, JOB, IFAULT
      REAL TAB(NR, NC), LAMBDA, LR(NR), LC(NC), M(NR, * ), N(NC, * ),
*      P( * ), RWT(NR), CWT(NC), A(MNRC, NC), W( * ), V(NC, NC),
*      WORK(NR), E(NC), LTAB(NR, NC), LRM(NR), LCM(NC)
      INTEGER I, IA, J, L
      REAL EPS, ZERO
      DATA EPS / 0.1 / ZERO / 0.0 /
C
      DO 20 J = 1, NC
        DO 10 I = 1, NR
          IF (TAB(I, J) .LE. EPS) THEN
            LTAB(I, J) = LOG(EPS)
          ELSE
            LTAB(I, J) = LOG(TAB(I, J))
          END IF
10      CONTINUE
20     CONTINUE
C
      CALL MARGIN(LTAB, LRM, LCM, LAMBDA, NR, NC)
      LAMBDA = LAMBDA / (NR * NC)
C
      DO 30 I = 1, NR
        LR(I) = LRM(I) / NC - LAMBDA
30     CONTINUE
      DO 40 J = 1, NC
        LC(J) = LCM(J) / NR - LAMBDA
40     CONTINUE
C
      IF (NM .GE. 1) THEN
        DO 60 J = 1, NC
          DO 50 I = 1, NR
            A(I, J) = LTAB(I, J) - (LAMBDA + LR(I) + LC(J))
            A(I, J) = A(I, J) * SQRT(RWT(I)) * SQRT(CWT(J))
50          CONTINUE
60        CONTINUE
C
          IF (MNRC .GT. NR) THEN
            IA = NR + 1
            DO 80 J = 1, NC
              DO 70 I = IA, MNRC
                A(I, J) = ZERO
70              CONTINUE
80            CONTINUE
          END IF
C
          Call LINPACK SVD subroutine
C
          CALL SSVDC(A, MNRC, NR, NC, W, E, A, MNRC, V, NC, WORK, JOB,
*          IFAULT)
C
          DO 110 L = 1, NM
            P(L) = W(L)

```



```

          DO 90 I = 1, NR
            M(I, L) = A(I, L) / SQRT(RWT(I))
90      CONTINUE
C
          DO 100 J = 1, NC
            N(J, L) = V(J, L) / SQRT(CWT(J))
100     CONTINUE
110     CONTINUE
        END IF
C
        RETURN
        END
        SUBROUTINE LAMFIT(IFLAG, TAB, FIT, FF, LAMBDA, LAM1, LAM2, M1, M2,
*           P, RM, CM, ERM, ECM, TOT, NR, NC, N1, N2, NM)
C
C       ALGORITHM AS 253.5 APPL. STATIST. (1990) VOL.39, NO. 1
C
C       Update the estimates of the lambdas
C       IFLAG =1 => Update row parameters, else do column parameters
C
        INTEGER FF(NR, NC), IFLAG, NR, NC, NM, N1, N2
        REAL TAB(NR, NC), FIT(NR, NC), LAMBDA, LAM1(N1), LAM2(N2),
*         M1(N1, * ), M2(N2, * ), P( * ), RM(NR), CM(NC), ERM(NR),
*         ECM(NC), TOT
        INTEGER II, NN
        REAL ETOT
C
        IF (IFLAG .EQ. 1) THEN
            CALL EXPTAB(TAB, FIT, FF, LAMBDA, LAM1, LAM2, M1, M2, P, NR,
*             NC, NM)
            NN = NR
        ELSE
            NN = NC
            CALL EXPTAB(TAB, FIT, FF, LAMBDA, LAM2, LAM1, M2, M1, P, NR,
*             NC, NM)
        END IF
C
        CALL MARGIN(FIT, ERM, ECM, ETOT, NR, NC)
C
        DO 10 II = 1, NN
            IF (IFLAG .EQ. 1) THEN
                LAM1(II) = LAM1(II) + (RM(II) - ERM(II)) / ERM(II)
            ELSE
                LAM1(II) = LAM1(II) + (CM(II) - ECM(II)) / ECM(II)
            END IF
10     CONTINUE
C
        RETURN
        END
        SUBROUTINE SCRFIT(IFLAG, TAB, FIT, FF, LAMBDA, LAM1, LAM2, M1, M2,
*           P, NR, NC, NM, N1, N2)
C
C       ALGORITHM AS 253.6 APPL. STATIST. (1990) VOL.39, NO. 1
C
C       Update the estimates of the MU's and NU's
C       IFLAG = 1 => Update MU's, else do NU's
C
        INTEGER FF(NR, NC), IFLAG, NR, NC, NM, N1, N2
        REAL TAB(NR, NC), FIT(NR, NC), LAMBDA, LAM1(N1), LAM2(N2),
*         M1(N1, * ), M2(N2, * ), P( * )
        INTEGER I1, I2, L

```

```

REAL C1, C2, X, XX, ZERO
DATA ZERO / 0.0 /
C
DO 30 L = 1, NM
  IF (IFLAG .EQ. 1) THEN
    N1 = NR
    N2 = NC
    CALL EXPTAB(TAB, FIT, FF, LAMBDA, LAM1, LAM2, M1, M2, P, NR,
*              NC, NM)
  ELSE
    N1 = NC
    N2 = NR
    CALL EXPTAB(TAB, FIT, FF, LAMBDA, LAM2, LAM1, M2, M1, P, NR,
*              NC, NM)
  END IF
C
DO 20 I1 = 1, N1
  X = ZERO
  XX = ZERO
  DO 10 I2 = 1, N2
    IF (IFLAG .EQ. 1) THEN
      C1 = TAB(I1, I2) - FIT(I1, I2)
      C2 = FIT(I1, I2)
    ELSE
      C1 = TAB(I2, I1) - FIT(I2, I1)
      C2 = FIT(I2, I1)
    END IF
    X = X + M2(I2, L) * C1
    XX = XX + M2(I2, L) * M2(I2, L) * C2
10  CONTINUE
    M1(I1, L) = M1(I1, L) + X / (XX * P(L))
20  CONTINUE
30  CONTINUE
RETURN
END
SUBROUTINE PHIFIT(TAB, FIT, FF, LAMBDA, LAM1, LAM2, M1, M2, P, NR,
*                NC, NM)
C
C      ALGORITHM AS 253.7  APPL. STATIST. (1990) VOL.39, NO. 1
C
C      Update the estimates of the PHI's
C
INTEGER FF(NR, NC), NR, NC, NM
REAL TAB(NR, NC), FIT(NR, NC), LAMBDA, LAM1(NR), LAM2(NC),
*     M1(NR, * ), M2(NC, * ), P( * )
INTEGER I, J, L
REAL X, XX, ZERO
DATA ZERO / 0.0 /
C
DO 30 L = 1, NM
  CALL EXPTAB(TAB, FIT, FF, LAMBDA, LAM1, LAM2, M1, M2, P, NR,
*            NC, NM)
  X = ZERO
  XX = ZERO
  DO 20 J = 1, NC
    DO 10 I = 1, NR
      X = X + M1(I, L) * M2(J, L) * (TAB(I, J) - FIT(I, J))
      XX = XX + M1(I, L) * M1(I, L) * M2(J, L) * M2(J, L) *
*      FIT(I, J)
10  CONTINUE
20  CONTINUE

```

```

      P(L) = P(L) + X / XX
30 CONTINUE
C
  RETURN
  END
  SUBROUTINE CENTRE(LAMBDA, LR, LC, MU, NU, P, RWT, CWT, NR, NC, NM)
C
C   ALGORITHM AS 253.8  APPL. STATIST. (1990) VOL.39, NO. 1
C
C   Centre (with respect to the row/column weights) the MUs/NU's
C   about zero
C
  INTEGER NR, NC, NM
  REAL LAMBDA, LR(NR), LC(NC), MU(NR, * ), NU(NC, * ), P( * ),
*     RWT(NR), CWT(NC)
  INTEGER I, J, L
  REAL C1, C2, X, XX, ZERO
  DATA ZERO / 0.0 /
C
  C1 = ZERO
  C2 = ZERO
C
  DO 10 I = 1, NR
    C1 = C1 + RWT(I)
10 CONTINUE
  DO 20 J = 1, NC
    C2 = C2 + CWT(J)
20 CONTINUE
C
  DO 70 L = 1, NM
    X = ZERO
    XX = ZERO
    DO 30 I = 1, NR
      X = X + MU(I, L) * RWT(I)
30 CONTINUE
    DO 40 J = 1, NC
      XX = XX + NU(J, L) * CWT(J)
40 CONTINUE
    DO 50 I = 1, NR
      LR(I) = LR(I) + (XX / C2 * P(L) * MU(I, L))
      MU(I, L) = MU(I, L) - X / C1
50 CONTINUE
    DO 60 J = 1, NC
      LC(J) = LC(J) + (X / C1 * P(L) * NU(J, L))
      NU(J, L) = NU(J, L) - XX / C2
60 CONTINUE
    LAMBDA = LAMBDA - (P(L) * X / C1 * XX / C2)
70 CONTINUE
  RETURN
  END
  SUBROUTINE SCALE(M, N, P, RWT, CWT, A, W, V, WORK, E, NR, NC, NM,
*     MNRC, JOB, IFAULT)
C
C   ALGORITHM AS 253.9  APPL. STATIST. (1990) VOL.39, NO. 1
C
C   Scale the MU's/NU's so that they satisfy the
C   identifying restrictions
C
  INTEGER NR, NC, NM, MNRC, JOB, IFAULT
  REAL M(NR, * ), N(NC, * ), P( * ), RWT(NR), CWT(NC), A(MNRC, NC),
*     W( * ), V(NC, NC), WORK(NR), E(NC)

```

```

      INTEGER I, IA, J, L
      REAL ZERO
      DATA ZERO / 0.0 /
C
      DO 30 J = 1, NC
        DO 20 I = 1, NR
          A(I, J) = ZERO
          DO 10 L = 1, NM
            A(I, J) = A(I, J) + P(L) * M(I, L) * N(J, L)
10          CONTINUE
            A(I, J) = A(I, J) * SQRT(RWT(I)) * SQRT(CWT(J))
20          CONTINUE
30          CONTINUE
C
      IF (MNRC .GT. NR) THEN
        IA = NR + 1
        DO 50 J = 1, NC
          DO 40 I = IA, MNRC
            A(I, J) = ZERO
40          CONTINUE
50          CONTINUE
        END IF
C
      Call LINPACK SVD subroutine
C
      CALL SSVDC(A, MNRC, NR, NC, W, E, A, MNRC, V, NC, WORK, JOB,
*             IFAULT)
      IF (IFAULT .NE. 0) RETURN
C
      DO 80 L = 1, NM
        P(L) = W(L)
        DO 60 I = 1, NR
          M(I, L) = A(I, L) / SQRT(RWT(I))
60        CONTINUE
C
        DO 70 J = 1, NC
          N(J, L) = V(J, L) / SQRT(CWT(J))
70        CONTINUE
80        CONTINUE
C
      RETURN
      END
      SUBROUTINE CONV(TAB, FIT, FF, WRK, LAMBDA, LR, LC, MU, NU, PHI,
*             IPT, TOT, TOL, SALE, NR, NC, NM, NW, ICON)
C
      ALGORITHM AS 253.10  APPL. STATIST. (1990) VOL.39, NO. 1
C
      Check for convergence of the algorithm to a solution
      of the likelihood equations
C
      INTEGER FF(NR, NC), IPT(6), NR, NC, NM, NW, ICON
      REAL TAB(NR, NC), FIT(NR, NC), WRK(NW), LAMBDA, LR(NR), LC(NC),
*       MU(NR, * ), NU(NC, * ), PHI( * ), TOT, TOL, SALE
      INTEGER I, J, L
      REAL ETOT, X, XX, ZERO
      DATA ZERO / 0.0 /
C
      CALL EXPTAB(TAB, FIT, FF, LAMBDA, LR, LC, MU, NU, PHI, NR, NC, NM)
C
      CALL MARGIN(FIT, WRK(IPT(2)), WRK(IPT(3)), ETOT, NR, NC)
C

```

```
      X = ZERO
C
      DO 10 I = 1, NR
        X = X + ABS(WRK(I) - WRK(IPT(2) + I - 1))
10    CONTINUE
C
      DO 20 J = 1, NC
        X = X + ABS(WRK(IPT(1) + J - 1) - WRK(IPT(3) + J - 1))
20    CONTINUE
C
      IF (NM .GT. 0) THEN
        DO 50 L = 1, NM
          XX = ZERO
          DO 40 J = 1, NC
            DO 30 I = 1, NR
              XX = XX + MU(I, L) * NU(J, L) *
*              (TAB(I, J) - FIT(I, J))
30          CONTINUE
40          CONTINUE
          X = X + ABS(XX)
50        CONTINUE
C
          DO 80 L = 1, NM
            DO 70 I = 1, NR
              XX = ZERO
              DO 60 J = 1, NC
                XX = XX + NU(J, L) * (TAB(I, J) - FIT(I, J))
60            CONTINUE
              X = X + ABS(XX * PHI(L))
70            CONTINUE
80          CONTINUE
C
          DO 110 L = 1, NM
            DO 100 J = 1, NC
              XX = ZERO
              DO 90 I = 1, NR
                XX = XX + MU(I, L) * (TAB(I, J) - FIT(I, J))
90            CONTINUE
              X = X + ABS(XX * PHI(L))
100           CONTINUE
110          CONTINUE
        END IF
C
      SALE = X
      IF (SALE .LT. TOL) THEN
        ICON = 1
      ELSE
        ICON = 0
      END IF
C
      RETURN
      END
```

C This file starts with a test driver program.  
C It includes all auxiliary routines required by the algorithm  
C

```
PROGRAM TESTMGT
DIMENSION X(19),N(19),XBAR(10),PI(10),VAR(10),PSE(10),XSE(10),
*          VSE(10),WK(500)
DATA N/10,21,56,79,114,122,110,85,85,
*      61,47,49,47,44,31,20,11,4,4/
```

C  
C TEST DATA FOR MGT OBTAINED FROM:  
C  
C EVERITT B.S. AND HAND D.J. (1981) FINITE MIXTURE DISTRIBUTIONS.  
C CHAPMAN AND HALL. P.46.

C PUBLISHED PARAMETER ESTIMATES

C MEANS: 19.96 ,26.16  
C VARIANCES: 4.6225, 7.6176  
C PROPORTIONS: 0.65 , 0.35  
C  
C

```
LOUT = 6
NG = 2
NR = 19
X0 = 14.5
DO 10 I = 1,19
  FI = FLOAT(I)
  X(I) = X0+FI
```

```
10 CONTINUE
KW = 500
PI(1) = .5
PI(2) = .5
XBAR(1) = 20.0
XBAR(2) = 26.0
VAR(1) = 4.0
VAR(2) = 8.0
TOL = 1.0E-8
ITRUNC = 1
ITER = 200
CALL MGT(NG,NR,ITRUNC,X0,X,NL,NU,N,WK,KW,
* PI,XBAR,VAR,PSE,XSE,VSE,TOL,XLOGL,ITER,IFAUULT)
WRITE(LOUT,35)
WRITE(LOUT,20)IFAUULT
WRITE(LOUT,20)ITER
20 FORMAT(I10,/)
30 FORMAT(2F14.7)
40 FORMAT(E14.7)
35 FORMAT(//)
WRITE(LOUT,35)
WRITE(LOUT,30)(XBAR(I),XSE(I),I=1,2)
WRITE(LOUT,35)
WRITE(LOUT,30)(VAR(I),VSE(I),I=1,2)
WRITE(LOUT,35)
WRITE(LOUT,30)(PI(I),PSE(I),I=1,2)
WRITE(LOUT,35)
WRITE(LOUT,40)XLOGL
WRITE(LOUT,35)
STOP
END
```

C  
C SUBROUTINE MGT(NG, NR, ITRUNC, X0, X, NL, NU, N, WK, KW, PI, XBAR,

```

      *          VAR, PSE, XSE, VSE, TOL, XLOGL, ITER, IFAULT)
C
C   ALGORITHM AS 254 APPL. STATIST. (1990), VOL. 39, NO. 2
C
C   Subroutine for fitting a mixture of normal distributions to
C   grouped and truncated data.
C
C   Auxiliary routines required: ALNORM (= AS66), CHOL (= AS6) and
C   SYMINV (= AS7)
C
      INTEGER NR, N(NR), NG, ITRUNC, NL, NU, KW, ITER, IFAULT
      REAL X(NR), WK(KW), PI(NG), XBAR(NG), VAR(NG), PSE(NG), XSE(NG),
      *   VSE(NG), X0, TOL, XLOGL
      INTEGER I1, I2, I3, IFA, IG, IG1, II1, IL, IP, IQ, IR, IR1,
      *   IT, IU, J1, J2, J3, JG, JG1, K1, K2, KG, KG1, LOC1, LOC2,
      *   LOC3, LOC4, LOC5, LOC6, MAXITR, NG1, NG3, NN, NPAR, NR1,
      *   NR2, NROW, NTOT, NULL
      REAL FNT(2), AA, AB, ARG, BA, BB, CA, CB, CONST, FN, ONE, R1, R2,
      *   RATIO, SMALL, SMALLM, SUMPI, T, TOT, TOTN, TRUNC, TWO, TXBAR,
      *   TXLOGL, UFLO, WW,XS,ZERO
      EXTERNAL ALNORM
      REAL ALNORM
      DATA ZERO, ONE, TWO / 0.0, 1.0, 2.0 /
      DATA CONST / 0.398942280401432 /
      DATA UFLO / -87.0 /
      DATA SMALL / -1.0E30 /
      DATA SMALLM / 1.0E-37 /
C
      Check on initial parameter estimates
C
      IFAULT = 0
      IF(NG.GT.NR)IFAULT = 1
      IF(IFAULT.NE.0)RETURN
      SUMPI = ZERO
      DO 1 IG = 1,NG
          IF(PI(IG).LT.ZERO.OR.PI(IG).GT.ONE)IFAULT = 2
          IF(IFAULT.NE.0)RETURN
          IF(VAR(IG).LE.ZERO)IFAULT = 4
          IF(IFAULT.NE.0)RETURN
          SUMPI = SUMPI+PI(IG)
1 CONTINUE
      IF(SUMPI.NE.ONE)IFAULT = 3
      IF(IFAULT.NE.0)RETURN
C
      Set storage location pointers
C
      NG3 = 3*NG
      NPAR = NG3-1
      NPAR = 3*NG-1
      NG1 = NG-1
      NR1 = NR+1
      NR2 = NR+2
      LOC1 = NG*NR2
      LOC2 = 2*LOC1
      LOC3 = 3*LOC1
      LOC4 = LOC3+3*NG
      LOC5 = LOC4+NR2
      LOC6 = LOC5+NPAR+1
      IF(ITRUNC.EQ.1)GOTO 20
      FNT(1) = NL
      FNT(2) = NU

```

```
20 CONTINUE
   NTOT = 0
   DO 30 IR = 1,NR
30  NTOT = NTOT+N(IR)
   FN = NTOT

C
C      Begin iteration loop
C
   XLOGL = SMALL
   MAXITR = ITER
   ITER = 1

C
C      Calculate the A, B and C's
C
40  DO 60 IG = 1,NG
   I1 = LOC3+IG
   I2 = I1+NG
   I3 = I2+NG
   WK(I1) = ZERO
   WK(I2) = ZERO
   WK(I3) = ZERO
   AA = ZERO
   BA = ZERO
   CA = ZERO
   DO 50 IR = 1,NR1
   IF(IR.EQ.1)THEN
     XS = X0
   ELSE
     IR1 = IR-1
     XS = X(IR1)
   ENDIF
   WW = SQRT(VAR(IG))
   ARG = (XS-XBAR(IG))/WW
   IF(ARG.LE.ZERO)THEN
     AB = ALNORM(ARG,.FALSE.)
   ELSE
     AB = ONE-ALNORM(ARG,.TRUE.)
   ENDIF
   ARG = -ARG*ARG/TWO
   IF(ARG.GT.UFLO)THEN
     ARG = EXP(ARG)
   ELSE
     ARG = ZERO
   ENDIF
   BB = ARG*CONST/WW
   CB = XS*BB
   J1 = (IG-1)*NR2+IR
   J2 = LOC1+J1
   J3 = LOC2+J1
   WK(J1) = AB-AA
   WK(J2) = BB-BA
   WK(J3) = CB-CA
   AA = AB
   BA = BB
   CA = CB
50  CONTINUE
   J1 = (IG-1)*NR2+NR2
   J2 = LOC1+J1
   J3 = LOC2+J1
   WK(J1) = ONE-AA
   WK(J2) = -BA
```



```

        WK(J3) = -CA
60 CONTINUE
C
C       Calculate the P's
C
      TRUNC = ZERO
      DO 80 IR = 1, NR2
        K1 = LOC4+IR
        WK(K1) = ZERO
        DO 70 IG = 1, NG
          J1 = (IG-1)*NR2+IR
          WK(K1) = WK(K1)+PI(IG)*WK(J1)
70 CONTINUE
        IF(WK(K1).LE.ZERO)IFAULT = 6
        IF(IFAULT.NE.0)RETURN
        TRUNC = TRUNC+WK(K1)
80 CONTINUE
C
C       Calculate the sums of the A, B and C's
C
      K1 = LOC4+1
      K2 = LOC4+NR2
      TRUNC = TRUNC-WK(K1)-WK(K2)
      TOT = ZERO
      TXLOGL = ZERO
      DO 110 IR = 1, NR2
        K1 = LOC4+IR
        IF(IR.EQ.1.OR.IR.EQ.NR2)THEN
          K2 = IR/NR2+1
          IF(ITRUNC.EQ.0)THEN
            T = FNT(K2)
          ELSE
            T = FN*WK(K1)/TRUNC
            FNT(K2) = T
          ENDIF
        ELSE
          IR1 = IR-1
          T = FLOAT(N(IR1))
        ENDIF
        IF(ITRUNC.EQ.1.AND.(IR.EQ.1.OR.IR.EQ.NR2))GOTO 90
        TXLOGL = TXLOGL+T*LOG(WK(K1))
90 CONTINUE
        TOT = TOT+T
        T = T/WK(K1)
        DO 100 IG = 1, NG
          I1 = LOC3+IG
          I2 = I1+NG
          I3 = I2+NG
          J1 = (IG-1)*NR2+IR
          J2 = LOC1+J1
          J3 = LOC2+J1
          WK(I1) = WK(I1)+T*WK(J1)
          WK(I2) = WK(I2)+T*WK(J2)
          WK(I3) = WK(I3)+T*WK(J3)
100 CONTINUE
110 CONTINUE
        IF(ITRUNC.NE.0) TXLOGL = TXLOGL-FN*LOG(TRUNC)
C
C       Calculate the new estimates
C
      DO 120 IG = 1, NG

```

```

      I1 = LOC3+IG
      I2 = I1+NG
      I3 = I2+NG
      WW = WK(I1)
      R1 = WK(I2)/WW
      R2 = WK(I3)/WW
      ARG = VAR(IG)
      TXBAR = XBAR(IG)-R1*ARG
      VAR(IG) = ARG*(ONE-R2+
*           (TWO*TXBAR-XBAR(IG))*R1)+
*           (TXBAR-XBAR(IG))**2
      XBAR(IG) = TXBAR
      PI(IG) = PI(IG)*WW/TOT
120 CONTINUE
C
C       If convergence criterion is not satisfied,
C       perform another iteration
C
      ARG = ABS((TXLOGL-XLOGL)/XLOGL)
      XLOGL = TXLOGL
      IF(ARG.LE.TOL)GOTO 130
      ITER = ITER+1
      IF(ITER.LE.MAXITR)GOTO 40
      IFAULT = 5
      RETURN
C
C       Calculate the standard errors of the estimates
C
130 IT = 0
      DO 150 IP = 1,NG3
          I1 = LOC5+IP
          WK(I1) = ZERO
          DO 140 IQ = 1,IP
              IT = IT+1
              I2 = LOC6+IT
              WK(I2) = ZERO
140      CONTINUE
150 CONTINUE
      IF(ITRUNC.EQ.0)THEN
          IL = 1
          IU = NR2
          TOTN = FN+FNT(1)+FNT(2)
      ELSE
          IL = 2
          IU = NR1
          TOTN = FN
      ENDIF
C
      DO 190 IR = IL,IU
          IR1 = IR-1
          IF(IR.EQ.1)NN = NL
          IF(IR.EQ.NR2)NN = NU
          IF(IR.NE.1.AND.IR.NE.NR2)NN = N(IR1)
          K1 = LOC4+IR
          K2 = NG1*NR2+IR
          WW = WK(K2)
C
      DO 160 IG = 1,NG
          J1 = (IG-1)*NR2+IR
          J2 = LOC1+J1
          J3 = LOC2+J1
```

```

        RATIO = PI(IG)/WK(K1)
        WK(J1) = (WK(J1)-WW)/WK(K1)
        WK(J2) = -RATIO*WK(J2)
        WK(J3) = -(WK(J2)*XBAR(IG)+RATIO*WK(J3))/(TWO*VAR(IG))
160    CONTINUE
C
        IT = 0
        DO 180 IG = 1,NG3
            IG1 = IG-1
            I1 = IG1*NR2+IR
            II1 = LOC5+IG
            WK(II1) = WK(II1)+NN*WK(I1)
            DO 170 JG = 1,IG
                IT = IT+1
                I2 = (JG-1)*NR2+IR
                I3 = LOC6+IT
                IF(LOG(ABS(WK(I1))+SMALLM)+
*           LOG(ABS(WK(I2))+SMALLM).LT.
*           LOG(SMALLM))GOTO 170
                WK(I3) = WK(I3)+NN*WK(I1)*WK(I2)
170    CONTINUE
180    CONTINUE
190    CONTINUE
C
        IF(ITRUNC.EQ.0)GOTO 220
C
        NL = FNT(1)
        NU = FNT(2)
        IT = 0
        DO 210 IG = 1,NG3
            I1 = LOC5+IG
            DO 200 JG = 1,IG
                IT = IT+1
                I2 = LOC5+JG
                I3 = LOC6+IT
                WK(I3) = WK(I3)-WK(I1)*WK(I2)/TOTN
200    CONTINUE
210    CONTINUE
C
220    IT = 0
        IP = 0
        DO 240 IG = 1,NG3
            DO 230 JG = 1,IG
                IT = IT+1
                IF(IG.EQ.NG.OR.JG.EQ.NG)GO TO 230
                IP = IP+1
                I1 = LOC6+IT
                WK(IP) = WK(I1)
230    CONTINUE
240    CONTINUE
C
        NROW = NPAR
        NN = NPAR*(NPAR+1)/2
        CALL SYMINV(WK,NROW,NN,WK,WK(LOC3),NULL,IFA)
        IF(NG.EQ.1)THEN
            PSE(1) = ZERO
        ELSE
            IT = 0
            PSE(NG) = ZERO
            DO 260 IG = 1,NG1
                KG = IG*(IG+1)/2

```

```

        PSE(IG) = WK(KG)
        PSE(NG) = PSE(NG)-PSE(IG)
        PSE(IG) = SQRT(PSE(IG))
        DO 250 JG = 1,IG
            IT = IT+1
            PSE(NG) = PSE(NG)+TWO*WK(IT)
250     CONTINUE
260     CONTINUE
        PSE(NG) = SQRT(PSE(NG))
    ENDIF
C
    DO 270 IG = 1,NG
        JG = IG+NG-1
        JG1 = (JG+1)*JG/2
        KG = JG+NG
        KG1 = (KG+1)*KG/2
        XSE(IG) = SQRT(WK(JG1))
        VSE(IG) = SQRT(WK(KG1))
270     CONTINUE
    RETURN
    END
C
    REAL FUNCTION ALNORM(X,UPPER)
C
C     ALGORITHM AS66 APPLIED STATISTICS (1973) VOL22 NO.3
C
C     EVALUATES THE TAIL AREA OF THE STANDARDISED NORMAL CURVE
C     FROM X TO INFINITY IF UPPER IS .TRUE. OR
C     FROM MINUS INFINITY TO X IF UPPER IS .FALSE.
C
    REAL LTONE, UTZERO, ZERO, HALF, ONE, CON,
$     A1, A2, A3, A4, A5, A6, A7, B1, B2, B3, B4, B5, B6,
$     B7, B8, B9, B10, B11, B12, X, Y, Z, ZEXP
    LOGICAL UPPER,UP
C
C     LTONE AND UTZERO MUST BE SET TO SUIT THE PARTICULAR COMPUTER
C     (SEE INTRODUCTORY TEXT)
C
    DATA LTONE, UTZERO /7.0, 12.5/
    DATA ZERO, HALF, ONE, CON /0.0, 0.5, 1.0, 1.28/
    DATA
$     A1,          A2,          A3,
$     A4,          A5,          A6,
$     A7
$     /0.398942280444, 0.399903438504, 5.75885480458,
$     29.8213557808,  2.62433121679, 48.6959930692,
$     5.92885724438/
    DATA
$     B1,          B2,          B3,
$     B4,          B5,          B6,
$     B7,          B8,          B9,
$     B10,         B11,         B12
$     /0.398942280385,  3.8052E-8,  1.00000615302,
$     3.98064794E-4,  1.98615381364, 0.151679116635,
$     5.29330324926,  4.8385912808,  15.1508972451,
$     0.742380924027, 30.789933034,  3.99019417011/
C
    ZEXP(Z) = EXP(Z)
C
    UP=UPPER
    Z=X
    IF(Z.GE.ZERO)GOTO 10
    UP=.NOT.UP

```

```

      Z=-Z
10  IF(Z.LE.LTONE.OR.UP.AND.Z.LE.UTZERO)GOTO 20
      ALNORM=ZERO
      GOTO 40
20  Y=HALF*Z*Z
      IF(Z.GT.CON) GOTO 30
C
      ALNORM=HALF-Z*(A1-A2*Y/(Y+A3-A4/(Y+A5+A6/(Y+A7))))
      GOTO 40
30  ALNORM=B1*ZEXP(-Y)/(Z-B2+B3/(Z+B4+B5/(Z-B6+B7/(Z+B8-B9/
      $    (Z+B10+B11/(Z+B12))))))
40  IF(.NOT.UP)ALNORM=ONE-ALNORM
      RETURN
      END
C
      SUBROUTINE SYMINV(A, N, NN, C, W, NULLTY, IFAULT)
C
C      ALGORITHM AS7, APPLIED STATISTICS, VOL.17, 1968, P.198.
C
C      FORMS IN C( ) AS LOWER TRIANGLE, A GENERALISED INVERSE
C      OF THE POSITIVE SEMI-DEFINITE SYMMETRIC MATRIX A( )
C      ORDER N, STORED AS LOWER TRIANGLE.
C
      REAL A(NN), C(NN), W(N), X, ZERO, ONE
C
      DATA ZERO, ONE /0.0, 1.0/
C
C      CHOLSKY FACTORIZATION OF A, RESULT IN C
C
      CALL CHOL(A, N, NN, C, NULLTY, IFAULT)
      IF(IFAULT.NE.0) RETURN
C
C      INVERT C & FORM THE PRODUCT (CINV)'*CINV, WHERE CINV IS THE INVERSE
C      OF C, ROW BY ROW STARTING WITH THE LAST ROW.
C      IROW = THE ROW NUMBER, NDIAG = LOCATION OF LAST ELEMENT IN THE ROW.
C
      IROW=N
      NDIAG=NN
10  L=NDIAG
      IF (C(NDIAG) .EQ. ZERO) GOTO 60
      DO 20 I=IROW,N
      W(I)=C(L)
      L=L+I
20  CONTINUE
      ICOL=N
      JCOL=NN
      MDIAG=NN
30  L=JCOL
      X=ZERO
      IF(ICOL.EQ.IROW) X=ONE/W(IROW)
      K=N
40  IF(K.EQ.IROW) GO TO 50
      X=X-W(K)*C(L)
      K=K-1
      L=L-1
      IF(L.GT.MDIAG) L=L-K+1
      GO TO 40
50  C(L)=X/W(IROW)
      IF(ICOL.EQ.IROW) GO TO 80
      MDIAG=MDIAG-ICOL
      ICOL=ICOL-1

```

```
JCOL=JCOL-1
GO TO 30
60 DO 70 J=IROW,N
   C(L)=ZERO
   L=L+J
70 CONTINUE
80 NDIAG=NDIAG-IROW
   IROW=IROW-1
   IF(IROW.NE.0) GO TO 10
   RETURN
   END

C
SUBROUTINE CHOL(A, N, NN, U, NULLTY, IFAULT)
C
C ALGORITHM AS6, APPLIED STATISTICS, VOL.17, (1968)
C
C GIVEN A SYMMETRIC MATRIX ORDER N AS LOWER TRIANGLE IN A( )
C CALCULATES AN UPPER TRIANGLE, U( ), SUCH THAT UPRIME * U = A.
C A MUST BE POSITIVE SEMI-DEFINITE. ETA IS SET TO MULTIPLYING
C FACTOR DETERMINING EFFECTIVE ZERO FOR PIVOT.
C
REAL A(NN), U(NN), ETA, ETA2, X, W, ZERO, ZABS, ZSQRT
C
C THE VALUE OF ETA WILL DEPEND ON THE WORD-LENGTH OF THE
C COMPUTER BEING USED. SEE INTRODUCTORY TEXT.
C
DATA ETA, ZERO /1.E-5, 0.0/
C
ZABS(X) = ABS(X)
ZSQRT(X) = SQRT(X)
C
IFault=1
IF(N.LE.0) GO TO 100
IFault=3
IF (NN .NE. N*(N+1)/2) RETURN
IFault=2
NULLTY=0
J=1
K=0
ETA2 = ETA*ETA
II=0
C
C FACTORIZE COLUMN BY COLUMN, ICOL = COLUMN NO.
C
DO 80 ICOL=1,N
  II=II+ICOL
  X=ETA2*A(II)
  L=0
  KK=0
C
C IROW = ROW NUMBER WITHIN COLUMN ICOL
C
DO 40 IROW=1,ICOL
  KK=KK+IROW
  K=K+1
  W=A(K)
  M=J
  DO 10 I=1,IROW
    L=L+1
    IF(I.EQ.IROW) GO TO 20
    W=W-U(L)*U(M)
```

```
      M=M+1
10    CONTINUE
20    IF(IROW.EQ.ICOL) GO TO 50
      IF(U(L).EQ.ZERO) GO TO 30
      U(K)=W/U(L)
      GO TO 40
30    IF (W*W .GT. ZABS(X*A(KK))) RETURN
      U(K)=ZERO
40    CONTINUE
50    IF (ZABS(W) .LE. ZABS(ETA*A(K))) GOTO 60
      IF(W.LT.ZERO) RETURN
      U(K)=ZSQRT(W)
      GO TO 70
60    U(K)=ZERO
      NULLTY=NULLTY+1
70    J=J+ICOL
80    CONTINUE
      IFAULT=0
100   RETURN
      END
```

```
'procedure' twoway(nrows, ncols, include, resval, baseval, rowval,
  colval, rxcval, init, rcfit, xfit, test, nsteps, evalue, ifault);
'comment' Algorithm AS 255.1 Appl. Statist. (1990) Vol.39, No.2;
'value' nrows, ncols, init, rcfit, xfit, evalue;
'integer' nrows, ncols, nsteps, ifault; 'Boolean' init, rcfit, xfit;
'real' baseval, rxcval, evalue; 'Boolean' 'array' include;
'real' 'array' resval, rowval, colval; 'Boolean' 'procedure' test;
'comment' Fits a two-dimensional array of numerical values to an
  additive model incorporating a row term, a column term, and
  an optional nonadditivity term;
'begin' 'integer' row, col, s0;
'real' sx, sy, sx2, sy2, sxy, rxctemp, xm, ym, newres, ssva, changeval;

'procedure' faultexit(i);
'value' i; 'integer' i;
'comment' Local procedure to exit on fault;
  'begin'
  ifault := i; 'goto' exit
  'end' faultexit;

'procedure' initcalc;
'comment' Local procedure to initialise the twoway model;
  'begin' 'integer' firstrow, lastrow, firstcol, lastcol, localrow, ndata;
  ndata := 0;
  'for' row := 1 'step' 1 'until' nrows 'do'
    'begin'
    firstcol := 0;
    'for' col := 1 'step' 1 'until' ncols 'do'
      'if' include[row, col] 'then'
        'begin'
        ndata := ndata + 1;
        'if' firstcol = 0 'then' firstcol := col 'else' lastcol := col
        'end';
      'if' firstcol = 0 'then' faultexit(4) 'else'
      'if' firstcol = lastcol 'then'
        'begin'
        firstrow := 0;
        'for' localrow := 1 'step' 1 'until' nrows 'do'
          'if' include[localrow, col] 'then'
            'begin'
            'if' firstrow = 0 'then' firstrow := localrow
            'else' lastrow := localrow
            'end';
          'if' firstrow = 0 'then' faultexit(4) 'else'
          'if' firstrow = lastrow 'then' faultexit(5)
          'end'
        'end' row;
      'if' ndata < nrows + ncols + ('if' xfit 'then' 1 'else' 0)
      'then' faultexit(3);
    'for' col := 1 'step' 1 'until' ncols 'do'
      'begin'
      firstrow := 0;
      'for' row := 1 'step' 1 'until' nrows 'do'
        'if' include[row, col] 'and' firstrow = 0 'then' firstrow := row;
        'if' firstrow = 0 'then' faultexit(4)
      'end' col;
  nsteps := 0; baseval := rxcval := 0.0;
  'for' row := 1 'step' 1 'until' nrows 'do' rowval[row] := 0.0;
  'for' col := 1 'step' 1 'until' ncols 'do' colval[col] := 0.0;
  s0 := 0; sy := 0.0;
  'for' row := 1 'step' 1 'until' nrows 'do'
```



```

'for' col := 1 'step' 1 'until' ncols 'do'
'if' include[row, col] 'then'
  'begin'
    s0 := s0 + 1; sy := sy + resval[row, col]
  'end';
changeval := sy / s0; baseval := baseval + changeval;
ssval := 0.0;
'for' row := 1 'step' 1 'until' nrows 'do'
'for' col := 1 'step' 1 'until' ncols 'do'
'if' include[row, col] 'then'
  'begin'
    newres := resval[row, col] := resval[row, col] - changeval;
    ssval := ssval + newres * newres
  'end';
ifault := 0;
test('true', nsteps, ssval, evalue, ifault);
'if' ifault > 5 'then' faultexit(ifault)
'end' initcalc;

'procedure' addstep(i1, i2, ni1, ni2, illevels);
'value' ni1, ni2; 'integer' i1, i2, ni1, ni2; 'real' 'array' illevels;
'comment' Local procedure to perform a row or column step. Actual
substitutions for i1, i2 are row, col or col, row. Note that
parameters i1, i2 must be called by name;
'begin'
ssval := 0.0;
'for' i1 := 1 'step' 1 'until' ni1 'do'
  'begin'
    s0 := 0; sy := 0.0;
    'for' i2 := 1 'step' 1 'until' ni2 'do'
      'if' include[row, col] 'then'
        'begin'
          s0 := s0 + 1; sy := sy + resval[row, col]
        'end' i2;
      'if' s0 > 0 'then'
        'begin'
          changeval := sy / s0;
          illevels[i1] := illevels[i1] + changeval;
          'for' i2 := 1 'step' 1 'until' ni2 'do'
            'if' include[row, col] 'then'
              'begin'
                newres := resval[row, col] := resval[row, col] - changeval;
                ssval := ssval + newres * newres
              'end' i2
            'end'
          'end' i1;
        nsteps := nsteps + 1;
        'if' test('false', nsteps, ssval, evalue, ifault) 'then' 'goto' rcdone;
        'if' ifault > 5 'then' 'goto' exit
        'end' addstep;

'procedure' rxccalc;
'comment' Local procedure to perform nonadditivity calculation;
'begin'
s0 := 0; sx := sy := 0.0;
'for' row := 1 'step' 1 'until' nrows 'do'
'for' col := 1 'step' 1 'until' ncols 'do'
'if' include[row, col] 'then'
  'begin'
    s0 := s0 + 1;
    sx := sx + rowval[row] * colval[col];

```

```
        sy := sy + resval[row, col]
        'end';
xm := sx / s0; ym := sy / s0;
sx2 := sxy := 0.0;
'for' row := 1 'step' 1 'until' nrows 'do'
'for' col := 1 'step' 1 'until' ncols 'do'
'if' include[row, col] 'then'
    'begin'
        rxctemp := rowval[row] * colval[col] - xm;
        sx2 := sx2 + rxctemp * rxctemp;
        sxy := sxy + rxctemp * (resval[row, col] - ym)
    'end';
changeval := ym - xm * sxy / sx2
'end' rxccalc;

'comment' Start of action of procedure twoway;
'if' nrows < 1 'or' ncols < 1 'then' faultexit(1);
'if' init 'and' xfit 'and' 'not' rcfit 'then' faultexit(2);
'if' init 'then' initcalc 'else'
'if' rcfit 'or' xfit 'then'
    'begin'
        'comment' Undo effect of any existing nonadditivity adjustment;
s0 := 0; sx := sy := 0.0;
'for' row := 1 'step' 1 'until' nrows 'do'
'for' col := 1 'step' 1 'until' ncols 'do'
'if' include[row, col] 'then'
resval[row, col] := resval[row, col] +
    rxcval * rowval[row] * colval[col];
rxccalc;
baseval := baseval - changeval;
'for' row := 1 'step' 1 'until' nrows 'do'
'for' col := 1 'step' 1 'until' ncols 'do'
'if' include[row, col] 'then'
resval[row, col] := resval[row, col] + changeval
'end';
'if' rcfit 'then'
    'begin'
        'comment' Fit for rows and columns alternately until fit
            criterion is satisfied;
rcloop:
    addstep(row, col, nrows, ncols, rowval);
    addstep(col, row, ncols, nrows, colval);
    'goto' rcloop
    'end' row + col fit;
rc done:
'if' xfit 'then'
    'begin'
        'comment' Apply nonadditive step;
rxccalc;
rxcval := sxy / sx2; ssva := 0.0;
baseval := baseval + changeval;
'for' row := 1 'step' 1 'until' nrows 'do'
'for' col := 1 'step' 1 'until' ncols 'do'
'if' include[row, col] 'then'
    'begin'
        resval[row, col] := newres := resval[row, col] - changeval
            - rxcval * rowval[row] * colval[col];
        ssva := ssva + newres * newres
    'end';
nsteps := nsteps + 1;
test('false', nsteps, ssva, evalue, ifault)
```

```

        'end' row * col fit;
exit:
    'end' twoway;

'procedure' ddplot(nrows, ncols, include, resval, baseval, rowval,
    colval, rxcval, rowxfit, colxfit, minx, maxx, miny, maxy, plotval);
'comment' Algorithm AS 255.2 Appl. Statist. (1990) Vol.39, No.2;
'value' nrows, ncols, baseval, rxcval, rowxfit, colxfit;
'integer' nrows, ncols; 'real' baseval, rxcval, minx, maxx, miny, maxy;
'Boolean' rowxfit, colxfit; 'Boolean' 'array' include;
'real' 'array' resval, rowval, colval, plotval;
    'comment' To produce a diagonal plot of the results of a
        two-way table analysis;
'begin' 'integer' row, col; 'real' temp, rc;
minx := maxx := 0.0; miny := maxy := baseval;
'for' row := 1 'step' 1 'until' nrows 'do'
'for' col := 1 'step' 1 'until' ncols 'do'
    'begin'
        rc := rxcval * rowval[row] * colval[col];
        temp := colval[col] - rowval[row];
        'if' rowxfit 'then'
            'begin'
                'if' 'not' colxfit 'then' temp := temp - rc
            'end'
        'else' 'if' colxfit 'then' temp := temp + rc;
        'if' temp < minx 'then' minx := temp
            'else' 'if' temp > maxx 'then' maxx := temp;
        plotval[row, col, 1] := temp;
        temp := baseval + rowval[row] + colval[col];
        'if' rowxfit 'or' colxfit 'then' temp := temp + rc;
        'if' temp < miny 'then' miny := temp
            'else' 'if' temp > maxy 'then' maxy := temp;
        plotval[row, col, 2] := temp;
        'if' include[row, col] 'then' temp := temp + resval[row, col];
        'if' temp < miny 'then' miny := temp
            'else' 'if' temp > maxy 'then' maxy := temp;
        plotval[row, col, 3] := temp
    'end'
'end' ddplot;

'Boolean' 'procedure' testex(init, nsteps, ssva, evaluate, ifault);
'comment' Algorithm AS 255.3 Appl. Statist. (1990) Vol.39, No.2;
'value' init, nsteps, sscal, evaluate;
'integer' nsteps, ifault; 'Boolean' init; 'real' ssva, evaluate;
    'comment' This particular implementation of the test procedure relies
        upon the ratio of the largest to the smallest of the 3 most
        recent values of ssva[ ]. The stack is implemented as an own
        array variable. No use is made of the nsteps parameter;
'if' ifault > 0 'then' testex := 'false' 'else'
'begin' 'integer' i; 'own' 'real' 'array' ssva[1:3];
'if' init 'then'
    'begin'
        'for' i := 1, 2, 3 'do' ssva[i] := -1; testex := 'false'
    'end'
'else' 'if' ssva < 0.0 'then'
    'begin'
        ifault := 6; testex := 'false'
    'end'
'else'
    'begin' 'real' ssva, ssvmax, ssvmin;
        'for' i := 3, 2 'do' ssva[i] := ssva[i - 1];

```

```
    ssvals[1] := ssva1;
    ssmax := -1; ssmi1 := ssva1;
    'for' i := 1, 2, 3 'do'
      'begin'
        ssva1ue := ssva1s[i];
        'if' ssva1ue < 0.0 'then'
          'begin'
            testex := 'false' ; 'goto' exit
          'end'
        'else' 'if' ssva1ue < ssmi1 'then' ssmi1 := ssva1ue
        'else' 'if' ssva1ue > ssmax 'then' ssmax := ssva1ue
        'end' i;
    testex := ssmax < ssmi1 * (1.0 + abs(evalue))
    'end';
exit:
  'end' testex;
```

```
FUNCTION imhofbd(lambda:realarray; mult:posintarray; delta:realarray;  
    noterms:units; eps1,eps2:real; VAR ifault:nonnegint):real;
```

```
{Algorithm AS 256.1 Appl. Statist. (1990) Vol.39, No.2}
```

```
{Pascal translation of Koerts and Abrahamse's procedure  
for evaluating Imhof's upper bound}
```

```
CONST pi=3.14159265;  
VAR i:units;  
    count,hold,range,sum1,sum2:real;
```

```
BEGIN  
IF (noterms < 1) OR (eps1 <= 0.0) OR (eps2 <= 0.0) THEN  
    BEGIN  
        ifault := 2; imhofbd := -2.0  
    END  
ELSE  
    BEGIN  
        count := 0.0;  
        sum1 := 0.0; sum2 := 0.0;  
        FOR i := 1 TO noterms DO  
            BEGIN  
                hold := abs(lambda[i]);  
                IF hold > eps2 THEN  
                    BEGIN  
                        count := count+mult[i];  
                        sum1 := sum1+mult[i]*ln(hold);  
                    END;  
                sum2 := sum2+delta[i]  
            END;  
        IF count < 0.9 THEN  
            BEGIN  
                ifault := 4; imhofbd := -4.0  
            END  
        ELSE  
            BEGIN  
                count := 0.5*count;  
                sum1 := 0.5*sum1+ln(pi*count);  
                range := exp(-(sum1+0.5*sum2+ln(eps1))/count);  
                IF sum2=0.0 THEN  
                    range := range+5.0/count  
                ELSE  
                    BEGIN  
                        REPEAT  
                            sum2 := 0.0;  
                            FOR i := 1 TO noterms DO  
                                BEGIN  
                                    hold := sqr(range*lambda[i]);  
                                    sum2 := sum2+delta[i]*hold/(1.0+hold)  
                                END;  
                            hold := exp(sum1+count*ln(range)+0.5*sum2);  
                            IF hold*eps1 <= 1.0 THEN range := range+5.0/count ELSE count := 0.0  
                            UNTIL count=0.0;  
                        END  
                    END  
            END  
        imhofbd := range  
    END  
END; {of imhofbd}
```

```
FUNCTION imhofint(lambda:realarray; mult:posintarray; delta:realarray;
```

```
noterms:units; arg,bound,eps3:real; VAR ifault:nonnegint):real;
```

```
{Algorithm AS 256.2 Appl. Statist. (1990) Vol.39, No.2}
```

```
{Pascal translation of Koerts and Abrahamse's procedure  
for evaluating Imhof's integral by Simpson's Rule}
```

```
CONST maxit=14;
```

```
pi=3.14159265;
```

```
VAR i,j,n:nonnegint;
```

```
eps4,hold,int1,int2,step,sum1,sum2,sum4:real;
```

```
cgd:boolean;
```

```
FUNCTION imhoffn(u:real):real;
```

```
{imhoffn evaluates Imhof's integrand}
```

```
VAR i:units;
```

```
hold2,hold3,rho,sum,theta:real;
```

```
BEGIN
```

```
rho := 0.0;
```

```
sum := 0.0;
```

```
theta := -u*arg;
```

```
FOR i := 1 TO noterms DO
```

```
  BEGIN
```

```
    hold := u*lambda[i];
```

```
    hold2 := sqr(hold);
```

```
    hold3 := 1.0+hold2;
```

```
    theta := theta+mult[i]*arctan(hold)+delta[i]*hold/hold3;
```

```
    sum := sum+delta[i]*hold2/hold3;
```

```
    rho := rho+mult[i]*ln(hold3)
```

```
  END;
```

```
imhoffn := sin(0.5*theta)/(u*exp(0.5*sum+0.25*rho))
```

```
END; {of imhoffn}
```

```
BEGIN
```

```
IF (noterms < 1) OR (bound <= 0.0) OR (eps3 <= 0.0) THEN
```

```
  BEGIN
```

```
    ifault := 2; imhofint := -2.0
```

```
  END
```

```
ELSE
```

```
  BEGIN
```

```
    ifault := 5;
```

```
    n := 2; step := 0.5*bound;
```

```
    eps4 := 3.0*pi*eps3;
```

```
    sum1 := -arg;
```

```
    FOR i := 1 TO noterms DO
```

```
      sum1 := sum1+lambda[i]*(mult[i]+delta[i]);
```

```
      sum1 := 0.5*sum1+imhoffn(bound);
```

```
      sum2 := 0.0;
```

```
      sum4 := imhoffn(step);
```

```
      int2 := (sum1+4.0*sum4)*step;
```

```
      i := 0; cgd := false;
```

```
      REPEAT
```

```
        i := i+1; n := n+n;
```

```
        step := 0.5*step;
```

```
        int1 := int2;
```

```
        sum2 := sum2+sum4;
```

```
        int2 := sum1+sum2+sum2;
```

```
        sum4 := 0.0; j := 1;
```

```
        REPEAT
        sum4 := sum4+imhoffn(j*step);
        j := j+2
        UNTIL j > n;
int2 := (int2+4.0*sum4)*step;
IF i > 3 THEN
    BEGIN
        IF abs(int1-int2) < eps4 THEN
            BEGIN
                IF abs(int2) > 1.5*pi THEN
                    ifault := 6 ELSE ifault := 0;
                    cgd := true
                END
            END;
        UNTIL (i=maxit) OR cgd;
        imhofint := 0.5-int2/(3.0*pi)
    END
END; {of imhofint}

FUNCTION imhof(lambda:realarray; mult:posintarray; delta:realarray;
noterms:units; arg,bound,eps1,eps2,eps3:real; VAR ifault:nonnegint):real;

{Algorithm AS 256.3 Appl. Statist. (1990) Vol.39, No.2}

{Pascal translation of Koerts and Abrahamse's implementation of
Imhof's procedure for evaluating the probability that a diagonal
form in normal variables is less than a given value, arg}

VAR i:units;

BEGIN

{check parameters}
IF (noterms < 1) OR (eps1 <= 0.0) OR (eps2 <= 0.0) OR (eps3 <= 0.0) THEN
    BEGIN
        ifault := 2; imhof := -2.0
    END
ELSE
    BEGIN
        ifault := 1; i := 1;
        WHILE ifault=1 DO
            BEGIN
                i := i+1;
                IF i=noterms THEN ifault := 0;
                IF (mult[i] < 1) OR (delta[i] < 0.0) THEN
                    BEGIN
                        ifault := 3; imhof := -i
                    END
                END;
            END;

{main body}
IF ifault=0 THEN
    BEGIN
        IF bound <= 0.0 THEN
            bound := imhofbd(lambda,mult,delta,noterms,eps1,eps2,ifault);
            IF ifault=0 THEN
                imhof := imhofint(lambda,mult,delta,noterms,arg,bound,eps3,ifault)
            ELSE imhof := -ifault
        END
    END
END; {of imhof}
```

```
FUNCTION imhotep(diag,subd:realarray; noterms:units;  
nc,arg,bound,eps0,eps1,eps2,eps3:real; VAR ifault:nonnegint):real;
```

```
{Algorithm AS 256.4 Appl. Statist. (1990) Vol.39, No.2}
```

```
{imhotep uses Imhof's procedure with real arithmetic  
to evaluate the probability that a tridiagonal form  
in normal variables is less than a given value, arg}
```

```
VAR i:units;  
hold:real;  
delta:realarray;  
mult:posintarray;
```

```
BEGIN
```

```
IF (noterms < 1) OR (nc < 0.0) OR  
(eps0 <= 0.0) OR (eps1 <= 0.0) OR (eps2 <= 0.0) OR (eps3 <= 0.0) THEN  
BEGIN  
ifault := 2; imhotep := -2.0  
END
```

```
ELSE
```

```
BEGIN
```

```
ifault := 0; delta[noterms] := 1.0;
```

```
IF noterms > 1 THEN
```

```
BEGIN
```

```
FOR i := noterms-1 DOWNTO 1 DO delta[i] := 0.0;
```

```
tql3(noterms,diag,subd,delta,eps0,ifault)
```

```
END;
```

```
IF ifault <> 0 THEN imhotep := -ifault
```

```
ELSE
```

```
BEGIN
```

```
FOR i := 1 TO noterms DO
```

```
BEGIN
```

```
hold := delta[i]; mult[i] := 1;
```

```
delta[i] := nc*sqr(hold)
```

```
END;
```

```
imhotep := imhof(diag,mult,delta,noterms,arg,bound,eps1,eps2,eps3,ifault)
```

```
END
```

```
END
```

```
END; {of imhotep}
```

```
FUNCTION sneekbd(diag,subd:realarray; noterms:units;  
nc,eps1,eps2:real; VAR ifault:nonnegint):real;
```

```
{Algorithm AS 256.5 Appl. Statist. (1990) Vol.39, No.2}
```

```
{sneekbd evaluates Imhof's upper bound  
by means of Sturm sequences}
```

```
CONST pi=3.14159265;
```

```
VAR i,j:nonnegint;
```

```
hold,sum1,sum2:real;
```

```
PROCEDURE sturm(eta:real; VAR det:real; VAR mult:nonnegint);
```

```
{sturm evaluates the determinant of a tridiagonal matrix  
and the number of roots less than a given value, eta}
```



```
VAR i:units;
    count:nonnegint;
    real0,real1,real2:real;

BEGIN
count := 0;
real1 := 1.0; real2 := 0.0;
FOR i := 1 TO noterms DO
    BEGIN
    real0 := real1*(diag[i]-eta)-real2*sqr(subd[i]);
    real2 := real1; real1 := real0;
    IF real1*real2 < 0.0 THEN count := count+1
    END;
det := real0;
mult := count
END; {of sturm}

BEGIN
IF (noterms < 1) OR (nc < 0.0) OR (eps1 <= 0.0) OR (eps2 <= 0.0) THEN
    BEGIN
    ifault := 2; sneekbd := -2.0
    END
ELSE
    BEGIN
    {trap small eigenvalues}
    sturm(-eps2,hold,i);
    sturm( eps2,hold,j);
    IF i <> j THEN
        BEGIN
        ifault := 7; sneekbd := -7.0
        END
    ELSE
        BEGIN
        {compute bound}
        ifault := 0;
        sturm(0.0,hold,j);
        sum1 := 0.5*noterms;
        sum2 := sqrt(abs(hold))*pi*sum1*eps1;
        sneekbd := exp(-(ln(sum2)+0.5*nc)/sum1)+5.0/sum1
        END
    END
END; {of sneekbd}

FUNCTION sneekint(diag,subd:realarray; noterms:units;
nc,arg,bound,eps3:real; VAR ifault:nonnegint):real;

{Algorithm AS 256.6 Appl. Statist. (1990) Vol.39, No.2}

{sneekint uses complex arithmetic to
evaluate Imhof's integral by Simpson's Rule}

CONST maxit=14;
    eta=0.0001;
    pi=3.14159265;
VAR    i,j,n:nonnegint;
        eps4,int1,int2,step,sum1,sum2,sum4:real;
        cgd:boolean;

FUNCTION sneekfn(u:real):real;

    {sneekfn evaluates Imhof's integrand}
```

```
VAR sgn:-1..1;
    i:units;
    hold1,hold2,imag0,imag1,imag2,pies,real0,real1,real2:real;

BEGIN

{evaluate determinant}
real1 := 1.0; imag1 := 0.0;
real2 := 0.0; imag2 := 0.0;
sgn := 1; pies := 0.0;
FOR i := 1 TO noterms DO
    BEGIN
    hold1 := u*diag[i]; hold2 := sqr(u*subd[i]);
    real0 := real1+imag1*hold1+real2*hold2;
    imag0 := imag1-real1*hold1+imag2*hold2;
    real2 := real1; real1 := real0;
    imag2 := imag1; imag1 := imag0;
    IF sgn*real0 < 0.0 THEN
        BEGIN
        sgn := -sgn;
        IF sgn*imag0 < 0.0
            THEN pies := pies+pi
            ELSE pies := pies-pi
        END
    END
END;

{evaluate exponent}
hold1 := -nc/(sqr(real1)+sqr(imag1));
real0 := nc+(real1*real2+imag1*imag2)*hold1;
imag0 := (real1*imag2-imag1*real2)*hold1;

{evaluate integrand}
hold1 := imag1/real1;
hold2 := sqr(hold1)+1.0;
hold2 := sqrt(hold2)*abs(real1);
hold2 := exp(-0.5*real0)/sqrt(hold2);
hold1 := arctan(hold1)+pies+imag0+u*arg;
sneekfn := sin(-0.5*hold1)*hold2/u
END; {of sneekfn}

BEGIN
IF (noterms < 1) OR (nc < 0.0) OR (bound <= 0.0) OR (eps3 <= 0.0) THEN
    BEGIN
    ifault := 2; sneekint := -2.0
    END
ELSE
    BEGIN
    ifault := 5;
    n := 2; step := 0.5*bound;
    eps4 := 3.0*pi*eps3;
    sum1 := sneekfn(eta*bound)+sneekfn(bound);
    sum2 := 0.0;
    sum4 := sneekfn(step);
    int2 := (sum1+4.0*sum4)*step;
    i := 0; cgd := false;
    REPEAT
        i := i+1; n := n+n;
        step := 0.5*step;
        int1 := int2;
        sum2 := sum2+sum4;
    UNTIL
```

```
int2 := sum1+sum2+sum2;
sum4 := 0.0; j := 1;
REPEAT
  sum4 := sum4+sneekfn(j*step);
  j := j+2
UNTIL j > n;
int2 := (int2+4.0*sum4)*step;
IF i > 3 THEN
  BEGIN
  IF abs(int1-int2) < eps4 THEN
    BEGIN
    IF abs(int2) > 1.5*pi THEN
      ifault := 6 ELSE ifault := 0;
      cgd := true
    END
    END
  UNTIL (i=maxit) OR cgd;
  sneekint := 0.5-int2/(3.0*pi)
END
END; {of sneekint}

FUNCTION sneek(diag,subd:realarray; noterms:units;
nc,arg,bound,eps1,eps2,eps3:real; VAR ifault:nonnegint):real;

{Algorithm AS 256.7 Appl. Statist. (1990) Vol.39, No.2}

{sneek uses Imhof's procedure with complex arithmetic
to evaluate the probability that a tridiagonal form
in normal variables is less than a given value, arg}

BEGIN
IF (noterms < 1) OR (nc < 0.0) OR
(eps1 <= 0.0) OR (eps2 <= 0.0) OR (eps3 <= 0.0) THEN
  BEGIN
  ifault := 2; sneek := -2.0
  END
ELSE
  BEGIN
  ifault := 0;
  IF bound <= 0.0 THEN
    bound := sneekbd(diag,subd,noterms,nc,eps1,eps2,ifault);
  IF ifault=0 THEN
    sneek := sneekint(diag,subd,noterms,nc,arg,bound,eps3,ifault)
  END
END; {of sneek}
```

```

SUBROUTINE ISRE(K, NH, XO, WO, X, Y, Z, WX, WY, WZ, XA, IFAULT)
C
C     ALGORITHM AS 257.1  APPL.STATIST. (1990), VOL.39, NO.3
C
C     Subroutine to compute isotonic regression for umbrella
C     ordering with known peak
C     Algorithm AMALGM (AS 149, Cran, 1980) is called
C
INTEGER K, NH, IFAULT
REAL XO(K), WO(K), X(K), Y(K), Z(K), WX(K), WY(K), WZ(K), XA(K)
INTEGER I, I1, IH, IH1, IHIGH, ILOW, IXMAX, J, L, N
REAL S, TOL, XMAX
DATA TOL / 1.0E-6 /
C
C     Check input data K, NH and WO
C
IFAULT = 1
IF (K .LT. 2) RETURN
IFAULT = 3
IF (NH .LT. 1 .OR. NH .GT. K) RETURN
IFAULT = 2
DO 10 I = 1, K
    IF (WO(I) .LE. TOL) RETURN
    X(I) = XO(I)
    WX(I) = WO(I)
10 CONTINUE
IFAULT = 0
N = K
IH = NH
C
C     Pool the active block with the next lower block
C     from X(1) to X(IH-1)
C
IF (IH .LE. 2) GO TO 40
DO 20 I = 1, IH - 1
    Y(I) = X(I)
    WY(I) = WX(I)
20 CONTINUE
CALL AMALGM(IH - 1, Y, WY, Z, WZ, XA, IFAULT)
DO 30 I = 1, IH - 1
    X(I) = XA(I)
30 CONTINUE
C
C     Pool the active block with the next higher block
C     from X(IH+1) to X(N)
C
40 IF (N - IH .LE. 1) GO TO 70
L = N - IH
DO 50 I = IH + 1, N
    Y(L) = X(I)
    WY(L) = WX(I)
    L = L - 1
50 CONTINUE
CALL AMALGM(N - IH, Y, WY, Z, WZ, XA, IFAULT)
L = N - IH
DO 60 I = IH + 1, N
    X(I) = XA(L)
    L = L - 1
60 CONTINUE
C
C     Pool adjacent violators such that X(IH) is largest

```

```

C
70 ILOW = MAX(1, IH - 1)
   IHIGH = MIN(N, IH + 1)
   XMAX = X(IH)
   IXMAX = IH
   DO 80 I = ILOW, IHIGH
       IF (I .EQ. IH .OR. XMAX .GE. X(I)) GO TO 80
       XMAX = X(I)
       IXMAX = I
80 CONTINUE
   IF (IXMAX .EQ. IH) GO TO 100
   IF (IXMAX .LT. IH) IH = IH - 1
   IH1 = IH + 1
   X(IH) = (WX(IH) * X(IH) + WX(IH1) * X(IH1)) / (WX(IH) + WX(IH1))
   WX(IH) = WX(IH) + WX(IH1)
   DO 90 I = IH1, N - 1
       X(I) = X(I + 1)
       WX(I) = WX(I + 1)
90 CONTINUE
   N = N - 1
   GO TO 70

C
C       Obtain XA(1), ..., XA(K) from X(1), ..., X(N)
C
100 I1 = 1
   DO 130 I = 1, N
       S = 0.0
       DO 110 J = I1, K
           S = S + WO(J)
           XA(J) = X(I)
           IF (ABS(S - WX(I)) .LT. TOL) GO TO 120
110 CONTINUE
120 I1 = J + 1
130 CONTINUE
   RETURN
   END
   SUBROUTINE ISREU(MAXK, K, XO, WO, X, Y, Z, WX, WY, WZ, MINVAL,
*           XMIN, XB, RES, IFAULT)

C
C       ALGORITHM AS 257.2 APPL.STATIST. (1990), VOL.39, NO.3
C
C       Subroutine to compute isotonic regression for umbrella
C       ordering with unknown peak
C       A subroutine ISRE given in this paper is called
C
   INTEGER MAXK, K, MINVAL, IFAULT
   REAL XO(K), WO(K), X(K), Y(K), Z(K), WX(K), WY(K), WZ(K), XMIN(K),
*       XB(MAXK, K), RES(K)
   INTEGER I, NH
   REAL RESMIN

C
C       Check that K .GE. 2
C
   IF (K .GE. 2) GO TO 10
   IFAULT = 1
   RETURN

C
C       For all cases with the peak NH = 1, ..., K
C
10 DO 30 NH = 1, K
   CALL ISRE(K, NH, XO, WO, X, Y, Z, WX, WY, WZ, XB(1, NH),

```

```
      *           IFAULT)
      IF (IFault .NE. 0) RETURN
C
C      Calculate square error to obtain min
C
      RES(NH) = 0.0
      DO 20 I = 1, K
          RES(NH) = RES(NH) + WO(I) * (XB(I, NH) - XO(I)) ** 2
20      CONTINUE
      IF (NH .NE. 1 .AND. RES(NH) .GT. RESMIN) GO TO 30
      MINVAL = NH
      RESMIN = RES(NH)
30      CONTINUE
      DO 40 I = 1, K
          XMIN(I) = XB(I, MINVAL)
40      CONTINUE
      RETURN
      END
```

```

SUBROUTINE ARL2(DELTA, K, H, S0, ARL, ARLFIR, IFAULT)
C
C   ALGORITHM AS 258.1  APPL.STATIST. (1990), VOL.39, NO.3
C
C   Computes the average run length for a cumulative
C   sum control scheme
C
REAL DELTA, K, H, S0, ARL, ARLFIR
INTEGER IFAULT
REAL ARLH, ARLHF, ARLL, ARLLF, BIGARL, BIGDEL
INTEGER JFAULT
DATA BIGARL / 1.E30 / , BIGDEL / 5.0 /
C
IFAULT = 0
IF (DELTA .LT. 0.0) THEN
  IFAULT = 1
ELSE
C
  Compute ARL's for upper tail.
C
  CALL ARL1(DELTA, K, H, S0, ARLH, ARLHF, IFAULT)
  IF (IFAULT .EQ. 0) THEN
C
  If DELTA=0, then ARL's for lower tail are the same as for
  the upper.
C
    IF (DELTA .EQ. 0.0) THEN
      ARLLF = ARLHF
      ARLL = ARLH
C
  If DELTA is too large, skip the low-side ARL calculation.
C
    ELSE IF (DELTA .GT. BIGDEL) THEN
      ARLL = BIGARL
      ARLLF = BIGARL
    ELSE
C
  Otherwise compute ARL's for lower tail.
C
    CALL ARL1(-DELTA, K, H, S0, ARLL, ARLLF, JFAULT)
C
  Set lower ARL's large if negative JFAULT .GT. 0
C
    IF (ARLL .LE. ARLH .OR. ARLLF .LE. ARLHF .OR.
*     ARLL .LT. ARLLF .OR. JFAULT .GT. 0) THEN
      ARLL = BIGARL
      ARLLF = BIGARL
    END IF
  END IF
C
  Compute two-sided ARL for S0=0.0
C
  ARL = ARLH / (1.0 + ARLH / ARLL)
C
  Compute two-sided ARL for specified value of S0.
C
  ARLFIR = ARLHF / (1.0 + ARLH / ARLL) +
*     ARLH / (ARLH / ARLLF + ARLL / ARLLF) - ARL
C
  Set IFAULT=3 if two-sided ARL's are lower bounds.
C

```

```

        IF (IFAUULT .EQ. 0 .AND. S0 .GT. H / 2.0 + K) IFAULT = 3
        END IF
    END IF
    RETURN
    END
    SUBROUTINE ARL1(DELTA, K, H, S0, ARL, ARLFIR, IFAULT)
C
C     ALGORITHM AS 258.2  APPL.STATIST. (1990), VOL.39, NO.3
C
    REAL DELTA, K, H, S0, ARL, ARLFIR
    INTEGER IFAULT
    INTEGER N, N1, N2, I, J
    REAL XN
    DOUBLE PRECISION XCOND
    PARAMETER (N=12, N1=N + 1, N2=N + 2, XN=N, XCOND=100.D0)
    INTEGER IPVT(N1)
    REAL P1, P2, ALNORM
    DOUBLE PRECISION A(N1, N1), B(N1), R(N1), W(N2),
*           C, E1, E2, RCOND, S, T
    EXTERNAL ALNORM
C
C     N is the degree of the polynomial approximation.
C     XCOND defines the criterion for singularity:
C           XCOND+RCOND .LE. XCOND,
C     where RCOND is the reciprocal of the condition number.
C
    IFAULT = 0
    IF (K .LT. 0.0 .OR. H .LT. 0.0 .OR. S0 .LT. 0.0 .OR.
*     S0 .GT. H) THEN
        IFAULT = 1
    ELSE IF (H .EQ. 0.0) THEN
        ARL = 1.0 / ALNORM(DELTA - K, .FALSE.)
        ARLFIR = ARL
    ELSE
C
C     Set C.
C
        C = MAX(0.0, K - DELTA)
C
C     For each point S at which the polynomial approximation is to be
C     evaluated...
C
        DO 40 I = 0, N
C
C     Compute S
C
            S = H * I / XN
C
C     Calculate necessary exponentials in S.
C
            E1 = EXP(C * S)
            E2 = EXP((S + DELTA - K) * C + C * C / 2.0)
C
C     Apply left-hand-side of integral equation.
C
            T = E1
            DO 10 J = 1, N + 1
                A(I + 1, J) = T
                T = T * S
            10 CONTINUE
C

```



```

C      Apply lower integration limit.
C
      CALL MOMENT(-S - DELTA - C + K, -S - DELTA - C + K, N, R, W)
      DO 20 J = 1, N + 1
        A(I + 1, J) = A(I + 1, J) - R(J) * E2
20     CONTINUE
C
C      Apply upper integration limit.
C
      CALL MOMENT(H - S - DELTA - C + K, -S - DELTA - C + K, N, R,
*         W)
      DO 30 J = 1, N + 1
        A(I + 1, J) = A(I + 1, J) + R(J) * E2
30     CONTINUE
C
C      Apply term '1 + L(0) F(-S-DELTA+K)'.
C
      A(I + 1, 1) = A(I + 1, 1) - ALNORM(REAL(-S - DELTA + K),
*         .FALSE.)
      B(I + 1) = 1.0
40     CONTINUE
C
C      Normalize the simultaneous equations
C
      DO 70 I = 1, N + 1
        S = 0.0
        DO 50 J = 1, N + 1
          S = MAX(S, ABS(A(I, J)))
50     CONTINUE
        B(I) = B(I) / S
        DO 60 J = 1, N + 1
          A(I, J) = A(I, J) / S
60     CONTINUE
70     CONTINUE
      DO 100 J = 1, N + 1
        W(J) = 0.0
        DO 80 I = 1, N + 1
          W(J) = MAX(W(J), ABS(A(I, J)))
80     CONTINUE
        DO 90 I = 1, N + 1
          A(I, J) = A(I, J) / W(J)
90     CONTINUE
100    CONTINUE
C
C      Factor matrix A.  If equations are singular to working
C      precision, IFAULT=2.
C
C      *****
C      SUBROUTINE DGECO(A,LDA,N,IPVT,RCOND,Z)
C      on entry:
C      A:      the matrix to be factored.
C      LDA:    the leading dimension of array A.
C      N:      the order of the matrix A.
C      on return:
C      A:      the lu factorization of A.
C      IPVT:   pivot indices.
C      RCOND:  an estimate of the reciprocal condition of A.
C      Z:      a working vector.
C      *****
C
      CALL DGECO(A, N + 1, N + 1, IPVT, RCOND, R)

```

```

      IF (XCOND + RCOND .EQ. XCOND) THEN
        IFAULT = 2
      ELSE
C
C      Solve for the polynomial coefficients
C
C      *****
C      SUBROUTINE DGESL(A,LDA,N,IPVT,B,JOB)
C      on entry:
C      A:      the output from dgeco.
C      LDA:    the leading dimension of array A.
C      N:      the order of the matrix A.
C      IPVT:   the pivot vector from dgeco.
C      B:      the right hand side vector.
C      JOB:    = 0          to solve A*X=B.
C              = nonzero to solve trans(A)*X=B.
C      on return:
C      B:      the solution vector X.
C      *****
C
C      CALL DGESL(A, N + 1, N + 1, IPVT, B, 0)
C
C      Get ARL and ARLFIR.
C
C      ARL = B(1) / W(1)
C      ARLFIR = 0.0
C      DO 110 I = 0, N
C          ARLFIR = S0 * ARLFIR + B(N - I + 1) / W(N - I + 1)
110    CONTINUE
C      ARLFIR = ARLFIR * EXP(C * S0)
C      END IF
C      END IF
C      RETURN
C      END
C      SUBROUTINE MOMENT(X, Y, N, R, W)
C
C      ALGORITHM AS 258.3  APPL.STATIST. (1990), VOL.39, NO.3
C
C      For k=0,...,n, computes the integral from x to
C      infinity of the quantity
C
C          
$$R(k+1) = \int_x^\infty (t - y)^{k} z(t) dt,$$

C      where
C          
$$z(t) = 1/\sqrt{2 \pi} \exp(-t^2 / 2) .$$

C
C      INTEGER N
C      DOUBLE PRECISION X, Y, R( * ), W( * )
C      INTEGER I, K
C      REAL ALNORM
C      DOUBLE PRECISION XMY, SQR2PI, FACT(19)
C      EXTERNAL ALNORM
C      DATA SQR2PI / 2.506628274631000502415765D0 /
C      DATA FACT / 2 * 1.D0, 2.D0, 6.D0, 24.D0, 120.D0, 720.D0, 5040.D0,
C      * 40320.D0, 362880.D0, 3628800.D0, 39916800.D0, 479001600.D0,
C      * 6227020800.D0, 87178291200.D0, 1307674368000.D0,
C      * 20922789888000.D0, 355687428096000.D0, 6402373705728000.D0 /
C
C      Compute first term of R.
C
C      W(1) = EXP(-X * X / 2.0) / SQR2PI
C      W(2) = ALNORM(REAL(-X), .FALSE.)

```

```

      R(1) = W(2)
      IF (N .GT. 0) THEN
        DO 10 I = 1, N
          W(I + 2) = (W(I) - X * W(I + 1)) / I
          R(I + 1) = W(I + 2) * FACT(I + 1)
10      CONTINUE
C
C      If X=Y, then R is already computed.
C
      IF (X .NE. Y) THEN
C
C      Compute R.
C
        DO 30 K = 0, N
          R(K + 1) = W(2) / FACT(K + 1)
          XMY = X - Y
          DO 20 I = 1, K
            R(K + 1) = R(K + 1) * XMY + W(I + 2) / FACT(K - I + 1)
20          CONTINUE
          R(K + 1) = R(K + 1) * FACT(K + 1)
30        CONTINUE
      END IF
      END IF
      RETURN
      END
```

```

SUBROUTINE RMCONF(EST, CONF, M, STEPK, MODSTP, LIML, SBOUND, LIMU,
*          BBOUND, LSTART, SLOLIM, SHILIM, ISTART, IRSTRT,
*          INDIC, CLIMLO, CLIMHI, CLLOSE, CLHISE, MLO, MHI,
*          PTHPLT, IFAULT)
C
C      ALGORITHM AS 259  APPL. STATIST. (1990) VOL. 39, NO. 3
C
C      Calculates Monte Carlo confidence intervals using the Robbins-
C      Monro process.  The intervals are asymptotically exact as the
C      number of steps tends to infinity under general conditions.
C
CHARACTER * 1 PTHPLT(76, 105)
INTEGER M, ISTART, INDIC, MLO, MHI, IFAULT
LOGICAL MODSTP, LIML, LIMU, LSTART, IRSTRT
REAL EST, CONF, STEPK, SBOUND, BBOUND, SLOLIM, SHILIM, CLIMLO,
*      CLIMHI, CLLOSE, CLHISE
CHARACTER * 1 DIGIT(0:9), SYMB
CHARACTER * 16 MIDPLT
CHARACTER * 28 HIPLT, LOPLT
CHARACTER * 30 MIDLIN
INTEGER IX(76), MULT(2)
REAL CVHI(20), CVLO(20), SEARCH(2, 2000)
INTEGER I, IERR, II, IIM, IPTH, IR, ISTRT, IY, J, JJ, JX, K,
*      KMULT, KOUNT, L, LIMIT, LL, LR, LX, LY, LYY, M0, M1, M2,
*      MID, MM, NPT
LOGICAL IRSTAR, ISTEP
REAL AL2, ALPHA, BB, BEGPOS, BIG, BOOTES, CONF2, D1, D2, DIV,
*      ENDPOS, FIFTY, HALF, HIPOS, HUN, ONE, ONEPSM, P95, POSN,
*      PTHREE, QUART, ROOT2, SB, SEPOSN, SEVFIV, SMALL, STEP,
*      STEP2, STEPC, STEPHI, TEN, THREP5, TRT2PI, TWO, X, YMAX,
*      YMIN, YSCALE, Z, Z1, ZA, ZERO
REAL PPND, SIMU
EXTERNAL PPND, SIMU
C
C      DATA DIGIT / '0', '1', '2', '3', '4', '5', '6', '7', '8', '9' /
C      DATA ZERO, QUART, PTHREE, HALF / 0.0, 0.25, 0.3, 0.5 /
C      DATA ONE, ROOT2, TWO, THREP5, TEN / 1.0, 1.414214, 2.0, 3.5,
*      10.0 /
C      DATA FIFTY, SEVFIV, P95, HUN / 50.0, 75.0, 95.0, 100.0 /
C      DATA SMALL, ONEPSM, BIG / 1.0E-6, 1.00001, 1.0E20 /
C      DATA HIPLT / 'Upper limit, number of steps' /
C      DATA LOPLT / 'Lower limit, number of steps' /
C      DATA MIDLIN / '-----' /
C      DATA MIDPLT / ' Point estimate ' /
C
C      TRT2PI is 2*SQRT(2*PI); Z1 is z st P(Z > z)=0.005,  Z is N(0,1)
C
C      DATA TRT2PI / 5.013257 / , Z1 / 2.576 /
C
C      IFAULT = 0
C      MULT(1) = 1
C      MULT(2) = 1
C      IF (CONF .GE. HUN .OR. CONF .LT. ZERO) THEN
C          IFAULT = 1
C          RETURN
C      END IF
C      CONF2 = CONF
C      IF (CONF .LT. SMALL) CONF2 = P95
C      ALPHA = (ONE - CONF2 / HUN) / TWO
C      MM = M
C      IF (M .EQ. 0) MM = 1000

```

```

M2 = MM / 2
IF (CONF2 .GE. FIFTY) THEN
  ISTEP = .FALSE.
  AL2 = ALPHA
ELSE
  ISTEP = .TRUE.
  AL2 = QUART
END IF
IF (AL2 * MM .LT. TEN / ONEPSM) THEN
  IFAULT = 5
  RETURN
END IF
IF (STEPK .LT. SMALL) THEN
C
C      PPND cannot fail since IFAULT=1 will have already
C      occurred if the conditions for IERR > 0 arise
C
      ZA = PPND(ONE - AL2, IERR)
      STEPC = TRT2PI * EXP(ZA ** 2 / TWO) / ZA
ELSE
  STEPC = STEPK
END IF
SB = SBOUND
BB = BBOUND
IF (LIML) SB = -BIG
IF (LIMU) BB = BIG
M1 = INT(TWO / ALPHA - HALF)
IF (M1 .LT. 39) M1 = 39
IF (ISTART .EQ. 0) THEN
  ISTRT = INT(HALF + PTHREE * M1)
  IF (ISTRT .GT. 50) ISTRT = 50
ELSE
  ISTRT = ISTART
END IF
IRSTAR = IRSTRT
IF (CONF2 .LT. SEVFIV .AND. IRSTRT) THEN
  IFAULT = 4
  IRSTAR = .FALSE.
END IF
KOUNT = 0
IF (LSTART .OR. ISTEP) THEN
C
C      Set starting points for search using the percentile method
C
      IR = INT((M1 + 1) * AL2 + HALF)
      DO 10 J = 1, IR
        CVHI(J) = -BIG
        CVLO(J) = BIG
10    CONTINUE
C
      DO 70 I = 1, M1
C
C      Generate a bootstrap estimate, assuming the true value of
C      the parameter is EST
C
        BOOTES = SIMU(EST)
        IF (BOOTES .LT. SB / ONEPSM) IFAULT = 2
        IF (BOOTES .GT. BB * ONEPSM) IFAULT = 3
        M0 = MIN(I, IR)
C
C      Extract the IR largest bootstrap estimates

```

```

C
      DO 30 J = 1, M0
        IF (CVHI(J) .LT. BOOTES) THEN
          IF (J .LT. M0) THEN
            DO 20 JJ = M0, J + 1, -1
              CVHI(JJ) = CVHI(JJ - 1)
20          CONTINUE
            END IF
            CVHI(J) = BOOTES
            GO TO 40
          END IF
30        CONTINUE
C
C      Similarly for the lower limit
C
40      DO 60 J = 1, M0
        IF (CVLO(J) .GT. BOOTES) THEN
          IF (J .LT. M0) THEN
            DO 50 JJ = M0, J + 1, -1
              CVLO(JJ) = CVLO(JJ - 1)
50          CONTINUE
            END IF
            CVLO(J) = BOOTES
            GO TO 70
          END IF
60        CONTINUE
70      CONTINUE
      IF (ISTEP) THEN
        STEPHI = (CVHI(IR) - EST) * STEPC
        STEP = (CVLO(IR) - EST) * STEPC
        CLIMHI = EST + CONF2 * (CVHI(IR) - EST) / FIFTY
        CLIMLO = EST - CONF2 * (EST - CVLO(IR)) / FIFTY
      ELSE
C
C      The starting point for the upper limit will be the IRth
C      largest of the M1 bootstrap estimates, and that for the
C      lower limit the IRth smallest.  For CONF2 > 87.5%, IR=2
C
        CLIMHI = CVHI(IR)
        CLIMLO = CVLO(IR)
      END IF
      END IF
      IF ( .NOT. LSTART) THEN
C
C      Starting points supplied by the user
C
        CLIMHI = SHILIM
        CLIMLO = SLOLIM
      END IF
      IF (IFAUULT .GT. 0 .AND. IFAUULT .NE. 4) RETURN
C
C      Start by searching for the lower limit
C
      POSN = CLIMLO
      SEARCH(1, 1) = POSN
      BEGPOS = POSN
      IF (IRSTAR) D1 = ABS(EST - BEGPOS)
      LIMIT = 1
80    I = ISTRT + 1
      II = 1
C

```

```
C      Generate a bootstrap estimate assuming the true value of the
C      parameter is POSN, the current position of the search
C
90  BOOTES = SIMU(POSN)
    IF (BOOTES .LT. SB / ONEPSM) THEN
        IFAULT = 2
        RETURN
    ELSE IF (BOOTES .GT. BB * ONEPSM) THEN
        IFAULT = 3
        RETURN
    END IF
    IF (LIMIT .EQ. 1) THEN
        X = EST - BOOTES
    ELSE
        X = BOOTES - EST
    END IF
    IF (X .LT. SMALL * ABS(EST)) THEN
        X = ONE
    ELSE
        X = ZERO
    END IF
    IF ( .NOT. ISTEP) THEN
C
C      Calculate the current estimate of the steplength constant
C
        STEP = (POSN - EST) * STEPC
        IF (MODSTP) THEN
            STEP2 = BB - POSN
            IF (LIMIT .EQ. 1) STEP2 = POSN - SB
            STEP2 = (STEP2 / ALPHA) + STEP * FLOAT(ISTRN) / FLOAT(I)
            IF (STEP2 .LT. STEP) STEP = STEP2
        END IF
    END IF
C
C      Step to the next position in the search
C
    POSN = POSN + STEP * (X - ALPHA) / FLOAT(I)
C
C      Constrain the search to lie within the bounds to the
C      parameter space
C
    IF (POSN .LT. SB) POSN = SB
    IF (POSN .GT. BB) POSN = BB
    I = I + 1
    II = II + 1
    IIM = II / MULT(LIMIT)
    IF (II .EQ. MULT(LIMIT) * IIM) SEARCH(LIMIT, IIM) = POSN
C
C      If array SEARCH is full, reduce the number of points stored
C      by a factor of 10
C
    IF (IIM .EQ. 200) THEN
        MULT(LIMIT) = MULT(LIMIT) * 10
        DO 100 J = 1, 200
            SEARCH(LIMIT, J) = SEARCH(LIMIT, J * 10)
100    CONTINUE
    END IF
C
C      Restart search if distance between POSN and EST has halved
C      or doubled and IRSTAR=.TRUE.
C
    IF (IRSTAR) THEN
```

```
      D2 = ABS(EST - POSN)
      IF (D1 .GT. TWO * D2 .OR. D1 .LT. HALF * D2) THEN
        I = ISTRT
        BEGPOS = POSN
        D1 = D2
      END IF
END IF

C
C      Go to the next step if more steps are required
IF (I .LT. MM + ISTRT .AND. INDIC .EQ. 0) GO TO 90
IF (I .LT. M2 + ISTRT) GO TO 90

C
C      End current search
C

IF (INDIC .GT. 0) THEN
  SEPOSN = ABS(STEP) * SQRT(ALPHA * (ONE - ALPHA) / FLOAT(I - 1))
  I = ISTRT
  BEGPOS = POSN
  IF (IRSTAR) D1 = D2
  KOUNT = KOUNT + 1

C
C      Test whether endpoint of the current search differs
C      significantly from that of previous search
C

IF (KOUNT .GT. 1 .AND. INDIC .GT. 1) THEN
  IF (SEPOSN .LT. SMALL * POSN) THEN
    Z = ZERO
  ELSE
    Z = ABS(POSN - ENDPOS) / (ROOT2 * SEPOSN)
  END IF
  IF (Z .GT. Z1) THEN
    IF (INDIC .EQ. 2) THEN
      KOUNT = 4
    ELSE
      KOUNT = KOUNT - 1
    END IF
  END IF
END IF

C
C      Is a further search required?
C

IF (KOUNT .EQ. 1) THEN
  ENDPOS = POSN
  GO TO 90
ELSE IF (KOUNT .NE. 4) THEN

C
C      Average the two end points selected to obtain the estimated
C      confidence limit.  If current search is for the lower limit,
C      start the search for the upper limit
C

  HIPOS = CLIMHI
  CLIMHI = (POSN + ENDPOS) / TWO
  CLHISE = SEPOSN / ROOT2
  MHI = II
  IF (LIMIT .EQ. 1) THEN
    CLIMLO = CLIMHI
    CLLOSE = CLHISE
    MLO = MHI
    LIMIT = 2
    KOUNT = 0
    POSN = HIPOS
```



```

        SEARCH(2, 1) = POSN
        BEGPOS = POSN
        IF (IRSTAR) D1 = ABS(EST - BEGPOS)
        IF (ISTEP) STEP = STEPHI
        GO TO 80
    END IF
END IF
END IF
C
C      Use the final endpoint as the estimate of the confidence
C      limit.  If current search is for the lower limit, start the
C      search for the upper limit
C
IF (INDIC .EQ. 0 .OR. KOUNT .EQ. 4) THEN
    IF (INDIC .EQ. 0) SEPOSN = ABS(STEP) *
*           SQRT(ALPHA * (ONE - ALPHA) /
*           FLOAT(I - 1))
    IF (LIMIT .EQ. 1) THEN
        CLIMLO = POSN
        CLLOSE = SEPOSN
        MLO = II
        LIMIT = 2
        KOUNT = 0
        POSN = CLIMHI
        SEARCH(2, 1) = POSN
        BEGPOS = POSN
        IF (IRSTAR) D1 = ABS(EST - BEGPOS)
        IF (ISTEP) STEP = STEPHI
        GO TO 80
    ELSE
        CLIMHI = POSN
        CLHISE = SEPOSN
        MHI = II
    END IF
END IF
C
C      Enter the path of the search for each limit into the array
C      PTHPLT so that it may be checked by the user for convergence
C
DO 120 K = 1, 105
    DO 110 J = 1, 76
        PTHPLT(J, K) = ' '
110    CONTINUE
120    CONTINUE
    DO 130 J = 1, 28
        PTHPLT(J + 20, 1) = HIPLT(J:J)
        PTHPLT(J + 20, 105) = LOPLT(J:J)
130    CONTINUE
    YMAX = -BIG
    YMIN = BIG
    DO 150 I = 1, 2
        IF (I .EQ. 1) THEN
            NPT = MLO / MULT(1)
        ELSE
            NPT = MHI / MULT(2)
        END IF
        DO 140 J = 1, NPT
            IF (SEARCH(I, J) .GT. YMAX) YMAX = SEARCH(I, J)
            IF (SEARCH(I, J) .LT. YMIN) YMIN = SEARCH(I, J)
140        CONTINUE
150    CONTINUE

```

```
DIV = YMAX - YMIN
IF (DIV .LE. ZERO) DIV = ONE
MID = HUN * (YMAX - EST) / DIV + THREP5
YSCALE = HUN / DIV
DO 160 J = 1, 30
  PTHPLT(J, MID) = MIDLIN(J:J)
  PTHPLT(J + 46, MID) = MIDLIN(J:J)
  IF (J .LE. 16) PTHPLT(J + 30, MID) = MIDPLT(J:J)
160 CONTINUE
DO 210 I = 1, 2
  IF (I .EQ. 1) THEN
    NPT = MLO / MULT(1)
    LYY = YSCALE * (CLIMLO - YMIN) + HALF
    SYMB = '<'
  ELSE
    NPT = MHI / MULT(2)
    LYY = YSCALE * (CLIMHI - YMIN) + HALF
    SYMB = '>'
  END IF
DO 170 J = 1, 76
  LX = (NPT - 1) * (J - 1) / SEVFIV + ONE + HALF
  IX(J) = LX
  LY = YSCALE * (SEARCH(I, LX) - YMIN) + HALF
  PTHPLT(J, 103 - LY) = SYMB
  IF (PTHPLT(J, 103 - LYY) .EQ. ' ')
    * PTHPLT(J, 103 - LYY) = '.'
170 CONTINUE
DO 190 J = 1, 15
  JX = IX(5 * J)
  DO 180 L = 0, 4
    LL = 10 ** L
    IF (JX .GE. LL) THEN
      LR = JX / LL - 10 * (JX / (LL * 10))
      PTHPLT(5 * J - L, 2 + (2 - I) * 102) = DIGIT(LR)
    END IF
180 CONTINUE
190 CONTINUE
IF (MULT(I) .GT. 1) THEN
  KMULT = LOG10(FLOAT(MULT(I))) + HALF
  IY = 1 + (2 - I) * 104
  PTHPLT(50, IY) = '/'
  PTHPLT(52, IY) = '1'
  IPTH = 53
  DO 200 K = 1, KMULT
    PTHPLT(IPTH, IY) = '0'
    IPTH = IPTH + 1
200 CONTINUE
  END IF
210 CONTINUE
RETURN
END
```

```

REAL FUNCTION SQMCOR(X, IP, N, RHO2, IFAULT)
C
C     ALGORITHM AS 260  APPL. STATIST. (1991) VOL. 40, NO. 1
C
C     Computes the C.D.F. for the distribution of the
C     square of the multiple correlation coefficient
C     with parameters IP, N, and RHO2
C
C     The following auxiliary algorithms are required:
C     ALOGAM - Log-gamma function (CACM 291)
C     (or  ALNGAM  AS 245)
C     BETAIN - Incomplete beta function (AS 63)
C
REAL X, RHO2
INTEGER IP, N, IFAULT
REAL A, B, BETA, ERRBD, ERRMAX, GX, Q, SUMQ, TEMP, TERM, XJ,
*     ZERO, HALF, ONE
INTEGER ITRMAX
REAL ALOGAM, BETAIN
EXTERNAL ALOGAM, BETAIN
C
DATA ERRMAX, ITRMAX / 1.0E-6, 100 /
DATA ZERO, HALF, ONE / 0.0, 0.5, 1.0 /
C
SQMCOR = X
IFAULT = 2
IF (RHO2 .LT. ZERO .OR. RHO2 .GT. ONE .OR. IP .LT. 2 .OR.
*   N .LE. IP) RETURN
IFAULT = 3
IF (X .LT. ZERO .OR. X .GT. ONE) RETURN
IFAULT = 0
IF (X .EQ. ZERO .OR. X .EQ. ONE) RETURN
C
A = HALF * (IP - 1)
B = HALF * (N - IP)
C
C     Initialize the series
C
BETA = EXP(ALOGAM(A, IFAULT) + ALOGAM(B, IFAULT) -
*     ALOGAM(A + B, IFAULT))
TEMP = BETAIN(X, A, B, BETA, IFAULT)
C
C     There is no need to test IFAULT since all of the
C     parameter values have already been checked
C
GX = EXP(A * LOG(X) + B * LOG(ONE - X) - LOG(A)) / BETA
Q = (ONE - RHO2) ** (A + B)
XJ = ZERO
TERM = Q * TEMP
SUMQ = ONE - Q
SQMCOR = TERM
C
C     Perform recurrence until convergence is achieved
C
10 XJ = XJ + ONE
TEMP = TEMP - GX
GX = GX * (A + B + XJ - ONE) * X / (A + XJ)
Q = Q * (A + B + XJ - ONE) * RHO2 / XJ
SUMQ = SUMQ - Q
TERM = TEMP * Q
SQMCOR = SQMCOR + TERM

```

```
C
C      Check for convergence and act accordingly
C
      ERRBD = (TEMP - GX) * SUMQ
      IF ((INT(XJ) .LT. ITRMAX) .AND. (ERRBD .GT. ERRMAX)) GO TO 10
      IF (ERRBD .GT. ERRMAX) IFAULT = 1
      RETURN
      END
```

=====

The author of algorithms AS 260 & 261 has found an improved algorithm which has been published in the journal 'Computational Statistics & Data Analysis'. Here it is.

C-----

```
C
C The following code for the distribution function of R^2 (cdfr2.for)
C and for its probability density (pdfr2.for) is by the author of AS 260
C and uses an improved algorithm.
```

```
      REAL FUNCTION CDFR2(Y, M, SIZE, RHO2, IFAULT)
```

```
C
C Computes the distribution function of the square of the sample
C multiple correlation coefficient for given abscissa Y, number
C of random variables M, sample size SIZE, and square of the population
C multiple correlation coefficient RHO2
```

```
C Reference:
C Ding, C.G. (1996) 'On the computation of the distribution of
C the square of the sample multiple correlation coefficient',
C Comput. Statist. & Data Analysis, vol. 22, 345-350.
```

```
C IFAULT is a fault indicator:
C = 1 if any of the input values is illegal
C = 0 otherwise
```

```
C No auxiliary algorithm is required
```

```
C
      INTEGER SIZE
      REAL N
      DATA EPS / 1.0E-6 /
      DATA HALF, ZERO, ONE, TWO / 0.5, 0.0, 1.0, 2.0 /
      DATA RP / 1.772453850905516028 /
```

```
      CDFR2 = ZERO
      IFAULT = 1
      IF (M .LE. 1 .OR. SIZE .LE. M .OR. RHO2 .LT. ZERO .OR.
$      RHO2 .GT. ONE) RETURN
```

```
      IFAULT = 0
      IF (Y .LE. ZERO) RETURN
      CDFR2 = ONE
      IF (Y .GE. ONE) RETURN
      A = (M - 1) / TWO
      B = (SIZE - M) / TWO
      AB = (SIZE - 1) / TWO
      IF (MOD(M + 1, 2) .EQ. 0) THEN
```

```
          NA = A + HALF
          GA = ONE
          DO 10 I = 1, NA
10      GA = GA * I
```

```
      ELSE
          NA = A + ONE
          GA = RP
```

```
      DO 20 I = 1, NA
20     GA = GA * (I - HALF)
      ENDIF
      IF (MOD(SIZE - M, 2) .EQ. 0) THEN
          NB = B - HALF
          GB = ONE
          IF (NB .EQ. 0) GO TO 50
          DO 30 I = 1, NB
30     GB = GB * I
      ELSE
          NB = B
          GB = RP
          IF (NB .EQ. 0) GO TO 50
          DO 40 I = 1, NB
40     GB = GB * (I - HALF)
      ENDIF
      IF (MOD(SIZE - 1, 2) .EQ. 0) THEN
          NAB = AB - HALF
          GAB = ONE
          IF (NAB .EQ. 0) GO TO 80
          DO 60 I = 1, NAB
60     GAB = GAB * I
      ELSE
          NAB = AB
          GAB = RP
          DO 70 I = 1, NAB
70     GAB = GAB * (I - HALF)
      ENDIF
```

```
C
C     Evaluate the first term
```

```
80 N = ONE
   Q = (ONE - RHO2) ** AB
   V = Q
   T = Y ** A * (ONE - Y) ** B * GAB / GA / GB
   TERM = V * T
   CDFR2 = TERM
```

```
C
C     Check if  $a + n > (a + b + n)y$ 
```

```
90 IF (A + N .GT. (A + B + N) * Y) GO TO 100
```

```
C
C     Evaluate the next term of the expansion and then the
C     partial sum
```

```
   Q = Q * (A + B + N - ONE) * RHO2 / N
   V = V + Q
   T = T * Y * (A + B + N - ONE) / (A + N)
   TERM = V * T
   CDFR2 = CDFR2 + TERM
   N = N + ONE
   GO TO 90
```

```
C
C     Find the error bound and check for convergence
```

```
100 BOUND = T * Y * (A + B + N - ONE) / ((A + N) - (A + B + N) * Y)
    IF (BOUND .LE. EPS) RETURN
```

```
C
C     Evaluate the next term of the expansion and then the
C     partial sum
```

```

C
  Q = Q * (A + B + N - ONE) * RHO2 / N
  V = V + Q
  T = T * Y * (A + B + N - ONE) / (A + N)
  TERM = V * T
  CDFR2 = CDFR2 + TERM
  N = N + ONE
  GO TO 100
END

C
PROGRAM MAIN

C
  is a driver program that calls CDFR2 and produces output
C
  INTEGER SIZE
10 WRITE (*,11)
11 FORMAT (/1X,'ENTER Y, M (>1), N (>M), RHO2 (BETWEEN 0 AND 1)',
  $      /1X,'FOR CDFR2 ==>')
  READ (*,*) Y, M, SIZE, RHO2
  CDF = CDFR2(Y, M, SIZE, RHO2, IFAULT)
  IF (IFAULT .EQ. 0) THEN
    WRITE (*,21) Y, M, SIZE, RHO2, CDF
21  FORMAT (/1X, 'CDFR2(', E10.4, ', ', 2(I3, ', '), E10.4, ') =',
  $      E12.6)
  ELSE
    WRITE (*,31)
31  FORMAT (/1X,'THE INPUT VALUE IS ILLEGAL!')
  ENDIF
  WRITE(*,41)
41 FORMAT (/1X, 'ENTER 1 TO CONTINUE OR 0 TO QUIT ==> ')
  READ (*,*)K
  IF (K .EQ. 1) GOTO 10
  STOP
  END

C-----
C

  REAL FUNCTION PDFR2(Y, M, SIZE, RHO2, IFAULT)
C
C Computes the density (pdf) of the square of the sample multiple
C correlation coefficient for given abscissa Y, number of random
C variables M, sample size SIZE, and square of the population
C multiple correlation coefficient RHO2
C
C Reference:
C Ding, C.G. (1996) `On the computation of the distribution of
C the square of the sample multiple correlation coefficient',
C Comput. Statist. & Data Analysis, vol. 22, 345-350.
C
C IFAULT is a fault indicator:
C = 1 if any of the input values is illegal
C = 0 otherwise
C
C No auxiliary algorithm is required
C
  INTEGER SIZE
  REAL N
  DATA EPS / 1.0E-6 /

```

```
DATA HALF, ZERO, ONE, TWO / 0.5, 0.0, 1.0, 2.0 /  
DATA RP / 1.772453850905516028 /
```

```
PDFR2 = ZERO  
IFAULT = 1  
IF (M .LE. 1 .OR. SIZE .LE. M .OR. RHO2 .LT. ZERO .OR.  
$ RHO2 .GT. ONE) RETURN  
IFAULT = 0  
IF (Y .LE. ZERO .OR. Y .GE. ONE) RETURN  
A = (M - 1) / TWO  
B = (SIZE - M) / TWO  
AB = (SIZE - 1) / TWO  
IF (MOD(M - 1, 2) .EQ. 0) THEN  
    NA = A - HALF  
    GA = ONE  
    IF (NA .EQ. 0) GO TO 25  
    DO 10 I = 1, NA  
10    GA = GA * I  
ELSE  
    NA = A  
    GA = RP  
    IF (NA .EQ. 0) GO TO 25  
    DO 20 I = 1, NA  
20    GA = GA * (I - HALF)  
ENDIF  
25 IF (MOD(SIZE - M, 2) .EQ. 0) THEN  
    NB = B - HALF  
    GB = ONE  
    IF (NB .EQ. 0) GO TO 50  
    DO 30 I = 1, NB  
30    GB = GB * I  
ELSE  
    NB = B  
    GB = RP  
    IF (NB .EQ. 0) GO TO 50  
    DO 40 I = 1, NB  
40    GB = GB * (I - HALF)  
ENDIF  
50 IF (MOD(SIZE - 1, 2) .EQ. 0) THEN  
    NAB = AB - HALF  
    GAB = ONE  
    IF (NAB .EQ. 0) GO TO 80  
    DO 60 I = 1, NAB  
60    GAB = GAB * I  
ELSE  
    NAB = AB  
    GAB = RP  
    DO 70 I = 1, NAB  
70    GAB = GAB * (I - HALF)  
ENDIF  
  
C  
C    Evaluate the first term  
C  
80 N = ONE  
    Q = (ONE - RHO2) ** AB  
    V = Q  
    S = Y ** (A - ONE) * (ONE - Y) ** (B - ONE) * GAB / GA / GB  
    TERM = Q * S  
    PDFR2 = TERM  
  
C
```

```

C          Check if  $a + n > (a + b + n)y$ 
C
90 IF (A + N .GT. (A + B + N) * Y) GO TO 100
C
C          Evaluate the next term of the expansion and then the
C          partial sum
C
Q = Q * (A + B + N - ONE) * RHO2 / N
V = V + Q
S = S * Y * (A + B + N - ONE) / (A + N - ONE)
TERM = Q * S
PDFR2 = PDFR2 + TERM
N = N + ONE
GO TO 90
C
C          Find the error bound and check for convergence
C
100 BOUND = S * Y * (A + B + N - ONE) * (ONE - V) / (A + N - ONE)
    IF (BOUND .LE. EPS) RETURN
C
C          Evaluate the next term of the expansion and then the
C          partial sum
C
Q = Q * (A + B + N - ONE) * RHO2 / N
V = V + Q
S = S * Y * (A + B + N - ONE) / (A + N - ONE)
TERM = Q * S
PDFR2 = PDFR2 + TERM
N = N + ONE
GO TO 100
END
C
PROGRAM MAIN
C
C          is a driver program that calls PDFR2 and produces output
C
INTEGER SIZE
10 WRITE (*,11)
11 FORMAT (/1X,'ENTER Y, M (>1), N (>M), RHO2 (BETWEEN 0 AND 1)',
$          /1X,'FOR PDFR2 ==> ')
    READ (*,*) Y, M, SIZE, RHO2
    PDF = PDFR2(Y, M, SIZE, RHO2, IFAULT)
    IF (IFAULT .EQ. 0) THEN
        WRITE (*,21) Y, M, SIZE, RHO2, PDF
21    FORMAT (/1X, 'PDFR2(', E10.4, ', ', 2(I3, ', '), E10.4, ') = ',
$           E12.6)
    ELSE
        WRITE (*,31)
31    FORMAT (/1X, 'THE INPUT VALUE IS ILLEGAL!')
    ENDIF
    WRITE(*,41)
41 FORMAT (/1X, 'ENTER 1 TO CONTINUE OR 0 TO QUIT ==> ')
    READ (*,*)K
    IF (K .EQ. 1) GOTO 10
    STOP
    END

```



```
REAL FUNCTION SQMCQ(CDF, IP, N, RHO2, IFAULT)
C
C     ALGORITHM AS 261  APPL. STATIST. (1991) VOL. 40, NO. 1
C
C     Returns the quantile of the distribution of the square
C     of the sample multiple correlation coefficient for
C     given values of CDF, IP, N, and RHO2
C
C     A modification of the secant method, called the
C     Illinois method, is used
C
C     The auxiliary algorithm SQMCOR, used to compute the
C     C.D.F. of the square of the sample multiple correlation
C     coefficient, is required
C
C     INTEGER IP, N, IFAULT
C     REAL CDF, RHO2
C     REAL DIFF, EPS, F0, F1, F2, X0, X1, X2, ZERO, ONE, TWO
C     REAL SQMCOR
C     EXTERNAL SQMCOR
C     DATA ZERO, ONE, TWO / 0.0, 1.0, 2.0 /
C     DATA EPS / 1.0E-6 /
C
C     SQMCQ = CDF
C     IFAULT = 2
C
C     Perform domain check
C
C     IF (RHO2 .LT. ZERO .OR. RHO2 .GT. ONE .OR. IP .LT. 2 .OR.
*     N .LE. IP) RETURN
C     IFAULT = 3
C     IF (CDF .LT. ZERO .OR. CDF .GT. ONE) RETURN
C     IFAULT = 0
C     IF (CDF .EQ. ZERO .OR. CDF .EQ. ONE) RETURN
C
C     Use ONE and ZERO as two starting points for the
C     Illinois method
C
C     X0 = ONE
C     F0 = ONE - CDF
C     X1 = ZERO
C     F1 = -CDF
C
C     Continue iterations until convergence is achieved
C
10  DIFF = F1 * (X1 - X0) / (F1 - F0)
C     X2 = X1 - DIFF
C     F2 = SQMCOR(X2, IP, N, RHO2, IFAULT) - CDF
C     IF (IFAILT .NE. 0) RETURN
C
C     Check for convergence
C
C     IF (ABS(F2) .LE. EPS * CDF) GO TO 20
C     IF (ABS(DIFF) .LE. EPS * X2) GO TO 20
C     IF (F2 * F1 .GE. ZERO) THEN
C         F0 = F0 / TWO
C     ELSE
C         X0 = X1
C         F0 = F1
C     END IF
C     X1 = X2
```

```
F1 = F2
GO TO 10
```

```
C
  20 SQMCQ = X2
  RETURN
  END
```

```
=====
The author of algorithms AS 260 & 261 has found an improved algorithm
which has been published in the journal `Computational Statistics &
Data Analysis'. Here it is.
```

```
C-----
C
C The following code for calculating quantiles of R^2 (qr2.for)
C is by the author of AS 261 and uses an improved algorithm.
```

```
REAL FUNCTION QR2(M, SIZE, RHO2, P, IFAULT)
```

```
C
C Computes the quantile of the distribution of the square of the
C sample multiple correlation coefficient for given number of
C random variables M, sample size SIZE, square of the population
C multiple correlation coefficient RHO2, and lower tail area P
```

```
C Reference:
C Ding, C.G. (1996) `On the computation of the distribution of
C the square of the sample multiple correlation coefficient',
C Comput. Statist. & Data Analysis, vol. 22, 345-350.
```

```
C IFAULT is a fault indicator:
C = 1 if there is no convergence after 10 Newton's iterations
C = 2 if any of the input values is illegal
C = 0 otherwise
```

```
C No auxiliary algorithm is required
```

```
INTEGER SIZE
REAL N
DATA ZERO, HALF, ONE, TWO / 0.0, 0.5, 1.0, 2.0 /
DATA EPS, DELTA / 1.0E-6, 1.0E-4 /
DATA ITRMAX / 10 /
DATA RP / 1.772453850905516028 /
```

```
QR2 = P
```

```
C
C Test for admissibility of arguments
```

```
IFAULT = 2
IF (M .LE. 1 .OR. SIZE .LE. M .OR. RHO2 .LT. ZERO .OR.
$ RHO2 .GT. ONE .OR. P .LT. ZERO .OR. P .GT. ONE) RETURN
IFAULT = 0
IF (P .EQ. ZERO .OR. P .EQ. ONE) RETURN
```

```
C Calculate the constants needed for each Newton's iteration
```

```
C
C
A = (M - 1) / TWO
B = (SIZE - M) / TWO
AB = (SIZE - 1) / TWO
IF (MOD(M + 1, 2) .EQ. 0) THEN
  NA = A + HALF
  GA = ONE
  DO 10 I = 1, NA
10 GA = GA * I
```

```

    ELSE
      NA = A + ONE
      GA = RP
      DO 20 I = 1, NA
20    GA = GA * (I - HALF)
    ENDIF
    IF (MOD(SIZE - M, 2) .EQ. 0) THEN
      NB = B - HALF
      GB = ONE
      IF (NB .EQ. 0) GO TO 50
      DO 30 I = 1, NB
30    GB = GB * I
    ELSE
      NB = B
      GB = RP
      IF (NB .EQ. 0) GO TO 50
      DO 40 I = 1, NB
40    GB = GB * (I - HALF)
    ENDIF
50  IF (MOD(SIZE - 1, 2) .EQ. 0) THEN
      NAB = AB - HALF
      GAB = ONE
      IF (NAB .EQ. 0) GO TO 75
      DO 60 I = 1, NAB
60    GAB = GAB * I
    ELSE
      NAB = AB
      GAB = RP
      DO 70 I = 1, NAB
70    GAB = GAB * (I - HALF)
    ENDIF
75  Q0 = (ONE - RHO2) ** AB
    COEFF = GAB / GA / GB
C
C      Use 0.5 as a starting value for Newton's iterations
C
Y = HALF
C
C      Perform Newton's iterations
C
DO 120 ITER = 1, ITRMAX
C
C      Evaluate the first terms of the series for CDF (distribution
C      function) and PDF (density)
C
N = ONE
YP = ONE - Y
T = COEFF * Y ** A * YP ** B
S = A * T / Y / YP
Q = Q0
V = Q
CDF = V * T
PDF = Q * S
C
C      Check if  $a + n > (a + b + n)y$ 
C
80 IF (A + N .GT. (A + B + N) * Y) GO TO 90
C
C      Evaluate the next terms of two series and then the
C      partial sums
C

```

```

Q = Q * (A + B + N - ONE) * RHO2 / N
V = V + Q
S = T * (A + B + N - ONE) / YP
T = T * Y * (A + B + N - ONE) / (A + N)
CDF = CDF + V * T
PDF = PDF + Q * S
N = N + ONE
GO TO 80

```

```

C
C      Find the error bounds and check for convergence for both
C      series
C

```

```

90 BNDPDF = T * Y * (A + B + N - ONE) / (A + N - (A + B + N) * Y)
BNDPDF = T * (A + B + N - ONE) * (ONE - V) / YP
100 IF (BNDPDF .LE. EPS .AND. BNDPDF .LE. EPS) GO TO 110

```

```

C
C      Continue to update the terms and then accumulate
C

```

```

Q = Q * (A + B + N - ONE) * RHO2 / N
V = V + Q
IF (BNDPDF .LE. EPS) THEN
  S = S * Y * (A + B + N - ONE) / (A + N - ONE)
  PDF = PDF + Q * S
  N = N + ONE
  BNDPDF = S * Y * (A + B + N - ONE) * (ONE - V) / (A + N - ONE)
  GO TO 100
ELSE IF (BNDPDF .LE. EPS) THEN
  T = T * Y * (A + B + N - ONE) / (A + N)
  CDF = CDF + V * T
  N = N + ONE
  BNDPDF = T * Y * (A+B+N-ONE) / (A+N - (A+B+N)*Y)
  GO TO 100
ELSE
  S = T * (A + B + N - ONE) / YP
  T = T * Y * (A + B + N - ONE) / (A + N)
  CDF = CDF + V * T
  PDF = PDF + Q * S
  N = N + ONE
  GO TO 90

```

```

ENDIF

```

```

C
C      Obtain a new Y and make changes if it is illegal
C

```

```

110 DIFF = (CDF - P) / PDF
YNEW = Y - DIFF
IF (YNEW .LE. ZERO) THEN
  Y = Y / TWO
ELSE IF (YNEW .GE. ONE) THEN
  Y = (Y + ONE) / TWO
ELSE
  Y = YNEW

```

```

ENDIF

```

```

C
C      Check for convergence of Newton's iterations
C

```

```

IF (ABS(DIFF) .LE. DELTA * Y) THEN
  QR2 = Y
  RETURN
ENDIF

```

```

120 CONTINUE
IF AULT = 1

```

```
        RETURN
        END
C
        PROGRAM MAIN
C
        This is a driver program that calls QR2 and produces output
C
        INTEGER SIZE

10 WRITE (*,11)
11 FORMAT (/1X,'ENTER M (>1), N (>M), RHO2 (BETWEEN 0 AND 1), and',
$         /1X,'P (BETWEEN 0 AND 1) FOR QR2 ==> ')
        READ (*,*) M, SIZE, RHO2, P
        Y = QR2(M, SIZE, RHO2, P, IFAULT)
        ICODE = IFAULT + 1
        GO TO (20, 30, 40), ICODE
20 WRITE (*,21) M, SIZE, RHO2, P, Y
21 FORMAT (/1X, 'QR2(', I3, ',', I3, ',', E10.4, ',', E10.4, ') =',
$         E11.5)
        GO TO 60
30 WRITE (*,31)
31 FORMAT (/1X,43HNO CONVERGENCE AFTER 10 NEWTON'S ITERATIONS)
        GO TO 60
40 WRITE (*,41)
41 FORMAT (/1X,'THE INPUT VALUE IS ILLEGAL!')
60 WRITE (*,61)
61 FORMAT (/1X, 'ENTER 1 TO CONTINUE OR 0 TO QUIT ==> ')
        READ (*,*) K
        IF (K .EQ. 1) GO TO 10
        STOP
        END
```

```

SUBROUTINE WL(NR, N, NN, G, X, S, D, SIGMA, SIGINV, WLT, NRUNIV,
*           CHIOMB, NRSTOC, METHOD, KERROR, IFAULT)
C
C   ALGORITHM AS 262  APPL.STATIST. (1991), VOL.40, NO.1
C
C   Wei-Lachin multivariate generalization of the generalized
C   Wilcoxon test of Gehan and the log-rank test for incomplete
C   multivariate observations with censoring.
C
INTEGER NREP, NOBS
PARAMETER (NREP=10, NOBS=500)
C
C   NREP      the maximum number of repeat times
C   NOBS      the maximum number of observations
C
INTEGER NR, N(2), NN, G(NOBS), S(NOBS, NREP), METHOD, KERROR,
*           IFAULT
REAL X(NOBS, NREP), D(2, NREP), SIGMA(NN), SIGINV(NN), WLT(NREP),
*           NRUNIV(NREP), CHIOMB, NRSTOC
INTEGER Y(2, NOBS), I, IFAIL, IPOINT, NULLTY, J, J2, K, K1,
*           K2, NT
REAL EE(2, NREP), MU(2, NOBS, NREP), PSI(2, NOBS, NREP), QE(2),
*           SIG(2, NREP, NREP), WORK(NREP), Q, SIGSUM, SUM, TSUM, Z,
*           ZERO, ONE, TWO
C
DATA ZERO, ONE, TWO / 0.0, 1.0, 2.0 /
C
ZSQRT(I) = SQRT(Z)
ZREAL(Z) = REAL(I)
C
C   Initialization
C
IFAULT = 4
IF (NR .GT. NREP) RETURN
IFAULT = 5
NT = N(1) + N(2)
IF (NT .GT. NOBS) RETURN
IFAULT = 0
DO 30 K = 1, NR
  DO 20 I = 1, 2
    EE(I, K) = ZERO
    D(I, K) = ZERO
    DO 10 K2 = 1, NR
      SIG(I, K, K2) = ZERO
10    CONTINUE
20    CONTINUE
30  CONTINUE
C
C   Y      number at risk of failure
C   EE     partial sum used in equation 1
C   QE     Q*E (see equation 4)
C   Evaluate MU (equation 4)
C
DO 110 K = 1, NR
  DO 70 J = 1, NT
    DO 40 I = 1, 2
      Y(I, J) = 0
      MU(I, J, K) = ZERO
40    CONTINUE
    IF (S(J, K) .EQ. 1) THEN
      DO 50 J2 = 1, NT

```

```

                IF (X(J2, K) .GE. X(J, K))
*                   Y(G(J2), J) = Y(G(J2), J) + 1
50      CONTINUE
        SUM = Y(1, J) + Y(2, J)
        IF (SUM .EQ. ZERO) THEN
            IFAULT = 1
            RETURN
        END IF
        IF (METHOD .EQ. 1) Q = SUM / NT
        IF (METHOD .EQ. 2) Q = ONE
        DO 60 I = 1, 2
            QE(I) = Q * Y(I, J) / SUM
60      CONTINUE
        MU(2, J, K) = QE(1)
        MU(1, J, K) = QE(2)
        EE(G(J), K) = EE(G(J), K) + MU(G(J), J, K)
        D(G(J), K) = D(G(J), K) + ONE
        ELSE
            MU(1, J, K) = ZERO
            MU(2, J, K) = ZERO
        END IF
70      CONTINUE
C
C      Evaluate PSI (equation 5)
C
        DO 100 J = 1, NT
            DO 90 I = 1, 2
                PSI(I, J, K) = ZERO
                DO 80 J2 = 1, NT
                    IF (G(J2) .EQ. I .AND. X(J2, K) .LE. X(J, K)) THEN
                        IF (S(J2, K) .EQ. 1) THEN
*                               PSI(I, J, K) = PSI(I, J, K) +
*                                       MU(I, J2, K) / Y(I, J2)
                                END IF
                            END IF
80      CONTINUE
90      CONTINUE
100     CONTINUE
110    CONTINUE
C
C      Compute entries in covariance matrix (see equations 2 and 3)
C
        DO 140 K1 = 1, NR
            DO 130 K2 = 1, K1
                DO 120 J = 1, NT
                    I = G(J)
                    IF (N(I) .EQ. 0) THEN
                        IFAULT = 2
                        RETURN
                    END IF
                    SIG(I, K1, K2) = SIG(I, K1, K2) +
*                               (MU(I, J, K1) * S(J, K1) -
*                               PSI(I, J, K1)) * (MU(I, J, K2) *
*                               S(J, K2) - PSI(I, J, K2)) / N(I)
120     CONTINUE
                    IPOINT = K1 * (K1 - 1) / 2 + K2
                    SIGMA(IPOINT) = (N(1) * SIG(1, K1, K2) +
*                               N(2) * SIG(2, K1, K2)) / NT
130     CONTINUE
140    CONTINUE
C

```

```
C      Compute Wei-Lachin univariate test NRUNIV (see eqns 1 and 6)
C
DO 150 K = 1, NR
  WLT(K) = (EE(1, K) - EE(2, K)) / ZSQRT(ZREAL(NT))
  IPOINT = K * (K + 1) / 2
  IF (SIGMA(IPOINT) .EQ. ZERO) THEN
    IFAULT = 3
    KERROR = K
    RETURN
  END IF
  NRUNIV(K) = WLT(K) / ZSQRT(SIGMA(IPOINT))
150 CONTINUE
C
C      Compute inverse of covariance matrix and Wei-Lachin
C      multivariate statistics CHIOMB (for omnibus test) and
C      NRSTOC (for test of stochastic ordering) (see eqn 7)
C
CALL SYMINV(SIGMA, NR, NN, SIGINV, WORK, NULLTY, IFAIL)
CHIOMB = ZERO
TSUM = ZERO
SIGSUM = ZERO
DO 170 J = 1, NR
  TSUM = TSUM + WLT(J)
  IPOINT = J * (J + 1) / 2
  CHIOMB = CHIOMB + WLT(J) * WLT(J) * SIGINV(IPOINT)
  SIGSUM = SIGSUM + SIGMA(IPOINT)
  DO 160 J2 = 1, J - 1
    IPOINT = J * (J - 1) / 2 + J2
    CHIOMB = CHIOMB + TWO * WLT(J) * WLT(J2) * SIGINV(IPOINT)
    SIGSUM = SIGSUM + TWO * SIGMA(IPOINT)
160 CONTINUE
170 CONTINUE
NRSTOC = TSUM / ZSQRT(SIGSUM)
RETURN
END
```



```

SUBROUTINE IRRED(ITBTYP, NTAXA, NTESTS, NDIST, LSTAB, LGROUP,
*          GROUP, NBI, ISETS, LSETS, LTBP, IOUT, IFAULT)
C
C   ALGORITHM AS 263.1  APPL.STATIST. (1991), VOL.40, NO.1
C
C   Constructs irredundant test sets
C
INTEGER IFAULT, IOUT, ITBTYP, LSETS, LTBP, NBI, NDIST, NTAXA,
*       NTESTS
INTEGER GROUP(NTAXA), ISETS(LSETS)
LOGICAL LGROUP, LSTAB
INTEGER I, ITAX1, ITAX2, IT1LIM, JTLLIST, KPOWR2, LDBP, NIBP, NB0
C
C   Check parameters
C
IF ((NTAXA .LE. 0) .OR. (NTESTS .LE. 0) .OR. (NDIST .LE. 0) .OR.
*   (NBI .LE. 0) .OR. (IOUT .LT. 0)) GO TO 40
IFault = 0
C
C   Set number of integers to store each irredundant test set
C
NIBP = (NTESTS - 1) / NBI + 1
C
C   Set number of unused bits within each bit pattern
C
NB0 = NIBP * NBI - NTESTS
C
C   Set up Powers of 2 (2**0,1,2...) in
C   ISETS(KPOWR2...KPOWR2+NBI-1)
C
KPOWR2 = LSETS - NBI + 1
ISETS(KPOWR2) = 1
DO 10 I = KPOWR2 + 1, LSETS
    ISETS(I) = ISETS(I - 1) * 2
10 CONTINUE
C
C   Initialise taxon indices and limits
C
ITAX1 = ITBTYP
IT1LIM = NTAXA
IF (ITBTYP .GT. 0) THEN
    IF (LGROUP) THEN
C
C   Find 1st taxon of group ITBTYP (to be distinguished from
C   other groups)
C
        DO 20 ITAX1 = 1, NTAXA
            IF (GROUP(ITAX1) .EQ. ITBTYP) GO TO 30
20 CONTINUE
C
C   No taxa in group
C
            IFAULT = 3
            RETURN
        ELSE
C
C   Test sets to distinguish an individual taxon
C
            IF ((ITBTYP .LT. 0) .OR. (ITBTYP .GT. NTAXA)) GO TO 40
            IT1LIM = ITAX1
            END IF
        END IF
    END IF

```

```

      END IF
C
C      Form irredundant sets
C
30 LDBP = NIBP
C
C      Initialise b.p. (i.e. bit pattern) of essential tests
C
      CALL SETVAL(ISETS(1), 0, NIBP)
      I = ITAX1
      ITAX2 = 0
      CALL IRRDTB(ITBTYP, NTAXA, NTESTS, NDIST, LSTAB, LGROUP, GROUP,
*              NBI, ISETS, LSETS, IOUT, IFAULT, ITAX1, ITAX2, IT1LIM,
*              NIBP, NB0, KPOWR2, 0, NIBP, LDBP, JTTLIST, KPOWR2 - 1,
*              .FALSE.)
      IF (IFAUULT .NE. 0) RETURN
      ITAX1 = I
      ITAX2 = 0
      CALL IRRMLT(ITBTYP, NTAXA, NTESTS, NDIST, LSTAB, LGROUP, GROUP,
*              NBI, ISETS, LSETS, LTBP, IOUT, IFAULT, ITAX1, ITAX2,
*              IT1LIM, NIBP, NB0, KPOWR2, 0, NIBP, LDBP, JTTLIST,
*              KPOWR2 - 1)
      RETURN
40 IFAULT = 1
      RETURN
      END
      SUBROUTINE IRRDTB(ITBTYP, NTAXA, NTESTS, NDIST, LSTAB, LGROUP,
*              GROUP, NBI, ISETS, LSETS, IOUT, IFAULT, ITAX1,
*              ITAX2, IT1LIM, NIBP, NB0, KPOWR2, KBPEST, KDBP,
*              LDBP, JTTLIST, LTTLIST, LNEXT)
C
C      ALGORITHM AS 263.2  APPL.STATIST. (1991), VOL.40, NO.1
C
C      Forms entries of the taxon x taxon table of sets of tests
C      that distinguish each pair of taxa.  LNEXT is .TRUE. on entry
C      if required to form tests in next non-null entry (by IRRMLT
C      when taxon x taxon table not stored)
C
      INTEGER IFAULT, IOUT, ITAX1, ITAX2, ITBTYP, IT1LIM, JTTLIST,
*          KBPEST, KDBP, KPOWR2, LDBP, LSETS, LTTLIST, NBI, NB0,
*          NDIST, NIBP, NTAXA, NTESTS
      INTEGER GROUP(NTAXA), ISETS(LSETS)
      LOGICAL LGROUP, LNEXT, LSTAB
      INTEGER IBT, JBT, J1, J2, K1, K2, K3, NTD, NTE
      INTEGER IAND, ICNT, IOR
      LOGICAL LTDIST
      EXTERNAL IAND, ICNT, IOR, LTDIST
C
      IF (ITAX1 .GT. 0) GO TO 20
C
C      Increment ITAX1/2 (scan rows/cols of table)
C
10 ITAX1 = ITAX1 + 1
      IF (ITAX1 .GT. IT1LIM) RETURN
      IF (LGROUP .AND. (ITBTYP .GT. 0)) THEN
          IF (GROUP(ITAX1) .NE. ITBTYP) GO TO 10
          ITAX2 = 0
      ELSE
C
C      Initialise ITAX2 (to scan across next line of table)
          ITAX2 = ITAX1

```

```

      END IF
C
C      Increment ITAX2
20 ITAX2 = ITAX2 + 1
   IF (ITAX2 .GT. NTAXA) GO TO 10
   IF (LGROUP) THEN
     IF (GROUP(ITAX1) .EQ. GROUP(ITAX2)) GO TO 20
   ELSE
     IF (ITAX1 .EQ. ITAX2) GO TO 20
   END IF
C
C      Form list of tests that distinguish between ITAX1 and ITAX2
C
JTLIST = LTLIST + 1
NTE = 0
NTD = 0
DO 30 J1 = 1, NTESTS
C
C      Exit to end of loop if test J1 does not distinguish ITAX1 and
C      ITAX2
C
   IF ( .NOT. LTDIST(J1, ITAX1, ITAX2)) GO TO 30
   NTD = NTD + 1
C
C      If NDIST tests already distinguish ITAX1 and ITAX2, and the
C      aim is merely to form the b.p. of essential tests, take the
C      next pair of taxa
C
   IF ((NTD .GT. NDIST) .AND. ( .NOT. (LNEXTE .OR.
*      LSTAB))) GO TO 20
C
C      Check whether J1 is an essential test
C
   JBT = (J1 + NB0 - 1) / NBI + 1
   IBT = ISETS(KPOWR2 + JBT * NBI - (J1 + NB0))
   IF (IAND(IBT, ISETS(KBPEST + JBT)) .GT. 0) THEN
C
C      Check whether sufficient essential tests already separate
C      ITAX1/2
C
     NTE = NTE + 1
     IF (NTE .GE. NDIST) GO TO 20
   END IF
C
C      Enter J1 in the list of tests that distinguish ITAX1 and ITAX2
C
   JTLIST = JTLIST - 2
   IF (JTLIST .LE. LDBP) GO TO 80
   ISETS(JTLIST) = JBT
   ISETS(JTLIST + 1) = IBT
30 CONTINUE
   IF (NTD .LE. NDIST) THEN
C
C      Taxa ITAX1 and ITAX2 distinguished by </= NDIST tests
C
     IF (LNEXTE) GO TO 20
     IF (NTD .EQ. 0) THEN
C
C      Taxa ITAX1 and ITAX2 cannot be distinguished
C
       WRITE (IOUT, '(A,I6,A,I6,A)') ' WARNING: TAXA', ITAX1,

```

```

*          ' AND', ITAX2,' CANNOT BE DISTINGUISHED'
      GO TO 20
      END IF
C
C      No more than NDIST tests distinguish ITAX1 and ITAX2
C
      IF (NTD .LT. NDIST) WRITE (IOUT,'(A,I6,A,I6,A,I6,A)')
*         ' WARNING: TAXA', ITAX1, ' AND', ITAX2,
*         ' DISTINGUISHED BY ONLY', NTD, ' TEST(S)'
C
C      Add to set of essential tests
C
      DO 40 J1 = JTTLIST, LTLIST, 2
          ISETS(KBPEST + ISETS(J1)) = IOR(ISETS(KBPEST + JBT),
*                                     ISETS(J1 + 1))
40      CONTINUE
C
C      Delete any sets containing >/= NDIST essential tests
C
      IF (KDBP .GE. LDBP) GO TO 20
      K2 = KDBP
      K3 = LDBP
      LDBP = KDBP
      DO 60 K1 = KDBP, K3, NIBP
          IF (K1 .LT. K3) THEN
              IF (NDIST .EQ. 1) THEN
C
C          Check whether set contains new essential test (IBT/JBT from
C          loop 30)
C
                  IF (IAND(ISETS(K1 + JBT), IBT) .EQ. 0) GO TO 60
                  ELSE
C
C          Check whether set contains >/= NDIST essential tests
C
                      NTE = 0
                      DO 50 J2 = K1 + 1, K1 + NIBP
                          NTE = NTE + ICNT(IAND(ISETS(J2),
*                                     ISETS(J2 + KBPEST - K1)))
50          CONTINUE
                      IF (NTE .LT. NDIST) GO TO 60
                      END IF
                  END IF
C
C          All sets checked or current set deleted, compact the list
C
                      CALL CPSETS(ISETS, LSETS, LDBP, K2, K1 - K2)
                      LDBP = LDBP + K1 - K2
                      K2 = K1 + NIBP
60          CONTINUE
          ELSE
C
C          >NDIST tests distinguish ITAX1 and ITAX2
C
              IF (LNEXTE) RETURN
C
C          Form bit pattern for new set at LDBP
C
              IF (LDBP + NIBP .GE. JTTLIST) GO TO 80
              CALL SETVAL(ISETS(LDBP + 1), 0, NIBP)
              DO 70 J1 = JTTLIST, LTLIST, 2

```

```

          ISETS(LDBP + ISETS(J1)) = ISETS(LDBP + ISETS(J1)) +
*                                     ISETS(J1 + 1)
70    CONTINUE
C
C    Merge new set into list KDBP...LDBP
C
      J1 = LDBP
      CALL IRRMRG(KDBP, J1, LDBP, NIBP, ISETS, LSETS)
      END IF
      GO TO 20
C
C    Insufficient workspace
C
80    IFAULT = 2
      RETURN
      END
      SUBROUTINE IRRMLT(ITBTYP, NTAXA, NTESTS, NDIST, LSTAB, LGROUP,
*                    GROUP, NBI, ISETS, LSETS, LTBP, IOUT, IFAULT,
*                    ITAX1, ITAX2, IT1LIM, NIBP, NB0, KPOWR2, KBPEST,
*                    KDBP, LDBP, JTTLIST, LTTLIST)
C
C    ALGORITHM AS 263.3  APPL.STATIST. (1991), VOL.40, NO.1
C
C    'multiplies' entries in the taxon x taxon table of (sets of)
C    distinguishing tests, thus forming irredundant test sets
C
      INTEGER IFAULT, IOUT, ITAX1, ITAX2, ITBTYP, IT1LIM, JTTLIST,
*           KBPEST, KDBP, KPOWR2, LTBP, LDBP, LSETS, LTTLIST, NBI,
*           NIBP, NB0, NDIST, NTAXA
      INTEGER NTESTS, GROUP(NTAXA), ISETS(LSETS)
      LOGICAL LGROUP, LSTAB
      INTEGER IBT, INTD, JBT, J1, J2, J3, J4, KBPENL, KTBCAB, KTBMBE,
*           KTBP, KTBP2, K1, K2, K3, K4, LTBCAB, LTBMBE, LTBMRG,
*           LTBNAB, LTIAB, NTD
      INTEGER IAND, ICNT, IOR
      LOGICAL IRRWSP
      EXTERNAL IAND, ICNT, IOR, IRRWSP
C
C    Initial set contains just the essential tests
C
      KTBP = LDBP
      CALL CPSETS(ISETS, LSETS, KTBP, KBPEST, NIBP)
      LTBP = KTBP + NIBP
C
C    Get the next entry from the taxon x taxon table
C
10    KTBP2 = KTBP
      IF (LSTAB) THEN
C
C    Generate test list from stored bit pattern
C
          IF (KTBP .LE. KDBP) RETURN
          JTTLIST = LTTLIST + 1
          KTBP = KTBP - NIBP
          K2 = KPOWR2 + NBI - NB0 - 1
          DO 40 JBT = 1, NIBP
              K1 = ISETS(KTBP + JBT)
              DO 20 J1 = K2, KPOWR2, -1
                  IBT = ISETS(J1)
                  IF (IAND(K1, IBT) .EQ. 0) GO TO 20
                  JTTLIST = JTTLIST - 2

```

```

                IF (JTTLIST .LE. LTBP + NIBP) GO TO 180
                ISETS(JTTLIST) = JBT
                ISETS(JTTLIST + 1) = IBT
                K1 = K1 - IBT
                IF (K1 .LE. 0) GO TO 30
20             CONTINUE
30             K2 = KPOWR2 + NBI - 1
40             CONTINUE
            ELSE
                CALL IRRDTB(ITBTYP, NTAXA, NTESTS, NDIST, LSTAB, LGROUP, GROUP,
*                 NBI, ISETS, LSETS, IOUT, IFAULT, ITAX1, ITAX2,
*                 IT1LIM, NIBP, NB0, KPOWR2, KBPEST, KDBP, LDBP,
*                 JTTLIST, LTLIST, .TRUE.)
                IF ((ITAX1 .GT. IT1LIM) .OR. (IFAUULT .NE. 0)) RETURN
            END IF

C
C             Sort sets into (a) pass-cannot-absorb (in KTBP...LTBNAB),
C             (b) pass-can-absorb (in KTBCAB (initially LTBP)...LTBCAB),
C             (c/d) must-be-enlarged (in KTBMBE...LTBMBE); also, if NDIST=1,
C             sort tests into contained-in-can-absorb (JTTLIST...LTIAB-1)
C             and not-contained-in-can-absorb (LTIAB...LTLIST)
C
                LTBNAB = KTBP
                KTBCAB = LTBP
                LTBMBE = JTTLIST - 1

C
C             Leave space above LTBMBE for sets with none of the new tests(d)
C
                IF (NDIST .GT. 1) LTBMBE = LTBCAB + (JTTLIST - LTBCAB) / 2
                KTBMBE = LTBMBE
                LTIAB = JTTLIST
                DO 60 K1 = KTBP2, LTBP - 1, NIBP

C
C             Count number of tests from list already in each set
C
                NTD = 0
                DO 50 J1 = JTTLIST, LTLIST, 2
                    IF (IAND(ISETS(K1 + ISETS(J1)), ISETS(J1 + 1)) .EQ.
*                     0) GO TO 50
                    NTD = NTD + 1
                    K3 = J1
50             CONTINUE
                IF (NDIST .LT. NTD) THEN

C
C             Pass, cannot absorb
C
                    CALL CPSETS(ISETS, LSETS, LTBNAB, K1, NIBP)
                    LTBNAB = LTBNAB + NIBP
                ELSE
                    IF (NDIST .EQ. NTD) THEN

C
C             Pass, can absorb
C
                        LTBMBE = LTBMBE + NIBP
                        IF (LTBMBE .GT. KTBMBE) THEN
                            IF (IRRWSP(LTBMBE, KTBMBE, LTBMBE, JTTLIST, ISETS,
*                               LSETS)) GO TO 180
                        END IF
                        CALL CPSETS(ISETS, LSETS, LTBMBE - NIBP, K1, NIBP)
                        IF ((NDIST .EQ. 1) .AND. (K3 .GE. LTIAB)) THEN

```

```

        JBT = ISETS(K3)
        IBT = ISETS(K3 + 1)
        ISETS(K3) = ISETS(LTIAB)
        ISETS(K3 + 1) = ISETS(LTIAB + 1)
        ISETS(LTIAB) = JBT
        ISETS(LTIAB + 1) = IBT
        LTIAB = LTIAB + 2
    END IF
ELSE
C
C      Must be enlarged
C
        IF ((NDIST .EQ. 1) .OR. (NTD .GT. 0)) THEN
            KTBMBE = KTBMBE - NIBP
            IF (LTBCAB .GE. KTBMBE) THEN
                IF (IRRWSP(LTBCAB, KTBMBE, LTBMBE, JTTLIST, ISETS,
*                   LSETS)) GO TO 180
                END IF
                CALL CPSETS(ISETS, LSETS, KTBMBE, K1, NIBP)
                IF (NDIST .EQ. 1) GO TO 60
C
C      (NDIST>1) store number of new tests already in set
C
                ISETS(KTBMBE) = NTD
                KTBMBE = KTBMBE - 1
            ELSE
                LTBMBE = LTBMBE + NIBP + 1
                IF (LTBMBE .GE. JTTLIST) THEN
                    IF (IRRWSP(LTBCAB, KTBMBE, LTBMBE, JTTLIST, ISETS,
*                   LSETS)) GO TO 180
                    END IF
                    CALL CPSETS(ISETS, LSETS, LTBMBE - NIBP, K1, NIBP)
                    ISETS(LTBMBE - NIBP) = 0
                END IF
            END IF
        END IF
    END IF
60 CONTINUE
C
C      Copy down pass-can-absorb sets
C
        J3 = LTBCAB - KTBBCAB
        CALL CPSETS(ISETS, LSETS, LTBNAB, KTBBCAB, J3)
        KTBBCAB = LTBNAB
        LTBCAB = KTBBCAB + J3
        LTBP = LTBCAB
        IF (LTBMBE .LE. KTBMBE) GO TO 10
C
C      Form and check new b.p.'s from must-be-enlarged list
C
        IF (NDIST .EQ. 1) THEN
            NTD = 0
            K2 = JTTLIST
            K3 = LTLIST
            K4 = 2
        ELSE
C
C      Calc number of 'augmenting' patterns (no. combinations of
C      NDIST tests)
C
            J1 = (LTLIST - JTTLIST + 1) / 2
            J3 = 1

```

```

    J4 = 1
    DO 70 J2 = 1, NDIST
        J3 = J3 * J2
        J4 = J4 * J1
        J1 = J1 - 1
70    CONTINUE
C
C    Reserve space for 'augmenting' patterns
C
    KBPENL = JTTLIST - 1 - J4 * NIBP / J3
C
C    Copy must-be-enlarged patterns to below 'augmenting' patterns
C
    J1 = LTBMBE - KTBMBE
    KTBMBE = KBPENL - J1
    CALL CPSETS(ISETS, LSETS, KTBMBE, LTBMBE - J1, J1)
    LTBMBE = KTBMBE + J1
C
C    Form 'augmenting' patterns (all combinations of NDIST tests)
C
    K1 = KBPENL
    K4 = LTBP + NDIST
    IF (K4 .GT. KTBMBE) GO TO 180
    K3 = LTBP + 1
    K2 = LTBP
    J1 = JTTLIST - 2
80    K2 = K2 + 1
90    J1 = J1 + 2
    ISETS(K2) = J1
    IF (K2 .LT. K4) GO TO 80
    CALL SETVAL(ISETS(K1 + 1), 0, NIBP)
    DO 100 J1 = K3, K4
        J2 = ISETS(J1)
        ISETS(K1 + ISETS(J2)) = ISETS(K1 + ISETS(J2)) +
*           ISETS(J2 + 1)
100    CONTINUE
    K1 = K1 + NIBP
110    J1 = ISETS(K2)
    IF (LTTLIST - J1 .GT. (K4 - K2 + 1) * 2) GO TO 90
    K2 = K2 - 1
    IF (K2 .GE. K3) GO TO 110
    K2 = KBPENL
    K3 = K1 - 1
    K4 = NIBP
    INTD = 1
    END IF
C
C    Enlarge b.p.'s (and check for absorption)
C
120 IF (NDIST .GT. 1) THEN
    KTBMBE = KTBMBE + 1
    NTD = ISETS(KTBMBE)
    LTBMRG = LTBP
    IF ((NTD .EQ. 0) .AND. (INTD .EQ. 1)) THEN
C
C    Sets initially with 0 new tests may be absorbed by sets that
C    had >0
C
        LTBCAB = LTBP
        INTD = 0
    END IF

```



```

      END IF
      DO 170 K1 = K2, K3, K4
C
C      Check space
C
      IF (LTBP + NIBP .GT. KTBMBE) GO TO 180
      CALL CPSETS(ISETS, LSETS, LTBP, KTBMBE, NIBP)
      IF (NDIST .EQ. 1) THEN
C
C      Add 1 test
C
      ISETS(LTBP + ISETS(K1)) = IOR(ISETS(LTBP + ISETS(K1)),
*      ISETS(K1 + 1))
      IF (K1 .GE. LTIAB) GO TO 160
      ELSE
C
C      Add >1 tests
C
      J2 = 0
      DO 130 J1 = 1, NIBP
      J2 = J2 + ICNT(IAND(ISETS(LTBP + J1), ISETS(K1 + J1)))
      ISETS(LTBP + J1) = IOR(ISETS(LTBP + J1), ISETS(K1 + J1))
130     CONTINUE
C
C      Sets augmented with >NDIST-NTD tests will be absorbed
C
      IF (J2 .LT. NTD) GO TO 170
      END IF
C
C      Check whether absorbed by pass-can-absorb b.p. (b)
C
      DO 150 J2 = KTBCAB, LTBCAB - 1, NIBP
      DO 140 J3 = 1, NIBP
      IF (IAND(ISETS(LTBP + J3), ISETS(J2 + J3)) .NE.
*      ISETS(J2 + J3)) GO TO 150
140     CONTINUE
      GO TO 170
150     CONTINUE
160     IF (NTD .EQ. 0) THEN
      LTBP = LTBP + NIBP
      ELSE
C
C      Check whether contains/contained in b.p. formed from other
C      sets in (c)
C
      CALL IRRMRG(LTBCAB, LTBMRG, LTBP, NIBP, ISETS, LSETS)
      END IF
170 CONTINUE
C
C      Next set to be enlarged
C
      KTBMBE = KTBMBE + NIBP
      IF (KTBMBE - LTBMBE) 120, 10, 10
C
C      Insufficient workspace
C
180 IFAULT = 2
      RETURN
      END
      SUBROUTINE IRRMRG(KBP, LBP, KNBP, NIBP, ISETS, LSETS)
C

```

```
C      ALGORITHM AS 263.4  APPL.STATIST. (1991), VOL.40, NO.1
C
C      Checks new b.p. ISETS(KNBP+1...) vs list in ISETS(KBP+1...LBP):
C      deletes it if it contains any b.p. in the list; otherwise,
C      deletes b.p.'s that contain it, adjusts LBP & sets KNBP to
C      length of the full list
C
      INTEGER KBP, KNBP, LBP, LSETS, NIBP
      INTEGER ISETS(LSETS)
      INTEGER IBPINT, IBPL, IBPN, INCL, J1, K1, K2, K3
      INTEGER IAND
      EXTERNAL IAND
C
      K2 = KBP
      K3 = KBP
      DO 20 K1 = KBP, LBP - 1, NIBP
C
      Check whether new set contains/is contained in set at K1
      (INCL=-/+1)
C
      INCL = 0
      DO 10 J1 = 1, NIBP
        IBPL = ISETS(K1 + J1)
        IBPN = ISETS(KNBP + J1)
        IF (IBPL .EQ. IBPN) GO TO 10
        IBPINT = IAND(IBPL, IBPN)
        IF (IBPINT .EQ. IBPL) THEN
          IF (INCL .GT. 0) GO TO 20
          INCL = -1
        ELSE
          IF ((IBPINT .NE. IBPN) .OR. (INCL .LT. 0)) GO TO 20
          INCL = 1
        END IF
      10 CONTINUE
C
      Return if new set contains/is same as an already stored set
C
      IF (INCL .LE. 0) RETURN
      CALL CPSETS(ISETS, LSETS, K2, K3, K1 - K3)
C
      K2 is length of compacted list
      K2 = K2 + K1 - K3
C
      K3=origin of section to be copied down when next containing
      set found
      K3 = K1 + NIBP
      20 CONTINUE
      IF (K2 .GT. KBP) THEN
C
      Copy final section, intermediate b.p.'s (LBP...KNBP) and
      new b.p.
C
      CALL CPSETS(ISETS, LSETS, K2, K3, KNBP + NIBP - K3)
      LBP = LBP - K3 + K2
      KNBP = K2 + KNBP + NIBP - K3
      ELSE
C
      No contained/containing sets found
C
      KNBP = KNBP + NIBP
      END IF
```

```
      RETURN
      END
      LOGICAL FUNCTION IRRWSP(KWSP, KUSED, LUSED, LWSP, ISETS, LSETS)
C
C      ALGORITHM AS 263.5  APPL.STATIST. (1991), VOL.40, NO.1
C
C      Reorganises workspace to give room before and after
C      KUSED...LUSED; returns value .TRUE. if insufficient space
C
      INTEGER KUSED, KWSP, LSETS, LUSED, LWSP
      INTEGER ISETS(LSETS)
      INTEGER NUSED
C
      NUSED = LUSED - KUSED
      KUSED = KWSP + (KUSED - KWSP + LWSP - LUSED) / 2
      CALL CPSETS(ISETS, LSETS, KUSED, LUSED - NUSED, NUSED)
      LUSED = KUSED + NUSED
      IRRWSP = (KUSED .LE. KWSP) .OR. (LUSED .GE. LWSP)
      RETURN
      END
      SUBROUTINE CPSETS(IVAL, LVAL, KTO, KFROM, NVAL)
C
C      ALGORITHM AS 263.6  APPL.STATIST. (1991), VOL.40, NO.1
C
C      Copies IVAL(KFROM+1...+NVAL) to IVAL(KTO+1...)
C
      INTEGER KFROM, KTO, LVAL, NVAL
      INTEGER IVAL(LVAL)
      INTEGER FROMTO, INC, ITO, JTO, LTO
C
C      Check whether new location above, same as, or below old
C
      FROMTO = KFROM - KTO
      IF (FROMTO) 10, 50, 20
C
C      Values may overlap, copy in reverse order
C
10  INC = -1
      JTO = KTO + NVAL
      LTO = KTO + 1
      GO TO 30
C
C      Set/copy values from origin upwards
C
20  INC = 1
      JTO = KTO + 1
      LTO = KTO + NVAL
C
C      Copy values
C
30  DO 40 ITO = JTO, LTO, INC
          IVAL(ITO) = IVAL(ITO + FROMTO)
40  CONTINUE
50  RETURN
      END
      SUBROUTINE SETVAL(IVAL, ICON, NVAL)
C
C      ALGORITHM AS 263.7  APPL.STATIST. (1991), VOL.40, NO.1
C
C      Sets IVAL(1...NVAL) to ICON
C
```

```
INTEGER ICON, NVAL
INTEGER IVAL(NVAL)
INTEGER I
DO 10 I = 1, NVAL
    IVAL(I) = ICON
10 CONTINUE
RETURN
END
```

```

SUBROUTINE PRINBP(NBI, NFACT, NBP, NPRINT, IBPS, LIBPS, IOUT,
*
          IFAULT)
C
C   ALGORITHM AS 264  APPL.STATIST. (1991), VOL.40, NO.1
C
C   Prints bit patterns on unit IOUT
C
C   INTEGER IOUT, IFAULT, LIBPS, NBI, NPRINT, NBP, NFACT
C   INTEGER IBPS(LIBPS)
C   INTEGER JP2IT1, JTTLIST, J1, J2, J3, J4, J5, KPOWR2, K1, K2, K3,
*       K4, K5, LTLIST, N, NB0, NIBP, NMIN, NMAX, NSETP
C   INTEGER IAND, ICNT
C   EXTERNAL IAND, ICNT
C
C   IF ((NFACT .LE. 0) .OR. (NBP .LE. 0)) GO TO 160
C
C   Calculate number of integers to store each bit pattern
C
C   NIBP = (NFACT - 1) / NBI + 1
C
C   Set up powers of 2 (2**0,1,2...) in IBPS(KPOWR2...LIBPS)
C
C   KPOWR2 = LIBPS - NBI + 1
C   IBPS(KPOWR2) = 1
C   DO 10 J1 = KPOWR2 + 1, LIBPS
C       IBPS(J1) = IBPS(J1 - 1) * 2
10 CONTINUE
C
C   Address of the power of 2 used to represent the first item
C
C   JP2IT1 = KPOWR2 + NFACT - NBI * (NIBP - 1) - 1
C   LTLIST = KPOWR2 - 1
C   IF (NBP + NBP / NIBP .GE. LTLIST) GO TO 150
C   NSETP = 0
C   NMIN = NFACT
C   NMAX = 1
C
C   Store number of factors in each set in IBPS(NBP+1...K1)
C
C   K1 = NBP
C   DO 30 K3 = 1, NBP, NIBP
C       J2 = 0
C       DO 20 J1 = K3, K3 + NIBP - 1
C           J2 = J2 + ICNT(IBPS(J1))
20 CONTINUE
C       NMIN = MIN(NMIN, J2)
C       NMAX = MAX(NMAX, J2)
C       K1 = K1 + 1
C       IBPS(K1) = J2
30 CONTINUE
C   IF (NPRINT .LT. 0) NMAX = MIN(NMAX, NMIN - NPRINT - 1)
C   IF (NPRINT .GT. 0) NMAX = MIN(NMAX, NPRINT)
C
C   DO 140 N = NMIN, NMAX
C       JTTLIST = LTLIST - N + 1
C
C   Store addresses of sets with N factors in IBPS(K1+1...K2)
C
C   K2 = K1
C   J1 = NBP
C   DO 90 K3 = 1, NBP, NIBP

```

```

        J1 = J1 + 1
        IF (IBPS(J1) .NE. N) GO TO 90
C
C      Place address of set into list, according to
C      lexicographic order
C
        DO 70 J2 = K1 + 1, K2
          J3 = IBPS(J2)
          DO 60 J4 = K3, K3 + NIBP - 1
            J3 = J3 + 1
            IF (IBPS(J3) - IBPS(J4)) 40, 60, 70
C
C      Move other sets up and insert current set
C
40          DO 50 J5 = K2, J2, -1
            IBPS(J5 + 1) = IBPS(J5)
50          CONTINUE
            IBPS(J2) = K3 - 1
            GO TO 80
60          CONTINUE
70          CONTINUE
C
C      Insert set at end of list
C
        IBPS(K2 + 1) = K3 - 1
80          K2 = K2 + 1
          IF (K2 .GE. JTTLIST) GO TO 150
90          CONTINUE
C
C      Decode each bit pattern, store factors in
C      IBPS(JTTLIST...LTLIST), then print
C
        DO 130 J2 = K1 + 1, K2
          K3 = 0
          K4 = JTTLIST
          K5 = JP2IT1
          DO 110 J3 = IBPS(J2) + 1, IBPS(J2) + NIBP
            J4 = IBPS(J3)
            DO 100 J5 = K5, KPOWR2, -1
              K3 = K3 + 1
              IF (IAND(IBPS(J5), J4) .EQ. 0) GO TO 100
              IBPS(K4) = K3
              IF (K4 .EQ. LTLIST) GO TO 120
              K4 = K4 + 1
100          CONTINUE
            K5 = LIBPS
110          CONTINUE
C
C      Print contents of bit pattern (now stored
C      in IBPS(JTTLIST...LTLIST))
C
120          NSETP = NSETP + 1
C
C ***** Lines below can be modified to change the style of output *****
C
          WRITE (IOUT, 9000) NSETP, N, (IBPS(J3), J3=JTTLIST, LTLIST)
9000          FORMAT(1X, I6, ' '), I5, ' FACTOR(S): ', 20I4 / (27X, 20I4))
130          CONTINUE
140          CONTINUE
          RETURN
C

```

```
150 IFAULT = IFAULT + 1
160 IFAULT = IFAULT + 1
    RETURN
    END
```

```

SUBROUTINE GG1WT(WAIT, DUMM, N, H, CTRL, IFAULT)
C
C     ALGORITHM AS 265.1  APPL.STATIST. (1991), VOL.40, NO.2
C
C     Obtains the distribution of the stationary waiting time for
C     a G/G/1 queue on using the fast Fourier transform algorithm
C
C     Auxiliary routines required: FORRT and REVRT from AS 97.
C
C     INTEGER N, IFAULT
C     REAL WAIT(N), DUMM(N), H, CTRL(3)
C     INTEGER I, J, M, MM
C     REAL AN, CA, FOUR, HALF, ONE, PI, Q, SA, TINY, TSI, TSR, TWI,
*     TWO, TWR, XI, XR, XOLD, XNEW, YR, YI, Z, ZERO
C     REAL ARRIVE, SERVE
C     EXTERNAL ARRIVE, SERVE
C     DATA ZERO, HALF, ONE, TWO, FOUR / 0.0, 0.5, 1.0, 2.0, 4.0 /
C     DATA TINY / 1.0E-6 /
C
C     PI = FOUR * ATAN(ONE)
C     M = N / 2
C     MM = M + 1
C
C     Check admissibility of H and N
C
C     IFAULT = 1
C     IF (H .LE. ZERO) RETURN
C     IFAULT = 2
C     J = 4
C     DO 10 I = 2, 20
C         IF (J .EQ. N) GO TO 20
C         J = J * 2
10 CONTINUE
C     RETURN
C
C     Find tail transforms of interarrival
C     and service time distributions
C
20 IFAULT = 3
C     XOLD = ONE
C     DO 30 I = 1, M
C         DUMM(I) = ZERO
C         XNEW = ARRIVE((REAL(I) - HALF) * H)
C         IF ((XNEW .LT. ZERO) .OR. (XNEW .GT. XOLD)) RETURN
C         XOLD = XNEW
C         WAIT(I) = XNEW
30 CONTINUE
C     IFAULT = 4
C     XOLD = ZERO
C     DO 40 I = MM, N
C         WAIT(I) = ZERO
C         XNEW = SERVE((REAL(N - I) + HALF) * H)
C         IF ((XNEW .GT. ONE) .OR. (XNEW .LT. XOLD)) RETURN
C         XOLD = XNEW
C         DUMM(I) = -XNEW
40 CONTINUE
C     CTRL(1) = WAIT(M)
C     CTRL(2) = -DUMM(M + 1)
C     CALL TRANSF(WAIT, N)
C     CALL TRANSF(DUMM, N)
C

```



```
C      Find transform of normalized harmonic
C      renewal sequence and invert
C
      IFAULT = 5
      Z = WAIT(1) + DUMM(1)
      IF (Z .LE. ZERO) RETURN
      WAIT(1) = -LOG(Z)
      Z = WAIT(MM) + DUMM(MM) - TWO * WAIT(MM) * DUMM(MM)
      IF (Z .LE. ZERO) RETURN
      WAIT(MM) = -LOG(Z)
      DO 50 I = 2, M
        AN = PI * (REAL(I) - ONE) / REAL(M)
        SA = SIN(AN)
        CA = COS(AN)
        TSR = DUMM(I)
        TSI = DUMM(I + M)
        TWR = WAIT(I)
        TWI = WAIT(I + M)
        XR = ONE + (CA - ONE) * TSR - SA * TSI
        XI = (CA - ONE) * TSI + SA * TSR
        YR = TSR + XR * TWR - XI * TWI
        YI = TSI + XR * TWI + XI * TWR
        Z = YR * YR + YI * YI
        IF (Z .LE. TINY) RETURN
        Z = HALF * LOG(Z)
        AN = ATAN2(YI, YR)
        WAIT(I) = -Z
        WAIT(I + M) = -AN
50 CONTINUE
      CALL REVERT(WAIT, N)
C
C      Change appropriate elements to zero and transform
C
      DO 60 I = 2, M
        WAIT(I) = ZERO
60 CONTINUE
      CTRL(3) = ABS(WAIT(MM)) + ABS(WAIT(MM + 1)) + ABS(WAIT(MM + 5))
      CALL TRANSF(WAIT, N)
C
C      Find transform of first descending ladder height
C
      WAIT(1) = ONE - EXP(-WAIT(1))
      WAIT(MM) = ONE - EXP(-WAIT(MM))
      DO 70 I = 2, M
        TWR = WAIT(I)
        TWI = WAIT(I + M)
        WAIT(I) = ONE - EXP(-TWR) * COS(TWI)
        WAIT(I + M) = EXP(-TWR) * SIN(TWI)
70 CONTINUE
C
C      Find transform of associated random walk minimum
C
      Q = ONE - WAIT(1)
      WAIT(1) = ONE
      WAIT(MM) = Q / (ONE - WAIT(MM))
      DO 80 I = 2, M
        TWR = ONE - WAIT(I)
        TWI = WAIT(I + M)
        Z = Q / (TWR * TWR + TWI * TWI)
        WAIT(I) = Z * TWR
        WAIT(I + M) = Z * TWI
```

```
80 CONTINUE
C
C      Invert and shift
C
      CALL REVERT(WAIT, N)
      DO 90 I = 2, M
          WAIT(I) = WAIT(N - I + 2)
90 CONTINUE
      DO 100 I = MM + 1, N
          WAIT(I) = ZERO
100 CONTINUE
      IFAULT = 0
      RETURN
      END

      SUBROUTINE TRANSF(X, N)
C
C      ALGORITHM AS 265.2  APPL.STATIST. (1991), VOL.40, NO.2
C
C      Adapts transform to definition used in algorithm AS 97
C
      INTEGER N
      REAL X(N)
      INTEGER I, MM
      REAL Z
C
      Z = REAL(N)
      MM = N / 2 + 1
      DO 10 I = 1, N
          X(I) = Z * X(I)
10 CONTINUE
      CALL FORRT(X, N)
      DO 20 I = MM + 1, N
          X(I) = -X(I)
20 CONTINUE
      RETURN
      END

      SUBROUTINE REVERT(X, N)
C
C      ALGORITHM AS 265.3  APPL.STATIST. (1991), VOL.40, NO.2
C
C      Adapts transform to definition used in algorithm AS 97
C
      INTEGER N
      REAL X(N)
      INTEGER I, MM
      REAL ONE, Z
      DATA ONE / 1.0 /
C
      Z = ONE / REAL(N)
      MM = N / 2 + 1
      DO 10 I = MM + 1, N
          X(I) = -X(I)
10 CONTINUE
      CALL REVRT(X, N)
      DO 20 I = 1, N
          X(I) = Z * X(I)
20 CONTINUE
      RETURN
      END
```



```

      SUBROUTINE DIRICH(K, N, X, IX, INIT, ALPHA, RLOGL, V, G, NITER, S,
*          EPS, WORK, IFAULT)
C
C      ALGORITHM AS 266  APPL.STATIST. (1991), VOL.40, NO.2
C
C      Auxiliary routines required: ALOGAM (CACM algorithm 291 or AS 245),
C      DIGAMA (AS 103), GAMMAD (AS 239), PPCHI2 (AS 91), TRIGAM (AS 121).
C
      INTEGER K, N, IX, INIT, NITER, IFAULT
      REAL X(IX, K), ALPHA(K), RLOGL, V(K * (K + 1) / 2), G(K), S, EPS,
*      WORK(2 * K)
      INTEGER I, J, IF1, KK, I2, ITN, MAXIT
      REAL ALOGAM, AN, BETA, CHI2, DIGAMA, GAMMA, GAMMAD, GG, ONE,
*      PPCHI2, RK, SUM, SUM1, TEMP, TRIGAM, TWO, VARP1, X11, X12,
*      ZERO
      PARAMETER (GAMMA=0.0001, ZERO=0.0, ONE=1.0, TWO=2.0, MAXIT=100)
      INTRINSIC ABS, LOG, MIN, REAL
      EXTERNAL ALOGAM, DIGAMA, GAMMAD, PPCHI2, TRIGAM
C
C      Check input arguments
C
      AN = REAL(N)
      RK = REAL(K)
      IF (K .LT. 2) THEN
        IFAULT = 1
        RETURN
      ELSE IF (N .LE. K) THEN
        IFAULT = 2
        RETURN
      ELSE IF (IX .LT. N) THEN
        IFAULT = 3
        RETURN
      END IF
C
      IFAULT = 4
      DO 20 I = 1, N
        SUM = ZERO
        NITER = I
        DO 10 J = 1, K
          IF (X(I, J) .LE. ZERO) RETURN
          SUM = SUM + X(I, J)
10      CONTINUE
        IF (ABS(SUM - ONE) .GE. GAMMA) RETURN
20    CONTINUE
      IFAULT = 0
C
      IF (INIT .EQ. 1) THEN
C
C      Calculate initial estimates using the method of moments
C
        SUM = ZERO
        DO 40 J = 1, K - 1
          X12 = ZERO
          DO 30 I = 1, N
            X12 = X12 + X(I, J)
30      CONTINUE
          ALPHA(J) = X12 / AN
          SUM = SUM + ALPHA(J)
40      CONTINUE
C
        X12 = ZERO

```

```
        DO 50 I = 1, N
          X12 = X12 + X(I, 1) ** 2
50      CONTINUE
C
        ALPHA(K) = ONE - SUM
        X12 = X12 / AN
        VARP1 = X12 - ALPHA(1) ** 2
C
        X11 = (ALPHA(1) - X12) / VARP1
        DO 60 J = 1, K
          ALPHA(J) = X11 * ALPHA(J)
60      CONTINUE
C
        END IF
C
        IF (INIT .EQ. 2) THEN
C
          Calculate initial estimates using Ronning's suggestion
C
          SUM = X(1, 1)
          DO 80 J = 1, K
            DO 70 I = 1, N
              SUM = MIN(SUM, X(I, J))
70          CONTINUE
80          CONTINUE
          DO 90 J = 1, K
            ALPHA(J) = SUM
90          CONTINUE
C
          END IF
C
          Check whether any ALPHAs are negative or zero
C
          NITER = 0
          DO 100 J = 1, K
            IF (ALPHA(J) .LE. ZERO) THEN
              IFAULT = 6
              RETURN
            END IF
100        CONTINUE
C
          Calculate n * log(G(j)) for j = 1,2,...,k and store in WORK array
C
          DO 120 J = 1, K
            SUM = ZERO
            DO 110 I = 1, N
              SUM = SUM + LOG(X(I, J))
110          CONTINUE
            WORK(J) = SUM
120        CONTINUE
C
          Note that ALOGAM cannot fail
C
          GG = ALOGAM(RK / TWO, IFAULT)
C
          Call Algorithm AS 91 to compute chi-squared value
C
          CHI2 = PPCHI2(GAMMA, RK, GG, IFAULT)
          IF (IFAULT .GT. 0) THEN
            IFAULT = 5
            RETURN
```

```

      END IF
C
      DO 220 ITN = 1, MAXIT
C
          SUM = ZERO
          DO 130 J = 1, K
              SUM = SUM + ALPHA(J)
130          CONTINUE
C
          Note that TRIGAM and DIGAMA cannot fail if the first argument
          is positive
C
          BETA = TRIGAM(SUM, IFAULT)
          TEMP = DIGAMA(SUM, IFAULT)
          SUM1 = ZERO
          DO 140 J = 1, K
              WORK(K + J) = TRIGAM(ALPHA(J), IFAULT)
              SUM1 = SUM1 + ONE / WORK(K + J)
              G(J) = AN * (TEMP - DIGAMA(ALPHA(J), IFAULT)) + WORK(J)
140          CONTINUE
          BETA = AN * BETA / (ONE - BETA * SUM1)
C
          Calculate the lower triangle of the Variance-Covariance matrix
          (V)
C
          SUM = BETA / (AN * AN)
          DO 160 I = 1, K
              DO 150 J = 1, I
                  KK = I * (I - 1) / 2 + J
                  V(KK) = SUM / (WORK(K + I) * WORK(K + J))
                  IF (I .EQ. J) V(KK) = V(KK) + ONE / (AN * WORK(K + J))
150          CONTINUE
160          CONTINUE
C
          Postmultiply the Variance-Covariance matrix (V) by G and store
          in the last k elements of WORK
C
          DO 190 I = 1, K
              SUM = ZERO
              I2 = I * (I - 1) / 2
              DO 170 J = 1, I - 1
                  SUM = SUM + V(I2 + J) * G(J)
170          CONTINUE
              DO 180 J = I + 1, K
                  SUM = SUM + V(J * (J - 1) / 2 + I) * G(J)
180          CONTINUE
              WORK(K + I) = SUM + V(I * (I + 1) / 2) * G(I)
190          CONTINUE
C
          Update the ALPHAs
C
          NITER = ITN
          DO 200 J = 1, K
              ALPHA(J) = ALPHA(J) + WORK(K + J)
              IF (ALPHA(J) .LE. ZERO) THEN
                  IFAULT = 6
                  RETURN
              END IF
200          CONTINUE
C
          Test for convergence

```

```
C
      S = ZERO
      DO 210 J = 1, K
        S = S + G(J) * WORK(K + J)
210   CONTINUE
C
      IF (S .LT. CHI2) GO TO 230
C
220  CONTINUE
C
      IFAULT = 7
C
      Note that GAMMAD cannot fail
C
230  EPS = GAMMAD(S / TWO, RK / TWO, IF1)
      RLOGL = ZERO
      SUM = ZERO
      DO 240 J = 1, K
        SUM = SUM + ALPHA(J)
        RLOGL = RLOGL + (ALPHA(J) - ONE) * WORK(J) -
*          AN * ALOGAM(ALPHA(J), IF1)
240  CONTINUE
      RLOGL = RLOGL + AN * ALOGAM(SUM, IF1)
C
      END
```

```

      REAL FUNCTION DPROB(DIFF, NDF, NPOPS, MBEST, IFAULT)
C
C      ALGORITHM AS 267.1  APPL.STATIST. (1991), VOL.40, NO.3
C
C      Calculates the lower bound for the probability of correct
C      selection of a subset containing the best populations within
C      the set of NPOPS populations.
C
C      Auxiliary routines required: ALNORM (AS 66) and ALOGAM (CACM
C      algorithm 291 or AS 245).
C
      INTEGER IFAULT, MBEST, NDF, NPOPS
      REAL DIFF
C
      INTEGER I, J, K, JMAX, JMIN, KMAX, KMIN, L, MAXDF
      REAL DFW(2, 10), QW(2, 10), BEST, CLOG, CUTJ, CUTK, DF, DF2,
*      EHJ, GK, GSTEP, HALF, HJ, HSTEP, ONE, PJ, PK, PROB, PZ1, PZ2,
*      Q, R1, R2, W0, W2, ZERO
      REAL ALNORM, ALOGAM
      EXTERNAL ALNORM, ALOGAM
C
      DATA CUTK, CUTJ, GSTEP / 0.00003, 0.00001, 0.70 /
      DATA ZERO, HALF, ONE / 0.0, 0.5, 1.0 /
      DATA JMAX, JMIN, KMAX, KMIN, MAXDF / 10, 3, 15, 7, 120 /
C
      Check input arguments
C
10  PROB = ZERO
      IFAULT = 0
      IF (DIFF .LE. 0.0) IFAULT = 1
      IF (NDF .LE. 3) IFAULT = 20 + IFAULT
      IF (NPOPS .LT. 2 .OR. NPOPS .GT. 100) IFAULT = 300 + IFAULT
      IF (MBEST .LT. 1 .OR. MBEST .GE. NPOPS) IFAULT = 4000 + IFAULT
      IF (IFAULT .NE. 0) GO TO 100
C
      Transfer arguments and calculate constants.
C
20  Q = DIFF
      DF = NDF
      BEST = MBEST
      R1 = NPOPS - MBEST
      R2 = MBEST - 1
      CLOG = LOG(BEST * GSTEP) - 0.918938533
C
      IF (NDF .LE. MAXDF) THEN
          DF2 = DF * HALF
          HSTEP = GSTEP * DF ** (-HALF)
          HJ = ZERO
          CLOG = CLOG + LOG(HSTEP) - ALOGAM(DF2, IFAULT) -
*          DF2 * (ONE - LOG(DF)) + (ONE - DF2) * 0.693147181
          DO 30 J = 1, JMAX
              HJ = HJ + HSTEP
              EHJ = EXP(HJ)
              QW(1, J) = Q * EHJ
              QW(2, J) = Q / EHJ
              DFW(1, J) = DF * (HALF + HJ - HALF * EHJ * EHJ)
              DFW(2, J) = DF * (HALF - HJ - HALF / EHJ / EHJ)
          30  CONTINUE
      END IF
C
      Compute integral

```



```

C
40 DO 90 K = 1, KMAX
   PK = ZERO
   DO 80 L = 1, 2
     IF (L .EQ. 1) THEN
       GK = GSTEP * REAL(K)
     ELSE
       GK = -GSTEP * REAL(K - 1)
     END IF
     W0 = CLOG - GK * GK * HALF
     W2 = ZERO
     PZ1 = ALNORM(-GK - Q, .TRUE.)
     PZ2 = ONE
     IF (MBEST .GT. 1) THEN
       PZ2 = ALNORM(GK, .TRUE.)
       IF (PZ2 .GT. ZERO) W2 = R2 * LOG(PZ2)
     END IF
     IF (PZ1 .GT. ZERO .AND. PZ2 .GT. ZERO) PK = PK +
*       EXP(W0 + R1 * LOG(PZ1) + W2)
     IF (NDF .LE. MAXDF .AND. PZ2 .GT. ZERO) THEN
50       DO 70 J = 1, JMAX
         PJ = ZERO
         DO 60 I = 1, 2
           PZ1 = ALNORM(-GK - QW(I, J), .TRUE.)
           IF (PZ1 .GT. ZERO) PJ = PJ +
*             EXP(W0 + DFW(I, J) +
*             R1 * LOG(PZ1) + W2)
60         CONTINUE
         PK = PK + PJ
         IF ((J .GT. JMIN .OR. K .GT. KMIN) .AND.
*           PJ .LT. CUTJ) GO TO 80
70       CONTINUE
     END IF
80     CONTINUE
     PROB = PROB + PK
     IF (PROB .GT. ONE) THEN
       PROB = ONE
       GO TO 100
     END IF
     IF (K .GT. KMIN .AND. PK .LT. CUTK) GO TO 100
90 CONTINUE
100 DPROB = PROB
    RETURN
    END

```

```

REAL FUNCTION DVALU(PROB, NDF, NPOPS, MBEST, IFAULT)

```

```

C
C   ALGORITHM AS 267.2  APPL.STATIST. (1991), VOL.40, NO.3
C
C   Given a probability PROB, function DVALU calculates the
C   standardized difference required between the MBEST population
C   means and the remaining means when applying ranking and
C   selection procedures to NPOPS populations.
C
C

```

```

INTEGER IFAULT, MBEST, NDF, NPOPS
REAL PROB
INTEGER J, JMAX
REAL A, BEST, DF, DCUT, E1, E2, EDIF, ONE, P1, P2, PCUT1, PCUT2,
*   POPS, Q1, Q2, TWO, ZERO
REAL DPROB, DVALU0
EXTERNAL DPROB, DVALU0

```

```

C
  DATA JMAX, ZERO, ONE, TWO, DCUT, PCUT1, PCUT2 / 8, 0.0, 1.0, 2.0,
*    0.00001, 0.00015, 0.001 /
C
C    Check input arguments.
C
DVALU = ZERO
IFAUULT = 0
IF (PROB .LT. 0.80 .OR. PROB .GT. 0.995) IFAULT = 5
IF (NDF .LE. 3) IFAULT = 20 + IFAULT
IF (NPOPS .LT. 2 .OR. NPOPS .GT. 100) IFAULT = 300 + IFAULT
IF (MBEST .LT. 1 .OR. MBEST .GE. NPOPS) IFAULT = 4000 + IFAULT
IF (IFAUULT .NE. 0) GO TO 20
C
C    Obtain initial values.
C
DF = NDF
POPS = NPOPS
BEST = MBEST
Q2 = DVALU0(PROB, DF, POPS, BEST)
P2 = DPROB(Q2, NDF, NPOPS, MBEST, IFAULT)
E2 = P2 - PROB
A = (ONE - PROB) / (ONE - P2)
IF (E2 .GT. ZERO) A = PROB / P2
P1 = PROB - E2 * A
Q1 = DVALU0(P1, DF, POPS, BEST)
E1 = DPROB(Q1, NDF, NPOPS, MBEST, IFAULT) - PROB
DVALU = Q1
C
C    Refine and test approximation.
C
DO 10 J = 1, JMAX
  IF (ABS(E1) .LT. PCUT1) GO TO 20
  EDIF = E2 - E1
  IF (ABS(EDIF) .LT. DCUT) THEN
    DVALU = (Q1 + Q2) / TWO
    IFAULT = 6
    GO TO 20
  END IF
  DVALU = (Q1 * E2 - Q2 * E1) / EDIF
  IF (ABS(E1) .LT. PCUT2) GO TO 20
  Q2 = Q1
  E2 = E1
  Q1 = DVALU
  E1 = DPROB(Q1, NDF, NPOPS, MBEST, IFAULT) - PROB
10 CONTINUE
  IFAULT = 6
20 RETURN
END
REAL FUNCTION DVALU0(PROB, DF, POPS, BEST)
C
C    ALGORITHM AS 267.3 APPL.STATIST. (1991), VOL.40, NO.3
C
C    Calculates an initial value for the standardized difference.
C
REAL ALBEST, ALPOPS, BEST, DF, DFMAX, PROB, POPS, T
REAL GAUINV
EXTERNAL GAUINV
DATA DFMAX / 120.0 /
C
  T = GAUINV(PROB)

```

```
IF (DF .LT. DFMAX) T = T + (T * T * T + T) / DF / 4.0
ALBEST = LOG(AMIN1(BEST, POPS - BEST))
ALPOPS = LOG(POPS)
DVALU0 = (-0.5185 + 0.7927 / DF + (0.09494 - 0.1824 / DF) * T) * T
DVALU0 = DVALU0 + 1.193 - 0.05360 * ALPOPS - 0.08017 * ALBEST
DVALU0 = (1.0 + DVALU0 * ALPOPS * LOG(BEST + 1.7183)) * T
RETURN
END
```

```
      SUBROUTINE ALLRQR(R, NR, N, W1, NW1, W2, IW1, NW2, W3, NW3, W4,
*          IW2, NW4, IW3, NW5, IORD, IFIN, OUTR, IFAULT)
C
C      ALGORITHM AS 268.1  APPL.STATIST. (1991), VOL.40, NO.3
C
C      Calculates statistics for all possible subset regressions using
C      the R* matrix from a QR decomposition of (X|Y)
C
C      Auxiliary routine required: AS 164 must be called first to form
C      the orthogonal reduction.
C
      INTEGER NR, N, NW1, NW2, IW1(NW2), NW3, IW2(NW4), NW4,
*          IW3(NW5, 2), NW5, IORD, IFIN, IFAULT
      REAL R(NR), W1(NW1), W2(NW2, 2), W3(NW3), W4(NW4, 3)
      INTEGER I, J, J1, J2, J3, K, L, N1, N2, N3, N4, NB, NC, NF, NI,
*          NL, NS1, NS2, NS3
      REAL TSS, GC, GS, E1, E2, E3, E4, E5, ONE
      EXTERNAL OUTR
      DATA ONE / 1.E+0 /
C
      IFAULT = 0
C
      Checks on input arguments
C
      I = N * (N + 1) / 2
      IF (I.NE. NR) THEN
          IFAULT = 1
          RETURN
      END IF
      N1 = N - 1
      IF (N1.LT. 2) THEN
          IFAULT = 2
          RETURN
      END IF
      N2 = I - N
      IF (N2.GT. NW3) THEN
          IFAULT = 3
          RETURN
      END IF
      IF (N1.GT. NW4) THEN
          IFAULT = 4
          RETURN
      END IF
      IF (N.LT. 5) THEN
          J1 = 1
          J2 = 1
          J3 = 1
      ELSE
          J1 = N - 4
          J2 = J1 * (3 + NR / 3)
          J3 = I - 2 * (N + 1)
      END IF
      IF (J1.GT. NW5) THEN
          IFAULT = 5
          RETURN
      END IF
      IF (J2.GT. NW1) THEN
          IFAULT = 6
          RETURN
      END IF
      IF (J3.GT. NW2) THEN
```

```

        IFAULT = 7
        RETURN
    END IF
    IF ( IORD .LT. 1 .OR. IORD .GT. 2 ) THEN
        IFAULT = 8
        RETURN
    END IF
    IF ( IFIN .LT. 1 .OR. IFIN .GT. (N1 - 1) ) THEN
        IFAULT = 9
        RETURN
    END IF
C
C      Calculate RSS's & TSS from original R* matrix
C
    DO 10 I = 1, N1
        IW2(I) = I
    10 CONTINUE
C*****
    TSS = ONE/R(NR) * 1A *
C*****
    CALL OUTR(IW2, TSS, R, N2, R(N2 + 1), N1)
    J = N2
    DO 20 I = N1, 1, -1
C*****
        W4(I, 3) = R(N2 + I) * R(N2 + I) / R(J) * 2A *
C*****
        TSS = TSS + W4(I, 3)
        J = J - I
        IF ( I .GE. IFIN .AND. I .GT. 1 ) THEN
            CALL OUTR(IW2, TSS, R, J, R(N2 + 1), (I - 1))
        END IF
    20 CONTINUE
    DO 30 I = 2, N1
        W4(I, 3) = W4(I, 3) + W4(I - 1, 3)
    30 CONTINUE
C
C      Proceed dropping each column in turn
C
    IF ( IORD .EQ. 1 ) THEN
        NB = 1
        NI = 1
        NF = N1 - IFIN
        NL = 0
    ELSE
        NB = N1 - IFIN
        NI = -1
        NF = 1
    END IF
    40 NC = NB
    IF ( IORD .EQ. 2 ) THEN
        NL = NC
    END IF
C
C      Initialise temporary storage markers
C
    NS1 = 0
    NS2 = 0
    NS3 = 0
C
C      Start with original matrix.
C

```

```

DO 50 I = 1, N2
  W3(I) = R(I)
50 CONTINUE
DO 60 I = 1, N1
  W4(I, 1) = R(N2 + I)
  W4(I, 2) = W4(I, 3)
  IW2(I) = I
60 CONTINUE
C
C   Calculate givens rotation factors, perform rotations & fill
C   in elements of work matrix dropping the appropriate column.
C
  N4 = N - NC
70 N3 = (N4 - 1) * (N4 - 2) / 2
80 K = N3
  DO 110 L = 1, NC
    J = N4 + L - 2
    K = K + J
    J1 = N4 - NI * NC - NL - 2
C
C   Shift unchanged elements of R matrix
C
    IF (J1 .GE. 1) THEN
      J2 = K - J
      DO 90 I = 1, J1
        W3(J2 + I) = W3(K + I)
90    CONTINUE
      END IF
C
C   Calculate first diagonal element
C
    J2 = K + J
    GC = W3(K)
    GS = W3(J2 + 1)
    IF (L .EQ. 1) THEN
      E1 = W3(J2)
C*****
      E5 = E1 * E1 * GS + GC * 3A *
C*****
      ELSE
C*****
      E5 = GS + GC * 4A *
C*****
      END IF
C*****
      W3(K) = GC * GS / E5 * *
      GC = GC / E5 * 5A *
      GS = GS / E5 * *
C*****
      IF (L .EQ. 1) THEN
C*****
      GS = E1 * GS * 6A *
C*****
      END IF
C
C   Calculate second diagonal element & first off diagonal element
C
    IF (L .LT. NC) THEN
      J1 = J2 + J + 1
      E3 = W3(J1 + 1)
      IF (L .EQ. 1) THEN

```

```

      E2 = W3(J1)
      E4 = -E2 + E1 * E3
    ELSE
      E2 = W3(J2)
      E4 = -E2 + E3
    END IF
C*****
      W3(J2) = E2 * GS + E3 * GC * 7A *
      W3(J2 + 1) = E5 / (E4 * E4) * *
C*****
    END IF
C
C   Calculate elements of rest of R matrix
C
    IF (L .LT. (NC - 1)) THEN
      J2 = K + 2 * J + 1
      DO 100 I = 1, NC - L - 1
        J1 = J2 + J + I + 1
        E3 = W3(J1 + 1)
        IF (L .EQ. 1) THEN
          E2 = W3(J1)
          W3(J2 + 1) = (-E2 + E1 * E3) / E4
        ELSE
          E2 = W3(J2)
          W3(J2 + 1) = (-E2 + E3) / E4
        END IF
C*****
        W3(J2) = E2 * GS + E3 * GC * 8A *
C*****
        J2 = J1
      100 CONTINUE
    END IF
C
C   Apply rotation to vector of C's
C
    E2 = W4(J, 1)
    E3 = W4(J + 1, 1)
    IF (L .LT. NC) THEN
      IF (L .EQ. 1) THEN
        W4(J + 1, 1) = (-E2 + E1 * E3) / E4
      ELSE
        W4(J + 1, 1) = (-E2 + E3) / E4
      END IF
    END IF
C*****
    W4(J, 1) = E2 * GS + E3 * GC * 9A *
    W4(J, 2) = W4(J, 1) * W4(J, 1) / W3(K) * *
C*****
    IF (J .GT. 1) W4(J, 2) = W4(J, 2) + W4(J - 1, 2)
  110 CONTINUE
C
C   Remove deleted variable from list of variables in model
C
    DO 120 L = N4 - 1, J
      IW2(L) = IW2(L + 1)
    120 CONTINUE
C
C   Print RSS's etc.
C
C*****
    CALL OUTR(IW2, (TSS - W4(J, 2)), W3, K, W4(1, 1), J) * 1B *

```

```

C*****
      IF (NC .GT. 1) THEN
C*****
C
C
C*****
      J2 = K
      J1 = J + 1
      DO 130 L = 1, NC - 1
        I = J - L
        J2 = J2 - J1 + L
C*****
      CALL OUTR(IW2, (TSS - W4(I, 2)), W3, J2, W4(1, 1), I)      * 2B *
C*****
130    CONTINUE
      END IF

C
C      Storing required R matrices in temporary storage
C
      IF (NC .LE. 2) GO TO 160
      DO 140 J1 = 1, K
        NS1 = NS1 + 1
        W1(NS1) = W3(J1)
140    CONTINUE
      DO 150 J1 = 1, J
        NS2 = NS2 + 1
        W2(NS2, 1) = W4(J1, 1)
        W2(NS2, 2) = W4(J1, 2)
        IW1(NS2) = IW2(J1)
150    CONTINUE
      NS3 = NS3 + 1
      IF (IORD .EQ. 1) THEN
        IW3(NS3, 1) = 2
        N4 = N1 - NS3
        IW3(NS3, 2) = NC
        NC = 2
      ELSE
        IW3(NS3, 1) = NC - 2
        IW3(NS3, 2) = 1
      END IF
160    NC = NC - 1
      IF (IORD .EQ. 1 .AND. NC .EQ. 1) THEN
        GO TO 70
      END IF
      IF (IORD .EQ. 2 .AND. NC .NE. 0) THEN
        GO TO 80
      END IF

C
C      Working through R matrices in temporary storage
C
170    IF (NS3 .EQ. 0) GO TO 200
      J = N1 - NS3
      J1 = NS2
      DO 180 L = J, 1, -1
        W4(L, 1) = W2(J1, 1)
        W4(L, 2) = W2(J1, 2)
        IW2(L) = IW1(J1)
        J1 = J1 - 1
180    CONTINUE
      K = J * (J + 1) / 2
      J2 = NS1
      DO 190 L = K, 1, -1

```



```
        W3(L) = W1(J2)
        J2 = J2 - 1
190 CONTINUE
        NC = IW3(NS3, 1)
        N4 = N - NS3 - NC
        IF (NC .EQ. IW3(NS3, 2)) THEN
            NS1 = J2
            NS2 = J1
            NS3 = NS3 - 1
            IF (IORD .EQ. 1) THEN
                GO TO 170
            END IF
        ELSE
            IW3(NS3, 1) = IW3(NS3, 1) + NI
        END IF
        GO TO 70
200 IF (NB .NE. NF) THEN
        NB = NB + NI
        GO TO 40
    END IF
    RETURN
    END
    SUBROUTINE OUTR(IMV, RSS, R, NR, C, NC)
C
C     ALGORITHM AS 268.2  APPL.STATIST. (1991), VOL.40, NO.3
C
C     Version A: For all possible subsets regression
C
    INTEGER NC, NR, IMV(NC)
    REAL R(NR), C(NC), RSS
    WRITE (6, '(A,10(1X,I3))') ' MODEL VARIABLES ', IMV
    WRITE (6, '(A,F20.8)') ' RESIDUAL SUM OF SQUARES ', RSS
    WRITE (6, '(A, I3)') ' R MATRIX IN PACKED VECTOR FORM LENGTH ', NR
    WRITE (6, * ) R
    WRITE (6, '(A, I3)') ' C VECTOR LENGTH ', NC
    WRITE (6, * ) C
    RETURN
    END
    SUBROUTINE OUTR(IMV, RSS, R, NR, C, NC)
C
C     ALGORITHM AS 268.3  APPL.STATIST. (1991), VOL.40, NO.3
C
C     Version B: Best subsets
C
    INTEGER NR, NC, IMV(NC)
    REAL R(NR), C(NC), RSS
    INTEGER IMVB
    REAL BRSS
    COMMON / BEST / BRSS(20), IMVB(210)
    INTEGER I, J
C
    J = NC * (NC - 1) / 2
    DO 10 I = 1, NC
        IMVB(J + I) = IMV(I)
10 CONTINUE
    BRSS(NC) = RSS
    RETURN
    END
```

```
      SUBROUTINE CF(NORD, X, AC, A, D, H, P, DEL, IFAULT)
C
C      ALGORITHM AS 269 APPL.STATIST. (1992), VOL.41, NO.1
C
C      Calculates the Cornish-Fisher adjustment to the normal deviate.
C
      INTEGER NORD, IFAULT
      REAL X, AC(NORD), A(NORD), D(NORD), H(3 * NORD),
*      P(3 * NORD * (NORD+1)/2), DEL(NORD)
C
C      Local variables
C
      INTEGER J, JA, JAL, JB, JBL, K, L
      REAL AA, BC, CC, DD, FAC, LIMIT, ONE, ZERO
      DATA LIMIT, ONE, ZERO / 3.719017274, 1.0, 0.0 /
C
C      Check input arguments
C
      IFAULT = 0
      IF (NORD .GT. 18) THEN
        IFAULT = 1
      ELSE IF (X .LT. -LIMIT .OR. X .GT. LIMIT) THEN
        IFAULT = 2
      END IF
      IF (IFAULT .NE. 0) RETURN
C
C      Compute the adjusted cumulants
C
      CC = -ONE
      DO 10 J = 1, NORD
        A(J) = CC * AC(J) / ((J+1) * (J+2))
        CC = -CC
      10 CONTINUE
C
C      Compute the Hermite polynomial values.
C
      H(1) = -X
      H(2) = X * X - ONE
      DO 20 J = 3, 3 * NORD
        H(J) = - (X * H(J-1) + (J-1) * H(J-2))
      20 CONTINUE
C
C      Clear the polynomial array.
C
      DO 30 J = 1, 3 * NORD * (NORD+1)/2
        P(J) = ZERO
      30 CONTINUE
      D(1) = - A(1) * H(2)
      DEL(1) = D(1)
      P(1) = D(1)
      P(3) = A(1)
      JA = ZERO
      FAC = ONE
C
C      Main loop
C
      DO 70 J = 2, NORD
C
C      Initialize.
C
        FAC = FAC * J
```

JA = JA + 3 \* (J-1)

JB = JA

BC = ONE

C

C Calculate coefficients of Hermite polynomials.

C

DO 50 K = 1, J-1

DD = BC \* D(K)

AA = BC \* A(K)

JB = JB - 3 \* (J - K)

DO 40 L = 1, 3 \* (J - K)

JBL = JB + L

JAL = JA + L

P(JAL+1) = P(JAL+1) + DD \* P(JBL)

P(JAL+K+2) = P(JAL+K+2) + AA \* P(JBL)

40 CONTINUE

BC = BC \* (J - K) / K

50 CONTINUE

P(JA+J+2) = P(JA+J+2) + A(J)

C

C Calculate the adjustments.

C

D(J) = ZERO

DO 60 L = 2, 3 \* J

D(J) = D(J) - P(JA+L) \* H(L-1)

60 CONTINUE

P(JA+1) = D(J)

DEL(J) = D(J) / FAC

70 CONTINUE

C

RETURN

END

C

SUBROUTINE CUM(CU, MU, NORD)

C

C Calculates the cumulants from the moment series by a  
C recursion relation.

C

C This code was published in Appl. Statist. vol.42 (1993),  
C pp. 268-269.

C

INTEGER NORD

REAL CU(NORD), MU(NORD)

C

C Local variables

C

INTEGER J, JJ

REAL ONE, C

DATA ONE /1.0/

C

CU(1) = MU(1)

DO 1 J = 1, NORD - 1

C = ONE

CU(J+1) = MU(J+1)

DO 1 JJ = 0, J-1

CU(J+1) = CU(J+1) - C \* CU(JJ+1) \* MU(J-JJ)

C = C \* (J-JJ) / (JJ+1)

1 CONTINUE

RETURN

END

```
      SUBROUTINE PLYFIT(NN,Y,NINTS,NOBS,DIVBEG,DIVEND,NK,NC,NOTE,  
* AGUESS,BOUND,BOUNDU,DBOUND,UBOUND,GROUP,KIND,ITERMX,QUICK,  
* A,SEA,CORR,ALOG,LOGL,P,CHISQ,NDF,AINV,AMU,DMUDA,YFN,IFAUULT)
```

```
C  
C      ALGORITHM AS 270.1 APPL.STATIST. (1992), VOL.41, NO.1
```

```
C      Subroutine for fitting a parametric 'key' function to data  
C      (grouped or ungrouped) and for making polynomial adjustments  
C      to that fit. An iterative maximum likelihood routine, based  
C      on Newton-Raphson search, is employed.
```

```
C      Stephen T Buckland, Scottish Agricultural Statistics Service,  
C      Aberdeen Unit, MLURI, Craigiebuckler, Aberdeen AB9 2QJ, Scotland
```

```
C      January, 1991
```

```
C      Auxiliary routines required: LUDCMP and LUBKSB from Numerical  
C      Recipes by Press, Flannery, Teukolsky and Vetterling, Cambridge  
C      University Press, 1986.
```

```
C      To change the key function, edit subroutines STD & KEY
```

```
C      IFAULT = 0 if convergence achieved  
C              = 1 if convergence not achieved after ITERMX steps  
C              = 2 if at most one group contains observations  
C              = 3 if DIVBEG and/or DIVEND values are invalid  
C              = 4 if both NN=0 (grouped data) and GROUP=.FALSE.  
C              = 5 if AGUESS = 0.0 or lies outside specified bounds  
C                  for any key parameter  
C              = 6 if NK<1 or NK>3  
C              = 7 if NC<0 or NC>10  
C              = 8 if ITERMX < 10  
C              = 9 if QUICK=.TRUE. and NC=0  
C              = 10 if NOTE contains unexpected zeros or invalid values  
C              = 11 if values of NOTE are not ordered from smallest to  
C                  largest or if not all values of NOTE are unique  
C              = 12 if at least one correlation between parameter  
C                  estimates is very close to unity  
C              = 13 if fitted density is negative somewhere in the  
C                  range (DIVBEG(1),DIVEND(NINTS))
```

```
      PARAMETER (KEYMAX=3,NMAX=13,INTMAX=85,NOBMAX=1000,EPS=1.0E-6,  
* JMAX=10)
```

```
C      KEYMAX      maximum number of key parameters  
C      NMAX        maximum total number of parameters (key parameters and  
C                  adjustment terms)  
C      INTMAX      maximum number of intervals (groups)  
C      NOBMAX      maximum number of observations  
C      EPS         determines the level of precision of numerical integration  
C      JMAX        maximum number of iterations for numerical integration
```

```
      REAL DIVBEG(*),DIVEND(*),Y(*),AGUESS(*),DBOUND(*),UBOUND(*),  
* Y2(NOBMAX),YFN(0:50)
```

```
C      On a 32 bit machine, change REAL to DOUBLE PRECISION below:
```

```
      DOUBLE PRECISION DFNDA(NMAX),A(*),A2(NMAX),A3(NMAX),  
* A4(KEYMAX),ALOG,ALOG2,AMU,AINFO(NMAX,NMAX),AINV(NMAX,*),  
* DLLDA(NMAX),DPGDA(INTMAX,NMAX),DMUDA(*),DMUDA2(NMAX),
```

```
* SEA (*), CORR(NMAX, *), B(NMAX), P(*), ALL, FNEV, DPDA(INTMAX, NMAX),
* DLFDA(NMAX), DAREA(NMAX), DAREA2(NMAX), ODAREA(NMAX), SUMD(NMAX),
* BMAT(NMAX, NMAX), BINV(NMAX, NMAX), DKEYDA(KEYMAX), DXSDA(KEYMAX),
* BB(NMAX, NMAX)
INTEGER NOBS(*), NOTE(*), INDX(NMAX)
LOGICAL GROUP, KIND, QUICK, BOUND(*), BOUNDU(*)

DATA SMALL1, SMALL2, P999, BIG1/1.0E-3, 1.0E-8, 9.99E-1, 1.0E10/

C CALL GETTIM(IHR, IMIN, ISEC, I100TH)
C TSTRT=(IHR*3600)+(IMIN*60)+ISEC+I100TH/100.0
  IFAULT=0

C Check for errors in the input parameters

DO 10 J=1, NINTS
  IF(DIVEND(J).LE.DIVBEG(J)) IFAULT=3

  IF(J.NE.NINTS) THEN
    IF(DIVEND(J+1).LE.DIVEND(J)) IFAULT=3
    IF(DIVBEG(J+1).LE.DIVBEG(J)) IFAULT=3
    IF(DIVEND(J).GT.DIVBEG(J+1)+SMALL2) IFAULT=3
    IF(.NOT.GROUP.AND.DIVEND(J).LT.DIVBEG(J+1)-SMALL2) IFAULT=3
  ENDIF

10 CONTINUE

IF(.NOT.GROUP.AND.NN.EQ.0) IFAULT=4
IF(NK.LT.1.OR.NK.GT.3) IFAULT=6
IF(NC.LT.0.OR.NC.GT.10) IFAULT=7
IF(ITERMX.LT.10) IFAULT=8
IF(NC.EQ.0.AND.QUICK) IFAULT=9

IF(NC.GT.0) THEN

  DO 20 J=1, NC
    IF(NOTE(J).LE.0.OR.NOTE(J).GT.10) IFAULT=10
    IF(J.GT.1.AND.NOTE(J).LE.NOTE(J-1)) IFAULT=11
20 CONTINUE

ENDIF

DO 30 J=1, NK
  IF(ABS(AGUESS(J)).LT.SMALL2) IFAULT=5
  IF(BOUND(J).AND.AGUESS(J).LT.DBOUND(J)) IFAULT=5
  IF(BOUNDU(J).AND.AGUESS(J).GT.UBOUND(J)) IFAULT=5
30 CONTINUE

IF(IFAULT.NE.0) RETURN

IF(NN.GT.0) THEN

C Calculate group frequencies

DO 40 J=1, NINTS
40 NOBS(J)=0

  N=0

  DO 60 I=1, NN
```

```
      IF(Y(I).GT.DIVBEG(1)-SMALL2) THEN
        DO 50 J=1,NINTS
          IF(Y(I).LE.DIVEND(J)+SMALL2) THEN
            N=N+1
            Y2(N)=Y(I)
            NOBS(J)=NOBS(J)+1
            GOTO 60
          ENDIF
50      CONTINUE
        ENDIF
60      CONTINUE
      ELSE
        N=0
        DO 65 J=1,NINTS
65      N=N+NOBS(J)
        ENDIF
        NZ=0
        DO 70 J=1,NINTS
          IF(NOBS(J).EQ.0) NZ=NZ+1
70      CONTINUE
        IF(NZ.GE.NINTS-1) THEN
          IFAULT=2
          RETURN
        ENDIF
        NP=NK+NC
        KOUNT=0
        ITER2=0
        ITER3=0
        ICON=0
        IF(GROUP) THEN
C      Calculate the constant part of the log likelihood function
          CONST=0.0
          K=0
          DO 90 J=2,NINTS
            K=K+NOBS(J-1)
            DO 80 I=1,NOBS(J)
80      CONST=CONST+LOG(FLOAT(I+K))-LOG(FLOAT(I))
          CONTINUE
90      CONTINUE
        ENDIF
        DO 110 J=1,NP
```

```
        IF(J.LE.NK) A4(J)=-1.0

        DO 100 K=1,NP
100      CORR(J,K)=0.0

        B(J)=AGUESS(J)
110     CONTINUE

        IF(.NOT.QUICK) THEN

C         In MODE 2, the search is conditional on the current key parameter
C         estimates, and only the polynomial coefficients are updated

        MODE=2
        ELSE

C         In MODE 4, only the key parameters are estimated

        MODE=4
        ENDIF

        M=NP
        INIT=0

C         This initialising ensures that erroneous 'convergence'
C         cannot occur at the 1st iteration

        DO 120 J=1,M
120     A3(J)=-1.0

        ALOGL2=-BIG1

C         If there are no polynomial coefficients to be fitted, only a
C         single set of iterations to fit the key parameters is required

        IF(M.EQ.NK) MODE=3

        IF(QUICK) THEN
            MOLD=M
            M=NK
        ENDIF

        M2=M

130     ITER=0

140     ALOGL=ALL(CONST,P,NINTS,DIVBEG,DIVEND,B,DPGDA,AMU,DMUDA,DAREA,
* DFNDA,DAREA2,ODAREA,SUMD,DKEYDA,DXSDA,M2,NOTE,NK,N,Y2,NOBS,
* KIND,GROUP,INTMAX,EPS,JMAX)

C         If the log likelihood has decreased, enter the Marquardt
C         procedure to find a point at least as good as the previous one

        IF(ALOGL.LT.ALOGL2) THEN
            CALL MARQUA(B,A2,AINFO,DL LDA,NK,MM,MODE,KOUNT,NMAX,BMAT,BINV,
* BB,INDX)
            GOTO 230
        ENDIF

        INIT=1
```

```
C      The following subroutine call allows progress in the search to
C      be monitored.  The subroutine is only entered if the likelihood
C      has increased or stayed the same relative to the previous call.
C      If the user wishes to monitor progress, he/she should write a
C      short subroutine MONITR with the arguments listed below that
C      simply prints each argument to a file or to the screen.  Note
C      that, if double precision is used, the first line following the
C      SUBROUTINE statement should be  DOUBLE PRECISION ALOGL,B(*)
C      For single precision, replace DOUBLE PRECISION by REAL
```

```
C      ALOGL is the current value of the likelihood
C      MODE is the current mode of search
C      ITER is the number of iterations in the current mode
C      ITER3 is the total number of iterations
C      B(J), J=1,M, is the vector of estimated parameters and
C      polynomial coefficients
```

```
      CALL MONITR(ALOGL,MODE,ITER,ITER3,M,B)
```

```
C      CALL GETTIM(IHR,IMIN,ISEC,I100TH)
C      TIME=(IHR*3600)+(IMIN*60)+ISEC+I100TH/100.0
C      PRINT *,' Time =',TIME-TSTRT
C      ITER=ITER+1
C      ITER3=ITER3+1
```

```
      IF(ICON.EQ.1) ITER2=ITER2+1
      IF(ITER.EQ.1) GOTO 210
```

```
      IF(MODE.EQ.3.OR.QUICK) THEN
```

```
C      Has convergence occurred?  If so, GOTO statement 250.
C      If not, return to statement 210
```

```
      IF(M.GT.NK) THEN
```

```
          DO 150 J=NK+1,M
              IF(ABS(B(J)-A3(J))/(SMALL1+ABS(A3(J))).GT.
*              SMALL1/SQRT(FLOAT(N))) GOTO 210
150          CONTINUE
```

```
      ENDIF
```

```
      IF(MODE.NE.2) THEN
```

```
          DO 160 J=1,NK
              IF(ABS(B(J)-A3(J))/(SMALL1+ABS(A3(J))).GT.
*              SMALL1/SQRT(FLOAT(N))) GOTO 210
160          CONTINUE
```

```
      ENDIF
```

```
      GOTO 250
```

```
  ENDIF
```

```
C      Update parameter estimates
```

```
      DO 170 J=1,M
170      A(J)=B(J)
```

```
      IF(MODE.EQ.1) THEN
```



```
C          Search alternates between MODE 1 (in which the key parameters
C          are fitted conditional on the current polynomial coefficient
C          estimates) and MODE 2 (the converse).  If MODE 3 has already
C          been entered once, it is automatically returned to after
C          several cycles, provided convergence seems close.

          IF(ITER2.LE.3.AND.ICON.EQ.1) THEN
              MODE=2
              GOTO 190
          ENDIF

C          If convergence is close, enter MODE 3

          DO 180 J=1,NK

              IF(ABS(B(J)-A4(J))/(SMALL1+ABS(A4(J))).GT.SMALL1) THEN
                  MODE=2
                  GOTO 190
              ENDIF

180         CONTINUE

          MODE=3
          ITER=0
          GOTO 210

C          Array A4 is used to test for convergence when the search is
C          conditional on the polynomial coefficient estimates (MODE 1)

          190         DO 200 J=1,NK
          200         A4(J)=B(J)

          ELSEIF(.NOT.QUICK.AND.MODE.EQ.2) THEN

C          After one step in MODE 2, switch to MODE 1

          MODE=1
          ENDIF

          210         IF(ITER3.GT.ITERMX) THEN
              IFAULT=1
              RETURN
          ENDIF

C          If 12 iterations fail to bring convergence in MODE 3, and there is
C          at least one polynomial coefficient to be fitted, revert to
C          alternation between MODEs 1 and 2 for several cycles.

          IF(ITER.GE.12.AND.MODE.EQ.3.AND.NP.GT.NK) THEN
              MODE=2
              ITER2=0
              ICON=1
          ENDIF

C          Initialise variables for Newton-Raphson search

          ALOGL2=ALOGL

          DO 220 J=1,M
          220         A3(J)=B(J)
```

KOUNT=0

C MM is the number of parameters to be fitted at this stage of the search

MM=NK

IF(MODE.EQ.2) MM=M-NK

IF(MODE.EQ.3) MM=M

CALL INFO(P,NINTS,B,AINFO,DLLDA,DPGDA,AMU,DMUDA,DPDA,DLFDA,  
\* DFNDA,DKEYDA,DXSDA,M,MM,NOTE,NK,N,Y2,NOBS,KIND,GROUP,MODE,  
\* NMAX,INTMAX)

CALL NRAPH(B,A2,AINFO,AINV,DLLDA,NK,MM,MODE,BB,INDX,NMAX)

C If search exceeds bounds on the parameters, enter Marquardt routine

230 DO 240 J=1,NK

IF((BOUND(D(J)).AND.B(J).LT.DBOUND(J)).OR.(BOUND(U(J)).AND.  
\* B(J).GT.UBOUND(J))) THEN  
CALL MARQUA(B,A2,AINFO,DLLDA,NK,MM,MODE,KOUNT,NMAX,  
\* BMAT,BINV,BB,INDX)  
GOTO 230  
ENDIF

240 CONTINUE

C Otherwise, continue to the next iteration of Newton-Raphson

GOTO 140

C After convergence has occurred:

250 IF(MODE.EQ.4) THEN

C Store the results from fitting the key function, then GOTO  
C statement 130 to fit the polynomial coefficients

DO 270 K=1,M

DO 260 L=1,M  
260 CORR(K,L)=AINV(K,L)

IF(AINV(K,K).LT.0.0) AINV(K,K)=1.0E-20  
SEA(K)=SQRT(AINV(K,K))

270 CONTINUE

M=MOLD  
M2=M  
MODE=2

DO 280 J=1,NK  
280 A(J)=B(J)

GOTO 130  
ENDIF

IF(QUICK) THEN  
MINUS=NK  
ELSE  
MINUS=0

```
ENDIF

CHISQ=0.0

C Evaluate chi-square goodness-of-fit statistic; if analysis is of
C ungrouped data, first evaluate areas under the estimated probability
C density function corresponding to the divisions defined by the
C cutpoints DIVEND and DIVBEG

DO 290 J=1,NINTS

    IF(.NOT.GROUP) THEN

        CALL AREAS(P(J),DMUDA2,DFNDA,DAREA2,ODAREA,SUMD,DKEYDA,
*         DXSDA,DIVBEG(J),DIVEND(J),B,M,NOTE,NK,KIND,EPS,JMAX)

        P(J)=P(J)/AMU
    ENDIF

    PJN=P(J)*N
    CHISQ=CHISQ+(NOBS(J)-PJN)**2/ABS(PJN)
290 CONTINUE

C Degrees of freedom for chi-square test

NDF=NINTS-1-M

C Evaluations of the fitted probability density function at 51
C equally spaced points; may be used for plotting

DO 300 I=0,50
    YVAL=DIVBEG(1)+I*(DIVEND(NINTS)-DIVBEG(1))/50.0
    CALL FNEVAL(YVAL,B,M2,NOTE,NK,KIND,FNEV,DFNDA,DKEYDA,DXSDA)
    YFN(I)=FNEV/AMU
    IF(FNEV.LT.0.0) IFAULT=13
300 CONTINUE

C Standard errors of the parameter estimates

DO 310 K=1,M-MINUS
    IF(AINV(K,K).LT.0.0) AINV(K,K)=1.0E-20
    SEA(K+MINUS)=SQRT(AINV(K,K))
310 CONTINUE

C Transfer of parameter estimates from array B to A, and corresponding
C reassignment of the elements of the inverse of the information matrix
C and of the estimated derivatives of the normalising function (DMUDA)
C wrt each parameter

DO 330 K=1,M-MINUS

    DO 320 L=1,M-MINUS
320     CORR(K+MINUS,L+MINUS)=AINV(K,L)

330 CONTINUE

DO 350 K=MINUS+1,M
    A(K)=B(K)

    DO 340 L=MINUS+1,M
340     AINV(K,L)=CORR(K,L)
```

```
350    CONTINUE
      IF(MINUS.GT.0) THEN
        DO 370 K=1,MINUS
          DO 360 L=1,MINUS
360      AINV(K,L)=CORR(K,L)
          CONTINUE
370      CONTINUE
        DO 390 K=1,MINUS
          DO 380 L=MINUS+1,M
            AINV(K,L)=0.0
            AINV(L,K)=0.0
380      CONTINUE
          CONTINUE
390      CONTINUE
      ENDIF
C      Calculation of correlations between parameter estimates
      IF(MINUS.GT.0) THEN
        CORR(MINUS,MINUS)=1.0
        IF(MINUS.GT.1) THEN
          DO 410 K=1,MINUS-1
            CORR(K,K)=1.0
            DO 400 L=K+1,MINUS
              CORR(K,L)=AINV(K,L)/SEA(K)/SEA(L)
              CORR(L,K)=CORR(K,L)
              IF(ABS(CORR(K,L)).GT.P999) IFAULT=12
400          CONTINUE
            CONTINUE
410          CONTINUE
          ENDIF
        ENDIF
      CORR(M,M)=1.0
      IF(M.LE.MINUS+1) RETURN
      DO 430 K=MINUS+1,M-1
        CORR(K,K)=1.0
        DO 420 L=K+1,M
          CORR(K,L)=AINV(K,L)/SEA(K)/SEA(L)
          CORR(L,K)=CORR(K,L)
          IF(ABS(CORR(K,L)).GT.P999) IFAULT=12
420      CONTINUE
        CONTINUE
430      CONTINUE
      RETURN
      END
```

C\*\*\*\*\*

```

SUBROUTINE AREAS(AREA,DAREA,DFNDA,DAREA2,ODAREA,SUMD,DKEYDA,
* DXSDA,DIV1,DIV2,A,M2,NOTE,NK,KIND,EPS,JMAX)

```

C Calculation of area under the fitted curve and under the derivative  
C of the fitted curve wrt each parameter between DIV1 and DIV2  
C using Simpson's rule for numerical integration. The number of  
C intervals is increased until a level of precision, determined  
C by EPS, is achieved. The method is described by Press et al. (1986)

C On a 32 bit machine, change REAL to DOUBLE PRECISION below:

```

DOUBLE PRECISION AREA,DFNDA(*),A(*),DAREA(*),OAREA,OAREAT,
* AREA2,DAREA2(*),ODAREA(*),SUM,SUMD(*),FNEV,DKEYDA(*),DXSDA(*)
INTEGER NOTE(*)
LOGICAL KIND

```

```

OAREAT=-1.0E30
OAREA=-1.0E30

```

```

DO 10 K=1,M2
10 ODAREA(K)=-1.0E30

```

```

DO 100 J=1,JMAX

```

```

IF(J.EQ.1) THEN

```

```

* CALL FNEVAL(DIV1,A,M2,NOTE,NK,KIND,FNEV,DFNDA,DKEYDA,
DXSDA)
AREA2=FNEV

```

```

DO 20 K=1,M2
20 DAREA2(K)=DFNDA(K)

```

```

* CALL FNEVAL(DIV2,A,M2,NOTE,NK,KIND,FNEV,DFNDA,DKEYDA,
DXSDA)
CON=0.5*(DIV2-DIV1)
AREA2=CON*(AREA2+FNEV)

```

```

DO 30 K=1,M2
30 DAREA2(K)=CON*(DAREA2(K)+DFNDA(K))

```

```

IT=1
ELSE

```

```

TNM=IT
DIFF=(DIV2-DIV1)/TNM
ARG=DIV1+0.5*DIFF
SUM=0.0

```

```

DO 40 K=1,M2
40 SUMD(K)=0.0

```

```

DO 60 JJ=1,IT
* CALL FNEVAL(ARG,A,M2,NOTE,NK,KIND,FNEV,DFNDA,DKEYDA,
DXSDA)
SUM=SUM+FNEV

```

```

DO 50 K=1,M2
50 SUMD(K)=SUMD(K)+DFNDA(K)

```

```

        ARG=ARG+DIFF
60      CONTINUE

        AREA2=0.5*(AREA2+(DIV2-DIV1)*SUM/TNM)

        DO 70 K=1,M2
70      DAREA2(K)=0.5*(DAREA2(K)+(DIV2-DIV1)*SUMD(K)/TNM)

        IT=2*IT
        ENDIF

        AREA=(4.0*AREA2-OAREAT)/3.0

        DO 80 K=1,M2
80      DAREA(K)=(4.0*DAREA2(K)-ODAREA(K))/3.0

        IF(ABS(AREA-OAREA).LT.EPS*ABS(AREA+OAREA)) RETURN

        OAREA=AREA
        OAREAT=AREA2

        DO 90 K=1,M2
90      ODAREA(K)=DAREA2(K)

100    CONTINUE

        RETURN
        END

C*****

        SUBROUTINE PROBS(P,NINTS,DIVBEG,DIVEND,A,PTOTAL,DPGDA,DMUDA,
* DAREA,DFNDA,DAREA2,ODAREA,SUMD,DKEYDA,DXSDA,M2,NOTE,NK,KIND,
* INTMAX,EPS,JMAX)

C      Evaluation of the area under each section of the fitted
C      probability density function

        REAL DIVBEG(*),DIVEND(*)

C      On a 32 bit machine, change REAL to DOUBLE PRECISION below:

        DOUBLE PRECISION A(*),DAREA(*),DMUDA(*),AREA,PTOTAL,P(*),
* DPGDA(INTMAX,*),DFNDA(*),DAREA2(*),ODAREA(*),SUMD(*),
* DKEYDA(*),DXSDA(*)
        LOGICAL KIND
        INTEGER NOTE(*)

        PTOTAL=0.0

        DO 10 K=1,M2
10      DMUDA(K)=0.0

        DO 30 J=1,NINTS

C      Calculation of the area under section J of the fitted curve
C      before normalisation

        DIV2=DIVEND(J)
        DIV1=DIVBEG(J)

```

```

CALL AREAS (AREA, DAREA, DFNDA, DAREA2, ODAREA, SUMD, DKEYDA,
* DXSDA, DIV1, DIV2, A, M2, NOTE, NK, KIND, EPS, JMAX)

P(J)=AREA
PTOTAL=PTOTAL+P(J)

DO 20 K=1, M2
    DPGDA(J, K)=DAREA(K)
    DMUDA(K)=DMUDA(K)+DPGDA(J, K)
20 CONTINUE

30 CONTINUE

C PTOTAL is now the value that normalises the fitted curve, to make
C it a valid density function. DPGDA is the matrix of estimated
C derivatives of each of the NINTS non-normalised areas wrt the
C parameters, and DMUDA is the estimated derivative of the
C normalising value wrt the parameters. The following DO loop
C normalises the P's so that they sum to unity.

DO 40 J=1, NINTS
    IF(PTOTAL.NE.0.0) P(J)=P(J)/PTOTAL
40 CONTINUE

RETURN
END

C*****

C On a 32 bit machine, change REAL to DOUBLE PRECISION below:

DOUBLE PRECISION FUNCTION ALL(CONST, P, NINTS, DIVBEG, DIVEND, B,
* DPGDA, AMU, DMUDA, DAREA, DFNDA, DAREA2, ODAREA, SUMD, DKEYDA, DXSDA, M2,
* NOTE, NK, N, Y, NOBS, KIND, GROUP, INTMAX, EPS, JMAX)

C On a 32 bit machine, change REAL to DOUBLE PRECISION below:

DOUBLE PRECISION P(*), B(*), AMU, DPGDA(INTMAX, *), DMUDA(*),
* FNEV, DFNDA(*), DAREA2(*), ODAREA(*), SUMD(*), DKEYDA(*), DXSDA(*),
* DAREA(*)
REAL DIVBEG(*), DIVEND(*), Y(*)
INTEGER NOTE(*), NOBS(*)
LOGICAL KIND, GROUP
DATA SMALL/1.0E-10/

IF(GROUP) THEN

C Grouped data:

CALL PROBS(P, NINTS, DIVBEG, DIVEND, B, AMU, DPGDA, DMUDA, DAREA,
* DFNDA, DAREA2, ODAREA, SUMD, DKEYDA, DXSDA, M2, NOTE, NK, KIND,
* INTMAX, EPS, JMAX)

ALL=CONST

C Add the part of the log likelihood that varies with
C the parameter estimates to the constant part

DO 10 J=1, NINTS

C If an estimated probability < or = 0, set it equal

```

```

C          to a very small value

          IF(P(J).LT.SMALL) P(J)=SMALL
          ALL=ALL+NOBS(J)*LOG(P(J))
10        CONTINUE

        ELSE

C          Ungrouped data:

          CALL AREAS(AMU,DMUDA,DFNDA,DAREA2,ODAREA,SUMD,DKEYDA,
*          DXSDA,DIVBEG(1),DIVEND(NINTS),B,M2,NOTE,NK,KIND,EPS,JMAX)

C          Evaluate the log likelihood; if the estimated fit is
C          impossible, give the log likelihood a large -ve value

          IF(AMU.LE.0.0) AMU=1.0E25
          ALL=-N*LOG(AMU)

          DO 20 J=1,N

*          CALL FNEVAL(Y(J),B,M2,NOTE,NK,KIND,FNEV,DFNDA,DKEYDA,
          DXSDA)

          IF(FNEV.LT.SMALL) FNEV=SMALL
          ALL=ALL+LOG(FNEV)
20        CONTINUE

        ENDIF

        RETURN
        END

C*****

          SUBROUTINE INFO(P,NINTS,B,AINFO,DLLDA,DPGDA,AMU,DMUDA,DPDA,
*          DLFDA,DFNDA,DKEYDA,DXSDA,M,MM,NOTE,NK,N,Y,NOBS,KIND,MODE,
*          NMAX,INTMAX)

C          On a 32 bit machine, change REAL to DOUBLE PRECISION below:

          DOUBLE PRECISION AMU,AINFO(NMAX,*),DPGDA(INTMAX*),DMUDA(*),
*          DPDA(INTMAX*),DLFDA(*),DFNDA(*),P(*),B(*),DLLDA(*),FNEV,
*          DKEYDA(*),DXSDA(*)
          INTEGER NOTE(*),NOBS(*)
          REAL Y(*)
          LOGICAL KIND,GROUP

          DO 20 K=1,M
            DLLDA(K)=0.0

            DO 10 L=1,M
10              AINFO(K,L)=0.0

20            CONTINUE

          IF(GROUP) THEN

C          Grouped data:

C          Evaluate derivative wrt each parameter to be fitted of the area

```



```
C          under each section of the probability density function
          DO 40 K=1,M
              IF((MODE.EQ.1.AND.K.LE.NK).OR.(MODE.EQ.2.AND.K.GT.NK).
*              OR.MODE.GT.2) THEN
                  DO 30 J=1,NINTS
                      DPDA(J,K)=(DPGDA(J,K)-P(J)*DMUDA(K))/AMU
30                  CONTINUE
              ENDIF
          CONTINUE
          40
C          Evaluate derivative of the log likelihood function
C          wrt each parameter to be fitted
          DO 60 K=1,M
              IF((MODE.EQ.1.AND.K.LE.NK).OR.(MODE.EQ.2.AND.K.GT.NK).
*              OR.MODE.GT.2) THEN
                  DO 50 J=1,NINTS
                      DLLDA(K)=DLLDA(K)+NOBS(J)*DPDA(J,K)/P(J)
50                  CONTINUE
              ENDIF
          CONTINUE
          60
C          Calculate the information matrix
          DO 90 K=1,MM
              KK=K
              IF(MODE.EQ.2) KK=K+NK
              DO 80 L=1,MM
                  LL=L
                  IF(MODE.EQ.2) LL=L+NK
              DO 70 J=1,NINTS
                  AINFO(K,L)=AINFO(K,L)+N*DPDA(J,KK)*DPDA(J,LL)/P(J)
70                  CONTINUE
              80
          CONTINUE
          90
          ELSE
C          Ungrouped data:
          DO 130 J=1,N
C          For each observation, calculate its contribution to the
C          derivatives wrt each parameter to be fitted of the log of
C          the probability density function and of the log likelihood.
*          CALL FNEVAL(Y(J),B,M,NOTE,NK,KIND,FNEV,DFNDA,DKEYDA,
              DXSDA)
          DO 100 K=1,M
```

```

                IF ( (MODE.EQ.1.AND.K.LE.NK).OR.(MODE.EQ.2.AND.K.GT.NK) .
*              OR.MODE.GT.2) THEN
                DLFDA(K)=DFNDA(K)/FNEV -DMUDA(K)/AMU
                DLLDA(K)=DLLDA(K)+DLFDA(K)
                ENDIF

100            CONTINUE

C              Calculate the contribution of each observation to the
C              information matrix

                DO 120 K=1,MM
                KK=K
                IF(MODE.EQ.2) KK=K+NK

                DO 110 L=1,MM
                LL=L
                IF(MODE.EQ.2) LL=L+NK
                AINFO(K,L)=AINFO(K,L)+DLFDA(KK)*DLFDA(LL)
110            CONTINUE

120            CONTINUE

130            CONTINUE

                ENDIF

                RETURN
                END

```

C\*\*\*\*\*

```

                SUBROUTINE NRAPH(B,A2,AINFO,AINV,DLLDA,NK,MM,MODE,BB,INDX,
*              NMAX)

C              On a 32 bit machine, change REAL to DOUBLE PRECISION below:

                DOUBLE PRECISION B(*),A2(*),AINFO(NMAX,*),AINV(NMAX,*),
*              DLLDA(*),BB(NMAX,*),
                INTEGER INDX(*)

C              Invert the information matrix

                IF(MM.EQ.1) THEN
                AINV(1,1)=1.0/AINFO(1,1)
                ELSE
                CALL INVERS(AINFO,AINV,BB,INDX,MM,NMAX)
                ENDIF

C              For each parameter being fitted, update its estimate, using
C              Newton-Raphson

                DO 20 K=1,MM
                KK=K
                IF(MODE.EQ.2) KK=K+NK
                A2(KK)=B(KK)

                DO 10 L=1,MM
                LL=L
                IF(MODE.EQ.2) LL=L+NK

```

```

          B(KK)=B(KK)+AINV(K,L)*DLLDA(LL)
10      CONTINUE

20      CONTINUE

      RETURN
      END

C*****

      SUBROUTINE MARQUA(B,A2,AINFO,DLLDA,NK,MM,MODE,KOUNT,NMAX,
* BMAT,BINV,BB,INDX)

C      The Marquardt procedure, for when Newton-Raphson fails to increase
C      the value of the log likelihood. The procedure is very similar to
C      Newton-Raphson, but progressively adds larger values to the
C      diagonal elements of the information matrix until a point with a
C      larger log likelihood is found.

C      On a 32 bit machine, change REAL to DOUBLE PRECISION below:

      DOUBLE PRECISION B(*),A2(*),AINFO(NMAX,*),DLLDA(*),
* BMAT(NMAX,*),BINV(NMAX,*),BB(NMAX,*),
      INTEGER INDX(*)

      KOUNT=KOUNT+1

      DO 20 K=1,MM

          DO 10 L=1,MM
              BMAT(K,L)=AINFO(K,L)
              IF(K.EQ.L) BMAT(K,L)=BMAT(K,L)*(1.0+2.0**KOUNT)
10          CONTINUE

20      CONTINUE

      IF(MM.EQ.1) THEN
          BINV(1,1)=1.0/BMAT(1,1)
      ELSE
          CALL INVERS(BMAT,BINV,BB,INDX,MM,NMAX)
      ENDIF

      DO 40 K=1,MM
          KK=K
          IF(MODE.EQ.2) KK=K+NK
          B(KK)=A2(KK)

          DO 30 L=1,MM
              LL=L
              IF(MODE.EQ.2) LL=L+NK
              B(KK)=B(KK)+BINV(K,L)*DLLDA(LL)
30          CONTINUE

40      CONTINUE

      RETURN
      END

C*****

      SUBROUTINE POLY(XS,H)

```

C Simple polynomials up to order 10

C On a 32 bit machine, change REAL to DOUBLE PRECISION below:

```
DOUBLE PRECISION H(0:10),XS
```

```
H(0)=1.0  
H(1)=XS  
H(2)=XS*XS  
H(3)=XS**3  
H(4)=XS**4  
H(5)=XS**5  
H(6)=XS**6  
H(7)=XS**7  
H(8)=XS**8  
H(9)=XS**9  
H(10)=XS**10
```

```
RETURN  
END
```

C\*\*\*\*\*

```
SUBROUTINE HERM(XS,H)
```

C Hermite polynomials up to order 10

C On a 32 bit machine, change REAL to DOUBLE PRECISION below:

```
DOUBLE PRECISION H(0:10),XS
```

```
H(0)=1.0  
H(1)=XS  
H(2)=XS*XS-1.0  
H(3)=XS**3-3.0*XS  
H(4)=XS**4-6.0*XS*XS+3.0  
H(5)=XS**5-10.0*XS**3+15.0*XS  
H(6)=XS**6-15.0*XS**4+45.0*XS*XS-15.0  
H(7)=XS**7-21.0*XS**5+105.0*XS**3-105.0*XS  
H(8)=XS**8-28.0*XS**6+210.0*XS**4-420.0*XS*XS+105.0  
H(9)=XS**9-36.0*XS**7+378.0*XS**5-1260.0*XS**3+945.0*XS  
* -945.0
```

```
RETURN  
END
```

C\*\*\*\*\*

```
SUBROUTINE FNEVAL(X,A,M2,NOTE,NK,KIND,FNEV,DFNDA,  
* DKEYDA,DXSDA)
```

C Evaluates the function and its derivative wrt A (before  
C normalisation) at point X, using parameter estimates A

C On a 32 bit machine, change REAL to DOUBLE PRECISION below:

```
DOUBLE PRECISION A(*),DFNDA(*),DKEYDA(*),XS,DXSDA(*),  
* VALKEY,H(0:10),FNEV,TOP,DTOP  
INTEGER NOTE(*)
```

LOGICAL KIND

CALL STD(X,A,XS,DXSDA)

TOP=1.0

C VALKEY is the value of the key function

CALL KEY(X,A,VALKEY,DKEYDA)

IF(M2.GT.NK) THEN

IF(KIND) THEN

CALL HERM(XS,H)

ELSE

CALL POLY(XS,H)

ENDIF

C TOP is the contribution of the polynomial terms to the fitted  
C density, apart from the normalising value, which is a function  
C of the parameters alone

DO 10 J=NK+1,M2

10 TOP=TOP+A(J)\*H(NOTE(J-NK))

ENDIF

FNEV=VALKEY\*TOP

C Evaluate the derivative of the curve (before normalisation) at point  
C X, wrt each parameter, using parameter estimates A

TOP=1.0

DTOP=0.0

IF(M2.GT.NK) THEN

DO 20 J=NK+1,M2

20 DFNDA(J)=VALKEY\*H(NOTE(J-NK))

DO 30 J=NK+1,M2

TOP=TOP+A(J)\*H(NOTE(J-NK))

DTOP=DTOP+A(J)\*(NOTE(J-NK))\*H(NOTE(J-NK)-1)

30 CONTINUE

ENDIF

DO 40 J=1,NK

40 DFNDA(J)=VALKEY\*DTOP\*DXSDA(J)+DKEYDA(J)\*TOP

RETURN

END

C\*\*\*\*\*

SUBROUTINE INVERS(A,Y,B,INDX,N,NMAX)

C Calculates the inverse of a matrix.

C See 'Numerical Recipes', Press et al., 1986, p38.

C On a 32 bit machine, change REAL to DOUBLE PRECISION below:

```
DOUBLE PRECISION A,B,Y
DIMENSION A(NMAX,*),B(NMAX,*),Y(NMAX*),INDX(*)

DO 20 I=1,N

    DO 10 J=1,N
        B(I,J)=A(I,J)
        Y(I,J)=0.0
10    CONTINUE

    Y(I,I)=1.0
20    CONTINUE

CALL LUDCMP(B,N,NMAX,INDX,D)

DO 30 J=1,N
    CALL LUBKSB(B,N,NMAX,INDX,Y(1,J))
30    CONTINUE

RETURN
END

C*****

SUBROUTINE STD(X,A,XS,DXSDA)

C Reduces observations to standard measure, to avoid numerical
C problems, and differentiates the standardised observation wrt A

C On a 32 bit machine, change REAL to DOUBLE PRECISION below:

DOUBLE PRECISION A(*),XS,DXSDA(*)

XS=(X-A(1))/A(2)
DXSDA(1)=-1.0/A(2)
DXSDA(2)=-((X-A(1))/(A(2)**2))

RETURN
END

C*****

SUBROUTINE KEY(X,A,VALKEY,DKEYDA)

C Evaluates the fitted key function and its derivative wrt A at X

C On a 32 bit machine, change REAL to DOUBLE PRECISION below:

DOUBLE PRECISION A(*),VALKEY,DKEYDA(*)

DATA SMALL2,SMALL3/1.0E-8,1.0E-10/

VALKEY=1.0
D=0.0
IF(ABS(X-A(1)).GT.SMALL3) D=((X-A(1))/A(2))**2/2.0

IF(D.GT.20.0) THEN
    VALKEY=0.0
ELSEIF(D.GT.SMALL2) THEN
    VALKEY=EXP(-D)
```

ENDIF

C Estimate the differential at X of the key function wrt A

DKEYDA(1)=(X-A(1))\*VALKEY/(A(2)\*\*2)

DKEYDA(2)=((X-A(1))\*\*2)\*VALKEY/(A(2)\*\*3)

RETURN

END

```

SUBROUTINE MCE (N, KMAX, A1, PQ, PMIN, LKA, UPMQM, ICR, IFAULT)
C
C     ALGORITHM AS 271 APPL.STATIST. (1992), VOL.41, NO.1
C
C     Obtains the optimal (smallest misclassification probability)
C     joint classification procedure combining at most KMAX of N
C     independent marginal classification rules.
C
INTEGER N, KMAX, LKA(N + 2), ICR(2, N), IFAULT
REAL A1, PQ(2, N), PMIN, UPMQM(3, N * (N + 1) / 2)
C
INTRINSIC ABS, MIN
C
INTEGER HELP, HOLD, I, I0, I2, II, J, J0, JI, JJ, K, L, LL, M,
*     MM, N1, N2, UPPER, R
REAL A2, ERP, ERQ, NEGONE, ONE, PSTAR, SIGN, STORE, ZERO
C
PARAMETER (ZERO = 0.0E0, ONE = 1.0E0 , NEGONE = -1.0E0)
C
C     Check for errors in the input variables
C
IFAULT = 0
IF (N .LT. 2) IFAULT = 1
IF (A1 .LE. ZERO .OR. A1 .GE. ONE) IFAULT = IFAULT + 2
DO 10 I = 2, N
  IF (PQ(1, I - 1) .GT. PQ(1, I)) THEN
    IFAULT = IFAULT + 4
    GOTO 20
  ENDIF
10 CONTINUE
20 DO 30 I = 1, N
  IF (PQ(2, I) .LT. ZERO .OR. PQ(2, I) .GT. ONE) THEN
    IFAULT = IFAULT + 8
    GOTO 40
  ENDIF
30 CONTINUE
40 IF (PQ(1, 1) .LT. ZERO .OR. PQ(1, N) .GT. ONE)
*   IFAULT = IFAULT + 16
  IF (KMAX .LT. 1 .OR. KMAX .GT. N) IFAULT = IFAULT + 32
  IF (IFAULT .GT. 0) RETURN
C
C     Initialization step
C
A2 = ONE - A1
PMIN = ONE
R = 1
ICR(2, 1) = 1
DO 50 I = 2, N
  IF (PQ(2, I - 1) .GT. PQ(2, I)) R = R + 1
  ICR(2, I) = R
50 CONTINUE
UPMQM(1, 1) = ONE
UPMQM(1, 2) = NEGONE
UPMQM(1, 3) = ONE
I0 = 2
II = 4
DO 70 J = 3, N
  UPMQM(1, II) = -UPMQM(1, I0)
  SIGN = UPMQM(1, I0)
  II = II + 1
  DO 60 I = 3, J

```



```

        UPMQM(1, II) = SIGN * (ABS(UPMQM(1, I0)) +
*           ABS(UPMQM(1, I0 + 1)))
        SIGN = -SIGN
        I0 = I0 + 1
        II = II + 1
60     CONTINUE
        UPMQM(1, II) = ONE
        I0 = I0 + 1
        II = II + 1
70     CONTINUE
C
C           Start with the full candidate problem (1, 2, ..., N)
C
        K = N
        MM = N
        DO 80 I = 1, N
            ICR(1, I) = I
80     CONTINUE
        N1 = N + 1
        N2 = N + 2
C
C           Optimality check
C
90     M = K - MM
        HOLD = M + 1
        HELP = M + MM
        UPPER = MIN(HELP, KMAX)
        IF (HOLD .EQ. 1) THEN
            UPMQM(2, 1) = PQ(1, ICR(1, 1))
            UPMQM(3, 1) = PQ(2, ICR(1, 1))
            PSTAR = A1 * UPMQM(2, 1) + A2 * UPMQM(3, 1)
            IF (PSTAR .LT. PMIN) THEN
                PMIN = PSTAR
                LKA(N1) = 1
                LKA(N2) = 1
                LKA(1) = ICR(1, 1)
            ENDIF
            HOLD = 2
        ENDIF
        IF (HELP .NE. 1) THEN
            II = HOLD * (HOLD - 1) / 2 + 1
            I0 = II - HOLD + 1
            DO 110 J = HOLD, UPPER
                L = ICR(1, J)
                UPMQM(2, II) = UPMQM(2, I0) + PQ(1, L)
                UPMQM(3, II) = UPMQM(3, I0) + PQ(2, L)
                II = II + 1
                DO 100 I = 3, J
                    UPMQM(2, II) = UPMQM(2, I0 + 1) +
*                       UPMQM(2, I0) * PQ(1, L)
                    UPMQM(3, II) = UPMQM(3, I0 + 1) +
*                       UPMQM(3, I0) * PQ(2, L)
                    II = II + 1
                    I0 = I0 + 1
100             CONTINUE
                UPMQM(2, II) = UPMQM(2, I0) * PQ(1, L)
                UPMQM(3, II) = UPMQM(3, I0) * PQ(2, L)
                II = II + 1
                I0 = I0 + 1
110             CONTINUE
            ENDIF

```

```

      J0 = HOLD * (HOLD - 1) / 2
      DO 160 J = HOLD, UPPER
        I0 = 1
        DO 150 I = 1, J
          ERP = ZERO
          ERQ = ZERO
          II = I0
          JI = J0 + I
          DO 120 L = I, J
            ERQ = ERQ + UPMQM(1, II) * UPMQM(3, JI)
            II = II + L
            JI = JI + 1
120      CONTINUE
          LL = J - I + 1
          II = LL * (LL + 1) / 2
          JI = J0 + LL
          DO 130 L = LL, J
            ERP = ERP + UPMQM(1, II) * UPMQM(2, JI)
            II = II + L
            JI = JI + 1
130      CONTINUE
          I0 = I0 + I + 1
          PSTAR = A1 * ERP + A2 * ERQ
          IF (PSTAR .LT. PMIN .OR.
*          (PSTAR .EQ. PMIN .AND. LKA(N2) .GT. J)) THEN
            PMIN = PSTAR
            LKA(N2) = J
            LKA(N1) = I
            DO 140 L = 1, J
              LKA(L) = ICR(1, L)
140          CONTINUE
            ENDIF
150      CONTINUE
          J0 = J0 + J
160      CONTINUE
          MM = 0
C
C          Backward step
C
170      IF (ICR(2, ICR(1, 1)) .EQ. R) RETURN
          L = ICR(2, ICR(1, K))
180      K = K - 1
          IF (K .GT. 0) THEN
            IF (ICR(2, ICR(1, K)) .GE. L) GOTO 180
          ENDIF
          IF (K .GT. 0 .AND. L .EQ. R) THEN
            L = ICR(2, ICR(1, K))
            K = K - 1
          ENDIF
          L = L + 1
          K = K + 1
          HELP = ICR(1, K) + 1
          DO 190 I = HELP, N
            IF (ICR(2, I) .EQ. L) GOTO 200
190      CONTINUE
200      ICR(1, K) = I
C
C          Fathoming step
C
210      JJ = ICR(1, K) - 1
          J = 1

```

```
        STORE = PQ(2, ICR(1, K))
        DO 230 I = 1, JJ
            IF (ICR(1, J) .GT. I) THEN
                IF (PQ(2, I) .LE. STORE) THEN
                    IF (MM .EQ. 0) THEN
                        GOTO 170
                    ELSE
C
C          Side step
C
                        HOLD = ICR(2, ICR(1, K))
                        K = K - 1
                        IF (HOLD .EQ. R) GOTO 90
                        K = K + 1
                        HELP = ICR(1, K) + 1
                        DO 220 I2 = HELP, N
                            IF (ICR(2, I2) .NE. HOLD) THEN
                                ICR(1, K) = I2
                                GOTO 210
                            ENDIF
220          CONTINUE
                        ENDIF
                    ENDIF
                    ELSE
                        J = J + 1
                    ENDIF
230 CONTINUE
C
C          Forward step
C
                MM = MM + 1
                IF (ICR(1, K) .EQ. N) GOTO 90
                IF (ICR(1, K) .LT. N) THEN
                    K = K + 1
                    ICR(1, K) = ICR(1, K - 1) + 1
                    GOTO 210
                ENDIF
            RETURN
        END
```

```
      SUBROUTINE BXPLT(NG, RVALS, IVALS, SCALEX, SCALEY, NY, NX, XTYPE,
*      WIDTH, NOTCH, IWRITE, OUTARR, INTARR, IVALS2, IFAULT)
C
C      ALGORITHM AS 272.1 APPL.STATIST. (1992), VOL.41, NO.1
C
C      PRODUCES A BOX-PLOT USING SUPPLIED QUANTILES
C
      REAL RVALS(6, NG), SCALEX(2), SCALEY(2), OUTARR(*), VALS(20)
      INTEGER IVALS(6, NG), WIDTH, WID, NX, IVALS2(8, NG),
*      INTARR(*), POINTS, PNTR
      CHARACTER INTCH(0:9), COLON, DASH, DOT
      CHARACTER*19 IFORM1
      CHARACTER*20 IFORM2
      CHARACTER*120 IOUT
      LOGICAL LWIDOK, NOTCH, XTYPE
      EXTERNAL AXIS, SCALE
C
      DATA MPVX / 10 /, MPVY / 5 /, MAXHT / 66 /, MAXWID / 130 /
      DATA IFORM1 / '(1H ,F8.0,1X,120A1)' /
      DATA IFORM2 / '(1H ,5X,16(F8.0,2X))' /
      DATA COLON / ':' /, DASH / '-' /, DOT / '.' /
      DATA INTCH / '0', '1', '2', '3', '4', '5', '6', '7', '8', '9' /
C
C CHECK PARAMETERS
C
      IFAULT = 0
      IF (NG .LT. 1) GOTO 900
      XMIN = SCALEX(1)
      XMAX = SCALEX(2)
      YMIN = SCALEY(1)
      YMAX = SCALEY(2)
C
C CHECK IF NLX NLY ARE IN LEGAL RANGE
C
      NLX = NX
      NLY = NY
      IF (NLY + 5 .GT. MAXHT) NLY = MAXHT - 5
      IF (NLY .LT. MPVY) NLY = MPVY
      IF (NLX + 11 .GT. MAXWID) NLX = MAXWID - 11
      IF (NLX .LT. MPVX) NLX = MPVX
      IF (XTYPE) NLX = (NG + 1) * (NLX / (NG + 1))
      NOUT = 0
      DO 10 I = 1, NG
         NOUT = NOUT + IVALS(1, I) + IVALS(2, I)
10 CONTINUE
      WID = WIDTH
      IF (WIDTH .EQ. 0) WID = NLX / (2 * NG + 1) + 1
C
C CALCULATE WIDTH EQUAL MARK SPACE RATIO
C
      IF (XTYPE) THEN
C
C QUALITATIVE X SIMULATE CALL OF SCALE
C
         XMIN = 0.0
         XSTEP = 1.0 / (NLX / (NG + 1))
C
C MUST CALCULATE SCALE, FIRST CHOOSE XMIN AND XMAX
C
      ELSE IF (XMIN .GE. XMAX) THEN
         XMIN = RVALS(1, 1)
```

```

        XMAX = XMIN
        DO 20 I = 2, NG
        IF (RVALS(1, I) .LT. XMIN) THEN
            XMIN = RVALS(1, I)
        ELSE IF (RVALS(1, I) .GT. XMAX) THEN
            XMAX = RVALS(1, I)
        ENDIF
20    CONTINUE
        XMN = XMIN
        XMX = XMAX
30    CALL SCALE(XMN, XMX, NLX, MPVX, TEMP, XVSTEP, NXVALS, IRX,
        *        IFAIL)
        IF (IFAIL .GT. 0) GOTO 901
        XSTEP = XVSTEP / MPVX
        IF ((XMIN - TEMP) / XSTEP .LT. WID) THEN
C
C OFFPLOT ON LEFT
C
            XMN = XMN - XSTEP
            GOTO 30
        ENDIF
        IF ((XMAX - TEMP) / XSTEP .GT. (NLX - WID)) THEN
C
C OFFPLOT ON RIGHT
C
            XMX = XMX + XSTEP
            GOTO 30
        ENDIF
        XMIN = TEMP
    ELSE
        CALL SCALE(XMIN, XMAX, NLX, MPVX, TEMP, XVSTEP, NXVALS, IRX,
        *        IFAIL)
        IF (IFAIL .GT. 0) GOTO 901
        XMIN = TEMP
        XSTEP = XVSTEP / MPVX
    ENDIF
    IF (YMIN .GE. YMAX) THEN
C
C CHOOSE YMIN AND YMAX
C
        YMAX = RVALS(2, 1)
        YMIN = RVALS(3, 1)
        DO 40 I = 2, NG
        IF (RVALS(2, I) .GT. YMAX) THEN
            YMAX = RVALS(2, I)
        ELSE IF (RVALS(3, I) .LT. YMIN) THEN
            YMIN = RVALS(3, I)
        ENDIF
40    CONTINUE
C
C CHECK IN OUTLIER ARRAY, ADJUST YMIN AND YMAX
C
        DO 50 I = 1, NOUT
        IF (OUTARR(I) .GT. YMAX) THEN
            YMAX = OUTARR(I)
        ELSE IF (OUTARR(I) .LT. YMIN) THEN
            YMIN = OUTARR(I)
        ENDIF
50    CONTINUE
    ENDIF
    CALL SCALE(YMIN, YMAX, NLY, MPVY, TEMP, YVSTEP, NYVALS, IRY,
```

```

      * IFAIL)
      IF (IFAIL .GT. 0) GOTO 902
      YMIN = TEMP
      YSTEP = YVSTEP / MPVY
C
C CONVERT TO PLOT UNITS
C
      DO 70 I = 1, NG
      DO 60 J = 2, 6
      IVALS2(J, I) = (RVALS(J, I) - YMIN) / YSTEP + 0.5
60 CONTINUE
C
C NOTCHES AT MEDIAN +/- 1.57 * IQR/SQRT(N)
C
      IF(NOTCH .AND. IVALS(5, I) .GT. 0) THEN
      QR = (RVALS(4, I) - RVALS(5, I)) * 1.57/SQRT(REAL(IVALS(5, I)))
      YDIFF = RVALS(6, I) - YMIN
      IVALS2(7, I) = (YDIFF + QR)/YSTEP + 0.5
      IVALS2(8, I) = (YDIFF - QR)/YSTEP + 0.5
      ENDIF
70 CONTINUE
      DO 80 I = 1, NG
      IF(XTYPE) THEN
      IVALS2(1, I) = (I - XMIN) / XSTEP + 1.5
      ELSE
      IVALS2(1, I) = (RVALS(1, I) - XMIN) / XSTEP + 1.5
      ENDIF
80 CONTINUE
      DO 90 I = 1, NOUT
      INTARR(I) = (OUTARR(I) - YMIN) / YSTEP + 0.5
90 CONTINUE
C
C CHECK OVERPRINTING ONLY IF WIDTH CALCULATED
C
      IF (WIDTH .EQ. 0) THEN
100      IF (WID .GT. 1) THEN
      LWIDOK = (IVALS2(1, 1) .GE. WID / 2 + 1 .AND.
      *          IVALS2(1, NG) .LE. NLX - (WID / 2 + 1))
      IF (.NOT. LWIDOK) GOTO 903
      DO 110 I = 2, NG
C
C CHECK GAPS BETWEEN BOXES
C
      *          IF (IVALS2(1, I) - IVALS2(1, I - 1) .LT. WID)
      LWIDOK = .FALSE.
110      CONTINUE
      IF (LWIDOK) GOTO 120
      WID = WID - 2
      GOTO 100
      ENDIF
120      CONTINUE
C
C LIMIT MUST PROVIDE ROOM FOR NOTCHES
C
      LIMIT = 3
      IF (NOTCH) LIMIT = 5
      IF (WID .LT. LIMIT) GOTO 903
      ENDIF
      DO 130 I = 1, NG
      IF (WIDTH .GE. 0) IVALS(6, I) = WID
C

```

```
C WIDTH MUST BE ODD EVEN IF EVEN VALUE SUPPLIED
C
      IF (MOD(IVAL5(6, I), 2) .EQ. 0) IVAL5(6, I) = IVAL5(6, I) + 1
      IF (IVAL5(6, I) .LT. 1) IVAL5(6, I) = 1
130 CONTINUE
      CALL AXIS(YMIN, YVSTEP, NYVALS, 6, IRY, IRPR, OFFSET, IFACT,
*           VALS, 20, IFAIL)
      IF (IFAIL .GT. 0) GOTO 904
      IFORM1(9:9) = INTCH(IRPR)
      IF (IFACT .NE. 0) WRITE(IWRITE, 2) IFACT
      IF (OFFSET .NE. 0.0) WRITE(IWRITE, 3) OFFSET
      DO 170 I = 1, NLY
C
C MAIN LOOP TO BUILD PLOT STARTS HERE
C
      IY = NLY - I
      IOUT(1:NLY) = ' '
C
C FIND CORRECT CODE
C
      DO 160 J = 1, NG
      IF (IVAL5(5, J) .GE. 1) THEN
        IX = IVAL52(1, J)
        ICODE = 0
        IF (IY .LE. IVAL52(2, J) .AND. IY .GE. IVAL52(3, J)) ICODE = 1
        POINTS = 0
        IF (IVAL5(1, J) .GT. 0) THEN
          PNTR = IVAL5(3, J)
          DO 140 K = 1, IVAL5(1, J)
            IF (INTARR(PNTR) .EQ. IY) POINTS = POINTS + 1
            PNTR = PNTR + 1
140          CONTINUE
          ENDIF
          IF (IVAL5(2, J) .GT. 0) THEN
            PNTR = IVAL5(4, J)
            DO 150 K = 1, IVAL5(2, J)
              IF (INTARR(PNTR) .EQ. IY) POINTS = POINTS + 1
              PNTR = PNTR + 1
150            CONTINUE
          ENDIF
          IF (POINTS .EQ. 1) ICODE = 2
          IF (POINTS .GT. 1) ICODE = 3
          IF (IY .EQ. IVAL52(4, J) .OR. IY .EQ. IVAL52(5, J)) ICODE = 4
          IF (IY .LT. IVAL52(4, J) .AND. IY .GT. IVAL52(5, J)) THEN
            ICODE = 5
            IF (NOTCH) THEN
              IF ((IY .LE. IVAL52(7, J) .AND. IY .GE. IVAL52(8, J)))
*                 ICODE = 6
            ENDIF
          ENDIF
          IF (IY .EQ. IVAL52(6, J)) ICODE = 7
          CALL SETGR(IOUT, IVAL5(6, J), ICODE, IX, NOTCH, NLY, IFAIL)
          IF (IFAIL .EQ. 1) IFAULT = - 1
        ENDIF
      ENDIF
      IF (MOD(IY, MPVY) .EQ. 0) THEN
        WRITE(IWRITE, IFORM1) VALS(NYVALS), DASH, COLON,
*           (IOUT(IX:IX), IX = 1, NLY)
      ENDIF
C
C UNABLE TO FIT ON PLOT
C
160 CONTINUE
      IF (MOD(IY, MPVY) .EQ. 0) THEN
        WRITE(IWRITE, IFORM1) VALS(NYVALS), DASH, COLON,
*           (IOUT(IX:IX), IX = 1, NLY)
      ENDIF
```

```
        NYVALS = NYVALS - 1
    ELSE
        WRITE(IWRITE, 1)(IOUT(IX:IX), IX = 1, NLX)
    ENDIF
170 CONTINUE
    WRITE(IWRITE, 1)(DOT, I = 1, NLX)
    IF ( .NOT. XTYPE) THEN
        CALL AXIS(XMIN, XVSTEP, NXVALS, 6, IRX, IRPR, OFFSET, IFACT,
*           VALS, 20, IFAIL)
        IF (IFAIL .GT. 0) GOTO 905
        IFORM2(15:15) = INTCH(IRPR)
        WRITE(IWRITE, 6)(COLON, I = 1, NXVALS)
        WRITE(IWRITE, IFORM2)(VALS(I), I = 1, NXVALS)
        IF (IFACT .NE. 0) WRITE(IWRITE, 4) IFACT
        IF (OFFSET .NE. 0.0) WRITE(IWRITE, 5) OFFSET
    ENDIF
C
C CHECK POINTS AND PARTS OF BOXES LYING BEYOND Y LIMITS
C
        IFAIL = 0
        DO 180 I = 1, NG
            IF (IVALS2(2, I) .GT. NLY - 1 .OR. IVALS2(3, I) .LT. 0) GOTO 190
180 CONTINUE
            GOTO 200
190 IFAULT = IFAULT - 2
200 DO 210 I = 1, NOUT
            IF (INTARR(I) .GT. NLY - 1 .OR. INTARR(I) .LT. 0) GOTO 220
210 CONTINUE
            RETURN
220 IFAULT = IFAULT - 4
            RETURN
1  FORMAT(11X, ':', 120A1)
2  FORMAT(' TIMES 10**', I3)
3  FORMAT(' OFFSET', F10.0)
4  FORMAT(15X, 'TIMES 10**', I3)
5  FORMAT(15X, 'OFFSET', F10.0)
6  FORMAT(3X, 16(9X, A1))
900 IFAULT = 1
    RETURN
901 IFAULT = 2
    RETURN
902 IFAULT = 3
    RETURN
903 IFAULT = 4
    RETURN
904 IFAULT = 5
    RETURN
905 IFAULT = 6
    RETURN
END
C
C
    SUBROUTINE SETGR(IOUT, WID, ICODE, IX, NOTCH, NLX, IFAIL)
C
C ALGORITHM AS 272.2 APPL.STATIST. (1992), VOL.41, NO.1
C
C PLACES CHARACTERS INTO IOUT AT POSITION IX
C CURRENT PART OF BOX CODED BY ICODE
C
    INTEGER WID, ICODE, IX, IFAIL
    CHARACTER VERT, STAR, PLUS, HORIZ, DASH
```



```
CHARACTER*120 IOUT
LOGICAL NOTCH
DATA VERT / ':' / , STAR / 'X' / , PLUS / '+' / , HORIZ / '-' / ,
* DASH / '=' /
IFAIL = 1
IF (IX .LT. 1 .OR. IX .GT. NLX) RETURN
IFAIL = 0
IW = WID / 2
IF (ICODE .EQ. 0) RETURN
IF (ICODE .EQ. 1) IOUT(IX:IX) = VERT
IF (ICODE .EQ. 2) IOUT(IX:IX) = STAR
IF (ICODE .EQ. 3) IOUT(IX:IX) = PLUS
IF (ICODE .LT. 4) RETURN
IXMIN = MAX(IX - IW, 1)
IXPLUS = MIN(IX + IW, NLX)
IF (ICODE .EQ. 4) THEN
  DO 10 I = IXMIN, IXPLUS
    IOUT(I:I) = HORIZ
10  CONTINUE
  RETURN
ENDIF
IF (ICODE .LT. 7) THEN
C
C IF WID LT 3 NO SIDES OF BOX OR NOTCHES
C
  IF (IW .LE. 0) RETURN
  IF (ICODE .EQ. 5) THEN
    IF (IX - IW .GE. 1) IOUT(IXMIN:IXMIN) = VERT
    IF (IX + IW .LE. NLX) IOUT(IXPLUS:IXPLUS) = VERT
  ENDIF
  IF (ICODE .EQ. 6) THEN
C
C IF ROOM MOVE SIDES OF BOX IN TO FORM NOTCH
C
    IF (WID .GT. 3) IXPLUS = IXPLUS - 1
    IF (IX + IW .LE. NLX) IOUT(IXPLUS:IXPLUS) = VERT
    IF (WID .GT. 3) IXMIN = IXMIN + 1
    IF (IX - IW .GE. 1) IOUT(IXMIN:IXMIN) = VERT
  ENDIF
  RETURN
ENDIF
IF (NOTCH .AND. WID .GT. 3) THEN
C
C MEDIAN SHORTER IF NOTCHED
C
  IXPLUS = IXPLUS - 1
  IXMIN = IXMIN + 1
ENDIF
DO 20 I = IXMIN, IXPLUS
  IOUT(I:I) = DASH
20 CONTINUE
IF (IW .GT. 0) THEN
C
C IF WID LT 3 DO NOT PUT SIDES OF BOX AT MEDIAN
C
  IF (IX - IW .GE. 1) IOUT(IXMIN:IXMIN) = VERT
  IF (IX + IW .LE. NLX) IOUT(IXPLUS:IXPLUS) = VERT
ENDIF
RETURN
END
```

Notes on AS 273 "Comparing subsets of regressor variables" by Alan Miller

This algorithm allows two regression subsets to be compared. It uses the method of Spj0tvoll (Ann. Math. Statist. vol.43, 1076-1088, 1972). The algorithm will typically be used after the use of some subset selection procedure, to make comparisons between subsets. It is a Scheffe-type procedure which gives a confidence level which applies simultaneously to all pairs of subsets from the same data set. The subsets may be of different numbers of variables, and there is no requirement that some or all of the variables in one subset must be in the other. For more details of the algorithm see chapter 4 of 'Subset selection in regression' by Alan Miller, Chapman & Hall, 1990 (ISBN 0 412 35380 6).

The algorithm calculates upper and lower confidence limits for the difference in regression sums of squares for the two subsets. If both limits are positive then the first subset has a significantly larger regression sum of squares than the first. If the range includes zero, the subsets do not differ significantly.

The user must enter F-values for the confidence levels required. The number of degrees of freedom for the numerator is equal to the total number of variables less any (such as the optional constant) forced into all subsets. The number of degrees of freedom for the denominator is equal to the number of degrees of freedom of the residual variance, or NCASES - NP.

Before calling this algorithm, the user must have first performed an orthogonal reduction of the data using Gentleman's algorithm (AS 75 or 274), or an equivalent algorithm.

The calling arguments are (real/dp means real or double precision):

NP	Input, integer	No. of variables in the orthogonal reduction
NRBAR	Input, integer	No. of elements in array RBAR (at least NP(NP-1)/2).
D	Input, real/dp array	Row multipliers from AS 75 or AS 274
RBAR	Input, real/dp array	Upper triangle of Cholesky factor without the diagonal elements (which are implicit 1's)
THETAB	Input, real/dp array	The least-squares projections of the dependent variable on the NP orthogonal directions
RSS	Input, real/dp array	RSS(I) is the residual sum of squares with the first I variables in the model (output from SS of AS 274)
TOL	Input, real/dp array	Array of tolerances from TOLSET in AS 274
NCASES	Input, integer	The number of cases on which the orthogonal reduction was based
VORDER	Input, integer array	An array of integer identifiers, one per variable
NFORCE	Input, integer	The number of variables which were forced into all subsets in the subset selection procedure (often = 1 for the constant term in all models)
LIST1	Input, integer array	Array of identifying integers (see VORDER above) for the variables in the first subset to be compared. Include variables which are forced in.
N1	Input, integer	The number of variables in LIST1.
LIST2	Input, integer array	The list of variables in the second subset.
N2	Input, integer	The number of variables in the second subset.
FVAL	Input, integer array	Array of F-values for the required confidence levels.
NF	Input, integer	The number of confidence levels required, usually only 1 or 2.
A1	Output, real/dp	Array of lower confidence limits corresponding to the

```

                array          input F values.
A2      Output, real/dp  Array of the corresponding upper confidence limits.
                array
WK      --, real/dp     Workspace, must be dimensioned at least 2N(N+1) where
                array          N = the number of variables which are in one subset
                                but not both.
DIMWK   Input, integer  The dimension of WK in the calling program.
IWK     --, integer     Workspace, must be dimensioned at least N.
                array
DIMIWK  Input, integer  The dimension of IWK in the calling program.
IFAULT  Output, integer Error indicator
                                = 0, no error detected
                                = -NEED, insufficient workspace provided for WK,
                                    increase to NEED.
                                = 1  NP < 2
                                = 2  NRBAR < NP(NP-1)/2
                                = 4  NCASES <= NP
                                = 8  either N1 or N2 exceeds NP
                                = 16 either N1 or N2 is negative
                                = 32 NF < 1
                                = 64 either NFORCE < 0 or NFORCE >= NP
                                = 128 LIST1 = LIST2, i.e. identical subsets
                                = 129 error in both lists, e.g. a repeated number or
                                    a number which is not in array VORDER
                                = 130 as for error 129 but only in LIST1
                                = 131 as for error 129 but only in LIST2
                                = 132 inadequate integer work space

```

Auxiliary routines required: TRED2 and TQL2 from EISPACK, or AS 60 to calculate the eigenvalues and vectors for a symmetric matrix. REORDR and VMOVE from algorithm AS 274.

Alan Miller  
25 November 1991

C-----

```

SUBROUTINE CONREG(NP, NRBAR, D, RBAR, THETAB, RSS, TOL, NCASES,
+  VORDER, NFORCE, LIST1, N1, LIST2, N2, FVAL, NF, A1, A2, WK,
+  DIMWK, IWK, DIMIWK, IFAULT)
C
C  ALGORITHM AS273  APPL. STATIST. (1992) VOL. 41, NO. 2
C
C  Calculate the Spj0tvoll confidence limits for the difference in
C  regression sums of squares of two subsets of variables.
C
C  Auxiliary routines required: TRED2, TQL2 (from EISPACK or AS 60),
C  and REORDR, VMOVE (from AS 274).
C
C  INTEGER NP, NRBAR, NCASES, VORDER(NP), NFORCE, N1, LIST1(N1), N2,
+  LIST2(N2), NF, DIMWK, DIMIWK, IWK(DIMIWK), IER
C  DOUBLE PRECISION D(NP), RBAR(NRBAR), THETAB(NP), RSS(NP), TOL(NP),
+  FVAL(NF), A1(NF), A2(NF), WK(DIMWK)
C
C  Local variables
C
C  INTEGER N0, I, L, J, K, N10, N20, N10N20, NEED, POS2, INC, POS1,
+  ROW, COL, ID, ITHETA, IRSS, ITOL, ROWPN0, ROWL1, NVAR, IZ,
+  M, IVAL, IMAX, IMIN
C  DOUBLE PRECISION ZERO, ONE, HALF, SCALE, TEMP, SUM, DIFF, SUME,
+  EMAX, EMIN, VAR, TEMPS, X, X1, X2, XTOL, A, B, GAMMA2

```

```
C
DATA ZERO/0.D0/, ONE/1.D0/, HALF/0.5D0/, XTOL/0.001D0/
C
C Some checks.
C
IER = 0
IF (NP .LT. 2) IER = 1
IF (NRBAR .LT. NP*(NP-1)/2) IER = IER + 2
IF (NCASES .LE. NP) IER = IER + 4
IF (N1 .GT. NP .OR. N2 .GT. NP) IER = IER + 8
IF (N1 .LT. 0 .OR. N2 .LT. 0) IER = IER + 16
IF (NF .LT. 1) IER = IER + 32
IF (NFORCE .LT. 0 .OR. NFORCE .GE. NP) IER = IER + 64
IF (IER .NE. 0) RETURN
C
C Find which variable numbers are on both lists and move them to
C the start.
C
N0 = 0
IF (N1 .EQ. 0 .OR. N2 .EQ. 0) GO TO 70
DO 60 I = 1, N1
  L = LIST1(I)
  DO 10 J = N0+1, N2
    IF (L .EQ. LIST2(J)) GO TO 20
10  CONTINUE
    GO TO 60
20  N0 = N0 + 1
    IF (I .EQ. N0) GO TO 40
    K = I
30  LIST1(K) = LIST1(K-1)
    K = K - 1
    IF (K .GT. N0) GO TO 30
    LIST1(N0) = L
C
40  IF (J .EQ. N0) GO TO 60
    K = J
50  LIST2(K) = LIST2(K-1)
    K = K - 1
    IF (K .GT. N0) GO TO 50
    LIST2(N0) = L
60 CONTINUE
C
C Exit if LIST1 = LIST2.
C
70 N10 = N1 - N0
   N20 = N2 - N0
   N10N20 = N10 + N20
   IF (N10N20 .EQ. 0) THEN
     IER = 128
     RETURN
   END IF
C
C Re-order the orthogonal reduction so that the N0 variables common
C to both lists are at the start.
C
IF (N0 .GT. 0) CALL REORDR(NP, NRBAR, VORDER, D, RBAR, THETAB,
+      RSS, TOL, LIST1, N0, 1, IER)
IF (IER .NE. 0) THEN
  IER = 129
  RETURN
END IF
```

```
C
C   Follow with the rest of the variables, if any, in LIST1, then any
C   any remaining from LIST2.
C
C   IF (N10 .GT. 0) CALL REORDR(NP, NRBAR, VORDER, D, RBAR, THETAB,
+       RSS, TOL, LIST1(N0+1), N10, N0+1, IER)
C   IF (IER .NE. 0) THEN
C       IER = 130
C       RETURN
C   END IF
C   IF (N20 .GT. 0) CALL REORDR(NP, NRBAR, VORDER, D, RBAR, THETAB,
+       RSS, TOL, LIST2(N0+1), N20, N1+1, IER)
C   IF (IER .NE. 0) THEN
C       IER = 131
C       RETURN
C   END IF
C
C   Estimate residual variance.
C
C   VAR = RSS(NP) / (NCASES - NP)
C
C   If N10 > 0 and N20 > 0, calculate the product of planar rotations
C   needed to place the N10 variables from LIST1 after the N20 from
C   LIST2 instead of before them.
C
C   IF (N10 .EQ. 0 .OR. N20 .EQ. 0) GO TO 400
C
C   Check that adequate workspace has been provided.
C
C   NEED = 2 * N10N20 * (N10N20 + 1)
C   IF (DIMWK .LT. NEED) THEN
C       IER = -NEED
C       RETURN
C   END IF
C   IF (DIMWK .LT. N10N20) THEN
C       IER = 132
C       RETURN
C   END IF
C
C   Copy the triangle of RBAR for the N10N20 rows and columns of
C   interest into WK with an N10N20 x N10N20 identity matrix added
C   as additional columns to store the product. Thus the contents
C   of WK look like (for N10N20 = 4):
C
C       X  X  X  1  0  0  0
C         X  X  0  1  0  0
C           X  0  0  1  0
C             0  0  0  1
C
C   As row multipliers are used by the square-root free method, the
C   reciprocals of the square roots of these multipliers are stored
C   on the diagonal instead of 1's.
C   POS2 = position within RBAR; INC = number of columns of RBAR to
C   be skipped in each row.
C
C   POS2 = N0 * (NP + NP - N0 - 1)/2 + 1
C   INC = NP - N0 - N10N20
C   POS1 = 1
C   DO 100 ROW = 1, N10N20
C       DO 80 COL = ROW+1, N10N20
C           WK(POS1) = RBAR(POS2)
C           POS1 = POS1 + 1
```

```

      POS2 = POS2 + 1
80  CONTINUE
      POS2 = POS2 + INC
      DO 90 COL = 1, N10N20
        IF (COL .EQ. ROW) THEN
          WK(POS1) = ONE / SQRT(D(ROW+N0))
        ELSE
          WK(POS1) = ZERO
        END IF
        POS1 = POS1 + 1
      90  CONTINUE
100 CONTINUE
C
C   Set up dummy arrays in WK for D, THETAB, RSS and TOL, and in IWK
C   for VORDER.
C
      ID = POS1
      ITHETA = ID + N10N20
      IRSS = ITHETA + N10N20
      ITOL = IRSS + N10N20
      DO 110 ROW = 1, N10N20
        ROWPN0 = ROW + N0
        ROWL1 = ROW - 1
        WK(ID + ROWL1) = D(ROWPN0)
        WK(ITHETA + ROWL1) = ZERO
        WK(IRSS + ROWL1) = RSS(ROWPN0)
        WK(ITOL + ROWL1) = TOL(ROWPN0)
        IWK(ROW) = VORDER(ROWPN0)
      110 CONTINUE
C
C   Swap positions of the N10 and N20 variables in WK.
C
      NVAR = 2 * N10N20
      DO 120 ROW = N10, 1, -1
120  CALL VMOVE(NVAR, DIMWK, IWK, WK(ID), WK, WK(ITHETA), WK(IRSS),
+      ROW, N10N20+ROW-N10, WK(ITOL), IER)
C
C   Scale the first N20 rows of the product and place at the start of
C   WK.  This is (P1, P2).
C
      POS2 = N10N20
      POS1 = 1
      DO 140 ROW = 1, N20
        SCALE = SQRT(WK(ID))
        ID = ID + 1
        DO 130 COL = 1, N10N20
          WK(POS1) = SCALE * WK(POS2)
          POS1 = POS1 + 1
          POS2 = POS2 + 1
        130  CONTINUE
        POS2 = POS2 + N10N20 - ROW - 1
      140 CONTINUE
C
C   Construct the matrix, Z, in WK from position IZ.
C
      Z = ( I 0 ) - ( P1' ) ( P1 P2 )
          ( 0 0 )   ( P2' )
C
      IZ = N10N20**2 + 1
      POS1 = IZ
      POS2 = IZ
      DO 170 ROW = 1, N10N20

```

```

    TEMP = ZERO
    IF (ROW .LE. N10) TEMP = ONE
    DO 160 COL = ROW, N10N20
        L = ROW
        J = COL
        DO 150 I = 1, N20
            TEMP = TEMP - WK(L)*WK(J)
            L = L + N10N20
            J = J + N10N20
150     CONTINUE
        WK(POS1) = TEMP
        WK(POS2) = TEMP
        POS1 = POS1 + 1
        POS2 = POS2 + N10N20
        TEMP = ZERO
160     CONTINUE
        POS1 = POS1 + ROW
        POS2 = POS1
170 CONTINUE
C
C     Put a copy of Z at the start of WK.
C
    POS2 = IZ
    DO 180 I = 1, IZ-1
        WK(I) = WK(POS2)
        POS2 = POS2 + 1
180 CONTINUE
C
C     Calculate the eigenvalues (stored from location IVAL in WK), and
C     the normalized eigenvectors (stored from location IZ).
C
    IVAL = 2*IZ - 1
    L = IVAL + N10N20**2
    CALL TRED2(N10N20, N10N20, WK, WK(IVAL), WK(L), WK(IZ))
    CALL TQL2(N10N20, N10N20, WK(IVAL), WK(L), WK(IZ), IER)
C
C     Calculate the transformed projections (Spj0tvoll's gammas) and
C     store at the start of WK.  Put the sum of squares of gamma(i).
C     lambda(i) into SUME.
C
    L = IZ
    SUME = ZERO
    DO 250 I = 1, N10N20
        M = N0 + 1
        SUM = ZERO
        DO 240 J = 1, N10N20
            SUM = SUM + WK(L)*THETAB(M)*SQRT(D(M))
            L = L + 1
            M = M + 1
240     CONTINUE
        WK(I) = SUM
        SUME = SUME + (SUM*WK(IVAL+I-1))**2
250 CONTINUE
C
C     Find the max. and min. non-zero eigenvalues.
C
    EMAX = WK(IVAL)
    EMIN = EMAX
    IMAX = 1
    IMIN = 1
    L = IVAL + 1

```

```

DO 260 I = 2, N10N20
  TEMP = WK(L)
  L = L + 1
  IF (TEMP .GT. EMAX) THEN
    EMAX = TEMP
    IMAX = I
  ELSE IF (TEMP .LT. EMIN) THEN
    EMIN = TEMP
    IMIN = I
  END IF
260 CONTINUE
C
C   Cycle through the NF confidence levels.
C
DO 310 K = 1, NF
  TEMP = VAR * (NP - NFORCE) * FVAL(K)
  TEMPS = SQRT(TEMP)
C
C   Find largest and smallest roots of Spj0tvoll's equation (3.2).
C
  X1 = EMIN - ABS(EMIN * WK(IMIN)) / TEMPS
  X2 = EMIN - SQRT(SUME / TEMP)
DO 290 I = 1, 2
270   X = HALF * (X1 + X2)
      L = IVAL
      SUM = -TEMP
      DO 280 J = 1, N10N20
        SUM = SUM + (WK(L)*WK(J)/(WK(L) - X)**2
        L = L + 1
280   CONTINUE
      IF (SUM .LE. ZERO) THEN
        X2 = X
      ELSE
        X1 = X
      END IF
      IF (ABS(X1 - X2) .GT. XTOL) GO TO 270
      X = HALF * (X1 + X2)
      IF (I .EQ. 1) THEN
        A = - X
        X1 = EMAX + ABS(EMAX * WK(IMAX)) / TEMPS
        X2 = EMAX + SQRT(SUME / TEMP)
      ELSE
        B = X
      END IF
290   CONTINUE
C
C   Calculate A1 and A2.
C
  A1(K) = -TEMP
  A2(K) = TEMP
  L = IVAL
DO 300 I = 1, N10N20
  GAMMA2 = WK(I)**2
  TEMP = WK(L)
  L = L + 1
  A1(K) = A1(K) + TEMP * GAMMA2 / (A + TEMP)
  A2(K) = A2(K) + TEMP * GAMMA2 / (B - TEMP)
300   CONTINUE
  A1(K) = A * A1(K)
  A2(K) = B * A2(K)
310   CONTINUE

```



```
C
      RETURN
C-----
C      Special cases; either N10 or N20 = 0.
C
400  GAMMA2 = RSS(N0) - RSS(N1+N20)
      DO 410 K = 1, NF
          TEMP = SQRT(VAR * (NP - NFORCE) * FVAL(K))
          TEMPS = SQRT(GAMMA2)
          SUM = (TEMPS + TEMP)**2
          DIFF = MAX(ZERO, TEMPS-TEMP)
          DIFF = DIFF**2
          IF (N10 .EQ. 0) THEN
              A1(K) = -SUM
              A2(K) = -DIFF
          ELSE
              A1(K) = DIFF
              A2(K) = SUM
          END IF
      410  CONTINUE
C
      RETURN
      END
```

Notes on AS 274 "Least-squares routines to supplement those of Gentleman" by Alan Miller.

This algorithm provides a set of high accuracy least squares routines which expand upon those provided by Gentleman in AS 75. In particular, it includes facilities for (weighted) least-squares for a subset of the variables, for changing the order of the variables, for testing for singularities, and for calculating an estimated covariance matrix for the regression coefficients.

The algorithm is NOT consistent with those which have been published in the same journal by Clarke (AS 163), Stirling (AS 164) or Smith (AS 268), in that the orthogonal reduction is stored in a different way. It is unfortunate that these authors have not used the same format as Gentleman.

The basic algorithm is the same as Gentleman's. As each new case is added, the orthogonal reduction is updated. In traditional least-squares notation, the algorithm goes straight from the X-matrix (the 'design' matrix) to the Cholesky factorization WITHOUT the intermediate step of forming a sum of squares and products matrix. Thus it avoids squaring the condition number. To be pedantic, it is actually the Banachiewicz factorization which is used. We use:

$$Q X = \text{sqrt}(D) R$$

where Q is an orthonormal matrix such that  $Q'Q = I$ , D is a diagonal matrix ( $\text{sqrt}(D)$  is my crude way of indicating a diagonal matrix with elements on the diagonal which are the square roots of the elements stored in array D in the routines), and R is an upper triangular matrix with 1's on the diagonal. The array R is stored in a 1-dimensional array with elements stored by rows as shown below (the 1's on the diagonal are NOT stored).

```
Storage of R:  (1)  1  2  3  4  5
                (1)  6  7  8  9
                (1) 10 11 12
                (1) 13 14
                (1) 15
                (1)
```

N.B. The matrix Q is a product of planar-rotation matrices (Jacobi/Givens rotations); it is not calculated or stored.

N.B. If you want to fit a constant (intercept) in your model, you can do it by putting the first element of each row of X equal to 1.0.

N.B. You may like to dimension XROW as XROW(0:K) in your calling program, where K is the number of variables (other than the constant). The parameter NP passed to routine INCLUD (and others) then takes the value K+1.

To perform the calculation of regression coefficients (and nothing else), you need to call the following routines in the order given:

1. clear - initializes arrays
2. includ - call once for each case to update the orthogonal reduction
3. tolset - calculates tolerances for each variable
4. sing (optional) - tests for singularities
5. regcf - calculates regression coefficients for the first NREQ variables

You can then add extra data and recalculate the regression coefficients.

Other routines (all require that 1 and 2 above have been used first).

- ss calculates array RSS such that  $RSS(I) =$  the residual sum of squares with the first I variables in the model
- cov calculates the estimated covariance matrix of the regression coefficients (the user must input a value for the residual variance VAR, usually the

residual sum of squares SSERR divided by NOBS - NP for all variables, or RSS(I) divided by NOBS - I for the first I variables).

pcorr calculates partial correlations with the first IN variables in the model. If IN = 1 and the first variable is identically equal to 1 then these are the usual full correlations. If IN = 0 it gives the cross products (not centered) divided by the square root of the product of the second moments (about zero) of the two variables.

vmove moves the variable in position FROM to position TO.

reordr calls vmove repeatedly to re-order the variables from the current order in integer array VORDER to that in the integer array LIST.

hdiag calculates the diagonal elements of the 'hat' matrix used in various diagnostic statistics.

For vmove and reordr, the user must first set up an integer array VORDER which assigns a unique integer value with each variable. You may like to associate the value 0 with the constant in the model.

For cov, vmove, reordr and hdiag you must call tolset first.

\*\*\* Warning \*\*\* Routine INCLUD (from Gentleman's AS 75) overwrites the elements in array XROW.

Alan Miller  
25 November 1991

#### Notes on handling singularities

-----  
If there is a singularity amongst your X-variables and routine SING is not used, you will get wrong answers from most routines. The orthogonal reduction can be written as:

$$X = Q' \text{sqrt}(D) R$$

If we denote the columns of X as X1, X2, ..., Xk, and the columns of Q' as q1, q2, ..., qk, then we have:

$$\begin{aligned} x1 &= r(11).q1 \\ x2 &= r(12).q1 + r(22).q2 \\ x3 &= r(13).q1 + r(23).q2 + r(33).q3 \end{aligned}$$

etc., where r(ij) = the (i,j)-element of R multiplied by the square root of the i-th diagonal element of D. That is x1 is equal to the first orthogonal direction, q1, multiplied by a scaling factor. x2 = a projection of length r(12) in the first direction, q1, plus a projection of length r(22) in a new direction, q2, which is orthogonal to q1, etc. If the X-directions are all orthogonal then all of the r(ij)'s for off-diagonal elements of R will be zero.

Let us suppose that there is a singularity amongst the X-variables, that is that one of the X-variables is exactly linearly related to some of the others. For simplicity, let us suppose that  $x3 = a.x1 + b.x2$ . The direction q3 is formed from x3 by subtracting its projections in directions q1 and q2 and then scaling so that it has length equal to 1. When the projections in directions q1 and q2 are subtracted in this case, there should be nothing left. In practice, there will be almost always be small rounding errors. Direction q3 will be formed from these rounding errors. Thus we will have a rogue direction in the columns of Q'. The projections of the dependant variable on this direction can be large. It is like correlating the Y-variable on a variable formed by using random numbers or a column of numbers from the phone directory.

Routine SING sets the projections on this direction equal to zero.

In the case just mentioned, a full rank X could be obtained by removing any one of the variables x1, x2 or x3. In AS274, the equivalent to removing a variable is to move it to the last position and then to only use the first (k-1) variables in subsequent calculations. You still tell routines such as REGCF that there are NP variables, but you set NREQ = NP - 1.

If you just want properties of a subset of variables, then you use either VMOVE or REORDR to re-order the variables so that the first ones are those which you are interested in, and you set NREQ equal to the number of those variables. In most cases, the constant (intercept) will be included in the model and so will be included in the count of variables, NREQ (N-required).

Features NOT included in AS274

-----

There is no facility for removing or adding variables (columns). This could be done but adding variables requires the storage of the Q-matrix, or at least of the rotations used to form it.

There is no facility for two or more dependant variables, though this is fairly easy to program. The extra dependant variables can be treated as X-variables. Thus if we have dependant variables Y1, Y2 and Y3, then Y2 and Y3 can be added at the end of the list of X-variables. When looking at the properties of Y1 related to the X-variables, use only the first (NP-2) columns by setting NREQ = NP-2. When you want to look at Y2, just copy column (NP-1) of RBAR into THETAB - this requires a little thought to work out just where those elements are stored. You may want to first copy the original THETAB, or to copy the column of RBAR into a different array, perhaps THETAB2 say. The residual sum of squares, SSERR, for variable Y2 is D(NP-1).

Y3 is a little more difficult. You must first change the order of the variables so that Y3 is before Y2, otherwise you will be regressing Y3 on Y2, and you probably don't want to do that.

The easy way of thinking about the above is by considering each column of R (after scaling by the square roots of the diagonal elements of D) as the projections of the corresponding variable on all of those which have preceded it. The Y-variable is just another variable being projected upon a set of orthogonal directions formed by the variables which came before it. The vector THETAB is stored separately just for fast access as most users will have only one Y-variable; it could have been incorporated as the last column of RBAR.

Alan Miller  
2 May 1993

C-----

```
      SUBROUTINE INCLUD(NP, NRBAR, WEIGHT, XROW, YELEM, D, RBAR, THETAB,
+      SSERR, IER)
```

```
C
C   ALGORITHM AS274.1  APPL. STATIST. (1992) VOL 41, NO. 2
```

```
C
C   DOUBLE PRECISION VERSION
```

```
C
C   Calling this routine updates d, rbar, thetab and sserr by the
C   inclusion of xrow, yelem with the specified weight.
C   This version has been modified to make it slightly faster when the
C   early elements of XROW are not zeroes.
```

```
C
C   *** WARNING ***   The elements of XROW are over-written.
C
C   INTEGER NP, NRBAR, IER
C   DOUBLE PRECISION WEIGHT, XROW(NP), YELEM, D(NP), RBAR(*),
+   THETAB(NP), SSERR
C
C   Local variables
C
C   INTEGER I, K, NEXTR
C   DOUBLE PRECISION ZERO, W, Y, XI, DI, WXI, DPI, CBAR, SBAR, XK
C
C   DATA ZERO/0.DO/
C
C   Some checks.
C
C   IER = 0
C   IF (NP .LT. 1) IER = 1
C   IF (NRBAR .LT. NP*(NP-1)/2) IER = IER + 2
C   IF (IER .NE. 0) RETURN
C
C   W = WEIGHT
C   Y = YELEM
C   NEXTR = 1
C   DO 30 I = 1, NP
C
C   Skip unnecessary transformations.   Test on exact zeroes must be
C   used or stability can be destroyed.
C
C   IF (W .EQ. ZERO) RETURN
C   XI = XROW(I)
C   IF (XI .EQ. ZERO) THEN
C     NEXTR = NEXTR + NP - I
C     GO TO 30
C   END IF
C   DI = D(I)
C   WXI = W * XI
C   DPI = DI + WXI*XI
C   CBAR = DI / DPI
C   SBAR = WXI / DPI
C   W = CBAR * W
C   D(I) = DPI
C   IF (I .EQ. NP) GO TO 20
C   DO 10 K = I+1, NP
C     XK = XROW(K)
C     XROW(K) = XK - XI * RBAR(NEXTR)
C     RBAR(NEXTR) = CBAR * RBAR(NEXTR) + SBAR * XK
C     NEXTR = NEXTR + 1
10  CONTINUE
20  XK = Y
C     Y = XK - XI * THETAB(I)
C     THETAB(I) = CBAR * THETAB(I) + SBAR * XK
30  CONTINUE
C
C   Y * SQRT(W) is now equal to the Brown, Durbin & Evans recursive
C   residual.
C
C   SSERR = SSERR + W * Y * Y
C
C   RETURN
C   END
```

```
C
SUBROUTINE CLEAR(NP, NRBAR, D, RBAR, THETAB, SSERR, IER)
C
C ALGORITHM AS274.2 APPL. STATIST. (1992) VOL.41, NO.2
C
C Sets arrays to zero prior to calling AS75.1
C
C INTEGER NP, NRBAR, IER
C DOUBLE PRECISION D(NP), RBAR(*), THETAB(NP), SSERR
C
C Local variables
C
C INTEGER I
C DOUBLE PRECISION ZERO
C
C DATA ZERO/0.D0/
C
C Some checks.
C
C IER = 0
C IF (NP .LT. 1) IER = 1
C IF (NRBAR .LT. NP*(NP-1)/2) IER = IER + 2
C IF (IER .NE. 0) RETURN
C
C DO 10 I = 1, NP
C   D(I) = ZERO
C   THETAB(I) = ZERO
10 CONTINUE
C DO 20 I = 1, NRBAR
20 RBAR(I) = ZERO
C SSERR = ZERO
C RETURN
C END
C
C SUBROUTINE REGCF(NP, NRBAR, D, RBAR, THETAB, TOL, BETA, NREQ,
+ IER)
C
C ALGORITHM AS274.3 APPL. STATIST. (1992) VOL 41, NO.2
C
C Modified version of AS75.4 to calculate regression coefficients
C for the first NREQ variables, given an orthogonal reduction from
C AS75.1.
C
C INTEGER NP, NRBAR, NREQ, IER
C DOUBLE PRECISION D(NP), RBAR(*), THETAB(NP), TOL(NP), BETA(NP)
C
C Local variables
C
C INTEGER I, J, NEXTR
C DOUBLE PRECISION ZERO
C
C DATA ZERO/0.D0/
C
C Some checks.
C
C IER = 0
C IF (NP .LT. 1) IER = 1
C IF (NRBAR .LT. NP*(NP-1)/2) IER = IER + 2
C IF (NREQ .LT. 1 .OR. NREQ .GT. NP) IER = IER + 4
C IF (IER .NE. 0) RETURN
C
```

```
      DO 20 I = NREQ, 1, -1
        IF (SQRT(D(I)) .LT. TOL(I)) THEN
          BETA(I) = ZERO
          D(I) = ZERO
          GO TO 20
        END IF
        BETA(I) = THETAB(I)
        NEXTR = (I-1) * (NP+NP-I)/2 + 1
        DO 10 J = I+1, NREQ
          BETA(I) = BETA(I) - RBAR(NEXTR) * BETA(J)
          NEXTR = NEXTR + 1
10      CONTINUE
20     CONTINUE
C
      RETURN
      END
C
      SUBROUTINE TOLSET(NP, NRBAR, D, RBAR, TOL, WORK, IER)
C
C      ALGORITHM AS274.4  APPL. STATIST. (1992) VOL 41, NO.2
C
C      Sets up array TOL for testing for zeroes in an orthogonal
C      reduction formed using AS75.1.
C
      INTEGER NP, NRBAR, IER
      DOUBLE PRECISION D(NP), RBAR(*), TOL(NP), WORK(NP)
C
C      Local variables.
C
      INTEGER COL, ROW, POS
      DOUBLE PRECISION EPS, SUM
C
C      EPS is a machine-dependent constant.  For compilers which use
C      the IEEE format for floating-point numbers, recommended values
C      are 1.E-06 for single precision and 1.E-15 for double precision.
C
      DATA EPS/1.D-15/
C
C      Some checks.
C
      IER = 0
      IF (NP .LT. 1) IER = 1
      IF (NRBAR .LT. NP*(NP-1)/2) IER = IER + 2
      IF (IER .NE. 0) RETURN
C
C      Set TOL(I) = sum of absolute values in column I of RBAR after
C      scaling each element by the square root of its row multiplier.
C
      DO 10 COL = 1, NP
10     WORK(COL) = SQRT(D(COL))
      DO 30 COL = 1, NP
        POS = COL - 1
        SUM = WORK(COL)
        DO 20 ROW = 1, COL-1
          SUM = SUM + ABS(RBAR(POS)) * WORK(ROW)
          POS = POS + NP - ROW - 1
20      CONTINUE
        TOL(COL) = EPS * SUM
30     CONTINUE
C
      RETURN
```

```

      END
C
      SUBROUTINE SING(NP, NRBAR, D, RBAR, THETAB, SSERR, TOL, LINDEP,
+      WORK, IER)
C
C      ALGORITHM AS274.5  APPL. STATIST. (1992) VOL 41, NO.2
C
C      Checks for singularities, reports, and adjusts orthogonal
C      reductions produced by AS75.1.
C
      INTEGER NP, NRBAR, IER
      DOUBLE PRECISION D(NP), RBAR(NRBAR), THETAB(NP), SSERR, TOL(NP),
+      WORK(NP)
      LOGICAL LINDEP(NP)
C
C      Local variables
C
      DOUBLE PRECISION ZERO, TEMP
      INTEGER COL, POS, ROW, NP2, POS2
C
      DATA ZERO/0.DO/
C
C      Check input parameters
C
      IER = 0
      IF (NP .LE. 0) IER = 1
      IF (NRBAR .LT. NP*(NP-1)/2) IER = IER + 2
      IF (IER .NE. 0) RETURN
C
      DO 10 COL = 1, NP
10  WORK(COL) = SQRT(D(COL))
C
      DO 40 COL = 1, NP
C
C      Set elements within RBAR to zero if they are less than TOL(COL) in
C      absolute value after being scaled by the square root of their row
C      multiplier.
C
      TEMP = TOL(COL)
      POS = COL - 1
      DO 30 ROW = 1, COL-1
          IF (ABS(RBAR(POS)) * WORK(ROW) .LT. TEMP) RBAR(POS) = ZERO
          POS = POS + NP - ROW - 1
30  CONTINUE
C
C      If diagonal element is near zero, set it to zero, set appropriate
C      element of LINDEP, and use INCLUD to augment the projections in
C      the lower rows of the orthogonalization.
C
      LINDEP(COL) = .FALSE.
      IF (WORK(COL) .LT. TEMP) THEN
          LINDEP(COL) = .TRUE.
          IER = IER - 1
          IF (COL .LT. NP) THEN
              NP2 = NP - COL
              POS2 = POS + NP - COL + 1
              CALL INCLUD(NP2, NP2*(NP2-1)/2, D(COL), RBAR(POS+1),
+              THETAB(COL), D(COL+1), RBAR(POS2), THETAB(COL+1),
+              SSERR, IER)
          ELSE
              SSERR = SSERR + D(COL) * THETAB(COL)**2

```



```
        END IF
        D(COL) = ZERO
        WORK(COL) = ZERO
        THETAB(COL) = ZERO
    END IF
40 CONTINUE
RETURN
END

C
SUBROUTINE SS(NP, D, THETAB, SSERR, RSS, IER)
C
C ALGORITHM AS274.6 APPL. STATIST. (1992) VOL 41, NO.2
C
C Calculates partial residual sums of squares from an orthogonal
C reduction from AS75.1.
C
C INTEGER NP, IER
C DOUBLE PRECISION D(NP), THETAB(NP), SSERR, RSS(NP)
C
C Local variables
C
C INTEGER I
C DOUBLE PRECISION SUM
C
C Some checks.
C
C IER = 0
C IF (NP .LT. 1) IER = 1
C IF (IER .NE. 0) RETURN
C
C SUM = SSERR
C RSS(NP) = SSERR
C DO 10 I = NP, 2, -1
C     SUM = SUM + D(I) * THETAB(I)**2
C     RSS(I-1) = SUM
10 CONTINUE
RETURN
END

C
SUBROUTINE COV(NP, NRBAR, D, RBAR, NREQ, RINV, VAR, COVMAT,
+ DIMCOV, STERR, IER)
C
C ALGORITHM AS274.7 APPL. STATIST. (1992) VOL 41, NO.2
C
C Calculate covariance matrix for regression coefficients for the
C first NREQ variables, from an orthogonal reduction produced from
C AS75.1.
C
C Auxiliary routine called: INV
C
C INTEGER NP, NRBAR, NREQ, DIMCOV, IER
C DOUBLE PRECISION D(NP), RBAR(*), RINV(*), VAR, COVMAT(DIMCOV),
+ STERR(NP)
C
C Local variables.
C
C INTEGER POS, ROW, START, POS2, COL, POS1, K
C DOUBLE PRECISION ZERO, ONE, SUM
C
C DATA ZERO/0.D0/, ONE/1.D0/
C
```

```
C      Some checks.
C
      IER = 0
      IF (NP .LT. 1) IER = 1
      IF (NRBAR .LT. NP*(NP-1)/2) IER = IER + 2
      IF (DIMCOV .LT. NREQ*(NREQ+1)/2) IER = IER + 4
      DO 10 ROW = 1, NREQ
         IF (D(ROW) .EQ. ZERO) IER = -ROW
10 CONTINUE
      IF (IER .NE. 0) RETURN
C
      CALL INV(NP, NRBAR, RBAR, NREQ, RINV)
      POS = 1
      START = 1
      DO 40 ROW = 1, NREQ
         POS2 = START
         DO 30 COL = ROW, NREQ
            POS1 = START + COL - ROW
            IF (ROW .EQ. COL) THEN
               SUM = ONE / D(COL)
            ELSE
               SUM = RINV(POS1-1) / D(COL)
            END IF
            DO 20 K = COL+1, NREQ
               SUM = SUM + RINV(POS1) * RINV(POS2) / D(K)
               POS1 = POS1 + 1
               POS2 = POS2 + 1
20          CONTINUE
            COVMAT(POS) = SUM * VAR
            IF (ROW .EQ. COL) STERR(ROW) = SQRT(COVMAT(POS))
            POS = POS + 1
30          CONTINUE
            START = START + NREQ - ROW
40 CONTINUE
C
      RETURN
      END
C
      SUBROUTINE INV(NP, NRBAR, RBAR, NREQ, RINV)
C
C      ALGORITHM AS274.8  APPL. STATIST. (1992) VOL 41, NO.2
C
C      Invert first NREQ rows and columns of Cholesky factorization
C      produced by AS75.1.
C
      INTEGER NP, NRBAR, NREQ
      DOUBLE PRECISION RBAR(*), RINV(*)
C
C      Local variables.
C
      INTEGER POS, ROW, COL, START, K, POS1, POS2
      DOUBLE PRECISION SUM, ZERO
C
      DATA ZERO/0.D0/
C
C      Invert RBAR ignoring row multipliers, from the bottom up.
C
      POS = NREQ * (NREQ-1)/2
      DO 30 ROW = NREQ-1, 1, -1
         START = (ROW-1) * (NP+NP-ROW)/2 + 1
         DO 20 COL = NREQ, ROW+1, -1
```

```
        POS1 = START
        POS2 = POS
        SUM = ZERO
        DO 10 K = ROW+1, COL-1
            POS2 = POS2 + NREQ - K
            SUM = SUM - RBAR(POS1) * RINV(POS2)
            POS1 = POS1 + 1
10      CONTINUE
        RINV(POS) = SUM - RBAR(POS1)
        POS = POS - 1
20      CONTINUE
30      CONTINUE
C
        RETURN
        END
C
        SUBROUTINE PCORR(NP, NRBAR, D, RBAR, THETAB, SSERR, IN, WORK,
+          CORMAT, DIMC, YCORR, IER)
C
C      ALGORITHM AS274.9  APPL. STATIST. (1992) VOL 41, NO.2
C
C      Calculate partial correlations after the first IN variables
C      have been forced into the regression.
C
C      Auxiliary routine called: COR
C
        INTEGER NP, NRBAR, IN, DIMC, IER
        DOUBLE PRECISION D(NP), RBAR(*), THETAB(NP), SSERR, WORK(NP),
+          CORMAT(*), YCORR
C
C      Local variables.
C
        INTEGER START, IN1, I
        DOUBLE PRECISION ZERO
C
        DATA ZERO/0.DO/
C
C      Some checks.
C
        IER = 0
        IF (NP .LT. 1) IER = 1
        IF (NRBAR .LT. NP*(NP-1)/2) IER = IER + 2
        IF (IN .LT. 0 .OR. IN .GT. NP-1) IER = IER + 4
        IF (DIMC .LT. (NP-IN)*(NP-IN-1)/2) IER = IER + 8
        IF (IER .NE. 0) RETURN
C
        START = IN * (NP+NP-IN-1)/2 + 1
        IN1 = IN + 1
        CALL COR(NP-IN, D(IN1), RBAR(START), THETAB(IN1), SSERR, WORK,
+          CORMAT, YCORR)
C
C      Check for zeroes.
C
        DO 10 I = 1, NP-IN
            IF (WORK(I) .LE. ZERO) IER = -I
10      CONTINUE
C
        RETURN
        END
C
        SUBROUTINE COR(NP, D, RBAR, THETAB, SSERR, WORK, CORMAT, YCORR)
```

```
C
C   ALGORITHM AS274.10  APPL. STATIST. (1992) VOL 41, NO.2
C
C   Calculate correlations from an orthogonal reduction.  This
C   routine will usually be called from PCORR, which will have
C   removed the appropriate number of rows at the start.
C
C   INTEGER NP
C   DOUBLE PRECISION D(NP), RBAR(*), THETAB(NP), SSERR, WORK(NP),
+     CORMAT(*), YCORR(NP)
C
C   Local variables.
C
C   INTEGER ROW, POS, COL1, POS1, COL2, POS2, DIFF
C   DOUBLE PRECISION SUMY, SUM, ZERO
C
C   DATA ZERO/0.DO/
C
C   Process by columns, including the projections of the dependent
C   variable (THETAB).
C
C   SUMY = SSERR
C   DO 10 ROW = 1, NP
10  SUMY = SUMY + D(ROW) * THETAB(ROW)**2
C   SUMY = SQRT(SUMY)
C   POS = NP*(NP-1)/2
C   DO 70 COL1 = NP, 1, -1
C
C   Calculate the length of column COL1.
C
C   SUM = D(COL1)
C   POS1 = COL1 - 1
C   DO 20 ROW = 1, COL1-1
C     SUM = SUM + D(ROW) * RBAR(POS1)**2
C     POS1 = POS1 + NP - ROW - 1
20  CONTINUE
C   WORK(COL1) = SQRT(SUM)
C
C   If SUM = 0, set all correlations with this variable to zero.
C
C   IF (SUM .EQ. ZERO) THEN
C     YCORR(COL1) = ZERO
C     DO 30 COL2 = NP, COL1+1, -1
C       CORMAT(POS) = ZERO
C       POS = POS - 1
30  CONTINUE
C     GO TO 70
C   END IF
C
C   Form cross-products, then divide by product of column lengths.
C
C   SUM = D(COL1) * THETAB(COL1)
C   POS1 = COL1 - 1
C   DO 40 ROW = 1, COL1-1
C     SUM = SUM + D(ROW) * RBAR(POS1) * THETAB(ROW)
C     POS1 = POS1 + NP - ROW - 1
40  CONTINUE
C   YCORR(COL1) = SUM / (SUMY * WORK(COL1))
C
C   DO 60 COL2 = NP, COL1+1, -1
C     IF (WORK(COL2) .GT. ZERO) THEN
```

```
        POS1 = COL1 - 1
        POS2 = COL2 - 1
        DIFF = COL2 - COL1
        SUM = ZERO
        DO 50 ROW = 1, COL1-1
            SUM = SUM + D(ROW) * RBAR(POS1) * RBAR(POS2)
            POS1 = POS1 + NP - ROW - 1
            POS2 = POS1 + DIFF
50      CONTINUE
        SUM = SUM + D(COL1) * RBAR(POS2)
        CORMAT(POS) = SUM / (WORK(COL1) * WORK(COL2))
        ELSE
            CORMAT(POS) = ZERO
        END IF
        POS = POS - 1
60      CONTINUE
70      CONTINUE
C
        RETURN
        END
C
        SUBROUTINE VMOVE(NP, NRBAR, VORDER, D, RBAR, THETAB, RSS, FROM,
+      TO, TOL, IER)
C
C      ALGORITHM AS274.11 APPL. STATIST. (1992) VOL 41, NO.2
C
C      Move variable from position FROM to position TO in an
C      orthogonal reduction produced by AS75.1.
C
        INTEGER NP, NRBAR, VORDER(NP), FROM, TO, IER
        DOUBLE PRECISION D(NP), RBAR(*), THETAB(NP), RSS(NP), TOL(NP)
C
C      Local variables
C
        DOUBLE PRECISION ZERO, D1, D2, X, ONE, D1NEW, D2NEW, CBAR, SBAR, Y
        INTEGER M, FIRST, LAST, INC, M1, M2, MP1, COL, POS, ROW
C
        DATA ZERO/0.D0/, ONE/1.D0/
C
C      Check input parameters
C
        IER = 0
        IF (NP .LE. 0) IER = 1
        IF (NRBAR .LT. NP*(NP-1)/2) IER = IER + 2
        IF (FROM .LT. 1 .OR. FROM .GT. NP) IER = IER + 4
        IF (TO .LT. 1 .OR. TO .GT. NP) IER = IER + 8
        IF (IER .NE. 0) RETURN
C
        IF (FROM .EQ. TO) RETURN
C
        IF (FROM .LT. TO) THEN
            FIRST = FROM
            LAST = TO - 1
            INC = 1
        ELSE
            FIRST = FROM - 1
            LAST = TO
            INC = -1
        END IF
        DO 70 M = FIRST, LAST, INC
C
```

C Find addresses of first elements of RBAR in rows M and (M+1).

C  
 $M1 = (M-1) * (NP+NP-M) / 2 + 1$   
 $M2 = M1 + NP - M$   
 $MP1 = M + 1$   
 $D1 = D(M)$   
 $D2 = D(MP1)$

C  
 C Special cases.

IF (D1 .EQ. ZERO .AND. D2 .EQ. ZERO) GO TO 40  
 $X = RBAR(M1)$   
 IF (ABS(X) \* SQRT(D1) .LT. TOL(MP1)) THEN  
 $X = ZERO$   
 END IF

IF (D1 .EQ. ZERO .OR. X .EQ. ZERO) THEN  
 $D(M) = D2$   
 $D(MP1) = D1$   
 $RBAR(M1) = ZERO$   
 DO 10 COL = M+2, NP  
 $M1 = M1 + 1$   
 $X = RBAR(M1)$   
 $RBAR(M1) = RBAR(M2)$   
 $RBAR(M2) = X$   
 $M2 = M2 + 1$

10 CONTINUE  
 $X = THETAB(M)$   
 $THETAB(M) = THETAB(MP1)$   
 $THETAB(MP1) = X$   
 GO TO 40  
 ELSE IF (D2 .EQ. ZERO) THEN  
 $D(M) = D1 * X**2$   
 $RBAR(M1) = ONE / X$   
 DO 20 COL = M+2, NP  
 $M1 = M1 + 1$   
 $RBAR(M1) = RBAR(M1) / X$

20 CONTINUE  
 $THETAB(M) = THETAB(M) / X$   
 GO TO 40  
 END IF

C  
 C Planar rotation in regular case.

$D1NEW = D2 + D1 * X**2$   
 $CBAR = D2 / D1NEW$   
 $SBAR = X * D1 / D1NEW$   
 $D2NEW = D1 * CBAR$   
 $D(M) = D1NEW$   
 $D(MP1) = D2NEW$   
 $RBAR(M1) = SBAR$   
 DO 30 COL = M+2, NP  
 $M1 = M1 + 1$   
 $Y = RBAR(M1)$   
 $RBAR(M1) = CBAR * RBAR(M2) + SBAR * Y$   
 $RBAR(M2) = Y - X * RBAR(M2)$   
 $M2 = M2 + 1$

30 CONTINUE  
 $Y = THETAB(M)$   
 $THETAB(M) = CBAR * THETAB(MP1) + SBAR * Y$   
 $THETAB(MP1) = Y - X * THETAB(MP1)$

C

```
C      Swap columns M and (M+1) down to row (M-1).
C
40     IF (M .EQ. 1) GO TO 60
        POS = M
        DO 50 ROW = 1, M-1
            X = RBAR(POS)
            RBAR(POS) = RBAR(POS-1)
            RBAR(POS-1) = X
            POS = POS + NP - ROW - 1
50     CONTINUE
C
C      Adjust variable order (VORDER), the tolerances (TOL) and
C      the vector of residual sums of squares (RSS).
C
60     M1 = VORDER(M)
        VORDER(M) = VORDER(MP1)
        VORDER(MP1) = M1
        X = TOL(M)
        TOL(M) = TOL(MP1)
        TOL(MP1) = X
        RSS(M) = RSS(MP1) + D(MP1) * THETAB(MP1)**2
70     CONTINUE
C
        RETURN
        END
C
        SUBROUTINE REORDR(NP, NRBAR, VORDER, D, RBAR, THETAB, RSS, TOL,
+          LIST, N, POS1, IER)
C
C      ALGORITHM AS274.12  APPL. STATIST. (1992) VOL 41, NO.2
C
C      Re-order the variables in an orthogonal reduction produced by
C      AS75.1 so that the N variables in LIST start at position POS1,
C      though will not necessarily be in the same order as in LIST.
C      Any variables in VORDER before position POS1 are not moved.
C
C      Auxiliary routine called: VMOVE
C
        INTEGER NP, NRBAR, VORDER(NP), N, LIST(N), POS1, IER
        DOUBLE PRECISION D(NP), RBAR(NRBAR), THETAB(NP), RSS(NP), TOL(NP)
C
C      Local variables.
C
        INTEGER NEXT, I, L, J
C
C      Check N.
C
        IER = 0
        IF (NP .LT. 1) IER = 1
        IF (NRBAR .LT. NP*(NP-1)/2) IER = IER + 2
        IF (N .LT. 1 .OR. N .GE. NP+1-POS1) IER = IER + 4
        IF (IER .NE. 0) RETURN
C
C      Work through VORDER finding variables which are in LIST.
C
        NEXT = POS1
        I = POS1
10     L = VORDER(I)
        DO 20 J = 1, N
            IF (L .EQ. LIST(J)) GO TO 40
20     CONTINUE
```

```
30 I = I + 1
   IF (I .LE. NP) GO TO 10
C
C   If this point is reached, one or more variables in LIST has not
C   been found.
C
   IER = 8
   RETURN
C
C   Variable L is in LIST; move it up to position NEXT if it is not
C   already there.
C
40 IF (I .GT. NEXT) CALL VMOVE(NP, NRBAR, VORDER, D, RBAR, THETAB,
+     RSS, I, NEXT, TOL, IER)
   NEXT = NEXT + 1
   IF (NEXT .LT. N+POS1) GO TO 30
C
   RETURN
   END
C
   SUBROUTINE HDIAG(XROW, NP, NRBAR, D, RBAR, TOL, NREQ, HII, WK,
+     IFAULT)
C
C   ALGORITHM AS274.13  APPL. STATIST. (1992) VOL.41, NO.2
C
   INTEGER NP, NRBAR, NREQ, IFAULT
   DOUBLE PRECISION XROW(NP), D(NP), RBAR(*), TOL(NP), HII, WK(NP)
C
C   Local variables
C
   INTEGER COL, ROW, POS
   DOUBLE PRECISION ZERO, SUM
C
   DATA ZERO /0.0D0/
C
C   Some checks
C
   IFAULT = 0
   IF (NP .LT. 1) IFAULT = 1
   IF (NRBAR .LT. NP*(NP-1)/2) IFAULT = IFAULT + 2
   IF (NREQ .GT. NP) IFAULT = IFAULT + 4
   IF (IFAULT .NE. 0) RETURN
C
C   The elements of XROW.inv(RBAR).sqrt(D) are calculated and stored
C   in WK.
C
   HII = ZERO
   DO 20 COL = 1, NREQ
     IF (SQRT(D(COL)) .LE. TOL(COL)) THEN
       WK(COL) = ZERO
       GO TO 20
     END IF
     POS = COL - 1
     SUM = XROW(COL)
     DO 10 ROW = 1, COL-1
       SUM = SUM - WK(ROW)*RBAR(POS)
       POS = POS + NP - ROW - 1
10    CONTINUE
     WK(COL) = SUM
     HII = HII + SUM**2 / D(COL)
20    CONTINUE
```



C

RETURN  
END

(File: LSQ.DOC)

The module LSQ is for unconstrained least-squares fitting. It is based upon Applied Statistics algorithm AS 274 (see comments at the start of the module). A planar-rotation algorithm is used to update the QR-factorization. This makes it suitable for updating regressions as more data become available.

By taking advantage of the MODULE facility, it has been possible to remove most of the arguments to routines. Apart from the new function VARPRD, and a back-substitution routine BKSUB2 which it calls, the routines behave as in AS 274.

This release, version 1.00 dated 24 May 1995, has only been tested using one Fortran 90 compiler, Lahey's LF90 versions up to 1.10c. It would be appreciated if users could report their findings with other compilers, or with the various translators to Fortran 77 and C.

The package as posted comprises:

LSQ.DOC	this brief note
LSQ.F90	the least-squares module
DEMO.F90	a simple demonstration program
FUELCONS.DAT	a file of data to be read by the demo program
TEST1.F90	another program which fits a cubic polynomial and has a deliberate singularity

Reference:

Miller, A.J. (1992). Algorithm AS 274: Least squares routines to supplement those of Gentleman. Appl. Statist., vol.41(2), 458-478.

!-----  
!-----

(File: LSQ.F90)

MODULE lsq

! Module for unconstrained linear least-squares calculations.  
! The algorithm is suitable for updating LS calculations as more  
! data are added. This is sometimes called recursive estimation.  
! Only one dependent variable is allowed.  
! Based upon Applied Statistics algorithm AS 274.  
! Translation from Fortran 77 to Fortran 90 by Alan Miller.  
! A subroutine, VARPRD, has been added for calculating the variances  
! of predicted values, and this uses a subroutine BKSUB2.

! Version 1.00, 25 May 1995  
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! The PUBLIC variables are:  
! lsq\_kind = a KIND parameter for the floating-point quantities calculated  
! in this module. See the more detailed explanation below.  
! This KIND parameter should be used for all floating-point  
! arguments passed to routines in this module.

! nobs = the number of observations processed to date.  
! ncol = the total number of variables, including one for the constant,

```

!           if a constant is being fitted.
!   r_dim   = the dimension of array r = ncol*(ncol-1)/2
!   vorder  = an integer vector storing the current order of the variables
!             in the QR-factorization.  The initial order is 0, 1, 2, ...
!             if a constant is being fitted, or 1, 2, ... otherwise.
!   initialized = a logical variable which indicates whether space has
!             been allocated for various arrays.
!   tol_set  = a logical variable which is set when subroutine TOLSET has
!             been called to calculate tolerances for use in testing for
!             singularities.
!   rss_set  = a logical variable indicating whether residual sums of squares
!             are available and usable.
!   d()      = array of row multipliers for the Cholesky factorization.
!             The factorization is  $X = Q.\text{sqrt}(D).R$  where Q is an ortho-
!             normal matrix which is NOT stored, D is a diagonal matrix
!             whose diagonal elements are stored in array d, and R is an
!             upper-triangular matrix with 1's as its diagonal elements.
!   rhs()    = vector of RHS projections (after scaling by  $\text{sqrt}(D)$ ).
!             Thus  $Q'y = \text{sqrt}(D).rhs$ 
!   r()      = the upper-triangular matrix R.  The upper triangle only,
!             excluding the implicit 1's on the diagonal, are stored by
!             rows.
!   tol()    = array of tolerances used in testing for singularities.
!   rss()    = array of residual sums of squares.  rss(i) is the residual
!             sum of squares with the first r variables in the model.
!             By changing the order of variables, the residual sums of
!             squares can be found for all possible subsets of the variables.
!             The residual sum of squares with NO variables in the model,
!             that is the total sum of squares of the y-values, can be
!             calculated as  $rss(1) + d(1)*rhs(1)^2$ .  If the first variable
!             is a constant, then rss(1) is the sum of squares of
!              $(y - \bar{y})$  where  $\bar{y}$  is the average value of y.
!   sserr    = residual sum of squares with all of the variables included.
!
!-----

```

```

!   General declarations

```

```

INTEGER                :: nobs, ncol, r_dim
INTEGER, ALLOCATABLE  :: vorder(:)
LOGICAL                :: initialized = .false.,                &
                       tol_set = .false., rss_set = .false.

```

```

!   Note. lsq_kind is being set to give at least 10 decimal digit
!   representation of floating point numbers.  This should be
!   adequate for most problems except the fitting of polynomials.
!   lsq_kind is being set so that the same code can be run on PCs
!   and Unix systems, which will usually represent floating-point
!   numbers in `double precision', and other systems with larger
!   word lengths which will give similar accuracy in `single
!   precision'.

```

```

INTEGER, PARAMETER    :: lsq_kind = SELECTED_REAL_KIND(10,70)
REAL (lsq_kind), ALLOCATABLE :: d(:), rhs(:), r(:), tol(:), rss(:)
REAL (lsq_kind)       :: sserr, zero = 0.D0, one = 1.D0,        &
                       vsmall = 1.d-69

```

```

PUBLIC                :: lsq_kind, nobs, ncol, r_dim, vorder,    &
                       initialized, tol_set, rss_set,          &
                       d, rhs, r, tol, rss, sserr
PRIVATE               :: zero, one, vsmall

```

```
SAVE                ! Save everything

CONTAINS

SUBROUTINE startup(nvar, fit_const)

!     Allocates dimensions for arrays and initializes to zero
!     The calling program must set nvar = the number of variables, and
!     fit_const = .true. if a constant is to be included in the model,
!     otherwise fit_const = .false.
!
!-----

IMPLICIT NONE
INTEGER, INTENT(IN)      :: nvar
LOGICAL, INTENT(IN)     :: fit_const

!     Local variable
INTEGER                  :: i

nobs = 0
IF (fit_const) THEN
  ncol = nvar + 1
ELSE
  ncol = nvar
END IF

IF (initialized) DEALLOCATE(d, rhs, r, tol, rss, vorder)
r_dim = ncol * (ncol - 1)/2
ALLOCATE( d(ncol), rhs(ncol), r(r_dim), tol(ncol), rss(ncol), vorder(ncol) )

d = zero
rhs = zero
r = zero
sserr = zero

IF (fit_const) THEN
  DO i = 1, ncol
    vorder(i) = i-1
  END DO
ELSE
  DO i = 1, ncol
    vorder(i) = i
  END DO
END IF ! (fit_const)

initialized = .true.
tol_set = .false.
rss_set = .false.

END SUBROUTINE startup
```

```
SUBROUTINE includ(weight, xrow, yelem)

!     ALGORITHM AS75.1  APPL. STATIST. (1974) VOL.23, NO. 3

!     Calling this routine updates D, R, RHS and SSERR by the
```

```
!      inclusion of xrow, yelem with the specified weight.

!      *** WARNING  Array XROW is overwritten.

!      N.B. As this routine will be called many times in most applications,
!            checks have been eliminated.
!
!-----
```

IMPLICIT NONE

```
REAL (lsq_kind),INTENT(IN)      :: weight, yelem
REAL (lsq_kind),INTENT(INOUT)  :: xrow(ncol)
```

! Local variables

```
INTEGER          :: i, k, nextr
REAL (lsq_kind)  :: w, y, xi, di, wxi, dpi, cbar, sbar, xk
```

```
nobs = nobs + 1
w = weight
y = yelem
rss_set = .false.
nextr = 1
DO i = 1, ncol
```

```
!      Skip unnecessary transformations.  Test on exact zeroes must be
!      used or stability can be destroyed.
```

```
IF (ABS(w) < vsmall) RETURN
xi = xrow(i)
IF (ABS(xi) < vsmall) THEN
  nextr = nextr + ncol - i
ELSE
  di = d(i)
  wxi = w * xi
  dpi = di + wxi*xi
  cbar = di / dpi
  sbar = wxi / dpi
  w = cbar * w
  d(i) = dpi
  DO k = i+1, ncol
    xk = xrow(k)
    xrow(k) = xk - xi * r(nextr)
    r(nextr) = cbar * r(nextr) + sbar * xk
    nextr = nextr + 1
  END DO
  xk = y
  y = xk - xi * rhs(i)
  rhs(i) = cbar * rhs(i) + sbar * xk
END IF
END DO ! i = 1, ncol
```

```
!      Y * SQRT(W) is now equal to the Brown, Durbin & Evans recursive
!      residual.
```

```
sserr = sserr + w * y * y
```

```
RETURN
END SUBROUTINE includ
```

```
SUBROUTINE regcf(beta, nreq, ifault)

!      ALGORITHM AS274  APPL. STATIST. (1992) VOL.41, NO. 2

!      Modified version of AS75.4 to calculate regression coefficients
!      for the first NREQ variables, given an orthogonal reduction from
!      AS75.1.
!
!-----

IMPLICIT NONE
INTEGER, INTENT(IN)          :: nreq
INTEGER, INTENT(OUT)         :: ifault
REAL (lsq_kind) ,INTENT(OUT) :: beta(nreq)

!      Local variables

INTEGER          :: i, j, nextr

!      Some checks.

ifault = 0
IF (nreq .LT. 1 .OR. nreq .GT. ncol) ifault = ifault + 4
IF (ifault .NE. 0) RETURN

IF (.NOT. tol_set) CALL tolset

DO i = nreq, 1, -1
  IF (SQRT(d(i)) .LT. tol(i)) THEN
    beta(i) = zero
    d(i) = zero
  ELSE
    beta(i) = rhs(i)
    nextr = (i-1) * (ncol+ncol-i)/2 + 1
    DO j = i+1, nreq
      beta(i) = beta(i) - r(nextr) * beta(j)
      nextr = nextr + 1
    END DO ! j = i+1, nreq
  END IF
END DO ! i = nreq, 1, -1

RETURN
END SUBROUTINE regcf
```

```
SUBROUTINE tolset

!      ALGORITHM AS274  APPL. STATIST. (1992) VOL.41, NO. 2

!      Sets up array TOL for testing for zeroes in an orthogonal
!      reduction formed using AS75.1.

!      Local variables.
!
!-----

IMPLICIT NONE
```

```
!      Local variables

INTEGER          :: col, row, pos
REAL (lsq_kind)  :: eps, ten = 10.0, total, work(ncol)

!      EPS is a machine-dependent constant.

eps = ten * EPSILON(ten)

!      Set tol(i) = sum of absolute values in column I of R after
!      scaling each element by the square root of its row multiplier,
!      multiplied by EPS.

work = SQRT(d)
DO col = 1, ncol
  pos = col - 1
  total = work(col)
  DO row = 1, col-1
    total = total + ABS(r(pos)) * work(row)
    pos = pos + ncol - row - 1
  END DO
  tol(col) = eps * total
END DO

tol_set = .TRUE.
RETURN
END SUBROUTINE tolset
```

```
SUBROUTINE sing(lindep, ifault)
```

```
!      ALGORITHM AS274  APPL. STATIST. (1992) VOL.41, NO. 2

!      Checks for singularities, reports, and adjusts orthogonal
!      reductions produced by AS75.1.

!      Auxiliary routine called: INCLUD
!  
!-----

IMPLICIT NONE
INTEGER, INTENT(OUT)      :: ifault
LOGICAL, INTENT(OUT)     :: lindep(ncol)
```

```
!      Local variables

REAL (lsq_kind)  :: temp, x(ncol), work(ncol), y, weight
INTEGER          :: col, pos, row, pos2

ifault = 0

work = SQRT(d)

DO col = 1, ncol

!      Set elements within R to zero if they are less than tol(col) in
!      absolute value after being scaled by the square root of their row
!      multiplier.
```

```
temp = tol(col)
pos = col - 1
DO row = 1, col-1
  IF (ABS(r(pos)) * work(row) .LT. temp) r(pos) = zero
  pos = pos + ncol - row - 1
END DO

!      If diagonal element is near zero, set it to zero, set appropriate
!      element of LINDEP, and use INCLUD to augment the projections in
!      the lower rows of the orthogonalization.

lindep(col) = .FALSE.
IF (work(col) .LE. temp) THEN
  lindep(col) = .TRUE.
  ifault = ifault - 1
  IF (col .LT. ncol) THEN
    pos2 = pos + ncol - col + 1
    x = zero
    x(col+1:ncol) = r(pos+1:pos2-1)
    y = rhs(col)
    weight = d(col)
    r(pos+1:pos2-1) = zero
    d(col) = zero
    rhs(col) = zero
    CALL includ(weight, x, y)
  ELSE
    sserr = sserr + d(col) * rhs(col)**2
  END IF ! (col .LT. ncol)
END IF ! (work(col) .LE. temp)
END DO ! col = 1, ncol
RETURN
END SUBROUTINE sing
```

SUBROUTINE ss

```
!      ALGORITHM AS274  APPL. STATIST. (1992) VOL.41, NO. 2

!      Calculates partial residual sums of squares from an orthogonal
!      reduction from AS75.1.
!
!-----

!      Local variables

IMPLICIT NONE
INTEGER          :: i
REAL (lsq_kind)  :: total

total = sserr
rss(ncol) = sserr
DO i = ncol, 2, -1
  total = total + d(i) * rhs(i)**2
  rss(i-1) = total
END DO

rss_set = .TRUE.
RETURN
END SUBROUTINE ss
```



```
SUBROUTINE cov(nreq, var, covmat, dimcov, sterr, ifault)

!     ALGORITHM AS274  APPL. STATIST. (1992) VOL.41, NO. 2

!     Calculate covariance matrix for regression coefficients for the
!     first nreq variables, from an orthogonal reduction produced from
!     AS75.1.

!     Auxiliary routine called: INV
!
!-----

IMPLICIT NONE
INTEGER, INTENT(IN)          :: nreq, dimcov
INTEGER, INTENT(OUT)         :: ifault
REAL (lsq_kind), INTENT(OUT) :: var, covmat(dimcov), sterr(nreq)

!     Local variables.

INTEGER                      :: dim_rinv, pos, row, start, pos2, col, pos1, k
REAL (lsq_kind)              :: total
REAL (lsq_kind), ALLOCATABLE :: rinv(:)

!     Check that dimension of array covmat is adequate.

IF (dimcov < nreq*(nreq+1)/2) THEN
  ifault = 1
  RETURN
END IF

!     Check for small or zero multipliers on the diagonal.

ifault = 0
DO row = 1, nreq
  IF (ABS(d(row)) .LT. vsmall) ifault = -row
END DO
IF (ifault .NE. 0) RETURN

!     Calculate estimate of the residual variance.

IF (nobs > nreq) THEN
  var = rss(nreq) / (nobs - nreq)
ELSE
  ifault = 2
  RETURN
END IF

dim_rinv = nreq*(nreq-1)/2
ALLOCATE ( rinv(dim_rinv) )

CALL INV(nreq, rinv)
pos = 1
start = 1
DO row = 1, nreq
  pos2 = start
  DO col = row, nreq
    pos1 = start + col - row
    IF (row .EQ. col) THEN
      total = one / d(col)
```

```
ELSE
  total = rinv(pos1-1) / d(col)
END IF
DO K = col+1, nreq
  total = total + rinv(pos1) * rinv(pos2) / d(k)
  pos1 = pos1 + 1
  pos2 = pos2 + 1
END DO ! K = col+1, nreq
covmat(pos) = total * var
IF (row .EQ. col) sterr(row) = SQRT(covmat(pos))
pos = pos + 1
END DO ! col = row, nreq
start = start + nreq - row
END DO ! row = 1, nreq

RETURN
END SUBROUTINE cov
```

```
SUBROUTINE inv(nreq, rinv)
```

```
! ALGORITHM AS274 APPL. STATIST. (1992) VOL.41, NO. 2
```

```
! Invert first nreq rows and columns of Cholesky factorization
! produced by AS 75.1.
```

```
!
!-----
```

```
IMPLICIT NONE
```

```
INTEGER, INTENT(IN) :: nreq
REAL (lsq_kind), INTENT(OUT) :: rinv(*)
```

```
! Local variables.
```

```
INTEGER :: pos, row, col, start, K, pos1, pos2
REAL (lsq_kind) :: total
```

```
! Invert R ignoring row multipliers, from the bottom up.
```

```
pos = nreq * (nreq-1)/2
DO row = nreq-1, 1, -1
  start = (row-1) * (ncol+ncol-row)/2 + 1
  DO col = nreq, row+1, -1
    pos1 = start
    pos2 = pos
    total = zero
    DO K = row+1, col-1
      pos2 = pos2 + nreq - K
      total = total - r(pos1) * rinv(pos2)
      pos1 = pos1 + 1
    END DO ! K = row+1, col-1
    rinv(pos) = total - r(pos1)
    pos = pos - 1
  END DO ! col = nreq, row+1, -1
END DO ! row = nreq-1, 1, -1
```

```
RETURN
```

```
END SUBROUTINE inv
```

```

SUBROUTINE partial_corr(in, cormat, dimc, ycorr, ifault)

!   Replaces subroutines PCORR and COR of:
!   ALGORITHM AS274  APPL. STATIST. (1992) VOL.41, NO. 2

!   Calculate partial correlations after the variables in rows
!   1, 2, ..., IN have been forced into the regression.
!   If IN = 1, and the first row of R represents a constant in the
!   model, then the usual simple correlations are returned.

!   If IN = 0, the value returned in array CORMAT for the correlation
!   of variables Xi & Xj is:
!       sum ( Xi.Xj ) / Sqrt ( sum (Xi^2) . sum (Xj^2) )

!   On return, array CORMAT contains the upper triangle of the matrix of
!   partial correlations stored by rows, excluding the 1's on the diagonal.
!   e.g. if IN = 2, the consecutive elements returned are:
!   (3,4) (3,5) ... (3,ncol), (4,5) (4,6) ... (4,ncol), etc.
!   Array YCORR stores the partial correlations with the Y-variable
!   starting with YCORR(IN+1) = partial correlation with the variable in
!   position (IN+1).
!
!-----

IMPLICIT NONE
INTEGER, INTENT(IN)           :: in, dimc
INTEGER, INTENT(OUT)          :: ifault
REAL (lsq_kind), INTENT(OUT) :: cormat(dimc), ycorr(ncol)

!   Local variables.

INTEGER           :: base_pos, pos, row, col, col1, col2, pos1, pos2
REAL (lsq_kind)  :: rms(in+1:ncol), sumxx, sumxy, sumyy, work(in+1:ncol)

!   Some checks.

ifault = 0
IF (in .LT. 0 .OR. in .GT. ncol-1) ifault = ifault + 4
IF (dimc .LT. (ncol-in)*(ncol-in-1)/2) ifault = ifault + 8
IF (ifault .NE. 0) RETURN

!   Base position for calculating positions of elements in row (IN+1) of R.

base_pos = in*ncol - (in+1)*(in+2)/2

!   Calculate 1/RMS of elements in columns from IN to (ncol-1).

IF (d(in+1) > zero) rms(in+1) = one / SQRT(d(in+1))
DO col = in+2, ncol
  pos = base_pos + col
  sumxx = d(col)
  DO row = in+1, col-1
    sumxx = sumxx + d(row) * r(pos)**2
    pos = pos + ncol - row - 1
  END DO ! row = in+1, col-1
  IF (sumxx > zero) THEN
    rms(col) = one / SQRT(sumxx)
  ELSE
    rms(col) = zero
    ifault = -col
  END IF
END DO

```

```
      END IF ! (sumxx > zero)
END DO ! col = in+1, ncol-1

!      Calculate 1/RMS for the Y-variable

sumyy = sserr
DO row = in+1, ncol
  sumyy = sumyy + d(row) * rhs(row)**2
END DO ! row = in+1, ncol
IF (sumyy > zero) sumyy = one / SQRT(sumyy)

!      Calculate sums of cross-products.
!      These are obtained by taking dot products of pairs of columns of R,
!      but with the product for each row multiplied by the row multiplier
!      in array D.

pos = 1
DO col1 = in+1, ncol
  sumxy = zero
  work(col1+1:ncol) = zero
  pos1 = base_pos + col1
  DO row = in+1, col1-1
    pos2 = pos1 + 1
    DO col2 = col1+1, ncol
      work(col2) = work(col2) + d(row) * r(pos1) * r(pos2)
      pos2 = pos2 + 1
    END DO ! col2 = col1+1, ncol
    sumxy = sumxy + d(row) * r(pos1) * rhs(row)
    pos1 = pos1 + ncol - row - 1
  END DO ! row = in+1, col1-1

!      Row COL1 has an implicit 1 as its first element (in column COL1)

  pos2 = pos1 + 1
  DO col2 = col1+1, ncol
    work(col2) = work(col2) + d(col1) * r(pos2)
    pos2 = pos2 + 1
    cormat(pos) = work(col2) * rms(col1) * rms(col2)
    pos = pos + 1
  END DO ! col2 = col1+1, ncol
  sumxy = sumxy + d(col1) * rhs(col1)
  ycorr(col1) = sumxy * rms(col1) * sumyy
END DO ! col1 = in+1, ncol-1

ycorr(1:in) = zero

RETURN
END SUBROUTINE partial_corr
```

```
SUBROUTINE vmove(from, to, ifault)
```

```
!      ALGORITHM AS274 APPL. STATIST. (1992) VOL.41, NO. 2
```

```
!      Move variable from position FROM to position TO in an
!      orthogonal reduction produced by AS75.1.
```

```
!
```

```
!-----
```

```
IMPLICIT NONE
INTEGER, INTENT(IN)          :: from, to
INTEGER, INTENT(OUT)         :: ifault

!      Local variables

REAL (lsq_kind)             :: d1, d2, X, dlnew, d2new, cbar, sbar, Y
INTEGER                      :: m, first, last, inc, m1, m2, mp1, col, pos, row

!      Check input parameters

ifault = 0
IF (from .LT. 1 .OR. from .GT. ncol) ifault = ifault + 4
IF (to .LT. 1 .OR. to .GT. ncol) ifault = ifault + 8
IF (ifault .NE. 0) RETURN

IF (from .EQ. to) RETURN

IF (.NOT. rss_set) CALL ss

IF (from .LT. to) THEN
  first = from
  last = to - 1
  inc = 1
ELSE
  first = from - 1
  last = to
  inc = -1
END IF

DO 70 m = first, last, inc

!      Find addresses of first elements of R in rows M and (M+1).

m1 = (m-1)*(ncol+ncol-m)/2 + 1
m2 = m1 + ncol - m
mp1 = m + 1
d1 = d(m)
d2 = d(mp1)

!      Special cases.

IF (d1 .LT. vsmall .AND. d2 .LT. vsmall) GO TO 40
X = r(m1)
IF (ABS(x) * SQRT(d1) .LT. tol(mp1)) THEN
  X = zero
END IF
IF (d1 .LT. vsmall .OR. ABS(x) .LT. vsmall) THEN
  d(m) = d2
  d(mp1) = d1
  r(m1) = zero
  DO col = m+2, ncol
    m1 = m1 + 1
    X = r(m1)
    r(m1) = r(m2)
    r(m2) = x
    m2 = m2 + 1
  END DO ! col = m+2, ncol
  X = rhs(m)
  rhs(m) = rhs(mp1)
  rhs(mp1) = x
```

```

        GO TO 40
ELSE IF (d2 .LT. vsmall) THEN
    d(m) = d1 * x**2
    r(m1) = one / x
    r(m1+1:m1+ncol-m-1) = r(m1+1:m1+ncol-m-1) / x
    rhs(m) = rhs(m) / x
    GO TO 40
END IF
!
!   Planar rotation in regular case.
!
dlnew = d2 + d1*x**2
cbar = d2 / dlnew
sbar = x * d1 / dlnew
d2new = d1 * cbar
d(m) = dlnew
d(mp1) = d2new
r(m1) = sbar
DO col = m+2, ncol
    m1 = m1 + 1
    y = r(m1)
    r(m1) = cbar*r(m2) + sbar*y
    r(m2) = y - x*r(m2)
    m2 = m2 + 1
END DO ! col = m+2, ncol
y = rhs(m)
rhs(m) = cbar*rhs(mp1) + sbar*y
rhs(mp1) = y - x*rhs(mp1)

!   Swap columns M and (M+1) down to row (M-1).

40  IF (m .EQ. 1) GO TO 60
    pos = m
    DO row = 1, m-1
        x = r(pos)
        r(pos) = r(pos-1)
        r(pos-1) = x
        pos = pos + ncol - row - 1
    END DO ! row = 1, m-1

!   Adjust variable order (VORDER), the tolerances (TOL) and
!   the vector of residual sums of squares (RSS).

60  m1 = vorder(m)
    vorder(m) = vorder(mp1)
    vorder(mp1) = m1
    x = tol(m)
    tol(m) = tol(mp1)
    tol(mp1) = x
    rss(m) = rss(mp1) + d(mp1) * rhs(mp1)**2
70  CONTINUE

RETURN
END SUBROUTINE vmove

```

```

SUBROUTINE reordr(list, n, pos1, ifault)

```

```

!   ALGORITHM AS274  APPL. STATIST. (1992) VOL.41, NO. 2

```

```
!      Re-order the variables in an orthogonal reduction produced by
!      AS75.1 so that the N variables in LIST start at position POS1,
!      though will not necessarily be in the same order as in LIST.
!      Any variables in VORDER before position POS1 are not moved.

!      Auxiliary routine called: VMOVE
!
!-----
```

```
IMPLICIT NONE
INTEGER, INTENT(IN)      :: n, list(n), pos1
INTEGER, INTENT(OUT)    :: ifault
```

```
!      Local variables.
```

```
INTEGER      :: next, i, l, j
```

```
!      Check N.
```

```
    ifault = 0
    IF (n .LT. 1 .OR. n .GT. ncol+1-pos1) ifault = ifault + 4
    IF (ifault .NE. 0) RETURN
```

```
!      Work through VORDER finding variables which are in LIST.
```

```
    next = pos1
    i = pos1
10  l = vorder(i)
    DO j = 1, n
        IF (l .EQ. list(j)) GO TO 40
    END DO
30  i = i + 1
    IF (i .LE. ncol) GO TO 10
```

```
!      If this point is reached, one or more variables in LIST has not
!      been found.
```

```
    ifault = 8
    RETURN
```

```
!      Variable L is in LIST; move it up to position NEXT if it is not
!      already there.
```

```
40  IF (i .GT. next) CALL vmove(i, next, ifault)
    next = next + 1
    IF (next .LT. n+pos1) GO TO 30
```

```
    RETURN
END SUBROUTINE reordr
```

```
SUBROUTINE hdiag(xrow, nreq, hii, ifault)
```

```
!      ALGORITHM AS274  APPL. STATIST. (1992) VOL.41, NO. 2
```

```
!-----
```

```
IMPLICIT NONE
INTEGER, INTENT(IN)      :: nreq
INTEGER, INTENT(OUT)    :: ifault
```

```
REAL (lsq_kind), INTENT(IN)  :: xrow(ncol)
REAL (lsq_kind), INTENT(OUT) :: hii

!      Local variables

INTEGER          :: col, row, pos
REAL (lsq_kind)  :: total, wk(ncol)

!      Some checks

ifault = 0
IF (nreq .GT. ncol) ifault = ifault + 4
IF (ifault .NE. 0) RETURN

!      The elements of xrow.inv(R).sqrt(D) are calculated and stored
!      in WK.

hii = zero
DO col = 1, nreq
  IF (SQRT(d(col)) .LE. tol(col)) THEN
    wk(col) = zero
  ELSE
    pos = col - 1
    total = xrow(col)
    DO row = 1, col-1
      total = total - wk(row)*r(pos)
      pos = pos + ncol - row - 1
    END DO ! row = 1, col-1
    wk(col) = total
    hii = hii + total**2 / d(col)
  END IF
END DO ! col = 1, nreq

RETURN
END SUBROUTINE hdiag
```

```
REAL (lsq_kind) FUNCTION varprd(x, nreq, var, ifault)

!      Calculate the variance of x'b where b consists of the first nreq
!      least-squares regression coefficients.
!
!-----

IMPLICIT NONE
INTEGER, INTENT(IN)          :: nreq
INTEGER, INTENT(OUT)         :: ifault
REAL (lsq_kind), INTENT(IN)  :: x(*)
REAL (lsq_kind), INTENT(OUT) :: var

!      Local variables

INTEGER          :: row
REAL (lsq_kind)  :: wk(nreq)

!      Check input parameter values

varprd = zero
ifault = 0
IF (nreq .LT. 1 .OR. nreq .GT. ncol) ifault = ifault + 4
```



```
IF (nobs .LE. nreq) ifault = ifault + 8
IF (ifault .NE. 0) RETURN

!      Calculate the residual variance estimate.

var = sserr / (nobs - nreq)

!      Variance of x'b = var.x'(inv R)(inv D)(inv R')x
!      First call BKSUB2 to calculate (inv R')x by back-substitution.

CALL BKSUB2(x, wk, nreq)
DO row = 1, nreq
  IF(d(row) .GT. tol(row)) varprd = varprd + wk(row)**2 / d(row)
END DO

varprd = varprd * var

RETURN
END FUNCTION varprd

SUBROUTINE bksub2(x, b, nreq)

!      Solve x = R'b for b given x, using only the first nreq rows and
!      columns of R, and only the first nreq elements of R.
!
!-----

IMPLICIT NONE
INTEGER, INTENT(IN)          :: nreq
REAL (lsq_kind), INTENT(IN) :: x(nreq)
REAL (lsq_kind), INTENT(OUT) :: b(nreq)

!      Local variables

INTEGER          :: pos, row, col
REAL (lsq_kind) :: temp

!      Solve by back-substitution, starting from the top.

DO row = 1, nreq
  pos = row - 1
  temp = x(row)
  DO col = 1, row-1
    temp = temp - r(pos)*b(col)
    pos = pos + ncol - col - 1
  END DO
  b(row) = temp
END DO

RETURN
END SUBROUTINE bksub2

END MODULE lsq

!-----
!-----
```

(File: DEMO.F90)

PROGRAM demo

```

!      Program to demonstrate the use of module LSQ for unconstrained
!      linear least-squares regression.
!      The data on fuel consumption are from:
!      Sanford Weisberg `Applied Linear Regression', 2nd edition, 1985,
!      pages 35-36.  Publisher: Wiley

!      The program is designed so that users can easily edit it for their
!      problems.  If you are likely to have more than 500 cases then increase
!      the value of maxcases below.  Similarly, if you may have more than
!      30 predictor variables, change maxvar below.

!      The subscript 0 is used to relate to the constant in the model.
!      Module LSQ treats the constant in the model, if there is one, just as
!      any other variable.  The numbering of all arrays starts from 1 in LSQ.

USE lsq                                ! Must be the first declaration in the program
IMPLICIT NONE

INTEGER, PARAMETER :: maxcases = 500, maxvar = 30,                                &
                    max_cdim = maxvar*(maxvar+1)/2, lout = 6
INTEGER              :: case, nvar, iostatus, nreq, ifault, i, list(maxvar), j, &
                    in
REAL ( lsq_kind )   :: xx(0:maxvar), yy, wt, one = 1.D0, beta(0:maxvar),        &
                    var, covmat(max_cdim), sterr(0:maxvar), hii,              &
                    cormat(max_cdim), ycorr(maxvar)
REAL (KIND(0.E0))   :: x(maxcases, maxvar), y(maxcases), t(0:maxvar), tmin,    &
                    r2, resid(maxcases), std_resid(maxcases), std_err_pred, &
                    fitted, stdev_res
CHARACTER           :: heading*80, vname(0:maxvar)*8, state(50)*2, y_name*8, key
LOGICAL             :: fit_const, lindep(0:maxvar)

WRITE(*, *) 'The data on fuel consumption are from:'
WRITE(*, *) 'Sanford Weisberg "Applied Linear Regression", 2nd edition, 1985,'
WRITE(*, *) 'pages 35-36.  Publisher: Wiley  ISBN: 0-471-87957-6'
WRITE(*, *)

OPEN(8, file='fuelcons.dat', status='old')

!      The first line of this file contains the names of the variables.

READ(8, '(a)') heading

vname(0) = 'Constant'

!      Read the heading to get the variable names & the number of variables

CALL separate_text(heading, vname(1), nvar)

nvar = nvar - 2                                ! nvar is the number of variables.
                                              ! 1 is subtracted as the first field in this
                                              ! file contains the abbreviated state name,
                                              ! & 1 is subtracted for the Y-variable.

vname(1:nvar) = vname(2:nvar+1)
y_name = vname(nvar+2)

WRITE(*, *) 'No. of variables =', nvar
WRITE(*, *) 'Predictor variables are:'
WRITE(*, '(1x, 9a9)') vname(1:nvar)
WRITE(*, *) 'Dependent variable is: ', y_name

```

```

fit_const = .true.          ! Change to .false. if fitting a model without
                           ! a constant.

CALL startup(nvar, fit_const)      ! Initializes the QR-factorization

!   Read in the data, one line at a time, and progressively update the
!   QR-factorization.

wt = one
case = 1

DO
  READ(8, *, IOSTAT=iostat) state(case), x(case, 1:nvar), y(case)
  IF (iostat > 0) CYCLE          ! Error in data
  IF (iostat < 0) EXIT          ! End of file

  xx(0) = one                   ! A one is inserted as the first
                               ! variable if a constant is being fitted.
  xx(1:nvar) = x(case, 1:nvar) ! New variables and transformed variables
                               ! will often be generated here.

  yy = y(case)
  CALL includ(wt, xx, yy)
  case = case + 1
END DO

WRITE(*, *)'No. of observations =', nobs

CALL sing(lindep, ifault)       ! Checks for singularities

IF (ifault == 0) THEN
  WRITE(*, *)'QR-factorization is not singular'
ELSE
  DO i = 1, nvar
    IF (lindep(i)) THEN
      WRITE(*, *) vname(i), ' is exactly linearly related to earlier variables'
    END IF
  END DO ! i = 1, nvar
END IF ! (ifault == 0)
WRITE(*, *)

!   Show correlations (IN = 1 for `usual' correlations)

in = 1
CALL partial_corr(in, cormat, max_cdim, ycorr, ifault)
CALL printc(in, cormat, max_cdim, ycorr, vname, y_name, 1, lout, ifault)
WRITE(*, *)
WRITE(*, *)'Press ENTER to continue'
READ(*, '(a)') key

!   Weisberg only uses variables TAX, INC, ROAD and DLIC.   These are
!   currently in positions 2, 4, 5 & 7.
!   We could have set NVAR = 4 and copied only these variables from X to
!   XX, but we will show how regressions can be performed for a subset
!   of the variables in the QR-factorization.   Routine REORDR will be used
!   to re-order the variables.

list(1:4) = (/ 2, 4, 5, 7/)
CALL reordr(list, 4, 2, ifault) ! Re-order so that the first 4 variables
                               ! appear in positions 2,3,4 & 5.
                               ! N.B. Though variables # 2, 4, 5 & 7

```

```

!      will occupy positions 2-5, they
!      may be in any order.
!      The constant remains in position 1.
WRITE(*, 910) (vname(vorder(1:ncol)))
910 FORMAT(1x, 'Current order of variables:'/1x, 8a9/)

!      Calculate regression coefficients of Y against the first variable, which
!      was just a constant = 1.0, and the next 4 predictors.

CALL tolset                ! Calculate tolerances before calling
                           ! subroutine regcf.
nreq = 5                    ! i.e. Const, TAX, INC, ROAD, DLIC
CALL regcf(beta, nreq, ifault)

CALL ss                    ! Calculate residual sums of squares

!      Calculate covariance matrix of the regression coefficients & their
!      standard errors.

CALL cov(nreq, var, covmat, max_cdim, sterr, ifault)

!      Calculate t-values

t(0:nreq-1) = beta(0:nreq-1) / sterr(0:nreq-1)

!      Output regression table, residual sums of squares, and R-squared.

WRITE(*, *)
WRITE(*, *)'Variable   Regn.coeff.   Std.error   t-value   Res.sum of sq.'
DO i = 0, nreq-1
  WRITE(*, 900) vname(vorder(i+1)), beta(i), sterr(i), t(i), rss(i+1)
  900 FORMAT(1x, a8, 2x, g12.4, 2x, g11.4, 1x, f7.2, 2x, g14.6)
END DO
WRITE(*, *)

!      Now delete the variable with the smallest t-value by moving it
!      to position 5 and then repeating the calculations for the constant
!      and the next 3 variables.

j = 1
tmin = ABS(t(1))
DO i = 2, nreq-1
  IF (ABS(t(i)) < tmin) THEN
    j = i
    tmin = ABS(t(i))
  END IF
END DO
j = j + 1                ! Add 1 as the t-array started at subscript 0

WRITE(*, *)'Removing variable in position', j
CALL vmove(j, nreq, ifault)
nreq = nreq - 1
CALL regcf(beta, nreq, ifault)
CALL ss
CALL cov(nreq, var, covmat, max_cdim, sterr, ifault)
t(0:nreq-1) = beta(0:nreq-1) / sterr(0:nreq-1)

!      Output regression table, residual sums of squares, and R-squared.

WRITE(*, *)
WRITE(*, *)'Variable   Regn.coeff.   Std.error   t-value   Res.sum of sq.'
```

```

DO i = 0, nreq-1
  WRITE(*, 900) vname(vorder(i+1)), beta(i), sterr(i), t(i), rss(i+1)
END DO
WRITE(*, *)
stdev_res = SQRT( rss(nreq)/(nobs - nreq) )
r2 = one - rss(nreq) / rss(1)          ! RSS(1) is the rss if only the constant
                                       ! is fitted; RSS(nreq) is the rss after
                                       ! fitting the requested NREQ variables.
WRITE(*, '(1x, "R^2 =", f8.4, 5x, "Std. devn. of residuals =", g12.4/))' &
  r2, stdev_res
WRITE(*, *)'N.B. Some statistical packages wrongly call the standard deviation'
WRITE(*, *)'  of the residuals the standard error of prediction'
WRITE(*, *)

!      Calculate residuals, hii, standardized residuals & standard errors of
!      prediction.

WRITE(*, *)'Press ENTER to continue'
READ(*, '(a)') key

WRITE(*, *)'State      Actual      Fitted  Residual  Std.resid.  SE(prediction)'
DO i = 1, nobs
  xx(0) = one
  DO j = 1, nreq-1
    xx(j) = x(i, vorder(j+1))          ! N.B. Regression coefficient j is for
                                       !      the variable vorder(j+1)
  END DO
  fitted = DOT_PRODUCT( beta(0:nreq-1), xx(0:nreq-1) )
  resid(i) = y(i) - fitted
  CALL hdiag(xx, nreq, hii, ifault)
  std_resid(i) = resid(i) / SQRT(var*(one - hii))
  std_err_pred = varprd(xx, nreq, var, ifault)
  WRITE(*, 920) state(i), y(i), fitted, resid(i), std_resid(i), std_err_pred
  920 FORMAT(3x, a2, 2x, 3f10.1, f9.2, 5x, f10.0)

  IF (i .EQ. 24) THEN
    WRITE(*, *)'Press ENTER to continue'
    READ(*, '(a)') key
    WRITE(*, *)'State      Actual      Fitted  Residual  Std.resid.
SE(prediction)'
  END IF
END DO ! i = 1, nobs

END PROGRAM demo

SUBROUTINE separate_text(text, name, number)

!      Takes the character string in `text' and separates it into `names'.
!      This version only allows spaces as delimiters.

IMPLICIT NONE
CHARACTER (LEN = *) , INTENT(INOUT)  :: text
CHARACTER (LEN = *) , INTENT(OUT)    :: name(*)
INTEGER, INTENT(OUT)                 :: number

!      Local variables

INTEGER  :: length, len_name, pos1, pos2, nchars

```

```
length = LEN_TRIM(text)
number = 0
IF (length == 0) RETURN

len_name = LEN(name(1))
IF (len_name < 1) RETURN

pos1 = 1
DO
  DO                                ! Remove any leading blanks
    IF (text(pos1:pos1) == ' ') THEN
      text(pos1:) = text(pos1+1:)
      length = length - 1
      CYCLE
    ELSE
      EXIT
    END IF
  END DO
  pos2 = INDEX(text(pos1:length), ' ') ! Find position of next blank
  IF (pos2 > 0) THEN
    pos2 = pos2 + pos1 - 1
  ELSE                                ! Last name, no blank found
    pos2 = length + 1
  END IF
  number = number + 1
  nchars = MIN(len_name, pos2-pos1)
  name(number) = text(pos1:pos1+nchars-1)
  pos1 = pos2 + 1                    ! Move past the blank
  IF (pos1 > length) RETURN
END DO

END SUBROUTINE separate_text
```

```
SUBROUTINE printc(in, cormat, dimc, ycorr, vname, yname, iopt, lout, ier)

!      Print (partial) correlations calculated using partial_corr to unit lout.
!      If IOPT = 0, print correlations with the Y-variable only.

USE lsq

IMPLICIT NONE
INTEGER, INTENT(IN)           :: in, dimc, iopt, lout
INTEGER, INTENT(OUT)          :: ier
REAL ( lsq_kind ), INTENT(IN) :: cormat(dimc), ycorr(ncol)
CHARACTER, INTENT(IN)         :: vname(0:ncol-1)*8, yname*8

!      Local variables.

INTEGER           :: nrows, j1, j2, i1, i2, row, upos, tpos, last
CHARACTER         :: text*74, empty*65 = ' ', char1*9 = ' 1.0'

!      Check validity of arguments

ier = 0
IF (in .GE. ncol) ier = 1
IF (ncol .LE. 1) ier = ier + 2
nrows = ncol - in
IF (dimc .LE. nrows*(nrows-1)/2) ier = ier + 4
IF (ier .NE. 0) RETURN
```

```

!      If iopt.NE.0 output heading

IF (iopt .EQ. 0) GO TO 30
WRITE(lout, 900)
900 FORMAT(/5x, 'Correlation matrix')
j1 = in + 1

DO
  j2 = MIN(j1+6, ncol)
  i1 = j1 - in
  i2 = j2 - in
  WRITE(lout, 910) vname(vorder(j1:j2))
  910 FORMAT(11X, 7(a8, 1x))

!      Print correlations for rows 1 to i2, columns i1 to i2.

DO row = 1, i2
  text = ' ' // vname(vorder(row+in)) // empty
  IF (i1 .GT. row) THEN
    upos = (row-1) * (nrows+nrows-row) /2 + (i1-row)
    last = upos + i2 - i1
    WRITE(text(12:74), '(7(F8.5, 1x))') cormat(upos:last)
  ELSE
    upos = (row-1) * (nrows+nrows-row) /2 + 1
    tpos = 12 + 9*(row-i1)
    text(tpos:tpos+8) = char1
    last = upos + i2 - row - 1
    IF (row .LT. i2) WRITE(text(tpos+9:74), '(6(F8.5, 1X))') cormat(upos:last)
  END IF
  WRITE(lout, '(a)') text
END DO ! row = 1, i2

!      Move onto the next block of columns.

  j1 = j2 + 1
  IF (j1 .GT. ncol) EXIT
END DO

!      Correlations with the Y-variable.

30 WRITE(lout, 920) yname
  920 FORMAT(/5x, 'Correlations with the dependent variable: ', a)
  j1 = in + 1

DO
  j2 = MIN(j1+7, ncol)
  WRITE(lout, 930) vname(vorder(j1:j2))
  930 FORMAT(/1X, 8(A8, 1X))
  WRITE(lout, 940) ycorr(j1:j2)
  940 FORMAT(1X, 8(F8.5, 1X))
  j1 = j2 + 1
  IF (j1 .GT. ncol) EXIT
END DO

END SUBROUTINE printc

!-----
!-----

(File: FUELCONS.DAT)
State Popn      Tax      NLic  Income  RoadMls FuelCon  DLic  Fuel_Pop

```

ME	1029.	9.00	540.	3.571	1.976	557.	52.5	541.
NH	771.	9.00	441.	4.092	1.250	404.	57.2	524.
VT	462.	9.00	268.	3.865	1.586	259.	58.0	561.
MA	5787.	7.50	3060.	4.870	2.351	2396.	52.9	414.
RI	968.	8.00	527.	4.399	.431	397.	54.4	410.
CN	3082.	10.00	1760.	5.342	1.333	1408.	57.1	457.
NY	18366.	8.00	8278.	5.319	11.868	6312.	45.1	344.
NJ	7367.	8.00	4074.	5.126	2.138	3439.	55.3	467.
PA	11926.	8.00	6312.	4.447	8.577	5528.	52.9	464.
OH	10783.	7.00	5948.	4.512	8.507	5375.	55.2	498.
IN	5291.	8.00	2804.	4.391	5.939	3068.	53.0	580.
IL	11251.	7.50	5903.	5.126	14.186	5301.	52.5	471.
MI	9082.	7.00	5213.	4.817	6.930	4768.	57.4	525.
WI	4520.	7.00	2465.	4.207	6.580	2294.	54.5	508.
MN	3896.	7.00	2368.	4.332	8.159	2204.	60.8	566.
IA	2883.	7.00	1689.	4.318	10.340	1830.	58.6	635.
MO	4753.	7.00	2719.	4.206	8.508	2865.	57.2	603.
ND	632.	7.00	341.	3.718	4.725	451.	54.0	714.
SD	579.	7.00	419.	4.716	5.915	501.	72.4	865.
NE	1525.	8.50	1033.	4.341	6.010	976.	67.7	640.
KS	2258.	7.00	1496.	4.593	7.834	1466.	66.3	649.
DE	565.	8.00	340.	4.983	.602	305.	60.2	540.
MD	4056.	9.00	2073.	4.897	2.449	1883.	51.1	464.
VA	4764.	9.00	2463.	4.258	4.686	2604.	51.7	547.
WV	1781.	8.50	982.	4.574	2.619	819.	55.1	460.
NC	5214.	9.00	2835.	3.721	4.746	2953.	54.4	566.
SC	2665.	8.00	1460.	3.448	5.399	1537.	54.8	577.
GA	4720.	7.50	2731.	3.846	9.061	2979.	57.9	631.
FL	7259.	8.00	4084.	4.188	5.975	4169.	56.3	574.
KY	3299.	9.00	1626.	3.601	4.650	1761.	49.3	534.
TN	4031.	7.00	2088.	3.640	6.905	2301.	51.8	571.
AL	3510.	7.00	1801.	3.333	6.594	1946.	51.3	554.
MS	2263.	8.00	1309.	3.063	6.524	1306.	57.8	577.
AR	1978.	7.50	1081.	3.357	4.121	1242.	54.7	628.
LA	3720.	8.00	1813.	3.528	3.495	1812.	48.7	487.
OK	2634.	6.58	1657.	3.802	7.834	1695.	62.9	644.
TX	11649.	5.00	6595.	4.045	17.782	7451.	56.6	640.
MT	719.	7.00	421.	3.897	6.385	506.	58.6	704.
ID	756.	8.50	501.	3.635	3.274	490.	66.3	648.
WY	345.	7.00	232.	4.345	3.905	334.	67.2	968.
CO	2357.	7.00	1475.	4.449	4.639	1384.	62.6	587.
NM	1065.	7.00	600.	3.656	3.985	744.	56.3	699.
AZ	1945.	7.00	1173.	4.300	3.635	1230.	60.3	632.
UT	1126.	7.00	572.	3.745	2.611	666.	50.8	591.
NV	527.	6.00	354.	5.215	2.302	412.	67.2	782.
WN	3443.	9.00	1966.	4.476	3.942	1757.	57.1	510.
OR	2182.	7.00	1360.	4.296	4.083	1331.	62.3	610.
CA	20468.	7.00	12130.	5.002	9.794	10730.	59.3	524.

!-----  
!-----

(File: TEST1.F90)

PROGRAM test1

! Test vmove.  
! The LS fit to the data is:  $Y = 1 + X + X^{**2} + X^{**3}$   
! i.e. all of the regression coefficients should be exactly 1.0.  
! An extra variable equal to  $X + X^{**2}$  is inserted to give a singularity.



```
USE lsq
IMPLICIT NONE

REAL ( lsq_kind ) :: x(11,4), y(11), xrow(5), yelem, beta(5), one = 1.D0
INTEGER           :: nvar, i, j, ifault
LOGICAL          :: fit_const, lindep(5)
CHARACTER (LEN=1) :: key

DATA y/65647., 70638., 75889., 81399., 87169., 93202., 99503., &
     106079., 112939., 120094., 127557./

WRITE(*, *)'Fitting nasty cubic'
WRITE(*, *)'1st 4 regression coefficients should equal 1.0'
WRITE(*, *)'Last variable = X + X^2, to introduce a deliberate singularity'
WRITE(*, *)

DO i = 1, 11
  x(i,1) = i + 39
  x(i,2) = x(i,1)**2
  x(i,3) = x(i,1) * x(i,2)
  x(i,4) = x(i,1) + x(i,2)
END DO

!      Use includ to form the orthogonal reduction.

nvar = 4
fit_const = .true.
CALL startup(nvar, fit_const)

DO i = 1, 11
  xrow(1) = one
  DO j = 1, 4
    xrow(j+1) = x(i,j)
  END DO
  yelem = y(i)
  CALL includ(one, xrow, yelem)
END DO

!      CALL tolset to set tolerances, then sing to detect singularities.

CALL tolset
CALL sing(lindep, ifault)
WRITE(*, *)'From routine SING, IFAULT =', ifault
WRITE(*, *)'Array LINDEP:', lindep
WRITE(*, *)
WRITE(*, *)'sserr = ', sserr, '   Should be 286.000'

!      Calculate residual sums of squares (RSS).

CALL ss

!      Calculate regression coefficients, using vmove to cycle through
!      the order of the variables.

DO i = 1, 6
  CALL regcf(beta, 5, ifault)
  WRITE(*, 920) vorder
920  FORMAT(1x, 'Variable order: '/ 1x, i10, 4i15)
  WRITE(*, 900) beta
900  FORMAT(' Regn. coeffs.:'/ 4x, 5g15.7)
  WRITE(*, 910) d, r, rhs, rss
```

```
910  FORMAT(' d: ', 5g15.7/ ' r: ', 4g15.7/19x,3g15.7/34x,2g15.7/ &  
      49x,g15.7/ ' rhs: '/4x, 5g15.7/ ' rss: '/4x, 5g15.7//)
```

```
WRITE(*, *)'Press ENTER to continue'
```

```
READ(*, '(a)') key
```

```
!      Move variable in 1st position to the last.
```

```
      CALL vmove(1, 5, ifault)
```

```
      END DO
```

```
END PROGRAM test1
```

```

      REAL FUNCTION CHI2NC(X, F, THETA, IFAULT)
C
C      ALGORITHM AS 275 APPL.STATIST. (1992), VOL.41, NO.2
C
C      Computes the noncentral chi-square distribution function
C      with positive real degrees of freedom f and nonnegative
C      noncentrality parameter theta
C
      REAL X, F, THETA
      INTEGER IFAULT
C
      INTEGER ITRMAX
      LOGICAL FLAG
      REAL ERRMAX, ZERO, ONE, TWO, LAM, N, U, V, X2, F2, T, TERM,
*      BOUND, ALOGAM
C
      EXTERNAL ALOGAM
C
      DATA ERRMAX, ITRMAX / 1.0E-6, 50 /
      DATA ZERO, ONE, TWO / 0.0, 1.0, 2.0 /
C
      CHI2NC = X
      IFAULT = 2
      IF (F .LE. ZERO .OR. THETA .LT. ZERO) RETURN
      IFAULT = 3
      IF (X .LT. ZERO) RETURN
      IFAULT = 0
      IF (X .EQ. ZERO) RETURN
      LAM = THETA / TWO
C
      Evaluate the first term
C
      N = ONE
      U = EXP(-LAM)
      V = U
      X2 = X / TWO
      F2 = F / TWO
      T = X2 ** F2 * EXP(-X2) / EXP(ALOGAM((F2 + ONE), IFAULT))
C
      There is no need to test IFAULT si
      already been checked
C
      TERM = V * T
      CHI2NC = TERM
C
      Check if (f+2n) is greater than x
C
      FLAG = .FALSE.
10 IF ((F + TWO * N - X) .LE. ZERO) GO TO 30
C
      Find the error bound and check for convergence
C
      FLAG = .TRUE.
20 BOUND = T * X / (F + TWO * N - X)
      IF (BOUND .GT. ERRMAX .AND. INT(N) .LE. ITRMAX) GO TO 30
      IF (BOUND .GT. ERRMAX) IFAULT = 1
      RETURN
C
      Evaluate the next term of the expansion and then the
      partial sum
C

```

```
30 U = U * LAM / N
   V = V + U
   T = T * X / (F + TWO * N)
   TERM = V * T
   CHI2NC = CHI2NC + TERM
   N = N + ONE
   IF (FLAG) GO TO 20
   GO TO 10
```

C

```
END
```

```

SUBROUTINE CCLASS (DD, DI, N1, N2, NP, KMAX, A1, COND, RAW, DATA,
*           SX, SY, TMV, CUT, ICC, PQ, PMIN, LKA, Z, UPMQM,
*           ICR, CGFE, IFAULT)
C
C   ALGORITHM AS 276.1 APPL.STATIST. (1992), VOL.41, NO.2
C
C   Obtains the optimal combinatoric classification procedure for
C   the two normal problem
C
C   INTEGER DD, DI, N1, N2, NP, KMAX, COND, RAW, ICC(NP), LKA(NP + 2),
*           ICR(2, NP), IFAULT
C   REAL A1, DATA(DD, NP), SX(DI, NP), SY(DI, NP), TMV(DI, 2),
*           CUT(NP), PQ(2, NP), PMIN, Z(DI, NP + 1), UPMQM(3, NP *
*           (NP + 1)/2), CGFE(DI, 3 * NP + 1)
C
C   EXTERNAL DIAG2, ERPROB, MCE, SWAP
C
C   INTEGER HOLD, I, IFLT, IZ, J, JP1, K, MX, MY, NDEN1, NDEN2, N1N2,
*           N1P1
C   REAL ONE, SSQ, STORE, SUM, XYMEAN, ZERO
C
C   PARAMETER (ZERO = 0.0E0, ONE = 1.0E0)
C
C   Initialise local variables
C
C   IZ = NP + 1
C   N1N2 = N1 + N2
C   MX = N1N2 + 1
C   MY = MX + 1
C   N1P1 = N1 + 1
C
C   Check for input failures
C
C
C   IFAULT = 0
C   IF (N1 .LT. 0 .OR. N2 .LT. 0 .OR. MY .GT. DD)
*   IFAULT = 1
C   IF (NP .LT. 2 .OR. NP .GT. DI) IFAULT = IFAULT + 2
C   IF (KMAX .LT. 1 .OR. KMAX .GT. NP) IFAULT = IFAULT + 4
C   IF (A1 .LE. ZERO .OR. A1 .GE. ONE) IFAULT = IFAULT + 8
C   IF (COND .LT. 1 .OR. COND .GT. 4) IFAULT = IFAULT + 16
C   IF (RAW .LT. 0 .OR. RAW .GT. 1) IFAULT = IFAULT + 32
C   IF (RAW .NE. 0 .AND. COND .EQ. 1) IFAULT = IFAULT + 64
C   IF (IFAULT .GT. 0) RETURN
C
C   Check for known population parameter
C
C   IF (RAW .EQ. 1) THEN
C     NDEN1 = N1
C     NDEN2 = N2
C     IF (COND.NE.2) THEN
C
C   Estimation of individual mean vector
C
C     DO 30 J = 1, NP
C       SUM = ZERO
C       DO 10 I = 1, N1
C         SUM = SUM + DATA(I, J)
10      CONTINUE
C       DATA(MX, J) = SUM / N1
C       SUM = ZERO

```

```

                DO 20 I = N1P1, N1N2
                  SUM = SUM + DATA(I, J)
20              CONTINUE
                DATA(MY, J) = SUM / N2
30              CONTINUE
C
C      Estimation of covariance matrices
C
                NDEN1 = N1 - 1
                NDEN2 = N2 - 1
                ENDIF
                DO 60 J = 1, NP
                  XYMEAN = DATA(MX, J)
                  DO 40 I = 1, N1
                    DATA(I, J) = DATA(I, J) - XYMEAN
40                CONTINUE
                  XYMEAN = DATA(MY, J)
                  DO 50 I = N1P1, N1N2
                    DATA(I, J) = DATA(I, J) - XYMEAN
50                CONTINUE
60              CONTINUE
                DO 100 J = 1, NP
                  DO 90 K = 1, J
                    SSQ = ZERO
                    DO 70 I = 1, N1
                      SSQ = SSQ + DATA(I, J) * DATA(I, K)
70                  CONTINUE
                    SX(J, K) = SSQ / NDEN1
                    SSQ = ZERO
                    DO 80 I = N1P1, N1N2
                      SSQ = SSQ + DATA(I, J) * DATA(I, K)
80                  CONTINUE
                    SY(J, K) = SSQ / NDEN2
90                CONTINUE
100             CONTINUE
                DO 120 J = 2, NP
                  DO 110 K = 1, J - 1
                    SX(K, J) = SX(J, K)
                    SY(K, J) = SY(J, K)
110             CONTINUE
120             CONTINUE
                IF (COND .EQ. 3) THEN
C
C      Estimation of common mean vector
C
                DO 130 J = 1, NP
                  DATA(MX, J) = (N1 * DATA(MX, J) + N2 * DATA(MY, J)) /
*                               N1N2
                  DATA(MY, J) = DATA(MX, J)
130             CONTINUE
                ENDIF
                ENDIF
C
C      Simultaneous diagonalisation of the covariance matrices
C
                CALL DIAG2 (DI, NP, SX, SY, TMV(1, 2), Z, CGFE(1, 1),
*              CGFE(1, NP+1), CGFE(1, 2*NP+1), CGFE(1, 3*NP+1), IFLT)
                IF (IFLT .GT. 0) THEN
                  IFAULT = 128
                  RETURN
                ENDIF

```

```

C
C      Compute population 2 mean vector (transformed)
C
      IF (COND .EQ. 3) THEN
        DO 140 I = 1, NP
          TMV(I, 1) = ZERO
140      CONTINUE
        ELSE
          DO 160 I = 1, NP
            STORE = ZERO
            DO 150 J = 1, NP
              STORE = Z(J, I) * (DATA(MY, J) - DATA(MX, J)) + STORE
150          CONTINUE
            TMV(I, 1) = STORE
160          CONTINUE
        ENDIF

C
C      Compute Z' * XBAR
C
      DO 180 I = 1, NP
        STORE = ZERO
        DO 170 J = 1, NP
          STORE = STORE + Z(J, I) * DATA(MX, J)
170      CONTINUE
        Z(I, IZ) = STORE
180      CONTINUE

C
C      Determination of marginal misclassification probabilities
C
      CALL ERPROB (DI, NP, TMV, A1, PQ, ICC, CUT)

C
C      Re-indexing the variables such that the values of p are
C      increasing
C
      DO 210 I = 1, NP - 1
        DO 200 J = 1, NP - I
          JP1 = J + 1
          IF ( (PQ(1, J) .EQ. PQ(1, JP1) .AND. PQ(2, J) .GT.
*           PQ(2, JP1)) .OR. PQ(1, J) .GT. PQ(1, JP1)) THEN
            CALL SWAP (PQ(1, J), PQ(1, JP1))
            CALL SWAP (PQ(2, J), PQ(2, JP1))
            CALL SWAP (CUT(J), CUT(JP1))
            HOLD = ICC(J)
            ICC(J) = ICC(JP1)
            ICC(JP1) = HOLD
            CALL SWAP (TMV(J, 2), TMV(JP1, 2))
            CALL SWAP (TMV(J, 1), TMV(JP1, 1))
            DO 190 K = 1, NP
              CALL SWAP (Z(K, J), Z(K, JP1))
190          CONTINUE
            CALL SWAP (Z(J, IZ), Z(JP1, IZ))
          ENDIF
        200      CONTINUE
      210      CONTINUE

C
C      Determination of the optimal joint classification rule
C
      CALL MCE (NP, KMAX, A1, PQ, PMIN, LKA, UPMQM, ICR, IFAULT)
      END

      SUBROUTINE DIAG2 (DI, NP, SX, SY, D, Z, C, G, F, E, IFAULT)

```

```

C
C      ALGORITHM AS 276.2 APPL.STATIST. (1992), VOL.41, NO.2
C
C      Simultaneously diagonalizes two covariance matrices such that
C       $Z'(SX)Z = I$  and  $Z'(SY)Z = D$  where  $D$  is a diagonal matrix
C
C      INTEGER DI, NP, IFAULT
C      REAL SX(DI, NP), SY(DI, NP), D(NP), Z(DI, NP), C(DI, NP),
*      G(DI, NP), F(DI, NP), E(NP)
C
C      EXTERNAL TQL2, TRED2
C
C      INTRINSIC SQRT
C
C      INTEGER I, IFLT, J, K
C      REAL ROOTD, SUM, ZERO
C      PARAMETER (ZERO = 0.0E0)
C
C      IFAULT = 0
C
C      Find G such that  $G' (SX) G = I$ 
C
C      CALL TRED2 (DI, NP, SX, D, E, G)
C      CALL TQL2 (DI, NP, D, E, G, IFLT)
C      IF (IFLT .NE. 0) THEN
C          IFAULT = 1
C          RETURN
C      ENDIF
C      DO 10 I = 1, NP
C          IF (D(I) .LE. ZERO) THEN
C              IFAULT = 2
C              RETURN
C          ENDIF
10  CONTINUE
C      DO 30 J = 1, NP
C          ROOTD = SQRT(D(J))
C          DO 20 I = 1, NP
C              G(I, J) = G(I, J) / ROOTD
20  CONTINUE
30  CONTINUE
C
C      Create matrix  $F = G' (SY) G$ 
C
C      DO 60 I = 1, NP
C          DO 50 J = 1, NP
C              SUM = ZERO
C              DO 40 K = 1, NP
C                  SUM = SY(I, K) * G(K, J) + SUM
40  CONTINUE
C              Z(I, J) = SUM
50  CONTINUE
60  CONTINUE
C      DO 90 I = 1, NP
C          DO 80 J = 1, NP
C              SUM = ZERO
C              DO 70 K = 1, NP
C                  SUM = Z(K, I) * G(K, J) + SUM
70  CONTINUE
C              F(I, J) = SUM
80  CONTINUE
90  CONTINUE

```



```
C
C      Find C such that C' F C = D
C
CALL TRED2 (DI, NP, F, D, E, C)
CALL TQL2 (DI, NP, D, E, C, IFLT)
IF (IFLT .NE. 0) THEN
  IFAULT = 3
  RETURN

ENDIF
DO 100 I = 1, NP
  IF (D(I) .LE. ZERO) THEN
    IFAULT = 4
    RETURN
  ENDIF
100 CONTINUE
C
C      Create matrix Z = GC
C
DO 130 I = 1, NP
  DO 120 J = 1, NP
    SUM = ZERO
    DO 110 K = 1, NP
      SUM = G(I, K) * C(K, J) + SUM
110    CONTINUE
    Z(I, J) = SUM
120  CONTINUE
130 CONTINUE
RETURN
END

SUBROUTINE ERPROB (DI, N, TMV, A1, PQ, ICC, CUT)
C
C      ALGORITHM AS 276.3 APPL.STATIST. (1992), VOL.41, NO.2
C
C      Gives the classification rules and misclassification
C      probabilities for each of the marginal classification
C      procedures in normal population combinatoric classification
C
INTEGER DI, N, ICC(N)
REAL TMV(DI, 2), A1, PQ(2, N), CUT(N)
C
REAL ALNORM, CHISQ1
C
EXTERNAL ALNORM, CHISQ1
C
INTRINSIC LOG, SQRT
C
INTEGER I
REAL B, G, H, HALF, ONE, S, T, TWO, VU, ZERO
C
PARAMETER (ONE = 1.0E0, ZERO = 0.0E0, TWO = 2.0E0, HALF = 0.5E0)
C
C      Misclassification probabilities for cases 1 and 2
C
B = ((ONE - A1) / A1) ** 2
DO 10 I = 1, N
  S = TMV(I, 2)
  T = TMV(I, 1)
  CUT(I) = ZERO
  IF (S .NE. ONE) THEN
```

```

      G = S * LOG(B / S) / (ONE - S) + (T / (ONE - S)) ** 2 * S
      IF (G .GT. ZERO) THEN
        VU = T / (S - ONE)
        CUT(I) = G
        ICC(I) = 1
        PQ(1, I) = ONE - CHISQ1(G, VU)
        G = G / S
        VU = (VU + T) / SQRT(S)
        PQ(2, I) = CHISQ1(G, VU)
        IF (S .LT. ONE) THEN
          ICC(I) = 2
          PQ(1, I) = ONE - PQ(1, I)
          PQ(2, I) = ONE - PQ(2, I)
        ENDIF
      ENDIF

```

```

C
C      Misclassification probabilities for cases 3 and 4
C

```

```

      ELSE IF (S .GT. ONE) THEN
        ICC(I) = 3
        PQ(1, I) = ONE
        PQ(2, I) = ZERO
      ELSE
        ICC(I) = 4
        PQ(1, I) = ZERO
        PQ(2, I) = ONE
      ENDIF

```

```

C
C      Misclassification probabilities for cases 5 and 6
C

```

```

      ELSE IF (T .EQ. ZERO) THEN
        IF (A1 .LT. HALF) THEN
          ICC(I) = 5
          PQ(1, I) = ONE
          PQ(2, I) = ZERO
        ELSE
          ICC(I) = 6
          PQ(1, I) = ZERO
          PQ(2, I) = ONE
        ENDIF
      ENDIF

```

```

C
C      Misclassification probabilities for cases 7 and 8
C

```

```

      ELSE
        H = T / TWO - LOG(B) / TWO / T
        CUT(I) = H
        ICC(I) = 7
        PQ(1, I) = ALNORM(H, .TRUE.)
        H = H - T
        PQ(2, I) = ALNORM(H, .FALSE.)
        IF (T .LT. ZERO) THEN
          ICC(I) = 8
          PQ(1, I) = ONE - PQ(1, I)
          PQ(2, I) = ONE - PQ(2, I)
        ENDIF
      ENDIF

```

```

      ENDIF
10 CONTINUE
      RETURN
      END

```

```

      SUBROUTINE SWAP (X, Y)

```

```

C

```

```
C      ALGORITHM AS 276.4 APPL.STATIST. (1992), VOL.41, NO.2
C
C      Interchanges the values of two real variables : X and Y
C
REAL X, Y
C
REAL STORE
C
STORE = X
X = Y
Y = STORE
RETURN
END

REAL FUNCTION CHISQ1(G, VU)
C
C      ALGORITHM AS 276.5 APPL.STATIST. (1992), VOL.41, NO.2
C
C      Calculates the probability that a noncentral chi-square
C      variable is less than G (with DF=1 and noncentrality parameter
C      VU**2)
C
REAL G, VU
C
REAL ALNORM
EXTERNAL ALNORM
INTRINSIC SQRT
C
REAL X, Y, ZERO
PARAMETER (ZERO = 0.0E0)
C
IF (G .GT. ZERO) THEN
  X = SQRT(G) - VU
  Y = -SQRT(G) - VU
  CHISQ1 = ALNORM(X, .FALSE.) - ALNORM(Y, .FALSE.)
  RETURN
ELSE
  CHISQ1 = ZERO
  RETURN
ENDIF
END
```

C-----

```

SUBROUTINE MEDIAN(X, Y, N, IWS, XMED, YMED, IFAULT)
C
C     ALGORITHM AS 277.1 APPL.STATIST. (1992) VOL.41, NO.3
C
C     On exit (XMED, YMED) will contain the bivariate median
C     of the points (X(i),Y(i)), i = 1, ... ,N.
C
C     *** WARNING ***
C     The routine as published in the journal contains at least three
C     errors. This version has been constructed by Alan Miller. It
C     appears to work correctly but no guarantee is given.
C     N.B. The name of this routine is MEDIAN, not MED as specified in
C     the Structure description given in the journal.
C
C     Auxiliary routines required: M01DAF and M01ZAF from the NAG library.
C
C     INTEGER N, IWS(N), IFAULT
C     REAL X(N), Y(N), XMED, YMED
C
C     EXTERNAL M01DAF, M01ZAF
C
C     INTEGER I, J, K, KQ, L, LL, NDIF, NT, NZ, NZERO
C     REAL D0, DP, EPS, SMALL, SMALLD, T, TL, TU, W, WW, XKL,
*     XMAX, XMIN, YKL, YMAX, YMIN
C
C     DATA EPS / 1.0E-6 /
C
C     IFAULT=0
C     CALL M01DAF(X,1,N,'A',IWS,IFAU)
C     CALL M01ZAF(IWS,1,N,IFAU)
C     XMIN=X(IWS(1))
C     XMAX=X(IWS(N))
C
C     CALL M01DAF(Y,1,N,'A',IWS,IFAU)
C     CALL M01ZAF(IWS,1,N,IFAU)
C     YMIN=Y(IWS(1))
C     YMAX=Y(IWS(N))
C
C     IFAULT=0
C     SMALL=EPS*(XMAX-XMIN)*(YMAX-YMIN)
C     SMALLD=SMALL*N
C
C     DO 40 NDIF=1,N
C         WW=0.0
C         DO 30 K=1,N-1
C             DO 20 L=K+1,N
C                 NT=0
C                 XKL=X(K)-X(L)
C                 YKL=Y(K)-Y(L)
C                 IF(ABS(XKL)+ABS(YKL).LT.SMALL) GO TO 15
C                 DO 10 I=1,N
C                     W=(Y(I)-Y(L))*XKL-(X(I)-X(L))*YKL
C                     WW=WW+ABS(W)
C                     IF(W.GT.0.0)NT=NT+1
C             CONTINUE
C         CONTINUE
C         IF((ABS(2*NT-N+2).LE.NDIF).AND.WW.GT.SMALLD) GO TO 50
C     CONTINUE
C     CONTINUE
C     IF(WW.LE.SMALLD) THEN

```

```

C      The data set is completely collinear.
C
      IF (MOD(N,2).EQ.0) THEN
          XMED=(X(IWS(N/2))+X(IWS(N/2+1)))/2
          YMED=(Y(IWS(N/2))+Y(IWS(N/2+1)))/2
      ELSE
          XMED=X(IWS((N+1)/2))
          YMED=Y(IWS((N+1)/2))
      END IF
      RETURN
END IF

C
40 CONTINUE

C
50 CALL TUTL(X,Y,N,XMIN,YMIN,XMAX,YMAX,K,L,SMALL,TU,TL)

C
C      Start the search along the line through the points (X(k),Y(k))
C      and (X(l),Y(l)), dividing the N-2 other points evenly.
C
60 KQ=1

C
C      Search for the minimum of the Oja objective function on the
C      line (X(k),Y(k)) to (X(l),Y(l)).
C
DO 80 I=1,N-1
    DO 70 J=I+1,N
        WW=(X(K)-X(L))*(Y(J)-Y(I))-(Y(K)-Y(L))*(X(J)-X(I))
        IF(ABS(WW).LT.SMALL) GO TO 70
        T=((X(L)-X(J))*(Y(I)-Y(J))-(Y(L)-Y(J))*(X(I)-X(J)))/WW
        IF(T.LT.TU.AND.T.GT.TL)THEN
            CALL DER(X,Y,N,K,L,T,IWS,SMALL,NZERO,KQ,DP,D0)
C            A=DP+D0 ! Redundant instruction
            IF(D0.GE.ABS(DP)-SMALLD) GO TO 90
            IF(DP+D0.LT.0.0)TL=T
            IF(DP+D0.GT.0.0)TU=T
        END IF
    70 CONTINUE
80 CONTINUE

C
C      The local minimum on the line (X(k),Y(k)) - (X(l),Y(l))
C      was not found.
C
IFAULT=IFAULT+2
IF(IFAULT.GT.6) RETURN
L=N-1
K=N
90 KQ=0
I=K
J=L

C
LL=1
NZ=NZERO
100 K=INT(IWS(LL)/REAL(N))
L=MOD(IWS(LL),N)+1
WW=(X(K)-X(L))*(Y(J)-Y(I))-(Y(K)-Y(L))*(X(J)-X(I))
IF(ABS(WW).GE.SMALL) THEN
    T=((X(L)-X(J))*(Y(I)-Y(J))-(Y(L)-Y(J))*(X(I)-X(J)))/WW
    CALL DER(X,Y,N,K,L,T,IWS,SMALL,NZERO,KQ,DP,D0)
    IF (D0.LT.ABS(DP)-SMALL) THEN
        CALL TUTL(X,Y,N,XMIN,YMIN,XMAX,YMAX,K,L,SMALL,TU,TL)
        IF(DP+D0.LT.0.0)THEN

```

```

        TL=T
        ELSE
            TU=T
        END IF
        GO TO 60
    END IF
    LL=LL+1
END IF
C
IF(LL.EQ.NZ+1)THEN
    XMED=X(L)+T*(X(K)-X(L))
    YMED=Y(L)+T*(Y(K)-Y(L))
    RETURN
END IF
C
GO TO 100
END
C
SUBROUTINE DER(X,Y,N,K,L,T,IWS,SMALL,NZERO,KQ,DP,D0)
C
C     ALGORITHM AS 277.2 APPL.STATIST. (1992) VOL.41, NO.3
C
C     DP-D0 and DP+D0 are the directional derivatives of the Oja
C     Objective function just before and after the point
C     (X(1)+t*(X(k)-X(1)),Y(1)+t*(Y(k)-Y(1)))
C
C     INTEGER N, K, L, IWS(N), NZERO, KQ
C     REAL X(N), Y(N), T, SMALL, DP, D0
C
C     REAL DIF, SGN, SMALLD, TT, WW, XKL, YKL
C     INTEGER II, JJ
C
C     DATA SMALLD / 1E-6 /
C
C     DP=0.0
C     D0=0.0
C     NZERO=0
C     XKL=X(K)-X(L)
C     YKL=Y(K)-Y(L)
C
DO 20 II=1,N-1
    DO 10 JJ=II+1,N
        WW=(Y(JJ)-Y(II))*XKL-(X(JJ)-X(II))*YKL
        IF(ABS(WW).LE.SMALL) GO TO 10
        TT=((X(L)-X(JJ))*(Y(II)-Y(JJ))-(Y(L)-Y(JJ))*(X(II)-X(JJ)))/WW
        DIF=T-TT
        IF(ABS(DIF).LE.SMALLD)THEN
            NZERO=NZERO+1
            NZERO=MIN(NZERO,N)
            IF(KQ.NE.0)IWS(NZERO)=N*II+JJ-1
            D0=D0+ABS(WW)
        ELSE
            DP=DP+ABS(WW)*SGN(DIF)
        END IF
    10 CONTINUE
    20 CONTINUE
    RETURN
END
C
FUNCTION SGN(X)
C

```

C           ALGORITHM AS 277.3 APPL.STATIST. (1992) VOL.41, NO.3

C

```
REAL SGN, X
SGN=1.0
IF (X.LT.0.0)SGN=-1.0
RETURN
END
```

C

```
SUBROUTINE TUTL(X,Y,N,XMIN,YMIN,XMAX,YMAX,K,L,SMALL,TU,TL)
```

C

C

C

C

C

C

C

C

```
ALGORITHM AS 277.4 APPL.STATIST. (1992) VOL.41, NO.3
```

```
This subroutine calculates the upper (TU) and lower limit (TL)
for parameter T on the line (X(l)+t*(X(k)-X(l)), Y(l)+t*(Y(k)-Y(l)))
inside the rectangle with vertices (XMIN,YMIN), (XMIN,YMAX),
(XMAX,YMIN) and (XMAX,YMAX).
```

```
INTEGER N, K, L
REAL X(N), Y(N), XMIN, YMIN, XMAX, YMAX, SMALL, TU, TL
REAL T1, T2, T3, T4, VBIG
DATA VBIG / 1E38 /
T1=-VBIG
T2=-T1
IF(ABS(X(K)-X(L)).GT.SMALL)THEN
  T1=-(X(L)-XMIN)/(X(K)-X(L))
  T2= (XMAX-X(L))/(X(K)-X(L))
END IF
T3=-VBIG
T4=-T3
IF(ABS(Y(K)-Y(L)).GT.SMALL)THEN
  T3=-(Y(L)-YMIN)/(Y(K)-Y(L))
  T4= (YMAX-Y(L))/(Y(K)-Y(L))
END IF
TU=MIN(MAX(T1,T2),MAX(T3,T4))+SMALL
TL=MAX(MIN(T1,T2),MIN(T3,T4))-SMALL
RETURN
END
```

```
REAL FUNCTION PSI2(X, P, Q, A2, DELTA, MAXITR, IFAULT)
C
C     ALGORITHM AS 278.1 APPL.STATIST. (1992) VOL.41, NO.3
C
C     Calculates the probability that a random variable distributed
C     according to the psi-square distribution with P and Q degrees
C     of freedom and A2 eccentricity parameter, is less than or
C     equal to X
C
REAL X, P, Q, A2, DELTA
INTEGER MAXITR, IFAULT
C
REAL ALNGAM, BETAIX
EXTERNAL ALNGAM, BETAIX
C
REAL AQAL, BL, CL, DAX, DJ, DJ1, ERP, ERR, EXPL, G,
*   GCJ, GCL, HALF, ONE, PQ2, PREC, P2, QQAL, Q2, R,
*   RL, SUM, SUMC, SUMCP, TWO, V, W, XLOW, XP, Y, YYL,
*   Z, ZERO, ZM, ZN
INTEGER IOK, J, JJ, JJJ, JOK, KOK
LOGICAL LALF
C
PARAMETER (ZERO=0.0E0, HALF=0.5E0, ONE=1.0E0, TWO=2.0E0)
C
C     machine-dependent constants
C
PARAMETER (PREC=1.0E-6, XLOW=1.2E-38, EXPL=-87.315E0)
PARAMETER (XP=XLOW/PREC)
C
IFAULT = 0
C
C     test for valid input arguments
C
IF (X .LT. ZERO .OR. A2 .LT. ZERO
*   .OR. P .LE. ZERO .OR. Q .LE. ZERO
*   .OR. DELTA .GE. ONE .OR. DELTA .LE. PREC) THEN
    IFAULT = 1
    PSI2 = -ONE
    RETURN
ENDIF
C
C     define usefull parameters
C
P2 = P * HALF
Q2 = Q * HALF
PQ2 = P2 + Q2
C
C     case A2 = 0
C
IF (A2 .LT. PREC) THEN
    PSI2 = BETAIX( P*X/(P*X+Q), P2, Q2, IOK )
    IF (IOK .NE. 0) THEN
        IFAULT = 4
        PSI2 = -ONE
    ENDIF
    RETURN
ENDIF
C
C     case P = 1
C
IF (ABS(P-ONE) .LT. PREC) THEN
```



```

        DAX  = TWO * SQRT( A2*X )
        PSI2 = HALF * ( SIGN( ONE, X-A2 ) *
*           BETAIX( (A2+X-DAX)/(A2+X-DAX+Q),HALF,Q2,IOK ) +
*           BETAIX( (A2+X+DAX)/(A2+X+DAX+Q),HALF,Q2,JOK ) )
        IF (IOK .NE. 0 .OR. JOK .NE. 0) THEN
            IFAULT = 4
            PSI2 = -ONE
        ENDIF
        RETURN
    ENDIF

C
Y = P*X / (A2+Q+P*X)

C
C     case P = Q and Y = 0.5
C
    IF (ABS(Y-HALF) .LT. PREC .AND. ABS(P-Q) .LT. PREC) THEN
        PSI2 = HALF
        RETURN
    ENDIF

C
C     calculate 1-F(X) or F(X) (LALF is the indicator)
C
    IF (Y .GT. HALF .OR. (Y .EQ. HALF .AND. P .GT. Q) ) THEN
        LALF = .TRUE.
        Z    = ONE - Y
        ZM   = Q2
        ZN   = P2
    ELSE
        LALF = .FALSE.
        Z    = Y
        ZM   = P2
        ZN   = Q2
    ENDIF

C
C     Y near 0 or 1 ?
C
    IF (Z .LT. PREC) THEN
        IF( LALF )THEN
            PSI2 = ONE
        ELSE
            PSI2 = ZERO
        ENDIF
        RETURN
    ENDIF

C
C     General case (iterations)
C     G's are decreasing for J >= JJ = -V/W + 1
C     CL's are decreasing for J >= JJJ = A2/2 + 1
C     GCJ, SUMC, SUMCP are only used for stopping rule
C     logs are used to avoid underflows
C
    ERR = DELTA * HALF
    ERP = ERR / PREC
    YYL = LOG( Y*(ONE-Y) )
    QQAL = Q2 * LOG( Q/(Q+A2) )
    AQAL = LOG( A2/(Q+A2) )
    V    = PQ2 * Z - ZN
    W    = Z + Z - ONE

C
C     initialize
C

```

```

BL = ZERO
CL = QQAL
G = BETAIX( Z, ZM, ZN, IOK )
IF ( IOK .NE. 0 ) THEN
  IFAULT = 4
  PSI2 = -ONE
  RETURN
ENDIF
RL = P2 * LOG(Y) + Q2 * LOG(ONE-Y) + ALNGAM(PQ2, IOK)
* - ALNGAM(P2, JOK) - ALNGAM(Q2, KOK) - LOG(P2) - LOG(Q2)
IF ( IOK+JOK+KOK .NE. 0 ) THEN
  IFAULT = 5
  PSI2 = -ONE
  RETURN
ENDIF
IF (RL .GE. EXPL) THEN
  R = EXP( RL )
ELSE
  R = ZERO
ENDIF
SUM = ZERO
GCJ = ZERO
SUMC = ZERO
SUMCP = SUMC
DJ = ZERO
C
C   define minimum numbers of iterations (JJ and JJJ)
C
IF (ZM .GT. ZN .AND. W .NE. ZERO) THEN
  JJ = INT( -V/W ) + 1
ELSE
  JJ = 0
ENDIF
JJJ = INT( A2*HALF ) + 1
C
C   iteration loop
C
DO 10 J = 0, MAXITR
C
  IF (G .GT. ZERO) THEN
    GCL = LOG(G) + CL
    IF (GCL .GE. EXPL) THEN
      GCL = EXP( GCL )
      SUM = SUM + GCL
      GCJ = GCJ + GCL*DJ
C     check loss of accuracy
      IF (GCJ .GE. ERP) THEN
        IFAULT = 3
        GOTO 20
      ENDIF
    ENDIF
  ENDIF
  SUMC = SUMC + EXP(CL)
C
C   check accuracy (stopping rule)
C
IF (J .GE. JJ) THEN
C   XP is used to prevent possible underflow
  IF (GCJ .GE. XP) THEN
    IF (PREC*GCJ+G*(ONE-SUMC) .LT. ERR) GOTO 20

```

```

        ELSE
          IF (          G*(ONE-SUMC) .LT. ERR) GOTO 20
        ENDIF
        IF (J .GE. JJJ .AND. SUMC .EQ. SUMCP .AND.
*         ABS(ONE-SUMC) .GE. PREC) THEN
          IFAULT = 3
          GOTO 20
        ENDIF
      ENDIF
    ENDIF

C
C      prepare next iteration
C
      SUMCP = SUMC
      DJ1   = DJ + ONE
      BL    = BL + LOG( (Q2+DJ)/DJ1 )
      CL    = BL + QQAL + DJ1*AQAL
      G     = G  + (V+W*DJ)*R
      RL    = RL + YYL +
*         LOG( ((DJ+DJ+PQ2)/(DJ1+P2)) * ((DJ+DJ1+PQ2)/(DJ1+Q2)) )
      IF (RL .GE. EXPL) THEN
        R = EXP( RL )
      ELSE
        R = ZERO
      ENDIF
      DJ = DJ1

10 CONTINUE

C
C      we get here if maximum number of iterations is reached
C
      IFAULT = 2

C
C      the end
C

20 CONTINUE
      IF (LALF) THEN
        PSI2 = ONE - SUM
      ELSE
        PSI2 = SUM
      ENDIF

C
      END
      REAL FUNCTION BETAIX(X, P, Q, IFAULT)

C
C      ALGORITHM AS 278.2 APPL.STATIST. (1992) VOL.41, NO.3
C
      REAL X, P, Q
      INTEGER IFAULT

C
      REAL ALNGAM, BETAIN
      EXTERNAL ALNGAM, BETAIN

C
      REAL BETA, EXPL, ZERO
      INTEGER IOK, JOK, KOK

C
      PARAMETER (ZERO=0.0E0)

C
C      machine-dependent constant
C
      PARAMETER (EXPL=-87.315E0)
C

```

```
BETAIX = ZERO
C
C      calculate beta parameter for betain
C
BETA = ALNGAM(P,JOK) + ALNGAM(Q,KOK) - ALNGAM(P+Q,IOK)
IF (IOK+JOK+KOK .NE. 0) THEN
  IFAULT = 5
  RETURN
ENDIF
IF (BETA .GE. EXPL) THEN
  BETA = EXP(BETA)
ELSE
  IFAULT = 4
  RETURN
ENDIF
BETAIX = BETAIN(X, P, Q, BETA, IFAULT)
END
```

```
      SUBROUTINE DWPVAL (X, IAX, N, M, NCONST, LAG, IALT, E, C, P,  
*                      WS1, WS2, WS3, IFAULT)  
C  
C      ALGORITHM AS279 APPL. STATIST. (1993) VOL. 42, NO.1  
C  
C      P-VALUE FOR GENERALIZED/ALTERNATIVE DURBIN-WATSON STATISTIC WITH  
C      ARBITRARY LAG BY CHOLESKY TRANSFORMATION METHOD  
C  
C      ARGUMENT DECLARATIONS  
C  
C      INTEGER N, M, IAX, NCONST, LAG, IFAULT, IALT  
C      REAL X(IAX,*), E, C, P, WS1(*), WS2(*), WS3(*)  
C  
C      LOCAL VARIABLE DECLARATIONS  
C  
C      INTEGER J, K, MTOT, MNET, ITAIL  
C      REAL POINT5, POINT1, ZERO, ONE, E1, E2, E3, F1, F2, U, UJ,  
*      PI, RBD, UMAX, DELTA, ZFLOAT, ZLOG, ZIMAG, ZABS  
C      COMPLEX CF  
C  
C      CONSTANTS  
C  
C      DATA ZERO, ONE, POINT5, POINT1 / 0.E0, 1.E0, 5.E-1, 1.E-1 /  
C      DATA PI /3.14159265358979E0 /  
C  
C      STANDARD FUNCTIONS  
C  
C      ZFLOAT(J) = FLOAT(J)  
C      ZLOG(U) = ALOG(U)  
C      ZIMAG(CF) = AIMAG(CF)  
C      ZABS(CF) = CABS(CF)  
C  
C      INITIALIZATIONS  
C  
C      IFAULT = 0  
C      MTOT = M + NCONST  
C      IF (N .LE. MTOT) THEN  
C         IFAULT = -1  
C         RETURN  
C      ELSEIF (N .LT. 2 * LAG) THEN  
C         IFAULT = -3  
C         RETURN  
C      ENDIF  
C      E1 = E * POINT1  
C      E3 = (E - E1) * POINT1  
C      E2 = E - E1 - E3  
C      E3 = E3 * PI  
C  
C      INTERVAL SIZE AND TRUNCATION LIMIT FOR TRAPEZOIDAL RULE  
C  
C      MNET = MTOT - NCONST  
C      CALL GKPTRP (N, MNET, NCONST, LAG, IALT, C, E1, E2, DELTA, K,  
*                WS1, WS1(N+1), ITAIL, IFAULT)  
C      IF (IFAILT .NE. 0) RETURN  
C      IF (ITAIL .GT. 0) THEN  
C         P = ONE  
C         RETURN  
C      ELSEIF (ITAIL .LT. 0) THEN  
C         P = ZERO  
C         RETURN  
C      ENDIF
```

```
C
C      SCALE FACTOR FOR CHARACTERISTIC FUNCTION
C
CALL DWSCLE (X, IAX, N, M, NCONST, F1, F2, WS2, IFAULT)
IF (IFAULT .NE. 0) RETURN

C
C      NUMERICAL INTEGRATION
C
UMAX = ZFLOAT(K) + POINT5
RBD = ONE
P = ZERO
J = 0
50 IF (RBD .GT. E3 .AND. J .LE. K) THEN
    UJ = ZFLOAT(J) + POINT5
    U = UJ * DELTA
    CALL DWCHF(X, IAX, N, M, NCONST, LAG, IALT, U, C, F1, F2,
*           CF, WS2, WS3, IFAULT)
    IF (IFAULT .NE. 0) RETURN
    P = P + ZIMAG(CF) / UJ
    RBD = ZABS(CF) * ZLOG(UMAX / UJ)
    J = J + 1
    GOTO 50
ENDIF
P = POINT5 - P / PI
RETURN
END

C
C
SUBROUTINE DWCHF (X, IAX, N, M, NCONST, LAG, IALT, T, C, F1,
*           F2, CF, S, XT, IFAULT)

C
C      CHARACTERISTIC FUNCTION FOR GENERALIZED/ALTERNATIVE DURBIN-
C      WATSON STATISTIC AND EXACT LBI VERSIONS FOR ARBITRARY LAG
C
C      ARGUMENT DECLARATIONS:
C
INTEGER IAX, IALT, N, M, NCONST, IFAULT, LAG
REAL X(IAX,*), T, C, F1, F2
COMPLEX CF, S(*), XT(LAG+1,*)

C
C      LOCAL VARIABLE DECLARATIONS
C
INTEGER MTOT, I, J, K, MLAG, II, JJ, KK, NN, N1, IROW, JROW
REAL ZERO, ONE, TWO, D2
COMPLEX A1, A2, A, B, LB, ZCMLPX, ZSQRT, D1, LD, LLD

C
C      CONSTANTS
C
DATA ZERO,ONE,TWO / 0.E0,1.E0,2.E0 /

C
C      STANDARD FUNCTIONS
C
ZCMLPX(F1,F2) = CMPLX(F1,F2)
ZSQRT(A) = CSQRT(A)

C
C      INITIALIZATIONS
C
IFAULT = 0
CF = F1
MTOT = M + NCONST
K = 0
```

```

DO 20 I = 1,MTOT
DO 10 J = 1,I
K = K + 1
S(K) = ZERO
10 CONTINUE
20 CONTINUE
A1 = ZCMPLX(ONE,TWO * T * (C - ONE))
A2 = A1 - ZCMPLX(ZERO,TWO * T)
IF (IALT .NE. 0) A1 = A2
B = ZCMPLX(ZERO,TWO * T)
NN = (N - 1)/LAG + 1
N1 = N - LAG + 1
MLAG = LAG + 1
IROW = 0
KK = 0

C
C      CHOLESKY TRANSFORMATION CYCLE
C
DO 110 II = 1,NN
DO 100 JJ = 1,LAG
KK = KK + 1
IF (KK .LE. N) THEN
  IROW = IROW + 1
  IF (IROW .GT. MLAG) IROW = 1
  IF (II .EQ. 1) THEN
    IF (JJ .EQ. 1) LD = ONE / ZSQRT(A1)
    DO 30 I = 1,M
    XT(IROW,I) = X(KK,I) * LD
30 CONTINUE
    IF (NCONST .NE. 0) XT(IROW,MTOT) = LD
  ELSE
    IF (JJ .EQ. 1 .OR. KK .EQ. N1) THEN
      IF (JJ .NE. 1 .OR. KK .GT. N1) THEN
        LB = B * LLD
      ELSE
        LB = B * LD
      ENDIF
      LLD = LD
      A = A2
      IF (KK .GE. N1) A = A1
      LD = ONE / ZSQRT(A - LB * LB)
    ENDIF
    JROW = IROW - LAG
    IF (JROW .LE. 0) JROW = JROW + MLAG
    DO 40 I = 1,M
    XT(IROW,I) = LD * (X(KK,I) - LB * XT(JROW,I))
40 CONTINUE
    IF (NCONST .NE. 0) XT(IROW,MTOT) = LD * (ONE - LB * XT(JROW,MTOT))
  ENDIF
  CF = CF * LD

C
C      UPDATE CROSS-PRODUCT MATRIX
C
IF (MTOT .GT. 0) THEN
  K = 0
  DO 60 I = 1,MTOT
  DO 50 J = 1,I
  K = K + 1
  S(K) = S(K) + XT(IROW,I) * XT(IROW,J)
50 CONTINUE
60 CONTINUE

```

```
        ENDIF
    ENDIF
100 CONTINUE
110 CONTINUE
C
C     DETERMINANT OF CROSS-PRODUCT MATRIX
C
    IF (MTOT .GT. 0) THEN
        CALL CCLSKY(S,MTOT,D1,D2,IFAU)
        CF = CF * D1 * TWO ** (D2 + F2)
    ENDIF
    RETURN
    END

C
C
    SUBROUTINE CCLSKY(S,M,D1,D2,IFAU)
C
C     CHOLESKY FACTORIZATION IN COMPLEX ARITHMETIC
C
C     ARGUMENT DECLARATIONS:
C
C     INTEGER M, IFAU
C     REAL D2
C     COMPLEX S(*), D1
C
C     LOCAL VARIABLE DECLARATIONS
C
C     INTEGER I, J, JJ, K, L, KK, KI, KJ
C     REAL EPS, ZERO, ONE, FOUR, SIXTEN, SIXNTH, ZABS
C     COMPLEX SUM, ZSQRT
C
C     CONSTANTS
C
C     DATA ZERO,ONE,FOUR,SIXTEN,SIXNTH / 0.E0,1.E0,4.E0,1.6E1,.625E-1 /
C     DATA EPS / 1.E-6 /
C
C     STANDARD FUNCTIONS
C
C     ZSQRT(SUM) = CSQRT(SUM)
C     ZABS(SUM) = CABS(SUM)
C
C     INITIALIZATIONS
C
C     IFAU = 0
C     D1 = ONE
C     D2 = ZERO
C
C     FACTORIZATION
C
C     K = 0
C     DO 60 I = 1,M
C     KK = 0
C     KI = K
C     DO 50 J = 1,I
C     K = K + 1
C     SUM = S(K)
C     IF (J .GT. 1) THEN
C     JJ = J - 1
C     KJ = KI
C     DO 10 L = 1,JJ
C     KK = KK + 1
```



```
      KJ = KJ + 1
      SUM = SUM - S(KK) * S(KJ)
10     CONTINUE
      ENDIF
      KK = KK + 1
      IF (J .LT. I) THEN
        S(K) = SUM * S(KK)
      ELSE
        IF (ZABS(SUM) .LT. ZABS(S(K)) * EPS) THEN
          IFAULT = -2
          D1 = ZERO
          RETURN
        ENDIF
        S(K) = ONE / ZSQRT(SUM)
        D1 = D1 * S(K)
20     IF (ZABS(D1) .LE. ONE) GOTO 30
        D1 = D1 * SIXNTH
        D2 = D2 + FOUR
        GOTO 20
30     IF (ZABS(D1) .GT. SIXNTH) GOTO 40
        D1 = D1 * SIXTEN
        D2 = D2 - FOUR
        GOTO 30
40     CONTINUE
      ENDIF
50     CONTINUE
60     CONTINUE
      RETURN
      END

C
C
      SUBROUTINE DWSCL (X, IAX, N, M, NCONST, F1, F2, S, IFAULT)
C
C     SCALE FACTOR FOR CHARACTERISTIC FUNCTION
C
C     ARGUMENT DECLARATIONS
C
      INTEGER IAX, N, M, NCONST, IFAULT
      REAL X(IAX,*), F1, F2, S(2,*)
C
C     LOCAL VARIABLE DECLARATIONS:
C
      INTEGER I, J, K, L, MTOT
      REAL EPS, TEMP, ONE, ZERO, ZREAL
      COMPLEX DET
C
C     CONSTANTS
C
      DATA ONE, ZERO / 1.E0, 0.E0 /
C
C     STANDARD FUNCTIONS
C
      ZREAL(DET) = REAL(DET)
C
C     INITIALIZATIONS
C
      IFAULT = 0
      K = 0
      MTOT = M + NCONST
      IF (MTOT .EQ. 0) THEN
        F1 = ONE
```

```

        F2 = ZERO
        RETURN
    ENDIF
    DO 20 I = 1,MTOT
    DO 10 J = 1,I
    K = K + 1
    S(1,K) = ZERO
    S(2,K) = ZERO
10    CONTINUE
20    CONTINUE
C
C        CROSS-PRODUCT MATRIX
C
    DO 50 L = 1,N
    K = 0
    DO 40 I = 1,MTOT
    TEMP = ONE
    IF (I .LE. M) TEMP = X(L,I)
    DO 30 J = 1,I
    K = K + 1
    IF (J .LE. M) THEN
        S(1,K) = S(1,K) + X(L,J) * TEMP
    ELSE
        S(1,K) = S(1,K) + TEMP
    ENDIF
30    CONTINUE
40    CONTINUE
50    CONTINUE
C
C        SCALE FACTOR: DETERMINANT OF CHOLESKY FACTOR
C
    CALL CCLSKY(S,MTOT,DET,F2,IFAU)
    IF (IFAU .NE. 0) RETURN
    F1 = ONE / ZREAL(DET)
    F2 = - F2
    RETURN
    END
C
C
C        SUBROUTINE GKFTRP (N, M, NCONST, LAG, IALT, C, E1, E2, DELTA, K,
*           WS1, WS2, ITAIL, IFAU)
C
C        INTERVAL SIZE AND TRUNCATION LIMIT FOR TRAPEZOIDAL RULE
C        EVALUATION OF GIL-PALAEZ FORMULA.
C
C        ARGUMENT DECLARATIONS
C
    INTEGER N, M, NCONST, IALT, K, LAG, ITAIL, IFAU
    REAL C, E1, E2, DELTA, WS1(*), WS2(*)
C
C        LOCAL VARIABLE DECLARATIONS
C
    INTEGER NNET, I, J, MAX, NG, K1
    REAL D2, ZERO, TWO, E, ZMIN1
C
C        CONSTANTS
C
    DATA MAX / 20 /
    DATA ZERO, TWO / 0.E0, 2.E0 /
C
C        STANDARD FUNCTIONS

```

```
C
      ZMIN1(E1,E2) = AMIN1(E1,E2)
C
C      INITIALIZATIONS
C
      IFAULT = 0
      IF (N .LE. M + NCONST) THEN
        IFAULT = -1
        RETURN
      ENDIF
      IF (IALT .EQ. 0) THEN
        NNET = N - M - NCONST
        K1 = NCONST
      ELSE
        NNET = N - M
        K1 = 0
      ENDIF
C
C      EIGENVALUES OF MATRIX DEFINING STATISTIC
C
      CALL EVALUE (WS1, N, LAG, IALT, C)
C
C      INITIAL CHECK FOR TAILS
C
      IF (WS1(K1 + 1) .GE. 0) THEN
        ITAIL = -1
        RETURN
      ELSEIF (WS1(N) .LE. 0) THEN
        ITAIL = 1
        RETURN
      ENDIF
C
C      INTERVAL SIZE
C
      E = E1 + E2
      IF (C .GT. TWO) THEN
        ITAIL = 1
        J = M + K1
      ELSE
        ITAIL = -1
        J = K1
      ENDIF
      DO 10 I = 1, NNET
        J = J + 1
        WS2(I) = WS1(J)
10 CONTINUE
        J = ITAIL
        CALL INTBD (WS2, NNET, E, E1, DELTA, ITAIL)
        IF (ITAIL .NE. 0) RETURN
        ITAIL = -J
        IF (ITAIL .EQ. 1) THEN
          J = M + K1
        ELSE
          J = K1
        ENDIF
      DO 20 I = 1, NNET
        J = J + 1
        WS2(I) = WS1(J)
20 CONTINUE
        CALL INTBD (WS2, NNET, E, E1, D2, ITAIL)
        IF (ITAIL .NE. 0) RETURN
```

```
      DELTA = ZMIN1 (DELTA, D2)
C
C      TRUNCATION POINT FOR TRAPEZOIDAL RULE
C
      CALL TBDWT (WS1, N, M, NCONST, IALT, WS2, NG)
      IF (NG .EQ. 0) THEN
        IFAULT = 2
        RETURN
      ENDIF
      CALL TBND1 (WS2, NG, E2, DELTA, K1, IFAULT)
      IF (IFAUULT .NE. 0) K1 = 0
      IFAULT = 0
      CALL TBND2 (WS2, NG, E2, DELTA, K)
      IF (K1 .GT. 0) K = MIN0(K,K1)
      RETURN
      END

C
C
      SUBROUTINE TBDWT (W, N, M, NCONST, IALT, G, NG)
C
C      WEIGHTS (SQUARED) FOR BOUNDING FUNCTION TO WHICH DAVIES' (APPL.
C      STATIST. 29, 1980, 323-333) TRUNCATION RULES ARE TO BE APPLIED.
C
C      ARGUMENT DECLARATIONS:
C
      INTEGER N, M, NCONST, IALT, NG
      REAL W(N), G(N)
C
C      LOCAL VARIABLE DECLARATIONS:
C
      INTEGER I, MTOT, NNET, L1, L2
      REAL ZERO
C
C      CONSTANTS
C
      DATA ZERO / 0.E0 /
C
C      NUMBER OF REGRESSORS, DEGREES OF FREEDOM
C
      MTOT = M + NCONST
      NNET = N - MTOT
C
C      WEIGHTS
C
      IF (IALT .EQ. 0 .AND. NCONST .NE. 0) THEN
        L1 = 1
      ELSE
        L1 = 0
      ENDIF
      L2 = MTOT
      NG = 0
      DO 30 I = 1, NNET
        L1 = L1 + 1
        L2 = L2 + 1
        IF (W(L1) .GT. ZERO) THEN
          NG = NG + 1
          G(NG) = W(L1) ** 2
        ELSEIF (W(L2) .LT. ZERO) THEN
          NG = NG + 1
          G(NG) = W(L2) ** 2
        ENDIF
      ENDIF
```

```
30 CONTINUE
  IF (NG .EQ. N) RETURN
  NNET = NG + 1
  DO 40 I = NNET, N
  G(I) = ZERO
40 CONTINUE
  RETURN
  END

C
C
  SUBROUTINE EVALUE (W, N, LAG, IALT, C)
C
C  EIGENVALUES OF DEFINING QUADRATIC FORM
C
C  ARGUMENT DECLARATIONS:
C
  INTEGER N, LAG, IALT
  REAL W(N), C
C
C  LOCAL VARIABLE DECLARATIONS:
C
  INTEGER I, J, K, L, NVAL, M1, M2
  REAL PI, D1, D2, TWO, C2, TEMP, ZFLOAT, ZCOS
C
C  STANDARD FUNCTIONS
C
  ZFLOAT(I) = FLOAT(I)
  ZCOS(D1) = COS(D1)
C
C  CONSTANTS
C
  DATA PI / 3.14159265358979E0 /
  DATA TWO / 2.E0 /
  C2 = TWO - C
C
C  FIRST-ORDER CASE
C
  IF (LAG .GT. 1) GOTO 20
  L = IALT
  IF (IALT .EQ. 0) D1 = PI / ZFLOAT(N)
  IF (IALT .NE. 0) D1 = PI / ZFLOAT(N + 1)
  DO 10 I = 1, N
  W(I) = C2 - TWO * ZCOS(L * D1)
  L = L + 1
10 CONTINUE
  RETURN
C
C  GENERAL-ORDER CASE
C
20 NVAL = (N - 1) / LAG + 1
  IF (IALT .EQ. 0) D1 = PI / ZFLOAT(NVAL)
  IF (IALT .NE. 0) D1 = PI / ZFLOAT(NVAL + 1)
  M1 = N - (NVAL - 1) * LAG
  M2 = M1 + 1
  IF (M1 .EQ. LAG) GOTO 30
  IF (IALT .EQ. 0) D2 = PI / ZFLOAT(NVAL - 1)
  IF (IALT .NE. 0) D2 = PI / ZFLOAT(NVAL)
30 K = 0
  L = IALT - 1
  DO 60 I = 1, NVAL
  L = L + 1
```

```
      TEMP = C2 - TWO * ZCOS(L * D1)
      DO 40 J = 1, M1
      K = K + 1
      W(K) = TEMP
40 CONTINUE
      IF (M1 .EQ. LAG .OR. K .EQ. N)GOTO 60
      TEMP = C2 - TWO * ZCOS(L * D2)
      DO 50 J = M2, LAG
      K = K + 1
      W(K) = TEMP
50 CONTINUE
60 CONTINUE
      RETURN
      END
```

C  
C

```
      SUBROUTINE LMGFEV (U, G, N, PSI, DPSI, D2PSI)
```

C  
C  
C  
C  
C  
C

```
      LOG MOMENT GENERATING FUNCTION FROM EIGENVALUES ADJUSTED FOR
      ARGUMENT OF DISTRIBUTION FUNCTION, AND DERIVATIVES
```

```
      ARGUMENT DECLARATIONS
```

```
      INTEGER N
      REAL U, G(N), PSI, DPSI, D2PSI
```

C  
C  
C

```
      LOCAL VARIABLE DECLARATIONS
```

```
      INTEGER I
      REAL U2, F, ZERO, ONE, TWO, ZLOG
```

C  
C  
C

```
      CONSTANTS
```

```
      DATA ZERO, ONE, TWO / 0.E0, 1.E0, 2.E0/
```

C  
C  
C

```
      STANDARD FUNCTIONS
```

```
      ZLOG(F) = ALOG(F)
```

C  
C  
C

```
      FUNCTION AND DERIVATIVES
```

```
      U2 = - TWO * U
      PSI = ZERO
      DPSI = ZERO
      D2PSI = ZERO
      DO 10 I = 1, N
      F = ONE + G(I) * U2
      PSI = PSI + ZLOG(F)
      F = G(I) / F
      DPSI = DPSI + F
      D2PSI = D2PSI + F ** 2
```

```
10 CONTINUE
      PSI = - PSI / TWO
      D2PSI = TWO * D2PSI
      RETURN
      END
```

C  
C

```
      SUBROUTINE INTBD (G, N, E, ET, DELTA, ITAIL)
```

C  
C

```
      INTERVAL FOR TRAPEZOIDAL RULE INTEGRATION TO LIMIT ERROR TO E
```

```

C      USING MOMENT GENERATING FUNCTION BOUND FOR WEIGHTED SUM OF CHI-
C      SQUARED(1) RANDOM VARIABLES
C
C      ARGUMENT DECLARATIONS
C
      INTEGER N, ITAIL
      REAL DELTA, G(N), E, ET
C
C      LOCAL VARIABLE DECLARATIONS:
C
      INTEGER I
      REAL ZERO, TWO, POINT1, POINT5, TWOPI, ULM, PSI, DPSI, D2PSI,
*      HB, U, U1, U2, ELOG, EPS, HM, HSD, SGN, ZABS, ZEXP, ZFLOAT,
*      ZLOG, ZMAX1, ZMIN1, ZSQRT
C
C      SET CONSTANTS (EPS = LOG(1.1))
C
      DATA ZERO, TWO, POINT1, POINT5 / 0.E0, 2.E0, .1E0, .5E0 /
      DATA TWOPI / 6.28318530717959E0 /
      DATA EPS / .09531E0 /
C
C      STANDARD FUNCTIONS
C
      ZABS(U) = ABS(U)
      ZEXP(U) = EXP(U)
      ZFLOAT(I) = FLOAT(I)
      ZLOG(U) = ALOG(U)
      ZMAX1(U,U1) = AMAX1(U,U1)
      ZMIN1(U,U1) = AMIN1(U,U1)
      ZSQRT(U) = SQRT(U)
C
C      TAIL CHECK
C
      SGN = ZFLOAT(ITAIL)
      IF (ITAIL .EQ. 1) THEN
        IF (G(N) .LE. ZERO) RETURN
        ULM = POINT5 / G(N)
      ELSE
        IF (G(1) .GE. ZERO) RETURN
        ULM = POINT5 / G(1)
      ENDIF
      HM = ZERO
      HSD = ZERO
      DO 10 I = 1, N
        HM = HM + G(I)
        HSD = HSD + G(I) ** 2
10 CONTINUE
C
C      NEWTON SEARCH FOR ZERO LOG(MGF) DERIVATIVE
C
      HSD = ZSQRT(HSD)
      U2 = ZERO
      IF ( SGN * HM .LT. ZERO .AND. - SGN * HM / HSD .GT. TWO) THEN
        DPSI = HM
20 IF (DPSI * SGN .LT. ZERO) THEN
        U1 = U2
        U2 = POINT5 * (U2 + ULM)
        CALL LMGFEV (U2, G, N, PSI, DPSI, D2PSI)
        GOTO 20
      ENDIF
25 IF (DPSI ** 2 .GE. POINT1 * D2PSI) THEN

```

```

        U2 = U2 - DPSI / D2PSI
        CALL LMGFEV (U2, G, N, PSI, DPSI, D2PSI)
    ENDIF
    IF (ZEXP(PSI) .LE. E) RETURN
ENDIF

```

```

C
C   BOUND EQUALITY
C

```

```

    ELOG = - ZLOG(ET)
    HB = POINT5
30 IF (HB .GT. ZERO) THEN
    U1 = U2
    U2 = POINT5 * (U2 + ULIM)
    CALL LMGFEV (U2, G, N, PSI, DPSI, D2PSI)
    HB = PSI - U2 * DPSI + ELOG
    GOTO 30
ENDIF

```

```

C
C   NEWTON/BINARY SEARCH SOLUTION
C

```

```

    U = U2
40 IF (ZABS(HB) .GE. EPS) THEN
    U = U - HB / (U * D2PSI)
    IF (U .LE. ZMIN1(U1,U2) .OR. U .GT. ZMAX1(U1,U2))
    *   U = POINT5 * (U1 + U2)
    CALL LMGFEV (U, G, N, PSI, DPSI, D2PSI)
    HB = PSI - U * DPSI + ELOG
    IF (HB .GT. ZERO) THEN
        U1 = U
    ELSE
        U2 = U
    ENDIF
    GOTO 40
ENDIF
IF (ITAIL .EQ. 1 .AND. DPSI .GT. ZERO) THEN
    DELTA = TWOPI / DPSI
    ITAIL = 0
ELSEIF (ITAIL .EQ. -1 .AND. DPSI .LT. ZERO) THEN
    DELTA = - TWOPI / DPSI
    ITAIL = 0
ENDIF
RETURN
END

```

```

C
C   SUBROUTINE TBND1 (G, N, E, DELTA, K, IFAULT)
C
C   UPPER BOUND ON NUMBER OF TERMS REQUIRED IN TRAPEZOIDAL RULE
C   INTEGRATION USING DAVIES' BOUND EQN (6), APPL. STATIST. 29 (1980)
C   P. 324. WEIGHTS G(J) ARE SQUARES OF DAVIES' COEFFICIENTS.
C

```

```

C   ARGUMENT DECLARATIONS
C

```

```

    INTEGER N, K, IFAULT
    REAL G(N), E, DELTA

```

```

C   LOCAL VARIABLE DECLARATIONS
C

```

```

    INTEGER I, M
    REAL PIBY2, ZERO, ONE, TWO, FOUR, S, F, DF, C, U, ULAST,
    *   FLAST, DFLAST, EPS, POINT5, ZABS, ZFLOAT, ZLOG, ZSQRT

```



```
C
C      CONSTANTS (EPS = 4 * LOG(1.1))
C
DATA PIBY2 / 1.57079632679490E0 /
DATA ZERO, ONE, TWO, FOUR, POINT5
* / 0.E0, 1.E0, 2.E0, 4.E0, 5.E-1 /
DATA EPS / .38124E0 /

C
C      STANDARD FUNCTIONS
C
ZABS(C) = ABS(C)
ZFLOAT(I) = FLOAT(I)
ZLOG(C) = ALOG(C)
ZSQRT(C) = SQRT(C)

C
C      INITIALIZATIONS
C
IFAUULT = 0
M = 0
C = ZERO
DO 10 I = 1, N
IF (G(I) .GT. ONE) THEN
    M = M + 1
    C = C + ZLOG(G(I))
ENDIF
10 CONTINUE
IF (M .EQ. 0) THEN
    IFAUULT = 1
    RETURN
ENDIF
S = ZFLOAT(M)
C = C + FOUR * ZLOG(S * PIBY2 * E)
I = 0
U = FOUR * FOUR * DELTA ** 2

C
C      INITIAL ESTIMATE OF BOUND FUNCTION SOLUTION
C
20 CALL FBND1 (G, N, C, S, U, F, DF)
IF (F .GT. ZERO .AND. I .EQ. -1) THEN
    U = ULAST
    F = FLAST
    DF = DFLAST
ELSEIF (F .GT. ZERO) THEN
    I = 1
    U = U * POINT5
    GOTO 20
ELSEIF (F .LE. ZERO .AND. I .NE. 1) THEN
    I = -1
    ULAST = U
    FLAST = F
    DFLAST = DF
    U = TWO * U
    GOTO 20
ENDIF

C
C      NEWTON'S METHOD SOLUTION FOR ARGUMENT OF BOUND FUNCTION
C
30 IF (ZABS(F) .GE. EPS) THEN
    U = U - F / DF
    CALL FBND1 (G, N, C, S, U, F, DF)
    GOTO 30
```

```
ENDIF  
K = ZSQRT(U / FOUR) / DELTA + POINT5  
RETURN  
END
```

C  
C

```
SUBROUTINE FBND1 (G, N, C, S, U, F, DF)
```

C

```
EVALUATION OF DAVIES' BOUND EQN (6), APPL. STATIST. 29 (1980)  
P. 324. WEIGHTS G(J) ARE SQUARES OF DAVIES' COEFFICIENTS, AND F  
IS - 4 * (LOG(BOUND) - LOG(MAX ERROR)).
```

C

```
ARGUMENT DECLARATIONS
```

C

```
INTEGER N  
REAL G(N), C, S, U, F, DF
```

C

```
LOCAL VARIABLE DECLARATIONS
```

C

```
INTEGER J  
REAL ONE, TEMP, ZLOG
```

C

```
CONSTANTS
```

C

```
DATA ONE / 1.E0 /
```

C

```
STANDARD FUNCTIONS
```

C

```
ZLOG(C) = ALOG(C)
```

C

```
F = C + S * ZLOG(U)  
DF = S / U  
DO 10 J = 1, N  
IF (G(J) .LE. ONE) THEN  
  TEMP = ONE + U * G(J)  
  F = F + ZLOG(TEMP)  
  DF = DF + G(J) / TEMP
```

```
ENDIF
```

```
10 CONTINUE
```

```
RETURN
```

```
END
```

C

C

```
SUBROUTINE TBND2 (G, N, E, DELTA, K)
```

C

```
UPPER BOUND ON NUMBER OF TERMS REQUIRED IN TRAPEZOIDAL RULE  
INTEGRATION USING DAVIES' BOUND EQN (8), APPL. STATIST. 29 (1980)  
P. 324. WEIGHTS G(J) ARE SQUARES OF DAVIES' COEFFICIENTS.  
LEADING CONSTANT IS 2/PI AS IN AKS (1990).
```

C

```
ARGUMENT DECLARATIONS:
```

C

```
INTEGER N, K  
REAL G(N), E, DELTA
```

C

```
LOCAL VARIABLE DECLARATIONS
```

C

```
INTEGER I, M  
REAL C1, ZERO, ONE, TWO, FOUR, F, DF, CONST, EPS,  
* POINT5, U, ULAST, FLAST, DFLAST, ZABS, ZLOG, ZSQRT
```

C

```

C      CONSTANTS (C1 = - 4 * LOG(2/PI), EPS = 4 * LOG(1.1))
C
DATA C1 / 1.80633E0 /
DATA ZERO, ONE, TWO, FOUR, POINT5 /
*      0.E0, 1.E0, 2.E0, 4.E0, 5.E-1 /
DATA EPS / .38124E0 /

C
C      STANDARD FUNCTIONS
C
ZABS(U) = ABS(U)
ZLOG(U) = ALOG(U)
ZSQRT(U) = SQRT(U)

C
C      INITIAL ESTIMATE OF BOUND FUNCTION SOLUTION
C
CONST = C1 + FOUR * ZLOG(E)
I = 0
U = FOUR * FOUR * DELTA ** 2
10 CALL FBND2 (G, N, CONST, U, F, DF)
IF (F .GT. ZERO .AND. I .EQ. -1) THEN
  U = ULAST
  F = FLAST
  DF = DFLAST
ELSEIF (F .GT. ZERO) THEN
  I = 1
  U = U * POINT5
  GOTO 10
ELSEIF (F .LE. ZERO .AND. I .NE. 1) THEN
  I = -1
  ULAST = U
  FLAST = F
  DFLAST = DF
  U = TWO * U
  GOTO 10
ENDIF

C
C      NEWTON'S METHOD SOLUTION FOR ARGUMENT OF BOUND FUNCTION
C
20 IF (ZABS(F) .GE. EPS) THEN
  U = U - F / DF
  CALL FBND2 (G, N, CONST, U, F, DF)
  GOTO 20
ENDIF

C
C      NUMBER OF INTERVALS
C
K = ZSQRT(U / FOUR) / DELTA + POINT5
RETURN
END

C
C      SUBROUTINE FBND2 (G, N, C, U, F, DF)
C
C      EVALUATION OF DAVIES' BOUND EQN (8), APPL. STATIST. 29 (1980)
C      P. 324, WITH CONSTANT 2/PI AS IN AKS (1990). WEIGHTS G(J) ARE
C      SQUARES OF DAVIES' COEFFICIENTS, AND F IS -4 * (LOG(BOUND)
C      - LOG(MAX ERROR)).
C
C      ARGUMENT DECLARATIONS
C
INTEGER N

```

```
      REAL G(N), C, U, F, DF
C
C      LOCAL VARIABLE DECLARATIONS
C
      INTEGER J
      REAL ZERO, ONE, TEMP, ZLOG
C
C      CONSTANTS
C
      DATA ZERO, ONE / 0.E0, 1.E0 /
C
C      STANDARD FUNCTIONS
C
      ZLOG(U) = ALOG(U)
C
C      FUNCTION AND DERIVATIVE
C
      F = C
      DF = ZERO
      DO 20 J = 1, N
      TEMP = ONE + G(J) * U
      F = F + ZLOG(TEMP)
      DF = DF + G(J) / TEMP
20 CONTINUE
      RETURN
      END
```

```

C      .. ULCC Toolpack/1 2.1
      DOUBLE PRECISION FUNCTION BINOM(N, LP1, LP2, LMP1, LMP2, X, R)
C
C      FAST BIVARIATE BINOMIAL DENSITY
C
      DOUBLE PRECISION ALNGAM, LP1, LP2, LMP1, LMP2, ONE, TWO
      INTEGER N, X, R, IER
      DATA ONE / 1.0 / , TWO / 2.0 /
C
      BINOM = DEXP(TWO * ALNGAM(N + ONE, IER) -
*      (ALNGAM(X + ONE, IER) + ALNGAM(N - X + ONE,
*      IER) + ALNGAM(R - X + ONE, IER) + ALNGAM(N - (R - X) +
*      ONE, IER)) + X * LP1 + (R - X) * LP2 + (N - X) * LMP1 +
*      (N - (R - X)) * LMP2)
      RETURN
      END

      INTEGER FUNCTION XFMAX(N, R, THETA)
C
C      RETURNS X SUCH THAT F(X,R) IS A MAXIMUM
C
      INTEGER N, R
      DOUBLE PRECISION THETA, A, B, C, Q, ONE, HALF, FOUR
      DATA ONE / 1.0 / , TWO / 2.0 / , HALF / 0.5 / , FOUR / 4.0 /
C
      IF (THETA .NE. ONE) THEN
          A = - (ONE - THETA)
          B = - ((R + N + TWO) * THETA + N - R)
          C = (N + ONE) * (R + ONE) * THETA
          Q = -HALF * (B - DSQRT(B * B - (FOUR * A * C)))
          XFMAX = INT(C / Q)
      ELSE
          XFMAX = (R + 1) / 2
      END IF
      RETURN
      END

      INTEGER FUNCTION CV(N, R, ALPHA)
C
C      RETURNS LARGEST X SUCH THAT PROB(X<=X) < ALPHA
C
      INTEGER N, R, XMIN, X, XSTART, IER
      DOUBLE PRECISION ALNGAM, ALPHA, HYPNUM, LNUM, LDEN, PROB, ONE,
*      HALF, TWO
      DATA ONE / 1.0 / , HALF / 0.5 / , TWO / 2.0 /
C
      LDEN = ALNGAM(2 * N + ONE, IER) - TWO * ALNGAM(N + ONE, IER) -
*      (ALNGAM(R + ONE, IER) + ALNGAM(2 * N - R + ONE, IER))
      XSTART = (R - 1) / 2
      X = XSTART + 1
      LNUM = - (ALNGAM(R - X + ONE, IER) +
*      ALNGAM(N - (R - X) + ONE, IER) + ALNGAM(X + ONE, IER) +
*      ALNGAM(N - X + ONE, IER))
      PROB = DEXP(LNUM - LDEN)
      HYPNUM = HALF
      IF (MOD(R, 2) .EQ. 0) HYPNUM = HYPNUM + HALF * PROB
      XMIN = 0
      IF (R .GT. N) XMIN = R - N
C

```

```

C          HYPERGEOMETRIC ADJACENCY
C
DO 10 X = XSTART, XMIN, -1
    PROB = PROB * (X + ONE) * (N - R + X + ONE) /
*        ((R - X) * ONE * (N - X))
    HYP SUM = HYP SUM + PROB
    IF (HYP SUM .GT. ONE - ALPHA) GO TO 20
10 CONTINUE
    X = XMIN
C
C          IF NO CRITICAL VALUE, RETURN -1
C
20 CV = -1
    IF (X - 1 .GE. XMIN) CV = X - 1
    RETURN
    END

DOUBLE PRECISION FUNCTION FSUM(FROM, TO, INC, F, FLIM, N, THETA,
*                               R, RCNT)
C
C          SUMS BINOMIAL PROBABILITIES ALONG FIXED R
C
DOUBLE PRECISION FP, F, FLIM, THETA, ONE, ZERO
INTEGER X, N, FROM, TO, R, INC, RCNT
DATA ONE / 1.0 / , ZERO / 0.0 /
C
FP = ZERO
RCNT = 0
X = FROM
10 IF (F .LT. FLIM) GO TO 20
    RCNT = RCNT + 1
    FP = FP + F
C
C          BINOMIAL ADJACENCY
C
IF (INC .GT. 0) F = F * THETA * (N - X) * (R - X) /
*        ((X + ONE) * (N - R + X + 1))
IF (INC .LE. 0) F = F * (ONE / THETA) * X * (N - R + X) /
*        ((N - X + ONE) * (R - X + 1))
X = X + INC
IF (X .NE. TO + INC) GO TO 10
20 FSUM = FP
    RETURN
    END

DOUBLE PRECISION FUNCTION FXPOWER(N, P1, P2, ALPHA, EPS, ERROR,
*                               COUNT, TOTAL, IFAULT)
C
C          POWER FOR FISHER'S EXACT TEST
C
C          RETURN THE POWER OF A LEVEL ALPHA TEST FOR A GIVEN
C          COMMON SAMPLE SIZE AND TRUE PROBABILITIES OF EVENTS P1 AND P2.
C
DOUBLE PRECISION P1, P2, ALPHA, EPS, ERROR, LP1, LP2, LMP1, LMP2,
*               F, FLIM, POWSUM, THETA, FMAX, FSUM, BINOM, ONE,
*               ZERO, TWO
INTEGER XM, N, TOTAL, COUNT, RMAX, XMAX, YMAX, XMIN, XCV, XFM, R,
*               I, J, RCNT, CV, XFMAX
DATA ONE / 1.0 / , ZERO / 0.0 / , TWO / 2.0 /

```

```

C
  IFAULT = 0
  ERROR = ZERO
  POWSUM = ZERO
  COUNT = 0
  TOTAL = 0

C
C   CHECK INPUT PARMS
C
  IF (N .LE. 0 .OR. P1 .LE. ZERO .OR. P1 .GE. ONE .OR.
*   P2 .LE. ZERO .OR. P2 .GE. ONE .OR. ALPHA .LE. ZERO .OR.
*   ALPHA .GE. ONE .OR. EPS .LE. ZERO .OR. EPS .GE. ONE) THEN
    IFAULT = 1
    RETURN
  END IF

C
  LP1 = DLOG(P1)
  LP2 = DLOG(P2)
  LMP1 = DLOG(ONE - P1)
  LMP2 = DLOG(ONE - P2)
  XMAX = (N + 1) * P1
  YMAX = (N + 1) * P2
  RMAX = XMAX + YMAX
  FMAX = BINOM(N, LP1, LP2, LMP1, LMP2, XMAX, RMAX)
  FLIM = FMAX * EPS
  THETA = P1 * (ONE - P2) / (P2 * (ONE - P1))
  XM = 0
  IF (RMAX .GT. N) XM = RMAX - N
  TOTAL = (N + 1 - RMAX + TWO * (CV(N, RMAX, ALPHA) - XM)) *
*         (N + 2 - RMAX + TWO * (CV(N, RMAX, ALPHA) - XM)) / 2
  R = RMAX
  I = 0
  J = 1

C
C   MAIN LOOP ON R
C
10 XMIN = 0
  IF (R .GT. N) XMIN = R - N
  XCV = CV(N, R, ALPHA)
  XFM = XFMAX(N, R, THETA)
  IF (XCV .LE. 0) GO TO 30
  IF (XCV .GT. XFM) GO TO 20

C
C   SUM FROM CRITICAL VALUE DOWN TO MINIMUM
C
  F = BINOM(N, LP1, LP2, LMP1, LMP2, XCV, R)
  POWSUM = POWSUM + FSUM(XCV, XMIN, -1, F, FLIM, N, THETA, R, RCNT)
  IF (RCNT .EQ. 0) GO TO 40
  COUNT = COUNT + RCNT
  GO TO 30

C
C   SUM FROM DENSITY MAX DOWN TO MINIMUM
C
20 F = BINOM(N, LP1, LP2, LMP1, LMP2, XFM, R)
  POWSUM = POWSUM + FSUM(XFM, XMIN, -1, F, FLIM, N, THETA, R, RCNT)
  IF (RCNT .EQ. 0) GO TO 40
  COUNT = COUNT + RCNT

C
C   SUM FROM DENSITY MAX UP TO CRITICAL VALUE
C
  F = BINOM(N, LP1, LP2, LMP1, LMP2, XFM + 1, R)

```

```
        POWSUM = POWSUM + FSUM(XFM + 1, XCV, 1, F, FLIM, N, THETA, R,  
*          RCNT)  
        COUNT = COUNT + RCNT  
C  
C          WORK OUT FROM RMAX ALTERNATING BETWEEN SMALLER AND LARGER R  
C  
30 I = I + 1  
   J = -1 * J  
   R = R + I * J  
   IF (R .GE. 0 .AND. R .LE. 2 * N) GO TO 10  
C  
C          CALCULATE ERROR BOUND AND RETURN  
C  
40 ERROR = ONE - POWSUM  
   IF (ONE - POWSUM .GT. (TOTAL - COUNT) * FLIM) ERROR = FLIM *  
*     (TOTAL - COUNT)  
   FXPOWER = POWSUM  
   RETURN  
   END
```



```

SUBROUTINE RCINT(N, RC, L, X, WT, Y, M, WORK, NS, WORK2)
C
C   ALGORITHM AS 281.1 APPL. STATIST. (1993) VOL.42, NO.1
C
C   Scaling and rounding regression coefficients to integers.
C
C   N.B. No checks of input parameters are made in this routine.
C   N.B. The published routine is in double precision contrary to
C       the rules of the journal.
C
C   INTEGER N, L, M, NS
C   DOUBLE PRECISION RC(N), X(N,L), WT(L), Y(L), WORK(3,M), WORK2(N)
C
C   Local variables
C
C   INTEGER I, J, NRC, JMIN, JMAX, K, NSC, KK
C   LOGICAL OK
C   DOUBLE PRECISION ZERO, EPS, HALF, BIG, SCMIN, RCSUM, RCT, SCMAX,
+   WTSUM, YSS, T, SC, RCSS, RCSP, SDP, SD, SDPP, SCP
C   EXTERNAL RCINT2      ! This is a subroutine, not a function!
C
C   DATA ZERO,  EPS,  HALF,  BIG
+   /0.D0, 1.D-08, 0.5D0, 1.D08/
C
C   Identify sums and range of coefficients
C
C   NS = 0
C   NRC = 0
C   SCMIN = BIG
C   RCSUM = ZERO
C   DO 10 I = 1, N
C       RCT = ABS( RC(I) )
C       IF ( RCT .EQ. ZERO ) GO TO 10
C       NRC = NRC + 1
C       RCSUM = RCSUM + RCT
C       IF ( RCT .LT. SCMIN ) SCMIN = RCT
10 CONTINUE
C   IF ( NRC .EQ. 0 ) RETURN
C
C   Derive range for scaling factor K.
C
C   SCMIN = HALF / SCMIN
C   SCMAX = SCMIN + M / RCSUM
C
C   Derive linear predictor, sum of squares and sum of weights.
C
C   WTSUM = ZERO
C   YSS = ZERO
C   DO 30 I = 1, L
C       IF (WT(I) .EQ. ZERO ) GO TO 30
C       T = ZERO
C       DO 20 J = 1, N
C           T = T + RC(J) * X(J,I)
20 CONTINUE
C       Y(I) = T
C       WTSUM = WTSUM + WT(I)
C       YSS = YSS + T * T * WT(I)
30 CONTINUE
C   IF ( WTSUM .LE. ZERO .OR. YSS .LE. ZERO ) RETURN
C   NSC = 0
C   DO 40 I = 1, M

```

```

      WORK(1,I) = ZERO
40  CONTINUE
C
C   For each coefficient in turn ...
C
      DO 130 I = 1, N
          RCT = ABS( RC(I) )
          IF ( RCT .EQ. ZERO ) GO TO 130
C
C   ... derive scaling factors at integer boundaries ...
C
          JMIN = NINT( RCT * SCMIN + EPS )
          JMAX = NINT( RCT * SCMAX + EPS )
          DO 120 J = JMIN, JMAX
              SC = ( J - HALF ) / RCT
              IF ( SC .LT. SCMIN .OR. SC .GT. SCMAX ) GO TO 120
C
C   ... derive sum of squares and sum of products for each
C   scaling factor.
C
          RCSS = ZERO
          RCSP = ZERO
          DO 50 K = 1, N
              WORK2(K) = NINT( RC(K) * SC + SIGN( EPS, RC(K) ) )
50      CONTINUE
C
          DO 70 K = 1, L
              IF ( WT(K) .EQ. ZERO ) GO TO 70
              T = ZERO
              DO 60 KK = 1, N
                  T = T + WORK2(KK) * X(KK,K)
60      CONTINUE
              RCSS = RCSS + T * T * WT(K)
              RCSP = RCSP + T * Y(K) * WT(K)
70      CONTINUE
C
C   Sort by scaling factor.
C
          NRC = 0
80      NRC = NRC + 1
          IF ( NRC .GT. M ) GO TO 120
          IF ( ABS( SC - WORK(1,NRC) ) .LT. SC * EPS ) GO TO 120
          IF ( NRC .LE. NSC .AND. SC .GT. WORK(1,NRC) ) GO TO 80
          IF ( NSC .LT. M ) NSC = NSC + 1
          IF ( NRC .EQ. NSC ) GO TO 110
          DO 100 K = NSC - 1, NRC, -1
              DO 90 KK = 1, 3
                  WORK(KK, K+1) = WORK(KK,K)
90      CONTINUE
100     CONTINUE
110     WORK(1,NRC) = SC
          WORK(2,NRC) = RCSS
          WORK(3,NRC) = RCSP
120     CONTINUE
130     CONTINUE
C
C   Identify optimal values for scaling factor.
C
          IF ( NSC .LE. 1 ) RETURN
          SDP = BIG
          DO 150 K = 1, NSC - 1

```

```
        RCSS = WORK(2,K)
        RCSP = WORK(3,K)
        IF ( RCSP .EQ. ZERO ) RETURN
C
C   Adjust scaling factor and derive residual sum of squares.
C
        SC = RCSS / RCSP
        IF ( SC .LT. WORK(1,K) ) THEN
            SC = WORK(1,K)
        ELSE IF ( SC .GT. WORK(1,K+1) ) THEN
            SC = WORK(1,K+1)
        END IF
        SD = YSS - 2 * RCSP / SC + RCSS / ( SC * SC )
        IF ( SD .LT. EPS * YSS ) SD = ZERO
        IF ( K .EQ. 1 .OR. SDP .GT. SD .OR. .NOT. OK
+         .OR. ( NS .GT. 0 .AND. SDP .GE. SDPP ) ) GO TO 140
        NS = NS + 1
        WORK(1,NS) = SCP
        WORK(2,NS) = SQRT( SDP / WTSUM )
        SDPP = SDP
140    OK = SD .LT. SDP
        SDP = SD
        SCP = SC
150    CONTINUE
C
        RETURN
        END
C
        SUBROUTINE RCINT2(N, RC, INT, SCALE)
C
C   ALGORITHM AS 281.2 APPL. STATIST. (1993) VOL.42, NO.1
C
        INTEGER N, INT(N)
        DOUBLE PRECISION RC(N), SCALE
C
C   Local variables
C
        INTEGER I
        DOUBLE PRECISION EPS
        DATA EPS / 1.D-08 /
C
        DO 10 I = 1, N
            INT(I) = NINT( RC(I) * SCALE + SIGN( EPS, RC(I) ) )
10    CONTINUE
C
        RETURN
        END
```

```
C
C THE FOLLOWING ROUTINES ARE WRITTEN IN DOUBLE PRECISION. IT IS STRONGLY
C RECOMMENDED THAT THEY BE RUN THIS WAY. IF IT IS DESIRED TO RUN THEM IN
C SINGLE PRECISION, ALL "IMPLICIT DOUBLE PRECISION (A-H,O-Z)" LINES SHOULD
C BE DELETED, ALL DOUBLE PRECISION CONSTANTS IN DATA STATEMENTS SHOULD BE
C CONVERTED TO REAL CONSTANTS, AND THE VALUE OF "TOLER" SET IN THE DATA
C STATEMENT IN ROUTINE MVELMS SHOULD BE CHANGED TO "1.E-5"
```

```
C
      SUBROUTINE MVELMS (X,Y,NCAS,NPRE,IOPTN,MAXTRY,NCLOW,NCHIGH,
1 COEFFS,EPRMIN,RESID,ROBDSQ,CVEMIN,DATA,IWORK,WORK,NVDIM,
2 NODIM,IFAUULT)
```

```
C
      ALGORITHM AS 282 APPL.STATIST. (1993), VOL.42, NO.2
      HIGH BREAKDOWN REGRESSION AND MULTIVARIATE ESTIMATION
```

```
C
      ROUTINE TO CALCULATE LEAST MEDIAN OF SQUARES REGRESSION, MINIMUM VOLUME
      ELLIPSOID, AND ASSOCIATED STATISTICS
```

```
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION X(NODIM,NVDIM), Y(NODIM), COEFFS(NVDIM,*),EPRMIN(*),
1 RESID(NODIM,*), CVEMIN(*), ROBDSQ(NODIM,*), DATA(0:NVDIM,*),
2 IWORK(*), WORK(*)
```

```
C
      OPTIONAL ADDITIONAL ARGUMENTS FOR MORE SPECIALIZED USE
```

```
C
      DIMENSION XINV(NVDIM,NVDIM*),ELSCAL(*),LMSBAS(NVDIM*),
1 MVEBAS(NVDIM,*)
```

```
C
      LOGICAL LMS,MVE,ISINT,EXH,EXACT
      DATA TOLER/1.D-9/,BIG/1.D30/,NFRESH/50/,ZERO/0.D0/,HALF/0.5D0/,
1 ONE/1.D0/,TEN/10.D0/
```

```
C
      EXTRACT THE OPTIONS REQUESTED
```

```
C
      ITEMP = IOPTN
      LMS = MOD(ITEMP,2) .EQ. 0
      ITEMP = ITEMP / 2
      MVE = MOD(ITEMP,2) .EQ. 0
      ITEMP = ITEMP / 2
      ISINT = MOD(ITEMP,2) .EQ. 0
      ITEMP = ITEMP / 2
      EXH = MOD(ITEMP,2) .EQ. 0
      IF (ISINT) THEN
        NVAR=NPRE+1
        ADDCON=ONE/FLOAT(NVAR)
        RPP1=SQRT(ADDCON)
        INT=1
      ELSE
        NVAR=NPRE
        ADDCON=ZERO
        RPP1=ONE
        INT=0
      END IF
```

```
C
      CHECK FAULT PARAMETERS
```

```
C
      IFAUULT=0
      IF ((NCLOW.LT.NVAR).OR.(NCLOW.GT.NCHIGH).OR.(NCHIGH.
1 GT.NCAS)) IFAUULT=2
```

```
      IF (NCAS.LT.NVAR) IFAULT=1
      IF ((ISINT).AND.(NVAR.EQ.1).AND.(MVE)) IFAULT=IFAULT+4
      IF (IFAULT.GT.0) GO TO 490
      EXACT=.FALSE.
      J2=NCAS
      J3=2*NCAS
      J4=3*NCAS
      I2=NVAR
      I3=2*NVAR
      I4=3*NVAR
      I5=I4+NCAS
      NVR2=2*NVAR
      DETER=RPP1
      POWMED=FLOAT(NPRE)*HALF
      DO 10 I=1,NVAR
10     IWORK(I)=NCAS+I-NVAR
      IPTR=1
      NCRANG=NCHIGH-NCLOW+1
      DO 20 I=1,NCRANG
      CVEMIN(I)=BIG
      EPRMIN(I)=BIG
20     CONTINUE
      LFRESH=0
      NCOUNT=0

C
C TARGET VARIABLE, IF PRESENT, IS TREATED IN STANDARDIZED FORM SO THAT EXACT
C FIT CAN BE DETECTED MORE EASILY
C
      IF (LMS) THEN
          IXLO=0
          DO 30 I=1,NCAS
30         WORK(I)=Y(I)
C
C THE USER-SUPPLIED SUBROUTINE SORTSUB(RA,N,ILOW) SORTS ENTRIES ILOW+1 THROUGH
C ILOW+N IN ASCENDING ORDER FROM A VECTOR RA
C
          CALL SORTSUB(WORK,NCAS,0)
          YMED=(WORK(NCAS/2+1)+WORK((NCAS+1)/2))*HALF
          DO 40 I=1,NCAS
40         WORK(I)=ABS(Y(I)-YMED)
          CALL SORTSUB(WORK,NCAS,0)
          YMAD=(WORK(NCAS/2+1)+WORK((NCAS+1)/2))*HALF
          IF (YMAD.EQ.ZERO) YMAD=ONE
      ELSE
          IXLO=1
      END IF
      DETADJ=ZERO
      DO 60 J=1,NPRE
      DO 50 I=1,NCAS
50     WORK(I)=ABS(X(I,J))
          CALL SORTSUB(WORK,NCAS,0)
          WORK(J4+J+INT)=(WORK(NCAS/2+1)+WORK((NCAS+1)/2))*HALF
          IF (WORK(J4+J+INT).EQ.ZERO) WORK(J4+J+INT)=WORK(NCAS)
          DETADJ=DETADJ+LOG10(WORK(J4+J+INT))
60     CONTINUE
          IF (ISINT) WORK(J4+1)=ONE

C
C DATA IS TRANSFERRED TO WORKAREA; INITIAL SIMPLEX TABLEAU IS SET UP
C
          CALL REFRESH(DATA,NODIM,NVDIM,IXLO,X,NCAS,NPRE,Y,YMAD,NVAR,WORK,
1     J4,IWORK,I2,I3,I5,0,ISINT,INT,LMS,DETER,LFRESH,TOLER)
```

```
C
C INITIAL BASIS IS SET UP. CHECKS ARE MADE THAT INITIAL BASIS MEMBERS ARE IN
C GENERAL POSITION
C
      IF (EXH) THEN
        IWORK(I2+1)=1
        DO 100 I=1,NVAR
70      J=IWORK(I2+I)
        DO 80 II=I,NVAR
          IF (ABS(DATA(II,J)).GE.TOLER) THEN
            CALL PIVOT(DATA,IXLO,NVAR,NCAS,IWORK,I5,II,J,DETER,
1          NVDIM)
            IWORK(I3+I)=J
            IF (II.NE.I) CALL SWAP(DATA,NVAR,NCAS,II,I,NVDIM)
            GO TO 90
          END IF
80      CONTINUE
          IF (J.EQ.NCAS) THEN
            IFAULT=IFAULT+8
            IF (IFAULT.GE.24) IFAULT=IFAULT-16
            GO TO 490
          ELSE
            IFAULT=16
            IWORK(I2+I)=IWORK(I2+I)+1
            GO TO 70
          END IF
90      IF (I.LT.NVAR) IWORK(I2+I+1)=IWORK(I2+I)+1
100     CONTINUE
        IPTR=NVAR
        GO TO 230
      ELSE
        DO 110 I=1,NCAS
110     IWORK(I4+I)=I
        CALL PERM(IWORK,I4,NCAS,0)
        INXPTR=0
        DO 140 I=1,NVAR
120     INXPTR=INXPTR+1
        J=IWORK(I4+INXPTR)
        DO 130 II=I,NVAR
          IF (ABS(DATA(II,J)).GE.TOLER) THEN
            CALL PIVOT(DATA,IXLO,NVAR,NCAS,IWORK,I5,II,J,DETER,
1          NVDIM)
            IWORK(I3+I)=J
            IF (II.NE.I) CALL SWAP(DATA,NVAR,NCAS,II,I,NVDIM)
            IWORK(I2+I)=J
            GO TO 140
          END IF
130     CONTINUE
          IF (INXPTR.EQ.NCAS) THEN
            IFAULT=IFAULT+8
            IF (IFAULT.GE.24) IFAULT=IFAULT-16
            GO TO 490
          ELSE
            IFAULT=16
            GO TO 120
          END IF
140     CONTINUE
        GO TO 230
      END IF
```

C

```
C MAIN ANALYSIS LOOP. GENERATE ALL SUBSETS (IF EXH) OR A SUBSET (IF
C NOT EXH)
C
150   IF (EXH) THEN
C
C IF EXHAUSTIVE, SUCCESSIVE BASES ARE CONSIDERED
C
160   IWORK(I2+IPTR)=IWORK(I2+IPTR)+1
      IF (IWORK(I2+IPTR).GT.IWORK(IPTR)) THEN
          IPTR=IPTR-1
          IF (IPTR.EQ.0) THEN
              GO TO 440
          ELSE
              GO TO 160
          END IF
      ELSE
C
C IF DATA IS NOT IN GENERAL POSITION, NEXT POSITION IN LIST MUST BE FOUND
C
          IF (ABS(DATA(IPTR,IWORK(I2+IPTR))).GE.TOLER) GO TO 210
          IF (LFRESH.GT.NVR2) THEN
              DETER=RPP1
              CALL REFRESH(DATA,NODIM,NVDIM,IXLO,X,NCAS,NPRE,Y,YMAD,
1              NVAR,WORK,J4,IWORK,I2,I3,I5,IPTR-1,ISINT,INT,LMS,DETER,
2              LFRESH,TOLER)
              IF (ABS(DATA(IPTR,IWORK(I2+IPTR))).GE.TOLER) GO TO 210
              IFAULT=16
              IF (IPTR.EQ.NVAR) THEN
                  GO TO 160
              ELSE
                  GO TO 170
              END IF
          END IF
          IFAULT=16
          IF (IPTR.EQ.NVAR) GO TO 160
          DETER=RPP1
          CALL REFRESH(DATA,NODIM,NVDIM,IXLO,X,NCAS,NPRE,Y,YMAD,
1              NVAR,WORK,J4,IWORK,I2,I3,I5,IPTR-1,ISINT,INT,LMS,DETER,
2              LFRESH,TOLER)
170      J=IWORK(I2+IPTR)
          DO 180 II=IPTR,NVAR
              IF (ABS(DATA(II,J)).GE.TOLER) THEN
                  CALL PIVOT(DATA,IXLO,NVAR,NCAS,IWORK,I5,II,J,DETER,
1                  NVDIM)
                  IWORK(I3+IPTR)=J
                  IF (II.NE.IPTR) CALL SWAP(DATA,NVAR,NCAS,II,IPTR,NVDIM)
                  GO TO 220
              END IF
          CONTINUE
180      IWORK(I2+IPTR)=IWORK(I2+IPTR)+1
          IF (IWORK(I2+IPTR).GT.IWORK(IPTR)) THEN
              IPTR=IPTR-1
              IF (IPTR.EQ.0) THEN
                  GO TO 440
              ELSE
                  IWORK(I2+IPTR)=IWORK(I2+IPTR)+1
                  END IF
              END IF
              GO TO 170
          END IF
      ELSE
```

```
C
C IF NOT EXHAUSTIVE, THE NEXT ENTRY IN RANDOM PERMUTATION VECTOR IS ENTERED
C INTO THE BASIS
C
      IF (NCOUNT.GT.MAXTRY) GO TO 440
      IPTR=MOD(IPTR,NVAR)+1
190    INXPTR=INXPTR+1
      IF (INXPTR.GT.NCAS) THEN
C
C IF COME TO THE END OF THE PERMUTATION VECTOR, GENERATE A NEW ONE
C
      DO 200 I=1,NVAR
      IWORK(I4+NCAS-NVAR+I)=IWORK(I4+I)
      IWORK(I4+I)=IWORK(I2+I)
200    CONTINUE
      CALL PERM(IWORK,I4,NCAS,NVAR)
      INXPTR=NVAR+1
      END IF
      NCOL=IWORK(I4+INXPTR)
      IF (ABS(DATA(IPTR,NCOL)).LT.TOLER) THEN
      IF (LFRESH.GT.NVR2) THEN
      DETER=RPP1
      CALL REFRESH(DATA,NODIM,NVDIM,IXLO,X,NCAS,NPRE,Y,YMAD,
1        NVAR,WORK,J4,IWORK,I2,I3,I5,IPTR-1,ISINT,INT,LMS,DETER,
2        LFRESH,TOLER)
      IF (ABS(DATA(IPTR,NCOL)).LT.TOLER) THEN
      IFAULT=16
      GO TO 190
      END IF
      ELSE
      IFAULT=16
      GO TO 190
      END IF
      END IF
      IWORK(I2+IPTR)=NCOL
      END IF
210    NCOUNT=NCOUNT+1
      LFRESH=LFRESH+1
C
C CARRY OUT NEXT PIVOT, THEREBY CREATING A NEW BASIS
C
      CALL PIVOT (DATA,IXLO,NVAR,NCAS,IWORK,I3,IPTR,
1    IWORK(I2+IPTR),DETER,NVDIM)
C
C RECOMPUTE THE INVERSE BASIS EVERY NFRESH SIMPLEX PIVOTS
C
      IF (LFRESH.GT.NFRESH) THEN
      DETER=RPP1
      CALL REFRESH(DATA,NODIM,NVDIM,IXLO,X,NCAS,NPRE,Y,YMAD,
1    NVAR,WORK,J4,IWORK,I2,I3,I5,NVAR,ISINT,INT,LMS,DETER,LFRESH,
2    TOLER)
      END IF
220    IF (EXH.AND.(IPTR.LT.NVAR)) THEN
      IPTR=IPTR+1
      IWORK(I2+IPTR)=IWORK(I2+IPTR-1)
      GO TO 150
      END IF
230    IF (LMS) THEN
C
C CHECK TO SEE IF THIS BASIS HAS A SMALLER LMS CRITERION VALUE THAN PREVIOUS
C BASES. IF THERE IS NO INTERCEPT, A PRELIMINARY COMPARISON IS MADE TO SEE IF
```



```
C THIS BASIS COULD BE OPTIMAL.
C
      IF (EXACT) GO TO 340
      IF (ISINT) THEN
        DO 240 J=1,NCAS
240     WORK(J)=DATA(0,J)
      ELSE
        DO 250 J=1,NCAS
250     WORK(J)=ABS(DATA(0,J))
        DO 270 KX=NLOW,NHIGH
          KXSTO=KX-NLOW+1
          TARGET=EPRMIN(KXSTO)
          ICOUNT=0
          DO 260 J=1,NCAS
260         IF (WORK(J).LE.TARGET) ICOUNT=ICOUNT+1
          IF (ICOUNT.GE.KX) GO TO 280
270         CONTINUE
          GO TO 340
        END IF
280     CALL SORTSUB(WORK,NCAS,0)
        DO 330 KX=NLOW,NHIGH
          KXSTO=KX-NLOW+1
          OFFS=ZERO
          IF (ISINT) THEN
C
C CALCULATE PROPER OFFSET FOR INTERCEPT TERM, IF REQUIRED, AND DETERMINE
C CRITERION FOR THIS BASIS
C
            SHORT=BIG
            DO 290 KX=KX,NCAS
              IF (WORK(KX)-WORK(KX-KX+1).LT.SHORT) THEN
                SHORT=WORK(KX)-WORK(KX-KX+1)
                CRITER=SHORT*HALF
                OFFS=(WORK(KX)+WORK(KX-KX+1))*HALF
              END IF
290             CONTINUE
            ELSE
              CRITER=WORK(KX)
            END IF
C
C UPDATE SUMMARY STATISTICS IF THIS BASIS IS CURRENTLY OPTIMAL
C
            IF (CRITER.LT.EPRMIN(KXSTO)) THEN
              EPRMIN(KXSTO)=CRITER
C
C DO 300 J=1,NVAR
C300     LMSBAS(J,KXSTO)=IWORK(I3+J)
              DO 310 J=1,NVAR
310         COEFFS(J,KXSTO)=-DATA(0,NCAS+J)*YMAD
              IF (ISINT) COEFFS(1,KXSTO)=COEFFS(1,KXSTO)+OFFS*YMAD
              DO 320 J=1,NCAS
320         RESID(J,KXSTO)=(DATA(0,J)-OFFS)*YMAD
C
C A CHECK FOR EXACT FIT IS MADE
C
              IF ((CRITER.LT.TOLER).AND.(KX.EQ.NHIGH)) THEN
                EXACT=.TRUE.
                IF (.NOT.MVE) GO TO 460
              END IF
            END IF
330     CONTINUE
C
```

```
C IF THIS IS A UNIVARIATE LOCATION PROBLEM, NO FURTHER ANALYSIS IS NEEDED
C
      IF ((ISINT).AND.(NVAR.EQ.1)) GO TO 460
      END IF
340   IF (MVE) THEN
C
C CHECK TO SEE IF THIS BASIS HAS A SMALLER MVE CRITERION VALUE THAN PREVIOUS
C BASES. A PRELIMINARY COMPARISON IS MADE TO SEE IF THIS BASIS COULD BE
C OPTIMAL.
C
      BASVOL=LOG10(ABS(DETER))
      DO 360 J=1,NCAS
      WORK(J+J2)=-ADDCON
      DO 350 I=1,NVAR
350   WORK(J+J2)=WORK(J+J2)+DATA(I,J)**2
      IF (WORK(J+J2).GT.ZERO) THEN
          WORK(J+J2)=LOG10(WORK(J+J2))
      ELSE
          WORK(J+J2)=-BIG
      END IF
      WORK(J+J3)=WORK(J+J2)
360   CONTINUE
      DO 380 KX=NLOW,NHIGH
      KXSTO=KX-NLOW+1
      TARGET=(CVEMIN(KXSTO)-BASVOL)/POWMED
      ICOUNT=0
      DO 370 J=1,NCAS
370   IF (WORK(J+J3).LE.TARGET) ICOUNT=ICOUNT+1
      IF (ICOUNT.GE.KX) GO TO 390
380   CONTINUE
      GO TO 150
390   CALL SORTSUB(WORK,NCAS,J3)
      DO 430 KX=NLOW,NHIGH
      KXSTO=KX-NLOW+1
      VOLU=BASVOL+POWMED*WORK(KX+J3)
      IF (VOLU.LT.CVEMIN(KXSTO)) THEN
C
C UPDATE SUMMARY STATISTICS IF THIS BASIS IS CURRENTLY OPTIMAL
C
          CVEMIN(KXSTO)=VOLU
C          ELSCAL(KXSTO)=WORK(KX+J3)
C          DO 400 J=1,NVAR
C400   MVEBAS(J,KXSTO)=IWORK(I3+J)
          DO 410 JJ=1,NCAS
410   ROBDSQ(JJ,KXSTO)=WORK(JJ+J2)-WORK(KX+J3)
C          DO 420 J=1,NVAR
C          DO 420 JJ=1,NVAR
C420   XINV(JJ,J,KXSTO)=DATA(J,JJ+NCAS)/WORK(J4+JJ)
          END IF
430   CONTINUE
      END IF
C
C END OF MAIN PROCESSING LOOP. GO TO BEGINNING AND GENERATE ANOTHER BASIS
C
      GO TO 150
440   IF (MVE) THEN
C
C CONVERT ROBUST DISTANCES AND SCALING BACK TO ORIGINAL SCALE
C
          DO 450 K=1,NCRANG
C          ELSCAL(K)=TEN**ELSCAL(K)
```

```

        CVEMIN(K)=CVEMIN(K)+DETADJ
        DO 450 J=1,NCAS
        IF (ROBDSQ(J,K).GT.(-BIG)) THEN
            ROBDSQ(J,K)=TEN**ROBDSQ(J,K)
        ELSE
            ROBDSQ(J,K)=ZERO
        END IF
450    CONTINUE
    END IF
460    IF (LMS) THEN
        DO 480 K=1,NCRANG
        EPRMIN(K)=EPRMIN(K)*YMAD
        DO 470 I=1,NPRE
470    COEFFS(I+INT,K)=COEFFS(I+INT,K)/WORK(I+J4+INT)
480    CONTINUE
        END IF
490    RETURN
    END
    SUBROUTINE REFRESH(DATA,NODIM,NVDIM,IXLO,X,NCAS,NPRE,Y,YMAD,
1  NVAR,WORK,J4,IWORK,I2,I3,I5,IUP,ISINT,INT,LMS,DETER,LFRESH,TOLER)
C
C SUBROUTINE TO REFRESH FIRST IUP ENTRIES OF SIMPLEX BASIS
C
    IMPLICIT DOUBLE PRECISION (A-H,O-Z)
    DIMENSION DATA(0:NVDIM,*), X(NODIM,NVDIM), Y(NODIM),
1  WORK(*),IWORK(*)
    LOGICAL ISINT,LMS
    DATA ZERO/0.DO/,ONE/1.DO/
    LFRESH=0
    IF (ISINT) THEN
        DO 10 I=1,NCAS
10    DATA(1,I)=ONE
        END IF
        DO 20 I=1,NCAS
        DO 20 J=1,NPRE
20    DATA(J+INT,I)=X(I,J)/WORK(J4+J+INT)
        DO 40 I=1,NVAR
        DO 30 J=1,NVAR
30    DATA(J,NCAS+I)=ZERO
        DATA(I,NCAS+I)=ONE
40    CONTINUE
        IF (LMS) THEN
            DO 50 I=1,NCAS
50    DATA(0,I)=Y(I)/YMAD
            DO 60 I=1,NVAR
60    DATA(0,NCAS+I)=ZERO
            END IF
            DO 80 I=1,IUP
            J=IWORK(I2+I)
            DO 70 II=I,NVAR
            IF (ABS(DATA(II,J)).GE.TOLER) THEN
                CALL PIVOT(DATA,IXLO,NVAR,NCAS,IWORK,I5,II,J,DETER,NVDIM)
                IF (II.NE.I) CALL SWAP(DATA,NVAR,NCAS,II,I,NVDIM)
                IWORK(I3+I)=J
                GO TO 80
            END IF
70    CONTINUE
80    CONTINUE
        RETURN
    END
    SUBROUTINE PIVOT(X,IXLO,NORD,NCAS,IWORK,I3,NROW,NCOL,DETER,

```

```

      1  NVDIM)
C
C SUBROUTINE TO PIVOT ENTRY CORRESPONDING TO (NROW,NCOL) INTO SIMPLEX TABLEAU
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION X(0:NVDIM,*),IWORK(*)
      DATA ZERO/0.DO/,ONE/1.DO/
      PIVT=X(NROW,NCOL)
      DETER=DETER*PIVT
      NHIGH=NORD+NCAS
      DO 20 J=1,NHIGH
      IF (J.NE.NCOL) THEN
          FMULT=X(NROW,J)/PIVT
          DO 10 I=IXLO,NORD
10      IF (I.NE.NROW) X(I,J)=X(I,J)-FMULT*X(I,NCOL)
          X(NROW,J)=FMULT
      END IF
20      CONTINUE
      DO 30 I=IXLO,NORD
30      X(I,NCOL)=ZERO
      X(NROW,NCOL)=ONE
      IWORK(I3+NROW)=NCOL
      RETURN
      END
      SUBROUTINE PERM(INDEX,IAA,N,IAB)
C
C SUBROUTINE TO RETURN PSEUDORANDOM PERMUTATION OF N - IAB ENTRIES IN
C VECTOR INDEX STARTING AT IAA+1
C
      DIMENSION INDEX(*)
      L=0
      M=N-IAB
C
C GENERATE A RANDOM DIGIT FROM 1 TO M USING THE PSEUDORANDOM U(0,1) VARIATE
C RANDOM() (SUCH AS FROM ALGORITHM AS 183)
C
10      J=INT(RANDOM()*FLOAT(M))+1
C
C SWAP ENTRIES IN INDEX CORRESPONDING TO J AND M, OFFSET BY IAB
C
      IF (J.NE.M) THEN
          ITEMP=INDEX(IAA+J+IAB)
          INDEX(IAA+J+IAB)=INDEX(IAA+M+IAB)
          INDEX(IAA+M+IAB)=ITEMP
      END IF
      M=M-1
      IF (M.GT.1) GO TO 10
      RETURN
      END
      SUBROUTINE SWAP(DATA,NVAR,NCAS,IR1,IR2,NVDIM)
C
C SUBROUTINE TO SWAP ROWS IR1 AND IR2 OF MATRIX DATA
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION DATA(0:NVDIM,*)
      NHIGH=NVAR+NCAS
      DO 10 I=1,NHIGH
10      TEMP=DATA(IR1,I)
          DATA(IR1,I)=DATA(IR2,I)
          DATA(IR2,I)=TEMP
      CONTINUE

```

RETURN

END

The file contains the following:

```
fishfun.c /* C-source of Fisher's symmetry test function + driver program */
groupfun.c /* C source of Pitman's 2 sample test function + driver program */
fishint.c /* exact (integer) version of fishfun.c */
groupint.c /* exact (integer) version of groupfun.c */
psydata /* data file of Rutter score data for fishfun */
agedata /* data file of age data for groupfun */
iagedat /* integer version of age data */

/* -----*/
/* fishfun.c */

#include <stdio.h>
#include <math.h>
#include <stdlib.h>

#define MAXNUM 200 /* max. sample size */
float fisherprob(float *,int,float,float *, long *);

#define NAMLEN 40 /* max. length of file-name */
int compare(int *x,int *y)
{
    return(*x-*y);
}

main()
{
    FILE *fp;
    char filename[NAMLEN]; /* array to hold filename */
    float a[MAXNUM],cv,p,ptol=.01; /* fractional error allowed on prob. */
    int scanval,n;
    long binsreq;

    puts("\nEnter input file name: ");
    scanf("%40s",filename); /* get file name (MAX 40 CHARS) */

    if ((fp = fopen(filename,"r")) == 0 ) /* open file */
    {
        puts ("Can't open input file"); /* unsuccessful */
        return;
    }

    n=0;
    while((scanval=fscanf(fp,"%f",&a[n])) != EOF && scanval != NULL )
    {
        printf("number %d is %f\n",n,a[n]);
        ++n;
    }
    close(fp);
    printf("read in %d numbers\n",n);

    p=fisherprob(a,n,ptol,&cv,&binsreq);
    if(p<0.)
    {
        printf("estimating probability to a CV of %f requires %ld
```

```

bins=sorry",ptol,binsreq);
        return;
    }
    printf("calculation used %ld histogram bins\n",binsreq);
    printf("1-tailed probability is %f\n",p);
    printf("Coefficient of variation on estimate of p is %f%\n",cv);
    /* can repeat with ptol less if cv is too large */
}

float fisherprob(float a[],int n,float ptol,float *cv,long *binsreq)
/* This function returns the 1-tailed probability from
Fisher's symmetry test, the permutation, i.e. distribution-free
analogue of the paired t-test. */

{
int numberpos=0,numberneg=0, *positive, *x,smallnum,topbin,
m, bin,i,ipossum=0,inegsum=0,s,n0,n0dash,ndash,ntop;
float possum=0,negsum=0,scale,sum,p,factor,mu,sigsq,term1,term2,tail,
*b;

*binsreq=n;
x=calloc(n,sizeof(int));
positive=calloc(n,sizeof(int)); /* allocate work arrays */
if(!x || !positive)return(-1.); /* and return -ve p-value if not
possible */

for(i=0,mu=0.,sigsq=0.;i<n;i++){
    sigsq+=a[i]*a[i]; /* accumulate permutation variance */
    if(a[i]>=0)
        {
            ++numberpos; /* count number of +ve values */
            possum+=a[i]; /* and accumulate their sum */
            positive[i]=1; /* flag value as +ve */
        }
    else
        {
            ++numberneg;
            negsum-=a[i];
            a[i]=-a[i];
            positive[i]=0;
        }
}

mu=(possum+negsum)/2.;
sigsq/=4.; /* permutation mean and variance */
sum=(possum<negsum)?possum:negsum; /* choose smaller sum as test
statistic */
m=(possum<negsum)?numberpos:numberneg;
factor=sqrt((n-(mu-sum)*(mu-sum)/sigsq)/48.); /*for error calculation */
term1=mu*(mu-sum)/(ptol*sigsq);
term2=2./ptol;
bin=factor*((term1>term2)?term1:term2);
/* no. of bins needed for required error on p*/

smallnum=(numberpos<numberneg)?numberpos:numberneg;
/* number in smaller group */
if(smallnum>0)
    scale=bin/sum; /* scale sample values so that smaller
sum is in bin number bin */
else

```

```

        scale=1.; /* if only one sign present calculation is trivial.
However,
just go through the usual motions */
    for (i=0;i<n;++i){
        x[i]=a[i]*scale+0.5; /* rescale sample values. Adding 0.5 rounds
to nearest integer rather than truncating*/
        if(positive[i])ipossum+=x[i];
        else
            inegsum+=x[i];
    }
    bin=(ipossum<inegsum)?ipossum:inegsum; /* rescale number of bins */

    *binsreq=bin+2;
    b=calloc(bin+2,sizeof(float)); /* allocate work array */
    if(!b)
        return(-1.); /* and return if not enough memory */

    qsort(x,n,sizeof(int),compare); /* sort sample values */
    for(i=0;i<n;++i)
        x[i]=(x[i]<bin+1)?x[i]:bin+1; /* any sample values
greater than bin are put into the
overflow bin */
    /* for(i=0;i<=bin+1;i++)b[i]=0.0; */
    ++b[0]; /* start histogram off - entries at zero and x0 */
    ++b[x[0]];
    n0=x[0];
    for(s=1;s<n;s++)
    {
        n0dash=n0+x[s];
        if(n0dash>bin)
        {
            b[bin+1]*=2.; /* just double entries in overflow bin */
        }
    }
    for(ndash=bin;ndash>=bin-x[s]+1;ndash--)b[bin+1]+=b[ndash];
    /* translate histogram */
    ntop=(bin>n0dash)?n0dash:bin;
    for(ndash=ntop;ndash>=x[s];ndash--)b[ndash]+=b[ndash-x[s]];
    n0=n0dash;
    }

    tail=0.; /* count entries in tail */
    for(i=0;i<=bin;++i)
        tail+=b[i];
    p=tail/(tail+b[bin+1]);
    *cv=100*b[bin]*factor/tail;
    free(b); /* free memory used for work arrays */
    free(x);
    free(positive);
    return(p);

}

/* -----*/
/* groupfun.c */

#include <stdio.h> /* for reading data file */
#include <math.h> /* for square root */
#include <stdlib.h>

```



```
#define MAXNUM 160 /* max. sample size */

#define LEN 40 /* max. length of filename */
int compare(int *x,int *y)
{
    return(*x-*y);
}

main()
{
    FILE *fp;
    int n,firstgroup[MAXNUM],scanval;
    float a[MAXNUM],p,cv,ptol=.05; /* fractional error required on prob. */
    long binsreq;
    float pitmanprob(float *,int *, int, float, float *, long *);
    char filename[LEN]; /* array to hold filename */

    puts("\nEnter input file name: ");
    scanf("%40s",filename); /* get file name (MAX 40 CHARS) */

    if ((fp = fopen(filename,"r")) == 0 ) /* open file */
    {
        puts ("Can't open input file"); /* unsuccessful */
        return;
    }

    n=0;
    while((scanval=fscanf(fp,"%f%d",&a[n],&firstgroup[n])) != EOF && scanval
    != NULL)
    {
        printf("number %d is %f group %d\n",n,a[n],firstgroup[n]);
        ++n;
        if(n>=MAXNUM)
        {
            printf("sample size too large. Maximum is %d\n",MAXNUM);
            return;
        }
    }
    close(fp);
    printf("read in %d numbers\n",n);

    p=pitmanprob(a,firstgroup,n,ptol,&cv,&binsreq); /* find tail probability
*/
    if(p<0.){
        printf("%ld array elements requested, which is too
many.\n",binsreq);
        return;
    }
    else
    {
        printf("%ld array elements used\n",binsreq);
        printf("1-tailed probability is %f\n",p);
        printf("CV of estimated probability is %f %%",cv);
    }
}

float pitmanprob(float a[],int firstgroup[],int n,float ptol,float *cv,long
*binsreq)
/* returns 1-tail probability from Pitman's 2-sample permutation test,
the distribution-free analogue of the grouped t-test */

{
    int numberone=0,numbertwo=0,
```

```

smallnum,k,j,smallgroup,ntop,kbot,topbin,
bin,i,isum=0,s,n0,n0dash,ndash,m,*dope,*x;
float onesum=0,twosum=0,scale,sum,p,tail,term1,term2,
minnum,maxnum,onemean,twomean,mu,sigsq,em,en,factor,*b;

*binsreq=n;
dope=calloc(n,sizeof(int));
x=calloc(n,sizeof(int)); /* allocate work area */
if(!dope || !x)return(-1.); /* return -ve p value if not possible */

for(i=0;i<n;i++){
    if(i == 0){
        minnum=a[i]; /* find max. and min. sample values */
        maxnum=a[i];
    }
    else {
        minnum=(a[i]>minnum)?minnum:a[i];
        maxnum=(a[i]>maxnum)?a[i]:maxnum;
    }
    if(firstgroup[i] ==1)
    {
        ++numberone; /* count numbers of in each group */
        onesum+=a[i]; /* and their sums */
    }
    else
    {
        ++numbertwo;
        twosum+=a[i];
    }
}

onemean=onesum/numberone; /* find means for each group */
twomean=twosum/numbertwo;
smallgroup=(onemean>twomean)?2:1;
for(i=0;i<n;i++)a[i]-=minnum; /* translate sample values to be >= 0 */
smallnum=(numberone<numbertwo)?1:2;
onesum-=numberone*minnum; /* and modify sums and maximum value */
twosum-=numbertwo*minnum;
maxnum-=minnum;

if(smallgroup != smallnum)
    { /* if necessary, reflect values so smaller group has smaller
mean */
        for(i=0;i<n;i++)a[i]=maxnum-a[i];
        onesum=numberone*maxnum-onesum;
        twosum=numbertwo*maxnum-twosum;
    }
sum=(smallnum == 1)?onesum:twosum;
m=(numberone<numbertwo)?numberone:numbertwo; /* number in smaller group
*/

em=m;
en=n;
for(mu=0.,sigsq=0.,i=0;i<n;i++){
    mu+=a[i];
    sigsq+=a[i]*a[i];
    for(j=i+1;j<n;j++)sigsq=sigsq-2.*a[i]*a[j]/(en-1.);
}
mu=(em/en)*mu;
sigsq=(em/en)*(1.-(em/en))*sigsq; /* permutation mean and variance */

```

```

factor=sqrt((em/en)*(1.-(em/en))*(en+(mu-sum)*(mu-sum)*(en+1.)/(en*sigsq))/12.);
term1=mu*(mu-sum)/(ptol*sigsq);
term2=2./ptol;
bin=factor*((term1>term2)?term1:term2); /* number of histogram bins
needed */

scale=bin/sum; /* scale sample values so that sum of smaller sample
is in bin
number bin */
for (i=0;i<n;i++){
x[i]=a[i]*scale+0.5; /* rescaling sample values.
Adding 0.5 rounds to
nearest bin rather than truncating */
if(firstgroup[i]==smallnum)isum+=x[i];
}
bin=isum; /* find exact histogram bin for start of reject H0 region */

*binsreq=(long)(bin+2)*m;
b=calloc(*binsreq,sizeof(float)); /* allocate and zero workspace */
if(!b)
return(-1.); /* not enough workspace */
qsort(x,n,sizeof(int),compare); /* sort sample */
for(i=0;i<n;i++)
x[i]=(x[i]<bin+1)?x[i]:bin+1; /* any sample values greater than
the test statistic "bin" will cause b[>bin] to be
occupied and are set
to bin+1, the overflow bin NOW rather than later so
as not to cause integer
overflow */

for(i=0;i<m;i++)dope[i]=i*(bin+2); /* offsets to mimick 2 dim. array */
++b[dope[0]+x[0]]; /* start histogram off */
/* for 2 dim. array code would be ++b[0][x[0]]; */

n0=x[0];
for(s=1;s<n;s++)
{
kbot=(m+s-n>1)?m+s-n:1;
n0dash=n0+x[s]; /* translate each level by x[s] */
for(k=(s>(m-1))?(m-1):s;k>=kbot;k--) /* only build up histograms
as far as mth level, which is the one we want */
{
if(n0dash>bin)for(ndash=bin-x[s]+1;ndash<=bin+1;ndash++)
/* translate k-1 th level onto kth level...these
terms go into overflow bin */
b[dope[k]+bin+1]+=b[dope[k-1]+ndash];
/* for 2 dim. array... b[k][bin+1]+=b[k-1][ndash]; */
ntop=(bin>n0dash)?n0dash:bin;
for(ndash=x[s];ndash<=ntop;ndash++){
/* these terms just translate along, but may go
into overflow bin */
b[dope[k]+ndash]+=b[dope[k-1]+ndash-x[s]];
/* for 2 dim. array...
b[k][ndash]+=b[k-1][ndash-x[s]]; */
}
}

++b[dope[0]+x[s]]; /* add new term to lowest level */
/* for 2 dim. array... ++b[0][x[s]]; */

```

```

        n0=n0dash;
    }

    tail=0.; /* find tail probability */
    for(i=0;i<=bin;i++)
        /* for 2 dim. array... tail+=b[m-1][i]; */
        tail+=b[dope[m-1]+i];

    *cv=100.*b[dope[m-1]+bin]*factor/tail; /* find coefficient of variation
*/
    /* for 2d array... *cv=100.*b[m-1][bin]*factor/tail; */
    free(x); /* free off workspace */
    free(dope);
    free(b);
    return(tail/(tail+b[dope[m-1]+bin+1]));
}

/* -----*/
/* fishint.c */

#include <stdio.h>
#include <math.h>
#include <stdlib.h>

#define MAXNUM 200 /* max. sample size */
float fishprob();

#define NAMLEN 40 /* max. length of file-name */
int comp(int *x,int *y)
{
return(*x-*y);
}
main()
{
FILE *fp;
char filename[NAMLEN]; /* array to hold filename */
float cv,p;
int scanval,n,a[MAXNUM];
long binsreq;

puts("\nEnter input file name: ");
scanf("%40s",filename); /* get file name (MAX 40 CHARS) */

if ((fp = fopen(filename,"r")) == 0 ) /* open file */
{
puts ("Can't open input file"); /* unsuccessful */
return;
}

n=0;
while((scanval=fscanf(fp,"%d",&a[n])) != EOF && scanval != NULL )
{
printf("number %d is %d\n",n,a[n]);
++n;
}
close(fp);
printf("read in %d numbers\n",n);

p=fishprob(a,n,&binsreq);
if(p<0.)
{

```

```

        printf("calculating probability requires %ld bins-sorry",binsreq);
        return;
    }
    printf("calculation used %ld histogram bins\n",binsreq);
    printf("1-tailed probability is %f\n",p);
}

float fishprob(int a[],int n,long *binsreq)
/* This function returns the 1-tailed probability from
Fisher's symmetry test, the permutation, i.e. distribution-free
analogue of the paired t-test. */

    {
    long bin,i,s,n0,n0dash,ndash,ntop;
    long possum=0,negsum=0,sum;
    float p,tail;
float *b;

    for(i=0;i<n;i++){
        if(a[i]>=0)
            {
            possum+=a[i]; /* and accumulate their sum */
            }
        else
            {
            negsum-=a[i];
            a[i]=-a[i];
            }
        }

    sum=(possum<negsum)?possum:negsum; /* choose smaller sum as test statistic
*/
    bin=sum;
    /* no. of bins needed */
b=calloc(bin+2,sizeof(float));
*binsreq=bin+2;
if(!b)
    return(-1.);

qsort(a,n,sizeof(int),comp);
for(i=0;i<n;++i)
    a[i]=(a[i]<bin+1)?a[i]:bin+1; /* any sample values
greater than bin are put into the overflow bin */
for(i=0;i<=bin+1;i++)b[i]=0.0;
++b[0]; /* start histogram off - entries at zero and x0 */
++b[a[0]];
n0=a[0];
for(s=1;s<n;s++)
    {
    n0dash=n0+a[s];
    if(n0dash>bin)
        {
        b[bin+1]=2*b[bin+1]; /* just double entries in overflow bin */
        for(ndash=bin;ndash>=bin-a[s]+1;ndash--)b[bin+1]+=b[ndash];
        }/* translate histogram */
    ntop=(bin>n0dash)?n0dash:bin;
    for(ndash=ntop;ndash>=a[s];ndash--)b[ndash]+=b[ndash-a[s]];
    n0=n0dash;
    }

    tail=0.; /* count entries in tail */

```

```
        for(i=0;i<=bin;++i)
            tail+=b[i];
        p=tail/(tail+b[bin+1]);
        free(b); /* free work space array */
        return(p);

    }

/* -----*/
/* groupint.c */

#include <stdio.h> /* for reading data file */
#include <math.h> /* for square root */
#include <stdlib.h>

#define MAXNUM 200 /* max. sample size */

#define LEN 40 /* max. length of filename */
int comp(int *x,int *y)
{
return(*x-*y);
}
void main()
{
FILE *fp;
int n,firstgroup[MAXNUM],scanval,x[MAXNUM];
long binsreq;
float p;
float grouprob();
char filename[LEN]; /* array to hold filename */

puts("\nEnter input file name: ");
scanf("%40s",filename); /* get file name (MAX 40 CHARS) */

if ((fp = fopen(filename,"r")) == 0 ) /* open file */
{
puts ("Can't open input file"); /* unsuccessful */
return;
}

n=0;
while((scanval=fscanf(fp,"%d%d",&x[n],&firstgroup[n])) != EOF && scanval
!= NULL)
{
printf("number %d is %d group %d\n",n,x[n],firstgroup[n]);
++n;
if(n>=MAXNUM)
{
printf("sample size too large. Maximum is %d\n",MAXNUM);
return;
}
}
close(fp);
printf("read in %d numbers\n",n);

p=grouprob(firstgroup,x,n,&binsreq); /* find tail probability */
if(p<0.){
printf("%ld array elements requested, which is too
many.\n",binsreq);
return;
}
```

```

    }
else {
    printf("%ld array elements used\n",binsreq);
    printf("1-tailed probability is %f\n",p);
}
}

```

```

float grouprob(int firstgroup[],int x[],int n,long *binsreq)
/* returns 1-tail probability from Pitman's 2-sample permutation test. */

{
    int numberone=0,numbertwo=0,
    smallnum,k,j,smallgroup,ntop,kbot,topbin,
    bin,i,s,n0,n0dash,ndash,m,onesum=0,twosum=0,sum,minnum,maxnum;
    float p,tail,onemean,twomean;
int *dope;
float *b;
*binsreq=n;
dope=calloc(n,sizeof(int));
if(!dope)return(-1.);
    for(i=0;i<n;i++){
        if(i == 0){
            minnum=x[i]; /* find max. and min. sample values */
            maxnum=x[i];
        }
        else {
            minnum=(x[i]>minnum)?minnum:x[i];
            maxnum=(x[i]>maxnum)?x[i]:maxnum;
        }
        if(firstgroup[i] ==1)
            {
                ++numberone; /* count numbers of in each group */
                onesum+=x[i]; /* and their sums */
            }
        else
            {
                ++numbertwo;
                twosum+=x[i];
            }
    }

    onemean=onesum/numberone; /* find means for each group */
    twomean=twosum/numbertwo;
    smallgroup=(onemean>twomean)?2:1;
    for(i=0;i<n;i++)x[i]-=minnum; /* translate sample values to be >= 0 */
    smallnum=(numberone<numbertwo)?1:2;
    onesum-=numberone*minnum; /* and modify sums and maximum value */
    twosum-=numbertwo*minnum;
    maxnum-=minnum;

    if(smallgroup != smallnum)
        { /* if necessary, reflect values so smaller group has smaller mean
*/
            for(i=0;i<n;i++)x[i]=maxnum-x[i];
            onesum=numberone*maxnum-onesum;
            twosum=numbertwo*maxnum-twosum;
        }
    sum=(smallnum == 1)?onesum:twosum;
    m=(numberone<numbertwo)?numberone:numbertwo; /* number in smaller group */

bin=sum;

```

```

    qsort(x,n,sizeof(int),comp);
    for(i=0;i<n;i++)
        x[i]=(x[i]<bin+1)?x[i]:bin+1; /* any sample values greater than
set                                     the test statistic "bin" will cause b[>bin] to be occupied and are
integer                                 to bin+1, the overflow bin NOW rather than later so as not to cause
                                        overflow */
        *binsreq=(bin+2)*m;
b=calloc(*binsreq,sizeof(float));
    if(!b)
        return(-1.); /* not enough workspace */
/*   for(i=0;i<*binsreq;i++)
        b[i]=0.0;  initialise work array */
    for(i=0;i<m;i++)dope[i]=i*(bin+2); /* offsets to mimic 2 dim. array */
    ++b[dope[0]+x[0]]; /* start histogram off */
/* for 2 dim. array code would be  ++b[0][x[0]]; */

    n0=x[0];
    for(s=1;s<n;s++)
        {
            kbot=(m+s-n>1)?m+s-n:1;
            n0dash=n0+x[s]; /* translate each level by x[s] */
            for(k=(s>(m-1))?m-1:s;k>=kbot;k--) /* only build up histograms
want */                                     as far as mth level, which is the one we
                                                {
                                                    if(n0dash>bin)for(ndash=bin-x[s]+1;ndash<=bin+1;ndash++)
go into overflow bin */
                                                        /* translate k-1 th level onto kth level...these terms
                                                            b[dope[k]+bin+1]+=b[dope[k-1]+ndash];
/* for 2 dim. array...  b[k][bin+1]+=b[k-1][ndash]; */
ntop=(bin>n0dash)?n0dash:bin;
for(ndash=x[s];ndash<=ntop;ndash++){
overflow bin */
                    /* these terms just translate along, but may go into
                        b[dope[k]+ndash]+=b[dope[k-1]+ndash-x[s]];
/* for 2 dim. array...  b[k][ndash]+=b[k-1][ndash-x[s]];
*/
                    }
                }

            ++b[dope[0]+x[s]]; /* add new term to lowest level */
            /* for 2 dim. array...  ++b[0][x[s]]; */
            n0=n0dash;
        }

    tail=0.; /* find tail probability */
    for(i=0;i<=bin;i++)
        /* for 2 dim. array...  tail+=b[m-1][i]; */
        tail+=b[dope[m-1]+i];

    return(tail/(tail+b[dope[m-1]+bin+1]));
}

/* -----*/
/* psydata */

```

```

-1 -2 1 -7 -5 0 3 0 -6 -1 -5 -1 -1 5 -1 -8 0 5 -2 -2 0 -4 -4 2
-1 -1 -1 4 0 1 -2 -2 -2 1 0 -4 -5 0 -5 -1 5 2 0

```



```
/* ----- */  
/* agedata */  
  
1.5 2  
2.5 2  
1 2  
6 2  
7 2  
2 2  
9 2  
8 1  
5 1  
6 1  
5 1  
6 1  
7 1  
4 1  
9 2  
6 2  
9 2  
7 2  
4 2  
4 2  
5 1  
5 1  
4 1  
7 1  
9 1  
6 1  
6 1  
6 1  
5 2  
3 2  
1 2  
3 2  
5 1  
4.5 1  
6 1  
4 1  
6 1  
4.5 1  
5 1  
9 1  
5 2  
3 2  
3.5 2  
5 2  
7 2  
3 2  
3.5 2  
7 2  
3 2
```

```
/* ----- */  
/* iagedat */  
  
3 2  
5 2  
2 2  
12 2
```

14 2  
4 2  
18 2  
16 1  
10 1  
12 1  
10 1  
12 1  
14 1  
8 1  
18 2  
12 2  
18 2  
14 2  
8 2  
8 2  
10 1  
10 1  
8 1  
14 1  
18 1  
12 1  
12 1  
12 1  
10 2  
6 2  
2 2  
6 2  
10 1  
9 1  
12 1  
8 1  
12 1  
9 1  
10 1  
18 1  
10 2  
6 2  
7 2  
10 2  
14 2  
6 2  
7 2  
14 2  
6 2

Program driver

```
C
C      Program to test and illustrate algorithm BEST.  Program
C      DRIVER is not necessary for using BEST.
C
C      At the prompt, input values for p, q, and x.  The value of
C      p is the dimension of the covariance matrix and the value
C      of q is the degrees of freedom.  The program outputs an
C      approximation to  $\Pr(GG < x)$ , where GG is the Greenhouse-
C      Geiser epsilon.
C
C      The program is intended to be run interactively.  It expects
C      that unit 5 is input and unit 6 is output.
C
```

```
real x,best,pval
integer ip,iq
write(6,10)
10  format(/,' To exit program, type Control C',/)
20  write(6,30)
30  format(/,' Input p, q, and x')
    read(5*,err=50) ip,iq,x
    pval=best(x,ip,iq,ifault)
    write(6,40) pval,ifault
40  format(' Pr(GG < x) = ',f7.5,', Ifault = ',i1)
    goto 20
50  stop
end
```

```
real function best(x,ip,iq,ifault)
```

```
C
C      ALGORITHM AS 284, APPL. STATIST. (1993), VOL. 42, NO. 3
C
C      Computes The Null Distribution Function of The Test
C      Statistic For The Locally Best Invariant Test of
C      Sphericity And Additivity
C
```

```
real x,p,q,a,b,t,s1,s2,s3,s4,s5,zero,one,two,three,four,epsi,
$ delta(4),fact(0:6),pocham,zreal,alogam,betain,beta,small,lag,
$ nbit,base
intrinsic abs,exp,log,sign,sqrt
```

```
C
C      Fixed Constants
C
```

```
data zero,one,two,three,four,small,(fact(i),i=0,6) /0.0e0,
$ 1.0e0, 2.0e0, 3.0e0, 4.0e0, 1.0e-2, 1.0e0, 1.0e0, 2.0e0,
$ 6.0e0, 2.4e1, 1.2e2, 7.2e2/
```

```
C
C      Machine Dependent Constants
C
```

```
data base,nbit/2.0e0, 23.0e0/
zreal(i)=real(i)
epsi=one/base**(nbit-one)
```

```
C
C      Check Validity of Input Arguments
C
```

```
best=one
ifault=4
if(ip.le.1.or.iq.lt.ip) return
p=zreal(ip)
```

```

    q=zreal(iq)
    ifault=5
    if(x.ge.one-epsi) return
    best=zero
    if(x*p.le.one+epsi) return
C
C          Use Chebyshev's Inequality to Check for Probabilities
C          Near 0 or 1
C
    ifault=3
    t=(one/x-one)/(p-one)
    a=(p+two)*(p*(p*q-q+two*four)-three*four)/(four*p*(q+two))
    b=(q-one)*a*p/(p+two)
    s1=a/(a+b)-t
    s2=(log(a)+log(b)-log(a+b+one))/two-log(a+b)-log(small)
    if(exp(s2).le.abs(s1)) then
        if(s1.lt.zero) then
            return
        else
            best=one
            return
        endif
    endif
    ifault=0
C
C          Use Exact Beta(1,(q-1)/2) Distribution if p = 2
C
    if(ip.eq.2) then
        best=exp((q-one)*log(one-t)/two)
C
C          Check Magnitude of Higher Order Terms.
C
    else
        call moment(p,q,delta)
        s1=abs(delta(1))+abs(delta(2))+abs(delta(3))+abs(delta(4))
        if(s1.ge.epsi**(one/three)) then
C
C          Use Exact Distribution from John (1972) if p = 3
C          and Magnitude of Higher Order Terms is Large
C
            if(ip.eq.3) then
                a=q/two
                b=q-one
C
C          Compute log Beta Function.  No Need to Check Error
C          Indicator, it is Known to be 0.
C
                beta=alogam(a,ier)+alogam(b,ier)-alogam(a+b,ier)
                s1=sqrt(t)
                s2=(one+two*s1)/three
                best=betain(s2,a,b,beta,ier)
$                -three*exp(a*log(s2)+b*log(one-s2)-beta)
                if(t.lt.one/four-epsi) then
                    s3=(one-two*s1)/three
C
C          Compute Probability.  No Need to Check Error
C          Indicator, it is Known to be 0.
C
                best=best-betain(s3,a,b,beta,ier)
$                +three*exp(a*log(s3)+b*log(one-s3)-beta)
            end if

```

```

                best=one-best
C
C      Use Six moment Jacobi Polynomial Expansion if p > 3
C      And Magnitude of Higher Order Terms is Large
C
      else
        ifault=1
C
C      Compute log Beta Function And Probability.  No Need to
C      Check Error Indicator, it is Known to be 0.
C
        beta=alogam(a,ier)+alogam(b,ier)-alogam(a+b,ier)
        best=betain(t,a,b,beta,ier)
        do 30 n=3,6
          s1=pocham(a,n-1)+pocham(a+b+zreal(n),n-1)
          $      -pocham(a+b,n)+pocham(a+b+zreal(n-1),n-1)
          $      -pocham(b,n)-log(fact(n))
          s2=zero
          do 10 i=0,n-3
            s3=pocham(zreal(n-i+1),i)-log(fact(i))
            $      +log(a+zreal(n-1))
            $      -pocham(a+b+zreal(2*n-i-1),i)
            $      +pocham(a+b+zreal(n-i),i)
            $      +log(abs(delta(n-i-2)))
            $      +log(a+b+zreal(2*n-2))
            s2=s2+exp(s3)*sign(one,delta(n-i-2))
            $      *(-one)**i
          10      continue
            if(abs(s2).le.epsi) goto 30
            s3=zero
            do 20 i=1,n
              s4=pocham(zreal(n-i+1),i)-log(fact(i))
              $      -pocham(a+b+zreal(2*n-i-1),i)
              $      +pocham(a+b+zreal(n-i),i)
              do 20 j=1,i
                s5=pocham(a+b,n-j)-pocham(a,n-j+1)
                $      +(a+zreal(n-j))*log(t)+b*log(one-t)
                $      -beta
                s3=s3+exp(s5+s4+log(a+b+zreal(2*n-1)))
                $      *(-one)**i
              20      continue
                if(abs(s3).le.epsi) goto 30
                s4=exp(s1+log(abs(s2))+log(abs(s3)))
                best=best+s4*sign(one,s2*s3)
            30      continue
              best=one-best
            end if
          end if
        end if
        if(best.lt.zero) best=zero
        if(best.gt.one) best=one
        return
        end

```

```

    real function lag(x,ip,iq,ifault)
C
C           Computes Three moment Laguerre Polynomial Approximation
C           to the Distribution Function
C
    real x,p,q,pq,a,b,s1,s2,t,delta,gammad,alogam,zreal,
$ zero,one,two,three,four,six,cn(9),cd(20)
    intrinsic abs,exp,log,sign
C
C           Fixed Constants
C
    data zero,one,two,three,four,six/ 0.0e0, 1.0e0, 2.0e0, 3.0e0,
$ 4.0e0, 6.0e0/
    data (cn(i),i=1,9)/ 0.0e0, 1.2e2, 1.8e1, 4.8e1, -1.2e1, -3.0e0,
$ 4.0e1, 0.0e0, -1.0e0/
    data (cd(i),i=1,20)/ 1.152e3, 3.84e2, -1.84e2, 1.2e1, -1.152e3,
$ -6.72e2, 6.4e1, 8.0e0, -2.88e2, -1.92e2, 5.4e1, 9.0e0, 2.88e2,
$ 2.96e2, 4.8e1, 2.0e0, 6.4e1, 8.8e1, 1.8e1, 1.0e0/
    zreal(i)=real(i)
    ifault=2
    p=zreal(ip)
    q=zreal(iq)
    pq=p*q
    a=two*four
    b=-log(a/pq+one)-log((a+two)/pq+one)-three*log(pq)
$ +log(q-one)+log(q+two)+log(zreal(32))
    b=-exp(b)
C
C           Compute Standardized Third moment
C
    n1=0
    n2=0
    s1=zero
    do 20 j=0,2
        a=zero
        do 10 k=0,2
            n1=n1+1
            a=a/pq+cn(n1)
10        continue
        s1=s1/p+a
20    continue
    s2=zero
    do 40 j=0,4
        a=zero
        do 30 k=0,3
            n2=n2+1
            a=a/pq+cd(n2)
30        continue
        s2=s2/p+a
40    continue
    delta=b*s1/s2
    a=(p-one)*(p+two)*(p*q+four)*(p*q+six)
$ /(four*(q-one)*(q+two)*p**2)
    b=(p*q+two)*a/(p+two)
    t=b*(one/x-one)/(p-one)
C
C           Compute Log Gamma Function.  No Need to Check Error
C           Indicator, it is Known to be 0.
C
    s1=a*log(t)-t-alogam(a,ier)+log(abs(delta))-log(six)
    s2=exp(s1+two*log(abs(t-a-two)))-exp(s1+log(abs(a-two)))

```

```

C
C      Compute Probability.  No Need to Check Error
C      Indicator, it is Known to be 0.
C
lag=one-gammad(t,a,ier)+s2*sign(one,delta)
return
end

```

```

real function pocham(x,i)
C
C      Compute Natural Log of Pochhammer's Symbol: (x) sub i
C
real x,zreal,zero
intrinsic log
data zero /0.0e0/
zreal(i)=real(i)
pocham=zero
if(i.eq.0) return
do 10 j=1,i
10 pocham=pocham+log(x+zreal(i)-zreal(j))
return
end

```

```

Subroutine moment(p,q,delta)
real p,q,pq,num,den,s,zero,one,two,three,four,cn(240),cd(154),
$ g(4),f(4),delta(4)
intrinsic exp,log

```

```

C
C      Compute Standardized moments of LBI Statistic
C
C      Fixed Constants
C

```

```

data zero,one,two,three,four /0.0e0, 1.0e0, 2.0e0, 3.0e0, 4.0e0/
data (g(i),i=1,4) /3.2e1, 1.28e2, 6.4e1, 1.28e2/
data (cn(i),i=1,110) / 0.0e0, -2.8e1, 0.0e0, 1.0e1, -5.0e0, -1.0e0,
$ 0.0e0, -1.12896e5, 1.94784e5, -3.3888e4, -3.2448e4, 0.0e0,
$ 4.032e4, -9.7968e4, 7.6856e4, 2.096e3, -1.732e4, -1.008e3,
$ 3.552e3, -1.4604e4, 1.002e4, 2.42e3, -3.268e3, -3.28e2, 3.28e2,
$ -4.34e2, 1.65e2, 3.19e2, -2.45e2, -3.7e1, -8.2e1, 1.16e2, -2.9e1,
$ 1.0e0, -5.0e0, -1.0e0, 0.0e0, -3.90168576e9, 1.4764032e10,
$ -1.7053949952e10, 3.842187264e9, 3.411984384e9, -9.30594816e8,
$ -3.29416704e8, 0.0e0, 1.3934592e9, -5.74580736e9, 1.010539008e10,
$ -8.198281728e9, 7.0906368e8, 2.382832128e9, -4.64467968e8,
$ -2.78255616e8, -9.068544e6, -3.787776e7, -5.95800576e8,
$ 1.800523008e9, -1.554594816e9, -2.6491904e7, 6.44580096e8,
$ -9.4626048e7, -9.609088e7, -5.374464e6, -1.525248e6, 4.829952e6,
$ 7.0553536e7, -9.968272e7, -1.3282944e7, 8.1219456e7, -8.673152e6,
$ -1.7555424e7, -1.35904e6, -6.517632e6, 1.8864096e7, -2.4434256e7,
$ 6.285264e6, 2.517872e6, 3.552544e6, -3.14064e5, -1.801424e6,
$ -1.7992e5, 2.71712e5, 1.948336e6, -4.017808e6, 1.359176e6,
$ 8.19112e5, -2.2064e5, -1.072e4, -9.9608e4, -1.2696e4, -9.7584e4,
$ 2.53584e5, -2.20896e5, 1.557e4, 7.9326e4, -2.446e4, -2.58e3,
$ -2.55e3, -4.1e2, 5.056e3, -1.1944e4, 8.55e3, -2.077e3, 8.75e2,
$ -3.7e2, -6.0e1, -2.5e1, -5.0e0, 0.0e0, -4.12018016256e13/
data (cn(i),i=111,170) / 2.544631676928e14, -5.8340956962816e14,
$ 5.799309115392e14, -1.667991011328e14, -1.0232596463616e14,
$ 5.784648155136e13, 9.4170710016e12, -5.5084843008e12,
$ -1.03842054144e12, 0.0e0, 1.4714929152e13, -8.270448427008e13,
$ 2.1422392786944e14, -3.36219910668288e14, 2.93880843804672e14,
$ -6.9645704552448e13, -7.5702487277568e13, 3.8893641228288e13,
$ 9.646000324608e12, -4.669805494272e12, -1.170392481792e12,

```

```
$ -2.569273344e10, -4.8813539328e12, 1.241719676928e13,  
$ 4.57903300608e12, -4.737808889856e13, 6.1560777191424e13,  
$ -1.9353568569344e13, -2.04090638848e13, 1.1918790731776e13,  
$ 3.827214399488e12, -1.7948152832e12, -5.66963986432e11,  
$ -2.1138112512e10, 1.2911837184e11, 2.002896101376e12,  
$ -5.52099796992e12, 2.399627067392e12, 4.85868078592e12,  
$ -4.4841321088e12, -2.005616851968e12, 2.151339017216e12,  
$ 7.65947608064e11, -4.0405611776e11, -1.56711717888e11,  
$ -7.879186432e9, -7.0632824832e10, 3.56417660928e11,  
$ -1.269488833536e12, 1.782649662464e12, -3.94358012672e11,  
$ -8.37563249024e11, 1.6834389056e11, 2.62308470784e11,  
$ 7.3064108032e10, -5.86671328e10, -2.7335101312e10,  
$ -1.713773312e9, 3.708598272e10, -5.6949588992e10/  
data (cn(i),i=171,240)/ -1.01034381696e11, 3.1574732672e11,  
$ -1.58358678688e11, -1.11234267456e11, 7.1553216224e10,  
$ 2.4591867072e10, -2.46103264e8, -5.746261696e9, -3.116678112e9,  
$ -2.36430272e8, -2.898390528e9, 3.32693408e9, -1.5851460992e10,  
$ 3.3324926128e10, -1.7291739616e10, -1.069476608e10,  
$ 8.859817856e9, 2.11305632e9, -8.7746096e8, -3.95701248e8,  
$ -2.31185472e8, -2.1039408e7, 4.6900352e8, -3.39609568e8,  
$ -8.90319408e8, 1.59414452e9, -7.83590964e8, -5.89984244e8,  
$ 5.16508044e8, 1.60988444e8, -9.91687e7, -2.0192284e7,  
$ -1.070398e7, -1.17714e6, -7.802352e7, 1.48137968e8, -2.5871288e7,  
$ -7.2898636e7, 2.0969796e7, -5.79076e5, 5.97858e6, 8.300068e6,  
$ -4.904884e6, -7.84316e5, -2.86284e5, -3.8408e4, 4.14784e6,  
$ -1.4920968e7, 2.0030724e7, -1.0498098e7, -8.32893e5, 2.605797e6,  
$ -5.28245e5, 1.13753e5, -9.6255e4, -1.6865e4, -4.115e3, -6.75e2,  
$ -8.3304e4, 2.76992e5, -3.30074e5, 1.73416e5, -5.7129e4, 2.7445e4,  
$ -6.681e3, 1.85e2, -6.75e2, -1.45e2, -2.5e1, -5.0e0/  
data (cd(i),i=1,124)/ 5.76e2, -7.68e2, -1.44e2, 2.56e2, 6.4e1,  
$ -1.92e2, 6.4e1, 4.8e1, 4.8e1, 1.6e1, 1.2e1, 8.0e0, 9.0e0, 2.0e0,  
$ 1.0e0, 1.3824e4, -3.456e4, 1.344e4, 1.632e4, -4.48e3, -3.84e3,  
$ -5.12e2, -1.0368e4, 1.4016e4, 2.528e3, -2.352e3, -2.096e3,  
$ -1.152e3, -1.92e2, 2.208e3, -5.92e2, -4.56e2, -8.6e2, -3.6e2,  
$ -1.08e2, -2.4e1, -1.2e2, -9.2e1, -1.1e2, -3.7e1, -2.1e1, -3.0e0,  
$ -1.0e0, 3.31776e5, -1.327104e6, 1.456128e6, 1.8432e5, -8.0256e5,  
$ -6.144e4, 1.61792e5, 4.9152e4, 4.096e3, -4.42368e5, 1.179648e6,  
$ -5.28384e5, -4.66944e5, 4.7104e4, 1.08544e5, 6.912e4, 2.048e4,  
$ 2.048e3, 1.98144e5, -2.79552e5, -4.6336e4, 1.6896e4, 5.5136e4,  
$ 3.7824e4, 1.2128e4, 3.072e3, 3.84e2, -3.3792e4, 8.192e3, 6.4e3,  
$ 1.6896e4, 8.064e3, 3.712e3, 1.056e3, 1.92e2, 3.2e1, 1.68e3,  
$ 1.408e3, 1.752e3, 7.2e2, 4.41e2, 1.0e2, 3.8e1, 4.0e0, 1.0e0,  
$ 7.962624e6, -4.644864e7, 9.068544e7, -4.902912e7, -3.9020544e7,  
$ 3.236352e7, 1.3006848e7, -5.44768e6, -3.35872e6, -5.7344e5,  
$ -3.2768e4, -1.65888e7, 7.133184e7, -8.626176e7, -8.41728e5,  
$ 3.8708736e7, 5.992192e6, -5.542144e6, -4.4032e6, -1.6896e6,  
$ -3.072e5, -2.048e4, 1.271808e7, -3.621888e7, 1.8376704e7,  
$ 1.2434432e7, 1.097984e6, -3.187328e6, -3.21408e6, -1.3088e6,  
$ -3.4944e5, -6.4e4, -5.12e3, -4.3776e6, 6.517248e6, 9.78944e5/  
data (cd(i),i=125,154)/ 8.0128e4, -1.564096e6, -1.15376e6,  
$ -5.1376e5, -1.768e5, -3.824e4, -6.4e3, -6.4e2, 6.48576e5,  
$ -1.53792e5, -1.22944e5, -3.89792e5, -2.0356e5, -1.1454e5,  
$ -3.78e4, -1.06e4, -2.28e3, -3.0e2, -4.0e1, -3.024e4, -2.7024e4,  
$ -3.4624e4, -1.612e4, -1.041e4, -2.961e3, -1.225e3, -2.1e2,  
$ -6.0e1, -5.0e0, -1.0e0/  
pq=p*q  
s=two*four  
f(1)=log(q-one)+log(q+two)+log(p-two)-log(pq)  
$ -log(p-one)-log(pq+s)-log(pq+s+two)  
do 10 i=2,4  
    s=s+four
```



```

      f(i)=f(i-1)+three*log(p)+two*log(q)
$      -log(p-one)-log(pq+s)-log(pq+s+two)
10  continue
      do 20 i=1,4
20  f(i)=exp(f(i)+log(g(i)))*(-one)**i
      n1=0
      n2=0
      do 70 ii=1,4
          i=ii+2
          num=zero
          ind=3*(i-3)+1
          do 40 j=0,ind
              s=zero
              do 30 k=0,ind+1
                  n1=n1+1
                  s=s/p+cn(n1)
30              continue
              num=num/pq+s
40              continue
              den=zero
              ind=i-1
              do 60 j=0,ind
                  s=zero
                  do 50 k=0,2*ind
                      n2=n2+1
                      s=s/p+cd(n2)
50                  continue
                  den=den/pq+s
60                  continue
              delta(ii)=f(ii)*num/den
70  continue
      return
      end

```

```

C
C
C *****
C *
C *   The remaining subprograms are included for referees use   *
C *   only.  They are not intended for publication.             *
C *
C *****

```

```

C
C      real function betain(x,p,q,beta,ifault)
C
C          Algorithm AS 63 Appl. Statist. (1973) Vol. 22, p. 409
C
C          Computes Incomplete Beta Function Ratio for Arguments
C          x between zero and one, p and q positive.
C          Log of Complete Beta Function, Beta, is Assumed to
C          be Known.
C
C          logical index
C          real acu,ai,beta,cx,one,p,pp,psq,q,qq,rx
C          real temp,term,x,xx,zero,zabs,zexp,zlog
C
C          Define Accuracy and Initialize
C
C          data acu,one,zero/1.0e-7, 1.0e0, 0.0e0/
C          zabs(X)=abs(X)

```

```
zexp(X)=exp(X)
zlog(X)=alog(X)
betain=x
```

```
C
C      Test for Admissibility of Arguments
C
```

```
Ifault=1
If(p.le.zero.or.q.le.zero) return
Ifault=2
If(x.lt.zero.or.x.gt.one) return
Ifault=0
if(x.eq.0.or.x.eq.one) return
```

```
C
C      Change Tail If Necessary and Determine s
C
```

```
psq=p+q
cx=one-x
if(p.ge.psq*x) goto 1
xx=cx
cx=x
pp=q
qq=p
index=.true.
goto 2
1
xx=x
pp=p
qq=q
index=.false.
2
term=one
ai=one
betain=one
ns=qq+cx*psq
```

```
C
C      Use Reduction Formulae of Soper
C
```

```
rx=xx/cx
3
temp=qq-ai
if(ns.eq.0) rx=xx
4
term=term*temp*rx/(pp+ai)
betain=betain+term
temp=zabs(term)
if(temp.le.acu.and.temp.le.acu*betain) goto 5
ai=ai+one
ns=ns-1
if(ns.ge.0) goto 3
temp=psq
psq=psq+one
goto 4
```

```
C
C      Calculate Result
C
```

```
5
betain=betain*zexp(pp*zlog(xx)+(qq-one)*zlog(cx)-beta)/pp
if(index) betain=one-betain
return
end
```

```
real function gammad(x,p,ifault)
```

```
C
C      Algorithm AS239 Appl. Statist. (1988) Vol. 37, No. 3
C
C      Computation of the Incomplete Gamma Integral
```

```
C
integer ifault
real pn1,pn2,pn3,pn4,pn5,pn6,x,tol,oflo,xbig,arg,c,rn,p,a,
$ b,one,zero,alogam,an,two,elimit,plimit,alnorm,three,nine
parameter (zero=0.0e0, one=1.0e0, two=2.0e0, oflo=1.3e19,
$ three=3.0e0, nine=9.0e0, tol=1.0e-7, plimit=1.0e3,
$ xbig=1.0e6, elimit=-8.8e1)
intrinsic abs,log,exp,sqrt,min
external alogam,alnorm

C
gammad=zero

C
      Check that we have valid values for X and P
C
C
if(p.le.zero.or.x.lt.zero) then
ifault=1
return
endif
ifault=0
if(x.eq.zero) then
gammad=zero
return
endif

C
      Use a Normal Approximation if P .gt. PLIMIT
C
C
if(p.gt.plimit) then
pn1=three*sqrt(p)*((x/p)**(one/three)+one/(nine*p)-one)
gammad=alnorm(pn1,.false.)
return
endif

C
      If X is extremely large compared to P then set GAMMAD to ONE
C
C
if(x.gt.xbig) then
gammad=one
return
endif

C
if(x.le.one.or.x.lt.p) then
C
      Use Pearson's series expansion (Note that P is not large enough
C      to force overflow in ALOGAM) No need to test IFAULT on exit
C      since P .gt. zero
C
arg=p*log(x)-x-alogam(p+one,ifault)
c=one
gammad=one
a=p
40 a=a+one
c=c*x/a
gammad=gammad+c
if(c.gt.tol) goto 40
arg=arg+log(gammad)
gammad=zero
if(arg.ge.elimit) gammad=exp(arg)

C
else
C
      Use a continued fraction expansion
C
```

```

        arg=p*log(x)-x-alogam(p,ifault)
        a=one-p
        b=a+x+one
        c=zero
        pn1=one
        pn2=x
        pn3=x+one
        pn4=x*b
        gammad=pn3/pn4
60      a=a+one
        b=b+two
        c=c+one
        an=a*c
        pn5=b*pn3-an*pn1
        pn6=b*pn4-an*pn2
        if(abs(pn6).gt.zero) then
        rn=pn5/pn6
        if(abs(gammad-rn).le.min(tol,tol*rn)) goto 80
        gammad=rn
        endif
C
        pn1=pn3
        pn2=pn4
        pn3=pn5
        pn4=pn6
        if(abs(pn5).ge.oflo) then
C
C          Re-scale terms in continued fraction if terms are large
C
        pn1=pn1/oflo
        pn2=pn2/oflo
        pn3=pn3/oflo
        pn4=pn4/oflo
        endif
        goto 60
80      arg=arg+log(gammad)
        gammad=one
        if(arg.ge.elimit) gammad=one-exp(arg)
        endif
C
        return
        end

real function alnorm(x,upper)
C
C      Algorithm AS 66 Appl. Statist. (1973) Vol. 22, p. 424
C
C      Evaluates the tail of the standardized normal curve
C      from x to infinity if .upper. is true or from minus
C      infinity to x if upper is .false.
C
        real ltone,utzero,zero,half,one,con,a1,a2,a3,a4,a5,a6,a7,
$      b1,b2,b3,b4,b5,b6,b7,b8,b9,b10,b11,b12,x,y,z,zexp
        logical upper,up
C
C      Ltone and utzero must be set to suit the particular computer
C      (See introductory text)
C
        data ltone,utzero/5.6e0, 1.2e1/
        data zero,half,one,con/ 0.0e0, 5.0e-1, 1.0e0, 1.28e0/
        data a1,a2,a3,a4,a5,a6,a7/ 3.98942280444e-1, 3.99903438504e-1,

```

```

$ 5.75885480458e0, 2.98213557808e1, 2.62433121679e0,
$ 4.86959930692e1, 5.92885724438e0/
data b1,b2,b3,b4,b5,b6,b7,b8,b9,b10,b11,b12/ 3.98942280385e-1,
$ 3.8052e-8, 1.00000615302e0, 3.98064794e-4, 1.98615381364e0,
$ 1.51679116635e-1, 5.29330324926e0, 4.8385912808e0,
$ 1.51508972451e1, 7.42380924027e-1, 3.0789933034e1,
$ 3.99019417011e0/
C
zexp(z)=exp(z)
C
up=upper
z=x
if(z.ge.zero) goto 10
up=.not. up
z=-z
10 if(z.le.ltone.or.up.and.z.le.utzero) goto 20
alnorm=zero
goto 40
20 y=half*z*z
if(z.gt.con) goto 30
C
alnorm=half-z*(a1-a2*y/(y+a3-a4/(y+a5+a6/(y+a7))))
goto 40
C
30 alnorm=b1*zexp(-y)/(z-b2+b3/(z+b4+b5/(z-b6+b7/
$ (z+b8-b9/(z+b10+b11/(z+b12))))))
C
40 if(.not.up) alnorm=one-alnorm
return
end
real function alogam(x,ifault)
C
Algorithm ACM 291, Comm. ACM. (1966) Vol. 9, p. 684
C
Evaluates Natural Logarithm of Gamma(x)
C
real a1,a2,a3,a4,a5,f,x,y,z,zlog,half,zero,one,seven
C
The Following Constants are Alog(2pi)/2,
C
1/1680, 1/1260, 1/360, and 1/12
C
data a1,a2,a3,a4,a5/ 9.18938533204673e-1, 5.95238095238e-4,
$ 7.93650793651e-4, 2.777777777778e-3,
$ 8.33333333333333e-2/
data half,zero,one,seven/ 0.5, 0.0, 1.0, 7.0/
C
zlog(f)=alog(f)
C
alogam=zero
ifault=1
if(x.le.zero) return
ifault=0
y=x
f=zero
if(y.ge.seven) goto 30
f=y
10 y=y+one
if(y.ge.seven) goto 20
f=f*y
goto 10
20 f=-zlog(f)

```

```
30  z=one/(y*y)
    alogam=f+(y-half)*zlog(y)-y+a1
    $ +((( -a2*z+a3)*z-a4)*z+a5)/y
    return
    end
```

ALGORITHM AS 285

-----

This file contains in order:

1. Some notes supplied by the author of the algorithm.
2. A MAKEFILE.
3. A driver program.
4. The algorithm.
5. User functions for various regions of integration - a cube, an ellipsoid, a rectangle, a sphere, a convex polynomial and a star shape.
6. The input data file FORT.1 needed by the driver program.

The sections are separated by the following:

C-----

1. Some notes supplied by the author of the algorithm.

The subroutines in this file compute the probability that a multivariate normal random vector falls within a prescribed region A. A is input to the program via a user-defined function subprogram.

The function should begin as follows:

```

real function f(n,v)
integer n
real v(n)

```

```

lines calculating f, which should take the value:
    = 0 if v is on the boundary of A
    < 0 if v is inside A
    > 0 if v is outside A

```

The following functions in this directory may be used to describe the boundary. Each must be altered to provide the specific boundary (or, the covariance matrix input into the driving program may be scaled appropriately).

- sphere      A is sphere of radius sqrt(radsq)
- cube        A is a cube with infinity-norm cubsz
- rect        x is in A if a(i) < x(i) < b(i) for all i
- ellipsoid   The boundary of A is x'ax + bx - c = 0
- convpoly    A is a convex polytope with faces described by the inequalities  
a(1,i)\*x(1) + a(2,i)\*x(2) +...+ a(n,i)\*x(n) <= 1  
for i=1,...,p.
- pentagram   A is a five-pointed star

Once an appropriate boundary function is selected or written, the program should be reloaded. This may be done quickly by editing the file "Makefile" so that the filename listed after "FNCN =" is the object file of the boundary function, e.g.

```
FNCN = sphere.o
```

To load the file, type

```
make FFLAGS=-O
```

and type

```
mulnor
```

to execute the program.

All input to the driving program should be in file fort.1, of the form

```
n          order of covariance matrix
stdev     desired standard deviation of estimate
rhigh    radius of sphere circumscribing region A
init      initial number of simulations to be run
ix,iy,iz  three integers between 1 and 50000 to initialize
          random normal generator
covar     lower triangle of the symmetric covariance matrix,
          stored row-wise as a one-dimensional array.
```

C-----

## 2. A MAKEFILE

```
FNCN = cube.o

MULNOR = mulnor.o chol.o zerovc.o chiprb.o orthp.o

RANDOM = rnortm.o normal.o alnorm.o random.o ppnd.o

AUX = drive.o tdiag.o lrvt.o

OBJECTS = $(MULNOR) $(RANDOM) $(AUX) $(FNCN)

mulnor: $(OBJECTS)
    f77 $(OBJECTS) -O0 -o mulnor

clean:
    rm *.o
```

C-----

## 3. A driver program.

```
C DRIVING PROGRAM
C
C REAL COVAR(1275),WORK(50,52),T(1275)
C INTEGER ISEED,N,IFault,J,IX,IY,IZ,ITER,INIT
C REAL F,SDEV,PROB,RHIGH,ETA
C COMMON /RAND/ IX,IY,IZ
C EXTERNAL F
C DATA ETA /1.0E-5/
C
C READ IN COVARIANCE AND INITIALIZE RANDOM NORMAL GENERATOR.
C
C With many Fortran compilers, you will need to insert a line such as:
C OPEN(1, file='FORT.1', status='old')
C before reading from unit 1.
C
C READ (1,*) N,SDEV,RHIGH,INIT,IX,IY,IZ
C READ (1,*) (COVAR(J),J=1,N*(N+1)/2)
C
```



```

C  FIND SMALLEST NONZERO EIGENVALUE OF COVARIANCE MATRIX
C
      NN = N*(N+1)/2
      CALL CHOL(COVAR,N,NN,T,NULLTY,IFAU)
      CALL TDIAG(N,ETA,COVAR,WORK(1,1),WORK(1,2),WORK(1,3),IFAU)
      CALL LRVT(N,ETA,WORK(1,1),WORK(1,2),WORK(1,3),IFAU)
      RHIGH = RHIGH/SQRT(WORK(NULLTY+1,1))
C
      CALL MULNOR(COVAR,N,F,SDEV,RHIGH,INIT,ISEED,T,WORK,PROB,
*      ITER,IFAU)
      PRINT *, 'ESTIMATED PROBABILITY IS', PROB,'WITH IFAULT = ',IFAU
      PRINT *, 'ITER = ',ITER
      STOP
      END

      SUBROUTINE TDIAG(N,TOL,A,D,E,Z,IFAU)
C
      REAL A(*),D(N),E(N),F,G,H,HH,TOL,Z(N,N),ZERO,
*      ONE,ZSQRT
      INTEGER I,J,K,L,N,IFAU,I1,J1
C
      DATA ZERO, ONE /0.0, 1.0/
C
      ZSQRT(H) = SQRT(H)
C
      IFAULT = 1
      IF (N .LE. 1) RETURN
      IFAULT = 0
      K = 0
      DO 10 I=1,N
      DO 10 J=1,I
      K = K+1
10     Z(I,J) = A(K)
      I=N
      DO 70 I1=2,N
      L = I-2
      F = Z(I,I-1)
      G=ZERO
      IF (L .LT. 1) GOTO 25
      DO 20 K=1,L
20     G=G+Z(I,K)**2
25     H=G+F*F
C
      IF (G .GT. TOL) GOTO 30
      E(I)=F
      D(I)=ZERO
      GOTO 65
30     L=L+1
      G=ZSQRT(H)
      IF (F .GE. ZERO) G=-G
      E(I) = G
      H = H-F*G
      Z(I,I-1)=F-G
      F=ZERO
      DO 50 J=1,L
      Z(J,I) = Z(I,J)/H
      G = ZERO
C
      DO 40 K=1,J
40     G = G+Z(J,K) *Z(I,K)
      IF (J .GE. L)GOTO 47

```

```

        J1 = J+1
        DO 45 K=J1,L
45      G=G + Z(K,J)*Z(I,K)
        C
47      E(J)=G/H
        F = F+G*Z(J,I)
50      CONTINUE
        C
        HH = F/(H+H)
        C
        DO 60 J=1,L
        F=Z(I,J)
        G=E(J)-HH*F
        E(J)=G
        DO 60 K=1,J
        Z(J,K) = Z(J,K) - F*E(K) - G*Z(I,K)
60      CONTINUE
        D(I)=H
65      I=I-1
70      CONTINUE
        D(1) = ZERO
        E(1) = ZERO
        C
        DO 110 I=1,N
        L=I-1
        IF (D(I) .EQ. ZERO .OR. L .EQ. 0) GO TO 100
        DO 90 J=1,L
        G=ZERO
        DO 80 K=1,L
80      G=G + Z(I,K)*Z(K,I)
        DO 90 K=1,L
        Z(K,J) = Z(K,J) - G*Z(K,I)
90      CONTINUE
100     D(I) = Z(I,I)
        Z(I,I) = ONE
        IF (L .EQ. 0) GO TO 110
        DO 105 J=1,L
        Z(I,J) = ZERO
        Z(J,I) = ZERO
105     CONTINUE
110     CONTINUE
        RETURN
        END

```

```

        SUBROUTINE LRVT(N,PRECIS,D,E,Z,IFAUULT)
        C
        REAL B,C,D(N),E(N),F,G,H,P,PR,PRECIS,R,S,
*          Z(N,N),ZERO,ONE,TWO,ZABS,ZSQRT
        INTEGER I,J,K,L,N,IFAUULT,MITS,N1,JJ,M1,M,I1
        C
        DATA MITS,ZERO,ONE,TWO /30,0.0,1.0,2.0/
        ZABS(B) = ABS(B)
        ZSQRT(B) = SQRT(B)
        C
        IFAUULT = 2
        IF (N .LE. 1) RETURN
        IFAUULT = 1
        N1 = N-1
        DO 10 I=2,N
10      E(I-1) = E(I)

```

```

      E(N) = ZERO
      B = ZERO
      F = ZERO
      DO 90 L=1,N
      JJ=0
      H = PRECIS * (ZABS(D(L)) + ZABS(E(L)))
      IF (B .LT. H) B = H
C
      DO 20 M1=L,N
      M=M1
      IF (ZABS(E(M)) .LE. B) GOTO 30
20    CONTINUE
30    IF (M .EQ. L) GOTO 85
40    IF (JJ .EQ. MITS) RETURN
      JJ = JJ+1
C
      P = (D(L+1) - D(L))/(TWO*E(L))
      R = ZSQRT(P*P + ONE)
      PR = P + R
      IF (P .LT. ZERO) PR = P - R
      H = D(L) - E(L)/PR
      DO 50 I=L,N
50    D(I) = D(I)-H
      F=F+H
C
      P=D(M)
      C=ONE
      S=ZERO
      M1=M-1
      I=M
      DO 80 I1=L,M1
      J=I
      I=I-1
      G=C*E(I)
      H=C*P
      IF(ZABS(P) .GE. ZABS(E(I))) GOTO 60
      C = P/E(I)
      R = ZSQRT(C*C+ONE)
      E(J) = S*E(I)*R
      S = ONE/R
      C = C/R
      GOTO 70
60    C=E(I)/P
      R=ZSQRT(C*C+ONE)
      E(J) = S*P*R
      S=C/R
      C=ONE/R
70    P=C*D(I)-S*G
      D(J)=H+S*(C*G+S*D(I))
C
      DO 80 K=1,N
      H=Z(K,J)
      Z(K,J)=S*Z(K,I) + C*H
      Z(K,I) = C*Z(K,I) - S*H
80    CONTINUE
      E(L)=S*P
      D(L)=C*P
      IF (ZABS(E(L)) .GT. B)GOTO 40
85    D(L) = D(L) + F
90    CONTINUE
C

```

```
      DO 120 I=1,N1
      K=I
      P=D(I)
      I1=I+1
      DO 100 J=I1,N
      IF (D(J) .GE. P) GOTO 100
      K=J
      P=D(J)
100    CONTINUE
      IF (K .EQ. I) GOTO 120
      D(K) = D(I)
      D(I) = P
      DO 110 J=1,N
      P=Z(J,I)
      Z(J,I)=Z(J,K)
      Z(J,K)=P
110    CONTINUE
120    CONTINUE
      IFAULT=0
      RETURN
      END
```

C-----

#### 4. The algorithm.

```
      SUBROUTINE MULNOR(COVAR,N,F,SDEV,RHIGH,INIT,ISEED,T,WORK,PROB,
*      ITER,IFAUULT)
C
C      ALGORITHM AS285 APPL. STATIST. (1993) VOL.42, NO.3
C
C      FINDS THE PROBABILITY THAT A NORMALLY DISTRIBUTED RANDOM
C      N-VECTOR WITH MEAN 0 AND COVARIANCE COVAR FALLS
C      IN AREA ENCLOSED BY THE EXTERNAL USER-DEFINED FUNCTION F.
C
      INTEGER N,ISEED,IFAUULT,INIT,INIT1,
*      K,II,KK,Q,ITER,NN,NULLTY,I,J,MAXITR
      REAL F,SDEV,RHIGH,PROB,P,VAR,ZERO,COX,
*      COVAR(*), WORK(N,*),T(*)
C
      EXTERNAL F
      DATA ZERO,MAXITR /0.0,10000/
C
      IFAUULT = 0
      INIT1 = INIT
      IF (INIT .LT. 25) INIT1 = 25
      IF (INIT .GT. 1000) INIT1 = 1000
      COX = 1.0 + 2.0/INIT1
C
C      FIND CHOLESKY DECOMPOSITION OF COVARIANCE MATRIX
C
      NN = N*(N+1)/2
      CALL CHOL(COVAR,N,NN,T,NULLTY,IFAUULT)
      Q = N - NULLTY
      IFAUULT = IFAUULT*IFAUULT
      IF (IFAUULT .NE. 0) RETURN
C
C      TRANSPOSE CHOLESKY FACTOR, OMITTING COLUMNS OF ZEROES.
C      RESULTING VECTOR IS PACKED FORM OF T'J,
C      WRITTEN ROWWISE BEGINNING WITH LAST ROW.
```

```
C
      DO 10 I = 1,N
      DO 10 J = 1,I
          WORK(J,I) = ZERO
10     CONTINUE
      II = 0
      DO 20 I = 1,N
      DO 20 J = 1,I
          II = II + 1
          WORK(I,J) = T(II)
20     CONTINUE
      J = 0
      DO 40 I = N,1,-1
          IF (J .EQ. NULLTY) GO TO 50
          IF (WORK(I,I) .EQ. ZERO) THEN
              J = J+1
              DO 30 K = I+1,N
              DO 30 KK = I, N-J
                  WORK(K,KK) = WORK(K,KK+1)
30         CONTINUE
          END IF
40     CONTINUE
50     CONTINUE
      K = 0
      DO 60 J = N,1,-1
      DO 60 I = 1,MIN0(J,Q)
          K = K + 1
          T(K) = WORK(J,I)
60     CONTINUE
C
C TAKE PILOT SAMPLE; ESTIMATE VARIANCE OF PROB FROM ORTHP.
C
      PROB = ZERO
      VAR = ZERO
      DO 70 K=1,INIT1
          CALL ORTHP(F,RHIGH,N,Q,T,WORK,P,ISEED,IFAU)
          IF (IFAU .NE. 0) RETURN
          PROB = PROB + P
          VAR = VAR + P*P
70     CONTINUE
      PROB = PROB/INIT1
      VAR = VAR/INIT1 - PROB*PROB
C
      ITER = INT(COX*VAR/(SDEV*SDEV)) + 1
      IF (ITER .GT. MAXITR) IFAU = 5
C
      DO 80 K=INIT1+1,ITER
          CALL ORTHP(F,RHIGH,N,Q,T,WORK,P,ISEED,IFAU)
          IF (IFAU .NE. 0) RETURN
          PROB = PROB + (P - PROB)/K
80     CONTINUE
C
      RETURN
      END

      SUBROUTINE CHOL(A,N,NN,U,NULLTY,IFAU)
      REAL A(NN),U(NN),ETA,ETA2,X,W,ZERO,ZABS,ZSQRT
      INTEGER N,NN,NULLTY,IFAU
      INTEGER J,K,II,ICOL,L,KK,M,IROW,I
C
      DATA ETA,ZERO /1.0E-05,0.0/
```

```
ZABS(X) = ABS(X)
ZSQRT(X) = SQRT(X)
```

C

```
IFAUULT = 1
IF (N .LE. 0) RETURN
IFAUULT = 3
IF (NN .NE. N*(N+1)/2) RETURN
IFAUULT = 2
NULLTY = 0
J = 1
K = 0
ETA2 = ETA*ETA
II = 0
DO 80 ICOL = 1,N
II = II + ICOL
X = ETA2 * A(II)
L = 0
KK = 0
DO 40 IROW = 1, ICOL
KK = KK + IROW
K = K+1
W = A(K)
M = J
DO 10 I = 1, IROW
L = L + 1
IF (I .EQ. IROW) GO TO 20
W = W - U(L) * U(M)
M = M + 1
10 CONTINUE
20 IF (IROW .EQ. ICOL) GO TO 50
IF (U(L) .EQ. ZERO) GO TO 30
U(K) = W / U(L)
GO TO 40
30 IF (W * W .GT. ZABS(X * A(KK))) RETURN
U(K) = ZERO
40 CONTINUE
50 IF (ZABS(W) .LE. ZABS(ETA * A(K))) GO TO 60
IF (W .LT. ZERO) RETURN
U(K) = ZSQRT(W)
GO TO 70
60 U(K) = ZERO
NULLTY = NULLTY + 1
70 J = J + ICOL
80 CONTINUE
IFAUULT = 0
RETURN
END
```

```
SUBROUTINE ORTHP(F,RHIGH,N,Q,T,Z,PROB,ISEED,IFAUULT)
```

C

C FINDS THE PSEUDO-MONTE CARLO ESTIMATE OF PROB USING AN  
C ORTHONORMAL SYSTEM OF VECTORS.

C

```
INTEGER N,ISEED,IFAUULT,Q,I,J,K,II,JP1,JP2
REAL T(*),RHIGH,Z(N,*),PROB,S,A,B,R,RT2RCP,ZERO,
* F,CHIPRB,FAB
```

C

```
EXTERNAL F
DATA ZERO,RT2RCP /0.0,0.707106781/
```

C

```
PROB = ZERO
```

```

      QP1 = Q+1
      QP2 = Q+2
C
C PUT RANDOMLY ORIENTED ORTHONORMAL SYSTEM OF Q-VECTORS IN Z.
C
      CALL RNORTM(N,Q, QP1, 1, 1, Z(1,QP1), 1, Z(1,QP1), ISEED, Z,
*      Z(1,QP1), FAB, Z(1,QP2), Z(1,QP2), IFAULT)
C
C REPLACE EACH COLUMN OF Z BY TRANS(CHOLESKY FACTOR)*J*COLUMN OF Z.
C
      DO 30 I=1,Q
        JJ = 0
        DO 20 J = N,1,-1
          S = ZERO
          DO 10 K=1,MIN0(J,Q)
            JJ = JJ + 1
            S = S + T(JJ)*Z(K,I)
10          CONTINUE
            Z(J,I) = S
20          CONTINUE
30          CONTINUE
C
C ESTIMATE THE PROBABILITY THAT N(0,COVAR) IS WITHIN THE
C BOUNDARY GIVEN BY F.
C
      DO 40 I = 1,Q
        A = ZERO
        B = RHIGH
        CALL ZEROVC (F,R,A,B,N,Z(1,I),Z(1,QP2),IFault)
        PROB = PROB - CHIPRB(R*R,Q)
40      CONTINUE
C
      DO 60 I = 1,Q
        A = ZERO
        B = RHIGH
        DO 50 K = 1,N
          Z(K,QP1) = -Z(K,I)
50          CONTINUE
          CALL ZEROVC (F,R,A,B,N,Z(1,QP1),Z(1,QP2),IFault)
          PROB = PROB - CHIPRB(R*R,Q)
60          CONTINUE
C
      DO 80 I = 1,Q-1
      DO 80 J = I+1,Q
      DO 80 JJ= -1,1,2
      DO 80 II = -1,1,2
        DO 70 K=1,N
          Z(K,QP1) = RT2RCP*(Z(K,I)*II + Z(K,J)*JJ)
70          CONTINUE
          A = ZERO
          B = RHIGH
          CALL ZEROVC (F,R,A,B,N,Z(1,QP1),Z(1,QP2),IFault)
          PROB = PROB - CHIPRB(R*R,Q)
80          CONTINUE
      PROB = PROB/(2.0*Q*Q) + 1.0
C
      RETURN
      END

```

```

SUBROUTINE RNORTM(LDA,N, NP1, IBCONF, NB, B, NDBI, DBI, ISEED, A,
* CHISQ, FAB, U, W, IFAULT)

```

```
C
C      ALGORITHM AS 127  APPL. STATIST.  (1978) VOL.27, NO.2
C
C      RNORMT GENERATES ORTHOGONAL MATRICES A FROM A DISTRIBUTION
C      WITH DENSITY FUNCTION DEFINED ON THE GROUP OF ORTHOGONAL
C      MATRICES.  WHEN THE INPUT PARAMETER IBCONF = 1 THE
C      MATRICES ARE GENERATED FROM THE INVARIANT HAAR MEASURE.
C
REAL B(NB), DBI(NDBI), A(LDA,N), CHISQ(N), U(NP1), W(N), FAB, UL,
*  WL, WIL, WWIL, T2, HV, HW, ZERO, ONE
INTEGER N, NP1, IBCONF, NB, NDBI, ISEED, IFAULT, I, J, IBSUB, L, NP1L
INTEGER LP1, LDA
C
DATA ZERO /0.0/, ONE /1.0/
C
C      STATEMENT FUNCTIONS FOR DOUBLE PRECISION
C      DOUBLE PRECISION SQRT, SIGN, ABS
C      SQRT(UL) = DSQRT(UL)
C      SIGN(UL, WL) = DSIGN(UL, WL)
C      ABS(UL) = DABS(UL)
C
C      SECTION 1 INITIALIZATION
C
C      IFAULT = 0
C      GO TO 4
C
C      ERROR RETURNS
C
C      IFAULT = 2
C      RETURN
C
C      INITIALIZE DENSITY, H(STORED IN A), AND IBSUB
C
C      4  FAB = ONE
C        DO 100 I=1,N
C          DO 50 J=1,N
C            50  A(I,J) = ZERO
C            A(I,I) = ONE
C          100  CONTINUE
C          IBSUB = 0
C
C      CONSTRUCT A ONE COLUMN AT A TIME
C
C      DO 315 L=1,N
C        NP1L = NP1 - L
C
C      SECTION 2
C      CONSTRUCT U(L..N) UNIFORMLY DISTRIBUTED ON THE SURFACE OF THE
C      (N+1-L)-SPHERE OF RADIUS UL = SQRT(CHISQ(L)).
C
C      CALL NORMAL(U(L),NP1L+1,ISEED, CHISQ(L))
C      UL = SQRT(CHISQ(L))
C      IF (UL .EQ. ZERO) GO TO 2
C      IF (L .EQ. N) GO TO 301
C
C      SECTION 3
C      CALCULATE W = B*U AND STORE ITS LENGTH IN WL.
C      SIGN OF WL PREVENTS LOSS OF SIGNIFICANCE IN WWIL.
C
C      B IS IDENTITY
C
```



```

        WL = SIGN(UL,-U(L))
        DO 219 J=L,N
219     W(J) = U(J)
C
C     SECTION 4
C     PROJECT W ONTO ORTHOGOANL COMPLEMENT OF FIRST L-1
C     COLUMNS OF A, NORMALIZE, AND STORE IN L COLUMN OF A.
C     A(L) = H(L) * W * WIL
C     CALCULATE PROJECTION MATRIX H(L) FOR ORTHOGOANL
C     COMPLEMENT OF FIRST L COLUMNS OF A AND STORE IN LAST
C     N-L COLUMNS OF A.
C
        LP1 = L+1
        WIL = ONE/WL
        WWIL = ONE/(WL - W(L))
        DO 250 I=1,N
        T2 = ZERO
        DO 230 J=L,N
230     T2 = T2 + A(I,J) * W(J)
        HV = T2 * WIL
        HW = (HV - A(I,L)) * WWIL
        A(I,L) = HV
        DO 240 J = LP1, N
240     A(I,J) = A(I,J) - HW*W(J)
250     CONTINUE
C
C     END OF L COLUMN OF MATRIX A
C
C     SECTION 5
C     WHEN L = N ONLY SIGN NEEDS TO BE CHOSEN
C     REMEMBER MATRIX H(N) IS STORED IN N COLUMN OF A.
C
301    IF (U(L) .GT. ZERO) GOTO 315
        DO 310 I=1,N
310    A(I,L) = -A(I,L)
C
C     FAB = ABS(B(LAST) * DBI(N)*FAB)
C
315    CONTINUE
320    FAB = ABS(FAB)
C
        RETURN
        END

        SUBROUTINE ZEROVC (F,R,R0,R1,N,V,Y,IFAU)
C
C     CALCULATES THE SOLUTION R TO F(R*V) = 0.
C
        INTEGER N,IFAU,I,J,NITER
        REAL F,R,R0,R1,ETA,V(N),Y(N),F0,F1,FR,HALF,ZABS,X
        EXTERNAL F
        DATA HALF, ETA /0.5,1.0E-05/ NITER /500/
        ZABS(X) = ABS(X)
C
        DO 10 I=1,N
            Y(I) = R0*V(I)
10     CONTINUE
        F0 = F(N,Y)
        DO 20 I=1,N
            Y(I) = R1*V(I)
20     CONTINUE

```

```

    F1 = F(N,Y)
    IF (SIGN(HALF,F1) .EQ. SIGN(HALF,F0)) THEN
        IFAULT = 3
        RETURN
    END IF
    DO 40 J = 1,NITER
        R = R1 - F1*(R1-R0)/(F1-F0)
        DO 30 I=1,N
            Y(I) = R*V(I)
30        CONTINUE
        FR = F(N,Y)
        IF (ZABS(R-R1) .LT. ETA) GO TO 50
        IF (SIGN(HALF,FR) .NE. SIGN(HALF,F1)) THEN
            R0=R1
            F0=F1
        ELSE
            F0 = F0 * HALF
        END IF
        R1 = R
        F1 = FR
40        CONTINUE
        IFAULT = 6
50        CONTINUE
        RETURN
    END

```

```

    REAL FUNCTION CHIPRB(X,DF)

```

```

C
C FINDS THE PROBABILITY THAT A CHI-SQUARED RANDOM VARIABLE
C WITH DF DEGREES OF FREEDOM EXCEEDS X.
C ADAPTED FROM HILL AND PIKE (1967) ALG. 299, CHI-SQUARED INTEGRAL,
C COMM. ACM, VOL.10, 243-244.
C

```

```

    REAL X,ZERFP1,ZSQRT,SQRT2,
*    A,SQRTA,Y,C,E,Z,S,BIG,SMALL,RTPIRP,ZERO,ONE,HALF,TWO
    INTEGER DF,ODD,N2,I
    REAL ALNORM

```

```

C    REAL ERF
C

```

```

    DATA RTPIRP /0.564189583547756/, SQRT2 /1.41421356237309/
    DATA BIG/88.03/,SMALL/-85.2/,ZERO/0.0/,ONE /1.0/,HALF/0.5/,
*    TWO /2.0/
    ZSQRT(A) = SQRT(A)
    ZERFP1(A) = TWO*ALNORM(SQRT2*A,.FALSE.)

```

```

C
C NOTE: IF THE FUNCTION "ERF" IS AVAILABLE, THE ABOVE STATEMENT
C FUNCTION MAY BE REPLACED BY
C    ZERFP1(A) = ERF(A) + ONE
C

```

```

    S = ZERO
    IF (X .GT. BIG) GO TO 50
    S = ONE
    IF (X .LT. SMALL) GO TO 50

```

```

C
    A = HALF*X
    Y = EXP(-A)
    ODD = MOD(DF,2)
    IF (ODD .EQ. 0) THEN
        S = Y
        E = ONE
        Z = ZERO

```

```

        ELSE
            SQRTA = ZSQRT(A)
            S = ZERFP1(-SQRTA)
            E = RTPIRP/SQRTA
            Z = -HALF
        END IF
        IF (DF .LT. 3) GO TO 50
C
        N2 = DF/2 - 1 + ODD
        C = ZERO
        DO 40 I = 1,N2
            Z = Z + 1
            E = E*(A/Z)
            C = C + E
40        CONTINUE
            S = S + C*Y
C
50        CONTINUE
        CHIPRB = S
        END

        SUBROUTINE NORMAL(U,NP1,ISEED, CHISQ)
C
C GENERATES AN (NP1-1)-VECTOR OF INDEPENDENT NORMAL VARIATES IN U.
C ON OUTPUT, CHISQ CONTAINS THE SQUARED LENGTH OF THE VECTOR.
C
        REAL U(NP1)
        INTEGER ISEED,NP1,I,IFAUULT,IX,IY,IZ
        REAL RANDOM,PPND,CHISQ,ZERO
C
        COMMON /RAND/ IX,IY,IZ
        DATA ZERO /0.0/
C
        CHISQ = ZERO
        DO 10 I = 1, NP1-1
            U(I) = PPND(RANDOM(ISEED),IFAUULT)
            CHISQ = CHISQ + U(I)*U(I)
10        CONTINUE
            RETURN
            END

        REAL FUNCTION PPND(P, IFAUULT)
C
C ALGORITHM AS 111 APPL. STATIST. (1977), VOL.26, NO.1
C
C PRODUCES NORMAL DEVIATE CORRESPONDING TO LOWER TAIL AREA OF P
C REAL VERSION FOR EPS = 2 **(-31)
C THE HASH SUMS ARE THE SUMS OF THE MODULI OF THE COEFFICIENTS
C THEY HAVE NO INHERENT MEANINGS BUT ARE INCLUDED FOR USE IN
C CHECKING TRANSCRIPTIONS
C STANDARD FUNCTIONS ABS, ALOG AND SQRT ARE USED
C
        REAL ZERO, SPLIT, HALF, ONE
        REAL A0, A1, A2, A3, B1, B2, B3, B4, C0, C1, C2, C3, D1, D2
        REAL P, Q, R
        INTEGER IFAUULT
        DATA ZERO /0.0E0/, HALF/0.5E0/, ONE/1.0E0/
        DATA SPLIT /0.42E0/
        DATA A0 / 2.50662823884E0/
        DATA A1 / -18.61500062529E0/
        DATA A2 / 41.39119773534E0/
    
```

```
DATA A3 / -25.44106049637E0/  
DATA B1 / -8.47351093090E0/  
DATA B2 / 23.08336743743E0/  
DATA B3 / -21.06224101826E0/  
DATA B4 / 3.13082909833E0/  
DATA C0 / -2.78718931138E0/  
DATA C1 / -2.29796479134E0/  
DATA C2 / 4.85014127135E0/  
DATA C3 / 2.32121276858E0/  
DATA D1 / 3.54388924762E0/  
DATA D2 / 1.63706781897E0/
```

C

```
IF AULT = 0  
Q = P - HALF  
IF (ABS(Q) .GT. SPLIT) GOTO 1  
R = Q*Q  
PPND = Q * (((A3*R + A2)*R + A1) * R + A0) /  
* (((B4*R + B3)*R + B2) * R + B1) * R + ONE)  
RETURN
```

1

```
R = P  
IF (Q .GT. ZERO) R = ONE - P  
IF (R .LE. ZERO) GOTO 2  
R = SQRT(-ALOG(R))  
PPND = ((C3 * R + C2) * R + C1) * R + C0 /  
* ((D2*R + D1) * R + ONE)  
IF (Q .LT. ZERO) PPND = -PPND  
RETURN
```

2

```
IF AULT = 1  
PPND = ZERO  
RETURN  
END
```

```
REAL FUNCTION RANDOM(L)
```

C

C ALGORITHM AS 183 APPL. STATIST. (1982) VOL. 31, NO. 2

C

C RETURNS A PSEUDO-RANDOM NUMBER RECTANGULARLY DISTRIBUTED  
C BETWEEN 0 AND 1.

C

C IX, IY, AND IZ SHOULD BE SET TO INTEGER VALUES BETWEEN  
C 1 AND 30000 BEFORE FIRST ENTRY

C

C INTEGER ARITHMETIC UP TO 30323 IS REQUIRED

C

```
INTEGER IX, IY, IZ, L  
COMMON /RAND/ IX,IY,IZ  
IX = 171 * MOD(IX, 177) - 2 * (IX / 177)  
IY = 172 * MOD(IY, 176) - 35 * (IY / 176)  
IZ = 170 * MOD(IZ,178) - 63 * (IZ / 178)
```

C

```
IF (IX .LT. 0) IX = IX + 30269  
IF (IY .LT. 0) IY = IY + 30307  
IF (IZ .LT. 0) IZ = IZ + 30323
```

C

```
RANDOM = MOD(FLOAT(IX) / 30269.0 + FLOAT(IY) / 30307.0 +  
* FLOAT(IZ) / 30323.0, 1.0)  
RETURN  
END
```

```
REAL FUNCTION ALNORM(X,UPPER)
```

C

```

C ALGORITHM AS 66 APPL. STATIST. (1973) VOL. 22, NO. 3
C
C EVALUATES THE TAIL AREA OF THE STANDARDIZED NORMAL CURVE
C FROM X TO INFINITY IF UPPER IS .TRUE. OR
C FROM MINUS INFINITY TO X IF UPPER IS .FALSE.
C
      REAL LTONE, UTZERO, ZERO, HALF, ONE, CON, Z, Y, X
      LOGICAL UPPER, UP
C
C LTONE AND UTZERO MUST BE SET TO SUIT THE PARTICULAR COMPUTER
C (SEE INTRODUCTORY TEXT)
C
      DATA LTONE, UTZERO /7.0, 18.66/
      DATA ZERO, HALF, ONE, CON /0.0,0.5,1.0,1.28/
      UP = UPPER
      Z = X
      IF (Z .GE. ZERO) GOTO 10
      UP = .NOT. UP
      Z = -Z
10    IF (Z .LE. LTONE .OR. UP .AND. Z .LE. UTZERO) GOTO 20
      ALNORM = ZERO
      GOTO 40
20    Y = HALF *Z * Z
      IF (Z .GT. CON) GOTO 30
C
      ALNORM = HALF - Z*(0.398942280444 - 0.399903438504 * Y /
1    (Y + 5.75885480458 - 29.8213557808 /
2    (Y + 2.62433121679 + 48.6959930692 /
3    (Y + 5.92885724438))))
      GO TO 40
C
30    ALNORM = 0.398942280385 * EXP(-Y) /
1    (Z - 3.8052E-08 + 1.00000615302 /
2    (Z + 3.98064794E-4 + 1.98615381364 /
3    (Z - 0.151679116635 + 5.29330324926 /
4    (Z + 4.8385912808 - 15.1508972451 /
5    (Z + 0.742380924027 + 30.789933034 / (Z + 3.99019417011))))))
C
40    IF (.NOT. UP) ALNORM = ONE - ALNORM
      RETURN
      END

```

C-----

5. Various user functions for different shapes of region of integration.

```

      REAL FUNCTION F(N,V)
      REAL V(N),CUBSZ
      INTEGER N,I
      DATA CUBSZ /3.00/
C
C BOUNDARY OF REGION IS AN N-DIMENSIONAL CUBE.
C CUBSZ IS THE DISTANCE FROM THE ORIGIN TO THE SIDE OF THE CUBE
C
      F = 0.0
      DO 20 I = 1,N
      F = AMAX1(F,ABS(V(I)))
20    CONTINUE
      F = F - CUBSZ
      RETURN
      END

```

```

REAL FUNCTION F(N,V)
REAL V(N)
INTEGER N
REAL A(200),B(10),C
INTEGER I,J,K
C
C THE BOUNDARY IS AN ELLIPSOID OF THE FORM X'AX + BX + C = 0
C THE UPPER TRIANGLE OF A IS STORED COLUMN-WISE IN PACKED FORM.
C IN THIS EXAMPLE, A = INVERSE (1 .3), B = 0, C = -1.
C                               (.3 1)
C
DATA A(1),A(2),A(3) /1.0989011,-.32967033,1.0989011/
*   B(1),B(2) /0.0,0.0/ C /-1.0/
C
F = C
K = 0
DO 20 I = 1,N
K = K + 1
F = F + (V(I)**2)*A(K)
DO 10 J = I+1,N
K = K + 1
F = F + 2.0*V(I)*V(J)*A(K)
10 CONTINUE
20 CONTINUE
DO 30 I = 1,N
F = F + B(I)*V(I)
30 CONTINUE
RETURN
END

```

```

REAL FUNCTION F(N,V)
REAL V(N)
INTEGER N,I
REAL TEMP,A(30),B(30)
C
C RECTANGLE IS GIVEN BY A < V < B FOR EACH COORDINATE.
C THIS SUBROUTINE MAY ALSO BE USED TO CALCULATE THE
C CDF BY MAKING THE APPROPRIATE SIDES OF THE RECTANGLE
C SUFFICIENTLY LARGE.
C THIS EXAMPLE IS THE FOUR-DIMENSIONAL RECTANGLE DEFINED
C BY -INFINITY (ALMOST) < V(I) < 2 FOR EACH I.
C
DATA A(1),A(2),A(3),A(4)
* /-20.0,-20.0,-20.0,-20.0/,
*   B(1),B(2),B(3),B(4)
* /2.0,2.0,2.0,2.0/
C
F = -1.0
DO 10 I=1,N
IF (V(I) .GT. 0.0) THEN
TEMP = V(I) - B(I)
ELSE
TEMP = A(I) - V(I)
END IF
F = AMAX1(F,TEMP)
10 CONTINUE
RETURN
END

```

```

REAL FUNCTION F(N,V)
REAL V(N),RADSQ
INTEGER N,I
DATA RADSQ /4.0/
C
C BOUNDARY IS SPHERE OF RADIUS SQRT(RADSQ).
C
    F = 0.0
    DO 20 I = 1,N
    F = F + V(I)*V(I)
20 CONTINUE
    F = F - RADSQ
    RETURN
    END

REAL FUNCTION F(N,V)
REAL V(N)
INTEGER N
INTEGER I,J,P
REAL TEMP, A(2,6)
C
C A CONVEX POLYTOPE WITH P FACES IS DEFINED BY THE INEQUALITIES
C  $A(1,I)*V(1) + A(2,I)*V(2) + \dots + A(N,I)*V(N) \leq 1$ 
C FOR  $I=1, \dots, P$ .
C
C THE FIGURE IN THIS DEMONSTRATION PROGRAM IS THE
C REGULAR PENTAGON WITH DISTANCE FROM CENTER TO POINT = 1.
C
    DATA P/5/
    *      A(1,1),A(2,1) /0.726542528, -1.0/
    *      A(1,2),A(2,2) /1.175570504, 0.381966011/
    *      A(1,3),A(2,3) /0.0, 1.236067978/
    *      A(1,4),A(2,4) /-0.726542528, -1.0/
    *      A(1,5),A(2,5) /-1.175570504, 0.381966011/
C
    F = -1.0
    DO 10 J=1,N
        F = F + A(J,1)*V(J)
10 CONTINUE
    DO 30 I=2,P
        TEMP = -1.0
        DO 20 J=1,N
            TEMP = TEMP + A(J,I)*V(J)
20 CONTINUE
        F = AMAX1(F,TEMP)
30 CONTINUE
    RETURN
    END

REAL FUNCTION F(N,V)
REAL V(N)
INTEGER I,J,P,INDEX,N
REAL A(2,6),TANG(5),X(2),TANGNT
C
C THE FIGURE IN THIS DEMONSTRATION PROGRAM IS THE
C REGULAR PENTAGRAM WITH DISTANCE FROM CENTER TO POINT = 2.618.
C

```

```

DATA P/5/
*      A(1,3),A(2,3) /0.726542528, -1.0/
*      A(1,2),A(2,2) /1.175570504, 0.381966011/
*      A(1,4),A(2,4) /0.0, 1.236067978/
*      A(1,1),A(2,1) /-0.726542528, -1.0/
*      A(1,5),A(2,5) /1.175570504, 0.381966011/
*      TANG(1) / -1.376381921/
*      TANG(2) / -0.3249196962329/
*      TANG(3) / 0.3249196962329/
*      TANG(4) / 1.376381921/

```

C

```

X(1) = ABS(V(1))
X(2) = V(2)
INDEX = P
IF (X(1) .EQ. 0.0) THEN
  INDEX = 3
ELSE
  TANGNT = X(2)/X(1)
  DO 10 I=1,P
    IF (TANGNT .LE. TANG(I)) THEN
      INDEX = I
      GO TO 20
    END IF
10  CONTINUE
20  CONTINUE
  END IF
  F = -1.0
  DO 30 J=1,2
    F = F + A(J,INDEX)*X(J)
30  CONTINUE
  RETURN
  END

```

C-----

6. The data input file FORT.1 needed by the driver program.

```

7  .0005  107.0  100  81501  19837  39470
1
0
1
0
0
1
0
0
0
1
0
0
0
0
1
0
0
0
0
0
1
0
0
0
1
0

```



















































```
C
C Park Reilly
C
C 1. EVM.FOR, THE GENERAL ALGORITHM
C
      SUBROUTINE EVM(B,BV,DATA,EST,F,G1,G2,G3,H,IFAULT,
*   NDAT,NEQ,NPAR,NVAR,PHI,Q1,Q2,RESID,S,T,THETA,V,XI,Z)
C
C PARAMETER ESTIMATION FOR THE ERROR-IN-VARIABLES MODEL
C
      REAL B(NEQ,NVAR), BV(NEQ,NVAR), CRIT1, DATA(NDAT,NVAR),
*   EST(NDAT,NVAR), F(NEQ), G1(NPAR,NPAR), G2(NPAR,NPAR),
*   G3(NPAR,NPAR), H(NEQ), ONE, PHI, Q1(NPAR), Q2(NPAR),
*   RESID(NDAT,NVAR), S(NEQ,NEQ), T(NEQ), THETA(NPAR),
*   V(NVAR,NVAR), WDIFF, W1, W2, XI(NVAR), Z(NEQ,NPAR), ZERO
      DIMENSION IFAULT(2)
      PARAMETER (CRIT1=1.E-6, NITER1=50, ZERO=0.E0, ONE=1.E0)
      IFAULT(1) = 0
      IFAULT(2) = 0
      DO 4 ITER = 1,NITER1
C
C EACH PASS THROUGH THIS LOOP PERFORMS A SINGLE OUTER ITERATION
C
      CALL INNER(B,BV,DATA,EST,F,G1,H,IFAULT,NDAT,
*   NEQ,NPAR,NVAR,PHI,Q1,RESID,S,T,THETA,V,XI,Z)
C
C PUT Q1 INTO Q2 AND G1 INTO G2
C
      DO 2 IPAR1 = 1,NPAR
        Q2(IPAR1) = Q1(IPAR1)
        DO 1 IPAR2 = IPAR1,NPAR
1          G2(IPAR1,IPAR2) = G1(IPAR1,IPAR2)
2        CONTINUE
C
C CALCULATE CORRECTION FOR THETA
C
      CALL CHOL(G2,Q2,NPAR)
      CALL BKSUB(G2,Q2,1,NPAR,1)
C
C CHECK FOR CONVERGENCE
C
      WDIFF = ZERO
      DO 3 IPAR = 1,NPAR
        W1 = Q2(IPAR)
        W2 = THETA(IPAR)
        WDIFF = MAX(WDIFF,ABS(W1/W2))
        THETA(IPAR) = W2-W1
3      CONTINUE
      IF(WDIFF.LE.CRIT1)GO TO 5
4      CONTINUE
      IFAULT(1) = 1
C
C FILL LOWER TRIANGLE OF G1 AND PREPARE G2
C FOR THE INVERSION OF G1
C
5      DO 7 IPAR1 = 1,NPAR
        DO 6 IPAR2 = IPAR1,NPAR
          W1 = G1(IPAR1,IPAR2)
          G1(IPAR2,IPAR1) = W1
```

```
        G2(IPAR1,IPAR2) = W1
        G3(IPAR1,IPAR2) = ZERO
6      CONTINUE
7      CONTINUE
C
C INVERT G1 INTO G3
C
      CALL CHOL(G2,Q2,NPAR)
      DO 8 IPAR1 = 1,NPAR
8      G3(IPAR1,IPAR1) = ONE/G2(IPAR1,IPAR1)
      CALL BKSUB(G2,G3,NPAR,NPAR,3)
      RETURN
      END

      SUBROUTINE INNER(B,BV,DATA,EST,F,G1,H,IFAULT,NDAT,NEQ,
*      NPAR,NVAR,PHI,Q1,RESID,S,T,THETA,V,XI,Z)
      REAL B(NEQ,NVAR), BV(NEQ,NVAR), CRIT2, DATA(NDAT,NVAR),
* EST(NDAT,NVAR), F(NEQ), G1(NPAR,NPAR), H(NEQ), HALF,
* PHI, Q1(NPAR), RESID(NDAT,NVAR), S(NEQ,NEQ),
* T(NEQ), THETA(NPAR),
* V(NVAR,NVAR), WDIFF, W1, XI(NVAR), Z(NEQ,NPAR), ZERO
      DIMENSION IFAULT(2)
      PARAMETER (CRIT2=1.E-6, HALF=.5E0, NITER2=20, ZERO=0.E0)
C
C INITIALIZE PHI, Q1, AND G1
C
      PHI = ZERO
      DO 2 IPAR1 = 1,NPAR
        Q1(IPAR1) = ZERO
        DO 1 IPAR2 = IPAR1,NPAR
1        G1(IPAR1,IPAR2) = ZERO
2      CONTINUE
C
C PERFORM INNER ITERATION TO CONVERGENCE FOR EACH IDAT
C
      DO 24 IDAT = 1,NDAT
        DO 3 IVAR1 = 1,NVAR
3        XI(IVAR1) = DATA(IDAT,IVAR1)
        DO 16 ITER = 1,NITER2
C
C THIS LOOP PERFORMS A SINGLE INNER ITERATION
C
          WDIFF = ZERO
          CALL BF(B,F,THETA,XI)
C
C CALCULATE BV
C
          DO 6 IEQ1 = 1,NEQ
            DO 5 IVAR1 = 1,NVAR
              W1 = ZERO
              DO 4 IVAR2 = 1,NVAR
4              W1 = W1 + B(IEQ1,IVAR2)*V(IVAR1,IVAR2)
              BV(IEQ1,IVAR1) = W1
5              CONTINUE
6              CONTINUE
C
C CALCULATE BVB' AND STORE IT IN S
C
          DO 9 IEQ1 = 1,NEQ
            DO 8 IEQ2 = IEQ1,NEQ
```



```

        W1 = ZERO
        DO 7 IVAR1 = 1,NVAR
7          W1 = W1 + BV(IEQ1,IVAR1)*B(IEQ2,IVAR1)
          S(IEQ1,IEQ2) = W1
8          CONTINUE
9          CONTINUE
C
C PUT F+B(X-XI) INTO H
C
        DO 11 IEQ1 = 1,NEQ
          W1 = F(IEQ1)
          DO 10 IVAR1 = 1,NVAR
10         W1 = W1 + B(IEQ1,IVAR1)*(DATA(IDAT,IVAR1)-XI(IVAR1))
          H(IEQ1) = W1
11        CONTINUE
C
C REPLACE S BY ITS TRIANGULAR FACTORIZATION
C AND SOLVE ST = H FOR T
C
        CALL CHOL(S,H,NEQ)
        DO 13 IEQ1 = 1,NEQ
          T(IEQ1) = H(IEQ1)
          DO 12 IEQ2 = IEQ1,NEQ
12         S(IEQ2,IEQ1) = S(IEQ1,IEQ2)
13        CONTINUE
        CALL BKSUB(S,T,1,NEQ,1)
C
C CALCULATE NEW XI AND PUT RELATIVE CHANGE IN XI INTO WDIFF
C
        DO 15 IVAR1 = 1,NVAR
          W1 = DATA(IDAT,IVAR1)
          DO 14 IEQ1 = 1,NEQ
14         W1 = W1 - BV(IEQ1,IVAR1)*T(IEQ1)
          WDIFF = MAX(WDIFF, ABS((W1-XI(IVAR1))/W1))
          XI(IVAR1) = W1
15        CONTINUE
C
C CHECK FOR CONVERGENCE
C
        IF(WDIFF.LE.CRIT2)GO TO 17
16        CONTINUE
        IFAULT(2) = 1
C
C ACCUMULATE PHI
C
17        DO 18 IEQ1 = 1,NEQ
18        PHI = PHI + H(IEQ1)**2
C
C CALCULATE FITTED VALUES AND RESIDUALS
C
        DO 19 IVAR1 = 1,NVAR
          W1 = XI(IVAR1)
          EST(IDAT,IVAR1) = W1
          RESID(IDAT,IVAR1) = DATA(IDAT,IVAR1)-W1
19        CONTINUE
C
C CALCULATE CONTRIBUTIONS TO Q1 AND G1 AND COMPLETE THE LOOPS
C
        CALL ZED(B,F,THETA,XI,Z)
        CALL BKSUB(S,Z,NPAR,NEQ,2)
        DO 23 IPAR1 = 1,NPAR

```

```
      W1 = Q1(IPAR1)
      DO 20 IEQ1 = 1,NEQ
20      W1 = W1 + Z(IEQ1,IPAR1)*H(IEQ1)
      Q1(IPAR1) = W1
      DO 22 IPAR2 = IPAR1,NPAR
      W1 = G1(IPAR1,IPAR2)
      DO 21 IEQ1 = 1,NEQ
21      W1 = W1 + Z(IEQ1,IPAR1)*Z(IEQ1,IPAR2)
      G1(IPAR1,IPAR2) = W1
22      CONTINUE
23      CONTINUE
24      CONTINUE
      PHI = PHI*HALF
      RETURN
      END
```

SUBROUTINE CHOL(A,B,N)

```
C
C PERFORM CHOLESKY DECOMPOSITION OF A AND PRELIMINARY TREATMENT OF B
C
```

```
      REAL A(N,N),B(N),W1,W2
      DO 5 IR1 = 1,N
      W1 = A(IR1,IR1)
      DO 1 IR2 = 1,IR1-1
1      W1 = W1 - A(IR2,IR1)**2
      W1 = SQRT(W1)
      A(IR1,IR1) = W1
      DO 3 IC1 = IR1+1,N
      W2 = A(IR1,IC1)
      DO 2 IR2 = 1,IR1-1
2      W2 = W2 - A(IR2,IR1)*A(IR2,IC1)
      A(IR1,IC1) = W2/W1
3      CONTINUE
      W2 = B(IR1)
      DO 4 IR2 = 1,IR1-1
4      W2 = W2 - A(IR2,IR1)*B(IR2)
      B(IR1) = W2/W1
5      CONTINUE
      RETURN
      END
```

SUBROUTINE BKSUB(A,B,M,N,JOB)

```
C
C PERFORM BACK-SOLUTION ACCORDING AS JOB = 1, 2, OR 3
C
```

```
      REAL A(N,N),B(N,M),W1
      DO 3 IC1 = M,1,-1
      IF(JOB.EQ.2) THEN
      K1 = 1
      K2 = N
      K3 = 1
      ELSE
      K2 = 1
      K3 = -1
      IF(JOB.EQ.1) THEN
      K1 = N
      ELSE
      K1 = IC1
      END IF
```

```

        END IF
        DO 2 IR1 = K1,K2,K3
            W1 = B(IR1,IC1)
            IF (JOB.EQ.2) THEN
                K2 = IR1-1
            ELSE
                K1 = N
                K2 = IR1+1
            END IF
            DO 1 IR2 = K1,K2,K3
1          W1 = W1 - A(IR1,IR2)*B(IR2,IC1)
            B(IR1,IC1) = W1/A(IR1,IR1)
            IF(JOB.EQ.3) B(IC1,IR1) = B(IR1,IC1)
2          CONTINUE
3          CONTINUE
        RETURN
    END

```

C-----

C  
C 2. EVMS.FOR, THE SPECIAL FORM FOR ONLY ONE FUNCTIONAL EQUATION

```

        SUBROUTINE EVMS(BS,BVS,DATA,EST,G1,G2,G3,IFAU,LT,
*          NDAT,NPAR,NVAR,PHI,Q1,Q2,RESID,THETA,V,XI,ZS)
C
C PARAMETER ESTIMATION FOR THE ERROR-IN-VARIABLES MODEL WITH M = 1
C 91/3/21 PMR
C
        REAL BS(NVAR), BVS(NVAR), BVB, CRIT1, DATA(NDAT,NVAR),
* EST(NDAT,NVAR), FS, G1(NPAR,NPAR), G2(NPAR,NPAR),
* G3(NPAR,NPAR), HS, ONE, PHI, Q1(NPAR), Q2(NPAR),
* RESID(NDAT,NVAR), THETA(NPAR),
* V(NVAR,NVAR), WDIFF, W1, W2, XI(NVAR), ZS(NPAR), ZERO
        DIMENSION IFAULT(2)
        PARAMETER (CRIT1=1.E-6, NITER1=50, ONE=1.E0, ZERO=0.E0)
C
        IFAULT(1) = 0
        IFAULT(2) = 0
        DO 4 ITER = 1,NITER1
C
C EACH PASS THROUGH THIS LOOP PERFORMS A SINGLE OUTER ITERATION
C
        CALL INNERS(BS,BVS,DATA,EST,G1,IFAU,LT,NDAT,
*          NPAR,NVAR,PHI,Q1,RESID,THETA,V,XI,ZS)
C
C PUT Q1 INTO Q2 AND G1 INTO G2
C
        DO 2 IPAR1 = 1,NPAR
            Q2(IPAR1) = Q1(IPAR1)
            DO 1 IPAR2 = IPAR1,NPAR
1          G2(IPAR1,IPAR2) = G1(IPAR1,IPAR2)
2          CONTINUE
C
C CALCULATE CORRECTION FOR THETA
C
        CALL CHOL(G2,Q2,NPAR)
        CALL BKSUB(G2,Q2,1,NPAR,1)
C
C CHECK FOR CONVERGENCE
C
        WDIFF = ZERO

```

```
      DO 3 IPAR = 1,NPAR
        W1 = Q2(IPAR)
        W2 = THETA(IPAR)
        WDIFF = MAX(WDIFF,ABS(W1/W2))
        THETA(IPAR) = W2-W1
3      CONTINUE
      IF(WDIFF.LE.CRIT1) GO TO 5
4      CONTINUE
      IFAULT(1) = 1
C
C FILL LOWER TRIANGLE OF G1 AND PREPARE G2 FOR THE INVERSION OF G1
C
5      DO 7 IPAR1 = 1,NPAR
        DO 6 IPAR2 = IPAR1,NPAR
          W1 = G1(IPAR1,IPAR2)
          G1(IPAR2,IPAR1) = W1
          G2(IPAR1,IPAR2) = W1
          G3(IPAR1,IPAR2) = ZERO
6        CONTINUE
7      CONTINUE
C
C INVERT G1 INTO G3
C
      CALL CHOL(G2,Q2,NPAR)
      DO 8 IPAR1 = 1,NPAR
8      G3(IPAR1,IPAR1) = ONE/G2(IPAR1,IPAR1)
      CALL BKSUB(G2,G3,NPAR,NPAR,3)
      RETURN
      END

      SUBROUTINE INNERS(BS,BVS,DATA,EST,G1,IFAU,NDAT,
*      NPAR,NVAR,PHI,Q1,RESID,THETA,V,XI,ZS)
C
C INNER ITERATION FOR M = 1
C
      REAL BS(NVAR),BVS(NVAR),BVB,CRIT2,DATA(NDAT,NVAR),
* EST(NDAT,NVAR),FS,HALF,G1(NPAR,NPAR),HS,
* PHI,Q1(NPAR),RESID(NDAT,NVAR),THETA(NPAR),
* V(NVAR,NVAR),WDIFF,W1,XI(NVAR),ZS(NPAR),ZERO
      DIMENSION IFAU(2)
      PARAMETER (CRIT2=1.E-5, HALF=.5E0, NITER2=15, ZERO=0.E0)
C
C INITIALIZE PHI, Q1, AND G1
C
      PHI = ZERO
      DO 2 IPAR1 = 1,NPAR
        Q1(IPAR1) = ZERO
        DO 1 IPAR2 = IPAR1,NPAR
1        G1(IPAR1,IPAR2) = ZERO
2      CONTINUE
C
C PERFORM INNER ITERATION TO CONVERGENCE FOR EACH IDAT
C
      DO 14 IDAT = 1,NDAT
C
C INITIALIZE XI
C
      DO 3 IVAR1 = 1,NVAR
3      XI(IVAR1) = DATA(IDAT,IVAR1)
      DO 9 ITER = 1,NITER2
```

```
C
C THIS LOOP PERFORMS A SINGLE INNER ITERATION
C
      WDIFF = ZERO
      CALL BF(BS,FS,THETA,XI)
C
C CALCULATE BVS
C
      DO 5 IVAR1 = 1,NVAR
        W1 = ZERO
        DO 4 IVAR2 = 1,NVAR
4          W1 = W1 + BS(IVAR2)*V(IVAR1,IVAR2)

          BVS(IVAR1) = W1
5        CONTINUE
C
C CALCULATE BVB
C
      BVB = ZERO
      DO 6 IVAR1 = 1,NVAR
6        BVB = BVB + BVS(IVAR1)*BS(IVAR1)
C
C PUT F+B(X-XI) INTO HS
C
      HS = FS
      DO 7 IVAR1 = 1,NVAR
7        HS = HS + BS(IVAR1)*(DATA(IDAT,IVAR1)-XI(IVAR1))
C
C CALCULATE NEW XI AND PUT RELATIVE CHANGE IN XI INTO WDIFF
C
      DO 8 IVAR1 = 1,NVAR
        W1 = DATA(IDAT,IVAR1) - BVS(IVAR1)*HS/BVB
        WDIFF = MAX(WDIFF, ABS((W1-XI(IVAR1))/W1))
        XI(IVAR1) = W1
8      CONTINUE
C
C CHECK FOR CONVERGENCE
C
      IF(WDIFF.LE.CRIT2) GO TO 10
9    CONTINUE
      IFAULT(2) = 1
C
C ACCUMULATE PHI
C
10   PHI = PHI+HS*HS/BVB
C
C CALCULATE FITTED VALUES AND RESIDUALS
C
      DO 11 IVAR1 = 1,NVAR
        W1 = XI(IVAR1)
        EST(IDAT,IVAR1) = W1
        RESID(IDAT,IVAR1) = DATA(IDAT,IVAR1) - W1
11  CONTINUE
C
C CALCULATE CONTRIBUTIONS TO Q1 AND G1 AND COMPLETE THE LOOPS
C
      CALL ZED(BS,FS,THETA,XI,ZS)
      DO 13 IPAR1 = 1,NPAR
        W1 = ZS(IPAR1)
        Q1(IPAR1) = Q1(IPAR1) + W1*HS/BVB
      DO 12 IPAR2 = IPAR1,NPAR
```

```
12      G1(IPAR1,IPAR2) = G1(IPAR1,IPAR2) + W1*ZS(IPAR2)/BVB
13      CONTINUE
14      CONTINUE
      PHI = PHI*HALF
      RETURN
      END
```

SUBROUTINE CHOL(A,B,N)

```
C
C PERFORM CHOLESKY DECOMPOSITION OF A AND PRELIMINARY TREATMENT
C OF B
C
```

```
      REAL A(N,N),B(N),W1,W2
      DO 5 IR1 = 1,N
        W1 = A(IR1,IR1)
        DO 1 IR2 = 1,IR1-1
1       W1 = W1 - A(IR2,IR1)**2
        W1 = SQRT(W1)
        A(IR1,IR1) = W1
        DO 3 IC1 = IR1+1,N
          W2 = A(IR1,IC1)
          DO 2 IR2 = 1,IR1-1
2         W2 = W2 - A(IR2,IR1)*A(IR2,IC1)
          A(IR1,IC1) = W2/W1
3        CONTINUE
        W2 = B(IR1)
        DO 4 IR2 = 1,IR1-1
4       W2 = W2 - A(IR2,IR1)*B(IR2)
        B(IR1) = W2/W1
5      CONTINUE
      RETURN
      END
```

SUBROUTINE BKSUB(A,B,M,N,JOB)

```
C
C PERFORM BACK-SOLUTION ACCORDING AS JOB = 1, 2, OR 3
C
```

```
      REAL A(N,N),B(N,M),W1
      DO 3 IC1 = M,1,-1
        IF(JOB.EQ.2) THEN
          K1 = 1
          K2 = N
          K3 = 1
        ELSE
          K2 = 1
          K3 = -1
          IF(JOB.EQ.1) THEN
            K1 = N
          ELSE
            K1 = IC1
          END IF
        END IF
      END IF
      DO 2 IR1 = K1,K2,K3
        W1 = B(IR1,IC1)
        IF (JOB.EQ.2) THEN
          K2 = IR1-1
        ELSE
          K1 = N
          K2 = IR1+1
        END IF
      END DO
```

```

      END IF
      DO 1 IR2 = K1,K2,K3
1      W1 = W1 - A(IR1,IR2)*B(IR2,IC1)
      B(IR1,IC1) = W1/A(IR1,IR1)
      IF(JOB.EQ.3) B(IC1,IR1) = B(IR1,IC1)
2      CONTINUE
3      CONTINUE
      RETURN
      END

```

```

C-----
C
C 3. EX1.FOR, EXAMPLE 1
C
C This example is fully described in the paper. The description is
C repeated here. The problem is a small artificial one (called the
C New Brunswick problem) in which it is wanted to obtain estimates
C for the elements of the parameter vector ~ in the following three
C functional equations which apply for all i=1,2,...,6
C
C      (see published paper)
C
C The parameters which describe the magnitude of the problem are:
C   the number of data vectors, NDAT=6
C   the number of equations, NEQ=3
C   the number of model parameters to be estimated, NPAR=4
C   the number of measured variables in a data vector, NVAR=5.
C The program parameters CRIT1 and CRIT2 were both set at 1.E-6 while NITER1
C and NITER2 were 50 and 20. The full Fortran code as used is listed in
C EX1.FOR. The data in the form required for input to the program are given
C in the file EX1.DAT. The same data are listed with descriptive headings at
C the beginning of the file EX1.OUT. The latter part of EX1.OUT shows the
C output from the program.
C
C EX1.FOR

```

```

C TEST PROGRAM FOR EVM USING NEW BRUNSWICK PROBLEM 91/3/27 PMR

```

```

      DIMENSION B(3,5), BV(3,5), DATA(6,5), EST(6,5), F(3), G1(4,4),
* G2(4,4), G3(4,4), H(3), IFAULT(2), Q1(4), Q2(4), RESID(6,5),
* S(3,3), T(3), THETA(4), V(5,5), XI(5), Z(3,4)
C
      READ(20,*) THETA
      READ(20,*) ((DATA(I,J),J=1,5),I=1,6)
      READ(20,*) V
      WRITE(30,1)
1      FORMAT(36X,'TABLE 1')
      WRITE(30,2)
2      FORMAT(//'DATA')
      WRITE(30,3) ((DATA(I,J),J=1,5),I=1,6)
3      FORMAT(5F9.2)
      WRITE(30,4)
4      FORMAT(//'V')
      WRITE(30,3) V
      WRITE(30,5) THETA
5      FORMAT(//'INITIAL PARAMETER ESTIMATES = ',4F9.2)
      CALL EVM(B,BV,DATA,EST,F,G1,G2,G3,H,IFAULT,
* 6,3,4,5,PHI,Q1,Q2,RESID,S,T,THETA,V,XI,Z)
      WRITE(30,6) THETA
6      FORMAT(//'FINAL PARAMETER ESTIMATES = ',4F9.6)
      WRITE(30,7) PHI

```

```
7      FORMAT(//'FINAL PHI = ',E13.7)
      WRITE(30,8) Q1
8      FORMAT(//'FINAL Q = ',4E16.7)
      WRITE(30,9)
9      FORMAT(//'ESTIMATED TRUE VALUES OF MEASUREMENTS')
      WRITE(30,10) ((EST(I,J),J=1,5),I=1,6)
10     FORMAT(5F9.4)
      WRITE(30,11)
11     FORMAT(//'RESIDUALS')
      WRITE(30,10) ((RESID(I,J),J=1,5),I=1,6)
      WRITE(30,12)
12     FORMAT(//'EXPECTED INFORMATION MATRIX')
      WRITE(30,13) G1
13     FORMAT(4F9.4)
      WRITE(30,14)
14     FORMAT(//'INVERSE OF EXPECTED INFORMATION MATRIX')
      WRITE(30,13) G3
      WRITE(30,15)
15     FORMAT(//'FAULT STATUS')
      WRITE(30,16) IFAULT
16     FORMAT(2I5)
      STOP
      END
```

```
      SUBROUTINE BF(B,F,THETA,XI)
      DIMENSION B(3,5), F(3), THETA(4), XI(5)
```

```
C
      F(1) = THETA(1)**2 + THETA(2)*XI(1) + THETA(3)*XI(2)**2 - XI(3)
      F(2) = THETA(2)**2 + (THETA(3)*XI(1))**2
*      + THETA(4)**3*XI(3)**2 - XI(4)
      F(3) = THETA(3)**2 + (THETA(1)*XI(2))**2 - XI(5)
      B(1,1) = THETA(2)
      B(1,2) = 2.E0*THETA(3)*XI(2)
      B(1,3) = -1.E0
      B(1,4) = 0.E0
      B(1,5) = 0.E0
      B(2,1) = 2.E0*THETA(3)**2*XI(1)
      B(2,2) = 0.E0
      B(2,3) = 2.E0*THETA(4)**3*XI(3)
      B(2,4) = -1.E0
      B(2,5) = 0.E0
      B(3,1) = 0.E0
      B(3,2) = 2.E0*THETA(1)**2*XI(2)
      B(3,3) = 0.E0
      B(3,4) = 0.E0
      B(3,5) = -1.E0
      RETURN
      END
```

```
      SUBROUTINE ZED(B,F,THETA,XI,Z)
      DIMENSION B(3,5), F(3), THETA(4), XI(5), Z(3,4)
      Z(1,1) = 2.E0*THETA(1)
      Z(1,2) = XI(1)
      Z(1,3) = XI(2)**2
      Z(1,4) = 0.E0
      Z(2,1) = 0.E0
      Z(2,2) = 2.E0*THETA(2)
      Z(2,3) = 2.E0*THETA(3)*XI(1)**2
      Z(2,4) = 3.E0*(THETA(4)*XI(3))**2
```



```
Z(3,1) = 2.E0*THETA(1)*XI(2)**2
Z(3,2) = 0.E0
Z(3,3) = 2.E0*THETA(3)
Z(3,4) = 0.E0
RETURN
END
```

```
      SUBROUTINE EVM(B,BV,DATA,EST,F,G1,G2,G3,H,IFAU,LT,
*      NDAT,NEQ,NPAR,NVAR,PHI,Q1,Q2,RESID,S,T,THETA,V,XI,Z)
```

```
C
C PARAMETER ESTIMATION FOR THE ERROR-IN-VARIABLES MODEL
C
      REAL B(NEQ,NVAR), BV(NEQ,NVAR), CRIT1, DATA(NDAT,NVAR),
* EST(NDAT,NVAR), F(NEQ), G1(NPAR,NPAR), G2(NPAR,NPAR),
* G3(NPAR,NPAR), H(NEQ), ONE, PHI, Q1(NPAR), Q2(NPAR),
* RESID(NDAT,NVAR), S(NEQ,NEQ), T(NEQ), THETA(NPAR),
* V(NVAR,NVAR), WDIFF, W1, W2, XI(NVAR), Z(NEQ,NPAR), ZERO
      DIMENSION IFAULT(2)
      PARAMETER (CRIT1=1.E-6, NITER1=50, ZERO=0.E0, ONE=1.E0)
      IFAULT(1) = 0
      IFAULT(2) = 0
      DO 4 ITER = 1,NITER1
C
C EACH PASS THROUGH THIS LOOP PERFORMS A SINGLE OUTER ITERATION
C
      CALL INNER(B,BV,DATA,EST,F,G1,H,IFAU,LT,NDAT,
*      NEQ,NPAR,NVAR,PHI,Q1,RESID,S,T,THETA,V,XI,Z)
C
C PUT Q1 INTO Q2 AND G1 INTO G2
C
      DO 2 IPAR1 = 1,NPAR
        Q2(IPAR1) = Q1(IPAR1)
        DO 1 IPAR2 = IPAR1,NPAR
1          G2(IPAR1,IPAR2) = G1(IPAR1,IPAR2)
2        CONTINUE
C
C CALCULATE CORRECTION FOR THETA
C
      CALL CHOL(G2,Q2,NPAR)
      CALL BKSUB(G2,Q2,1,NPAR,1)
C
C CHECK FOR CONVERGENCE
C
      WDIFF = ZERO
      DO 3 IPAR = 1,NPAR
        W1 = Q2(IPAR)
        W2 = THETA(IPAR)
        WDIFF = MAX(WDIFF,ABS(W1/W2))
        THETA(IPAR) = W2-W1
3      CONTINUE
      IF(WDIFF.LE.CRIT1)GO TO 5
4      CONTINUE
      IFAULT(1) = 1
C
C FILL LOWER TRIANGLE OF G1 AND PREPARE G2
C FOR THE INVERSION OF G1
C
5      DO 7 IPAR1 = 1,NPAR
        DO 6 IPAR2 = IPAR1,NPAR
          W1 = G1(IPAR1,IPAR2)
```

```
      G1(IPAR2,IPAR1) = W1
      G2(IPAR1,IPAR2) = W1
      G3(IPAR1,IPAR2) = ZERO
6      CONTINUE
7      CONTINUE
C
C      INVERT G1 INTO G3
C
      CALL CHOL(G2,Q2,NPAR)
      DO 8 IPAR1 = 1,NPAR
8      G3(IPAR1,IPAR1) = ONE/G2(IPAR1,IPAR1)
      CALL BKSUB(G2,G3,NPAR,NPAR,3)
      RETURN
      END

      SUBROUTINE INNER(B,BV,DATA,EST,F,G1,H,IFAULT,NDAT,NEQ,
* NPAR,NVAR,PHI,Q1,RESID,S,T,THETA,V,XI,Z)
      REAL B(NEQ,NVAR), BV(NEQ,NVAR), CRIT2, DATA(NDAT,NVAR),
* EST(NDAT,NVAR), F(NEQ), G1(NPAR,NPAR), H(NEQ), HALF,
* PHI, Q1(NPAR), RESID(NDAT,NVAR), S(NEQ,NEQ),
* T(NEQ), THETA(NPAR),
* V(NVAR,NVAR), WDIFF, W1, XI(NVAR), Z(NEQ,NPAR), ZERO
      DIMENSION IFAULT(2)
      PARAMETER (CRIT2=1.E-6, HALF=.5E0, NITER2=20, ZERO=0.E0)
C
C      INITIALIZE PHI, Q1, AND G1
C
      PHI = ZERO
      DO 2 IPAR1 = 1,NPAR
          Q1(IPAR1) = ZERO
          DO 1 IPAR2 = IPAR1,NPAR
1          G1(IPAR1,IPAR2) = ZERO
2      CONTINUE
C
C      PERFORM INNER ITERATION TO CONVERGENCE FOR EACH IDAT
C
      DO 24 IDAT = 1,NDAT
          DO 3 IVAR1 = 1,NVAR
3          XI(IVAR1) = DATA(IDAT,IVAR1)
          DO 16 ITER = 1,NITER2
C
C      THIS LOOP PERFORMS A SINGLE INNER ITERATION
C
          WDIFF = ZERO
          CALL BF(B,F,THETA,XI)
C
C      CALCULATE BV
C
          DO 6 IEQ1 = 1,NEQ
              DO 5 IVAR1 = 1,NVAR
                  W1 = ZERO
                  DO 4 IVAR2 = 1,NVAR
4                  W1 = W1+B(IEQ1,IVAR2)*V(IVAR1,IVAR2)
                  BV(IEQ1,IVAR1) = W1
5                  CONTINUE
6                  CONTINUE
C
C      CALCULATE BVB' AND STORE IT IN S
C
          DO 9 IEQ1 = 1,NEQ
```

```

      DO 8 IEQ2 = IEQ1,NEQ
        W1 = ZERO
        DO 7 IVAR1 = 1,NVAR
          W1 = W1+BV(IEQ1,IVAR1)*B(IEQ2,IVAR1)
          S(IEQ1,IEQ2) = W1
        CONTINUE
      CONTINUE
C
C PUT F+B(X-XI) INTO H
C
      DO 11 IEQ1 = 1,NEQ
        W1 = F(IEQ1)
        DO 10 IVAR1 = 1,NVAR
          W1 = W1+B(IEQ1,IVAR1)*(DATA(IDAT,IVAR1)-XI(IVAR1))
          H(IEQ1) = W1
        CONTINUE
      CONTINUE
C
C REPLACE S BY ITS TRIANGULAR FACTORIZATION
C AND SOLVE ST = H FOR T
C
      CALL CHOL(S,H,NEQ)
      DO 13 IEQ1 = 1,NEQ
        T(IEQ1) = H(IEQ1)
        DO 12 IEQ2 = IEQ1,NEQ
          S(IEQ2,IEQ1) = S(IEQ1,IEQ2)
        CONTINUE
      CALL BKSUB(S,T,1,NEQ,1)
C
C CALCULATE NEW XI AND PUT RELATIVE CHANGE IN XI INTO WDIFF
C
      DO 15 IVAR1 = 1,NVAR
        W1 = DATA(IDAT,IVAR1)
        DO 14 IEQ1 = 1,NEQ
          W1 = W1 - BV(IEQ1,IVAR1)*T(IEQ1)
          WDIFF = MAX(WDIFF, ABS((W1-XI(IVAR1))/W1))
          XI(IVAR1) = W1
        CONTINUE
      CONTINUE
C
C CHECK FOR CONVERGENCE
C
      IF(WDIFF.LE.CRIT2)GO TO 17
      CONTINUE
      IFAULT(2) = 1
C
C ACCUMULATE PHI
C
      DO 18 IEQ1 = 1,NEQ
        PHI = PHI + H(IEQ1)**2
      CONTINUE
C
C CALCULATE FITTED VALUES AND RESIDUALS
C
      DO 19 IVAR1 = 1,NVAR
        W1 = XI(IVAR1)
        EST(IDAT,IVAR1) = W1
        RESID(IDAT,IVAR1) = DATA(IDAT,IVAR1)-W1
      CONTINUE
C
C CALCULATE CONTRIBUTIONS TO Q1 AND G1 AND COMPLETE THE LOOPS
C
      CALL ZED(B,F,THETA,XI,Z)
      CALL BKSUB(S,Z,NPAR,NEQ,2)

```

```
DO 23 IPAR1 = 1,NPAR
  W1 = Q1(IPAR1)
  DO 20 IEQ1 = 1,NEQ
20    W1 = W1 + Z(IEQ1,IPAR1)*H(IEQ1)
    Q1(IPAR1) = W1
  DO 22 IPAR2 = IPAR1,NPAR
    W1 = G1(IPAR1,IPAR2)
    DO 21 IEQ1 = 1,NEQ
21    W1 = W1 + Z(IEQ1,IPAR1)*Z(IEQ1,IPAR2)
    G1(IPAR1,IPAR2) = W1
22  CONTINUE
23  CONTINUE
24  CONTINUE
  PHI = PHI*HALF
  RETURN
  END
```

```
      SUBROUTINE CHOL(A,B,N)
C
C  PERFORM CHOLESKY DECOMPOSITION OF A AND PRELIMINARY TREATMENT
C    OF B
C
```

```
  REAL A(N,N),B(N),W1,W2
  DO 5 IR1 = 1,N
    W1 = A(IR1,IR1)
    DO 1 IR2 = 1,IR1-1
1    W1 = W1 - A(IR2,IR1)**2
    W1 = SQRT(W1)
    A(IR1,IR1) = W1
    DO 3 IC1 = IR1+1,N
      W2 = A(IR1,IC1)
      DO 2 IR2 = 1,IR1-1
2      W2 = W2 - A(IR2,IR1)*A(IR2,IC1)
      A(IR1,IC1) = W2/W1
3    CONTINUE
    W2 = B(IR1)
    DO 4 IR2 = 1,IR1-1
4    W2 = W2 - A(IR2,IR1)*B(IR2)
    B(IR1) = W2/W1
5  CONTINUE
  RETURN
  END
```

```
      SUBROUTINE BKSUB(A,B,M,N,JOB)
C
C  PERFORM BACK-SOLUTION ACCORDING AS JOB = 1, 2, OR 3
C
```

```
  REAL A(N,N),B(N,M),W1
  DO 3 IC1 = M,1,-1
    IF(JOB.EQ.2) THEN
      K1 = 1
      K2 = N
      K3 = 1
    ELSE
      K2 = 1
      K3 = -1
      IF(JOB.EQ.1) THEN
        K1 = N
      ELSE
```

```

        K1 = IC1
        END IF
    END IF
    DO 2 IR1 = K1,K2,K3
        W1 = B(IR1,IC1)
        IF (JOB.EQ.2) THEN
            K2 = IR1-1
        ELSE
            K1 = N
            K2 = IR1+1
        END IF
        DO 1 IR2 = K1,K2,K3
1          W1 = W1 - A(IR1,IR2)*B(IR2,IC1)
            B(IR1,IC1) = W1/A(IR1,IR1)
            IF(JOB.EQ.3) B(IC1,IR1) = B(IR1,IC1)
2          CONTINUE
3          CONTINUE
        RETURN
    END

```

C-----

C  
C 4. EX1.DAT

```

1 1 1 1
-.78 1.39 3.99 11.7 3.44
-1.27 2 5.15 36.58 4.59
2.62 .38 5.77 16.49 .33
2.05 2.92 6.78 75.68 2.74
1.05 2.46 12.85 149.42 7.59
2.96 1.47 3.9 52.11 6.82
1 -.2 .1 .3 0
-.2 1 .2 -.1 0
.1 .2 2 .4 -.2
.3 -.1 .4 5 .4
0 0 -.2 .4 3

```

C-----

C  
C 5. EX1.OUT

TABLE 1

DATA

-0.78	1.39	3.99	11.70	3.44
-1.27	2.00	5.15	36.58	4.59
2.62	0.38	5.77	16.49	0.33
2.05	2.92	6.78	75.68	2.74
1.05	2.46	12.85	149.42	7.59
2.96	1.47	3.90	52.11	6.82

V

1.00	-0.20	0.10	0.30	0.00
-0.20	1.00	0.20	-0.10	0.00
0.10	0.20	2.00	0.40	-0.20
0.30	-0.10	0.40	5.00	0.40
0.00	0.00	-0.20	0.40	3.00

INITIAL PARAMETER ESTIMATES = 1.00 1.00 1.00  
1.00

FINAL PARAMETER ESTIMATES = 0.822474 0.445297 1.442967 1.001551

FINAL PHI = 0.7515061E+01

FINAL Q = -0.4954202E-05 0.1068151E-05 0.1989809E-05  
0.2217203E-04

ESTIMATED TRUE VALUES OF MEASUREMENTS

-0.6633	1.4147	3.2692	11.8515	3.4361
-1.3739	1.9729	5.6814	36.5576	4.7153
1.7831	1.0674	3.1146	16.5644	2.8529
2.9277	1.9753	7.6105	76.2357	4.7217
0.8652	2.7678	12.1155	149.2269	7.2642
3.1432	1.5559	5.5692	51.9294	3.7197

RESIDUALS

-0.1167	-0.0247	0.7208	-0.1515	0.0039
0.1039	0.0271	-0.5314	0.0224	-0.1253
0.8369	-0.6874	2.6554	-0.0744	-2.5229
-0.8777	0.9447	-0.8305	-0.5557	-1.9817
0.1848	-0.3078	0.7345	0.1931	0.3258
-0.1832	-0.0859	-1.6692	0.1806	3.1003

EXPECTED INFORMATION MATRIX

72.8418	-3.7697	4.1724	-58.4874
-3.7697	2.9379	0.7385	6.4070
4.1724	0.7385	10.2625	18.3139
-58.4874	6.4070	18.3139	334.4229

INVERSE OF EXPECTED INFORMATION MATRIX

0.0187	0.0197	-0.0157	0.0037
0.0197	0.3781	-0.0315	-0.0021
-0.0157	-0.0315	0.1218	-0.0088
0.0037	-0.0021	-0.0088	0.0042

FAULT STATUS

0 0

C-----

C  
C 6. EX2.FOR, EXAMPLE 2  
C

C The data for this example were obtained as digitized observations on the  
C outline of the nerve-head in a subject's eye. There are 32 data (NDAT),  
C one functional relation (NEQ), two variables (NVAR), and five parameters  
C (NPAR). The functional relation describes an ellipse with the following  
C equation

C

```
C F = T3*(XI1-T1)**2 + 2*T4*(XI1-T1)*(XI2-T2) + T5*(XI2-T2)**2 - 1 = 0
```

```
C
```

```
C where F is the functional value which numerically must be brought to zero,  
C T1,T2,T3,T4 and T5 are the functional parameters the values of which are  
C to be estimated. XI1 and XI2 are the estimated true values of the measured  
C variables. The T's are represented by the Greek letter theta in the paper  
C and the XI's by xi. The parameters which describe the magnitude of the  
C problem are NDAT = 32, NPAR = 4, NVAR = 2. The program parameters were  
C set at CRIT1 = 1.E-6 and CRIT2 = 1.E-5. NITER1 was 50 and NITER2 15. The  
C full Fortran code as used is listed under EX2.FOR. The data in the format  
C used by the program is under EX2.DAT. The output is listed under EX2.OUT.
```

```
C
```

```
C EX2.FOR
```

```
C FITTING OF ELLIPSE BY EVMS 91/3/25 PMR
```

```
      DIMENSION BS(2),BVS(2),DATA(32,2),EST(32,2),  
* G1(5,5),G2(5,5),  
* G3(5,5),IFAUULT(2),Q1(5),Q2(5),RESID(32,2),THETA(5),V(2,2),  
* XI(2),ZS(5)  
      DATA V/1,0,0,1/
```

```
C
```

```
      READ(21,*)((DATA(I,J),J=1,2),I=1,32)  
      DO 2 I = 1,32  
        DO 1 J = 1,2  
1          DATA(I,J) = .001*DATA(I,J)  
2          CONTINUE  
      READ(21,*) THETA  
      CALL EVMS(BS,BVS,DATA,EST,G1,G2,G3,IFAUULT,32,5,2,PHI,  
* Q1,Q2,RESID,THETA,V,XI,ZS)  
      DO 4 I = 1,32  
        DO 3 J = 1,2  
          DATA(I,J) = 1000.*DATA(I,J)  
          EST(I,J) = 1000.*EST(I,J)  
          RESID(I,J) = 1000.*RESID(I,J)
```

```
3
```

```
          CONTINUE
```

```
4
```

```
          CONTINUE
```

```
      WRITE(31,5)
```

```
5
```

```
      FORMAT(//'FAULT STATUS')
```

```
      WRITE(31,6) IFAUULT
```

```
6
```

```
      FORMAT(2I5)
```

```
      WRITE(31,7)
```

```
7
```

```
      FORMAT(//'PARAMETER ESTIMATES')
```

```
      WRITE(31,8) THETA
```

```
8
```

```
      FORMAT(5F9.4)
```

```
      WRITE(31,9)
```

```
9
```

```
      FORMAT(//'INFORMATION MATRIX')
```

```
      WRITE(31,8) G1
```

```
      WRITE(31,10)
```

```
10
```

```
      FORMAT(//'INVERSE OF INFORMATION MATRIX')
```

```
      WRITE(31,8) G3
```

```
      WRITE(31,11)
```

```
11
```

```
      FORMAT(//6X,'DATA',11X,'ESTIMATES',14X,'RESIDUALS')
```

```
      WRITE(31,12)((DATA(I,J),J=1,2),(EST(I,J),J=1,2),
```

```
* (RESID(I,J),J=1,2),I=1,32)
```

```
12
```

```
      FORMAT(2F7.0,2F11.4,1X,2F10.4)
```

```
      STOP
```

```
      END
```

```

SUBROUTINE BF(B,F,THETA,XI)
DIMENSION B(2),THETA(5),XI(2)
C
C CALCULATE F
W1 = XI(1)-THETA(1)
W2 = XI(2)-THETA(2)
F = THETA(3)*W1*W1 + 2.D0*THETA(4)*W1*W2 + THETA(5)*W2*W2 - 1.D0
C
C CALCULATE B
B(1) = 2.D0*(W1*THETA(3) + W2*THETA(4))
B(2) = 2.D0*(W1*THETA(4) + W2*THETA(5))
RETURN
END

```

```

SUBROUTINE ZED(B,F,THETA,XI,Z)
DIMENSION B(2),THETA(5),XI(2),Z(5)
C
W1 = XI(1)-THETA(1)
W2 = XI(2)-THETA(2)
Z(1) = -2.D0*(W1*THETA(3) + W2*THETA(4))
Z(2) = -2.D0*(W1*THETA(4) + W2*THETA(5))
Z(3) = W1*W1
Z(4) = 2.D0*W1*W2
Z(5) = W2*W2
RETURN
END

```

```

SUBROUTINE EVMS(BS,BVS,DATA,EST,G1,G2,G3,IFAUULT,
*   NDAT,NPAR,NVAR,PHI,Q1,Q2,RESID,THETA,V,XI,ZS)
C
C PARAMETER ESTIMATION FOR THE ERROR-IN-VARIABLES MODEL WITH M = 1
C 91/3/21 PMR
C
REAL BS(NVAR), BVS(NVAR), BVB, CRIT1, DATA(NDAT,NVAR),
* EST(NDAT,NVAR), FS, G1(NPAR,NPAR), G2(NPAR,NPAR),
* G3(NPAR,NPAR), HS, ONE, PHI, Q1(NPAR), Q2(NPAR),
* RESID(NDAT,NVAR), THETA(NPAR),
* V(NVAR,NVAR), WDIFF, W1, W2, XI(NVAR), ZS(NPAR), ZERO
DIMENSION IFAUULT(2)
PARAMETER(CRIT1=1.E-6,NITER1=50,ONE=1.E0,ZERO=0.E0)
C
IFAUULT(1) = 0
IFAUULT(2) = 0
DO 4 ITER = 1,NITER1
C
C EACH PASS THROUGH THIS LOOP PERFORMS A SINGLE OUTER ITERATION
C
CALL INNERS(BS,BVS,DATA,EST,G1,IFAUULT,NDAT,
*   NPAR,NVAR,PHI,Q1,RESID,THETA,V,XI,ZS)
C
C PUT Q1 INTO Q2 AND G1 INTO G2
C
DO 2 IPAR1 = 1,NPAR
Q2(IPAR1) = Q1(IPAR1)
DO 1 IPAR2 = IPAR1,NPAR
1 G2(IPAR1,IPAR2) = G1(IPAR1,IPAR2)
2 CONTINUE
C
C CALCULATE CORRECTION FOR THETA

```



```

C
      CALL CHOL(G2,Q2,NPAR)
      CALL BKSUB(G2,Q2,1,NPAR,1)
C
C CHECK FOR CONVERGENCE
C
      WDIFF = ZERO
      DO 3 IPAR = 1,NPAR
        W1 = Q2(IPAR)
        W2 = THETA(IPAR)
        WDIFF = MAX(WDIFF,ABS(W1/W2))
        THETA(IPAR) = W2-W1
3      CONTINUE
      IF(WDIFF.LE.CRIT1)GO TO 5
4      CONTINUE
      IFAULT(1) = 1
C
C FILL LOWER TRIANGLE OF G1 AND PREPARE G2
C FOR THE INVERSION OF G1
C
5      DO 7 IPAR1 = 1,NPAR
        DO 6 IPAR2 = IPAR1,NPAR
          W1 = G1(IPAR1,IPAR2)
          G1(IPAR2,IPAR1) = W1
          G2(IPAR1,IPAR2) = W1
          G3(IPAR1,IPAR2) = ZERO
6        CONTINUE
7      CONTINUE
C
C INVERT G1 INTO G3
C
      CALL CHOL(G2,Q2,NPAR)
      DO 8 IPAR1 = 1,NPAR
6      G3(IPAR1,IPAR1) = ONE/G2(IPAR1,IPAR1)
      CALL BKSUB(G2,G3,NPAR,NPAR,3)
      RETURN
      END

      SUBROUTINE INNERS(BS,BVS,DATA,EST,G1,IFAULT,NDAT,
*      NPAR,NVAR,PHI,Q1,RESID,THETA,V,XI,ZS)
C
C INNER ITERATION FOR M = 1
C
      REAL BS(NVAR), BVS(NVAR), BVB, CRIT2, DATA(NDAT,NVAR),
* EST(NDAT,NVAR), FS, HALF, G1(NPAR,NPAR), HS,
* PHI, Q1(NPAR), RESID(NDAT,NVAR), THETA(NPAR),
* V(NVAR,NVAR), WDIFF, W1, XI(NVAR), ZS(NPAR), ZERO
      DIMENSION IFAULT(2)
      PARAMETER (CRIT2=1.E-5, HALF=.5E0, NITER2=15, ZERO=0.E0)
C
C INITIALIZE PHI, Q1, AND G1
C
      PHI = ZERO
      DO 2 IPAR1 = 1,NPAR
        Q1(IPAR1) = ZERO
        DO 1 IPAR2 = IPAR1,NPAR
1          G1(IPAR1,IPAR2) = ZERO
2        CONTINUE
C
C PERFORM INNER ITERATION TO CONVERGENCE FOR EACH IDAT

```

```
C
      DO 14 IDAT = 1,NDAT
C
C   INITIALIZE XI
C
      DO 3 IVAR1 = 1,NVAR
3      XI(IVAR1) = DATA(IDAT,IVAR1)
      DO 9 ITER = 1,NITER2
C
C   THIS LOOP PERFORMS A SINGLE INNER ITERATION
C
      WDIFF = ZERO
      CALL BF(BS,FS,THETA,XI)
C
C   CALCULATE BVS
C
      DO 5 IVAR1 = 1,NVAR
        W1 = ZERO
        DO 4 IVAR2 = 1,NVAR
4          W1 = W1 + BS(IVAR2)*V(IVAR1,IVAR2)

          BVS(IVAR1) = W1
5        CONTINUE
C
C   CALCULATE BVB
C
      BVB = ZERO
      DO 6 IVAR1 = 1,NVAR
6        BVB = BVB + BVS(IVAR1)*BS(IVAR1)
C
C   PUT F+B(X-XI) INTO HS
C
      HS = FS
      DO 7 IVAR1 = 1,NVAR
7        HS = HS + BS(IVAR1)*(DATA(IDAT,IVAR1) - XI(IVAR1))
C
C   CALCULATE NEW XI AND PUT RELATIVE CHANGE IN XI INTO WDIFF
C
      DO 8 IVAR1 = 1,NVAR
        W1 = DATA(IDAT,IVAR1) - BVS(IVAR1)*HS/BVB
        WDIFF = MAX(WDIFF, ABS((W1-XI(IVAR1))/W1))
        XI(IVAR1) = W1
8      CONTINUE
C
C   CHECK FOR CONVERGENCE
C
      IF(WDIFF.LE.CRIT2)GO TO 10
9      CONTINUE
      IFAULT(2) = 1
C
C   ACCUMULATE PHI
C
10     PHI = PHI+HS*HS/BVB
C
C   CALCULATE FITTED VALUES AND RESIDUALS
C
      DO 11 IVAR1 = 1,NVAR
        W1 = XI(IVAR1)
        EST(IDAT,IVAR1) = W1
        RESID(IDAT,IVAR1) = DATA(IDAT,IVAR1) - W1
11    CONTINUE
```

```
C
C CALCULATE CONTRIBUTIONS TO Q1 AND G1 AND COMPLETE THE LOOPS
C
      CALL ZED(BS,FS,THETA,XI,ZS)
      DO 13 IPAR1 = 1,NPAR
        W1 = ZS(IPAR1)
        Q1(IPAR1) = Q1(IPAR1) + W1*HS/BVB
        DO 12 IPAR2 = IPAR1,NPAR
12          G1(IPAR1,IPAR2) = G1(IPAR1,IPAR2) + W1*ZS(IPAR2)/BVB
13        CONTINUE
14      CONTINUE
      PHI = PHI*HALF
      RETURN
      END
```

```
      SUBROUTINE CHOL(A,B,N)
C
C PERFORM CHOLESKY DECOMPOSITION OF A AND PRELIMINARY TREATMENT
C OF B
C
      REAL A(N,N),B(N),W1,W2
      DO 5 IR1 = 1,N
        W1 = A(IR1,IR1)
        DO 1 IR2 = 1,IR1-1
1          W1 = W1-A(IR2,IR1)**2
        W1 = SQRT(W1)
        A(IR1,IR1) = W1
        DO 3 IC1 = IR1+1,N
          W2 = A(IR1,IC1)
          DO 2 IR2 = 1,IR1-1
2            W2 = W2 - A(IR2,IR1)*A(IR2,IC1)
          A(IR1,IC1) = W2/W1
3          CONTINUE
        W2 = B(IR1)
        DO 4 IR2 = 1,IR1-1
4          W2 = W2 - A(IR2,IR1)*B(IR2)
        B(IR1) = W2/W1
5      CONTINUE
      RETURN
      END
```

```
      SUBROUTINE BKSUB(A,B,M,N,JOB)
C
C PERFORM BACK-SOLUTION ACCORDING AS JOB = 1, 2, OR 3
C
      REAL A(N,N),B(N,M),W1
      DO 3 IC1 = M,1,-1
        IF(JOB.EQ.2) THEN
          K1 = 1
          K2 = N
          K3 = 1
        ELSE
          K2 = 1
          K3 = -1
          IF(JOB.EQ.1) THEN
            K1 = N
          ELSE
            K1 = IC1
          END IF
        END IF
```

```
      END IF
      DO 2 IR1 = K1,K2,K3
        W1 = B(IR1,IC1)
        IF (JOB.EQ.2) THEN
          K2 = IR1-1
        ELSE
          K1 = N
          K2 = IR1+1
        END IF
      DO 1 IR2 = K1,K2,K3
1      W1 = W1-A(IR1,IR2)*B(IR2,IC1)
      B(IR1,IC1) = W1/A(IR1,IR1)
      IF(JOB.EQ.3) B(IC1,IR1) = B(IR1,IC1)
2      CONTINUE
3      CONTINUE
      RETURN
      END
```

C-----

7. EX2.DAT

```
1420 470
1188 476
1015 539
830 655
660 825
543 1041
468 1268
459 1528
510 1804
628 2063
795 2221
1040 2345
1303 2417
1452 2431
1738 2411
1901 2318
2091 2222
2230 2117
2311 1984
2385 1837
2451 1630
2467 1462
2472 1263
2446 1112
2387 963
2255 796
2109 696
1929 597
1846 556
1620 486
1418 437
1259 453
1 1 1 -.001 1
```

8. EX2.OUT

```
FAULT STATUS
  0      0
```

PARAMETER ESTIMATES

1.4594 1.4454 0.9582 0.0039 1.0186

INFORMATION MATRIX

14.6768	0.4050	-1.1978	0.2560	-0.2880
0.4050	17.3231	0.1325	-0.6215	1.2703
-1.1978	0.1325	3.1070	0.0154	0.9994
0.2560	-0.6215	0.0154	3.9975	0.1110
-0.2880	1.2703	0.9994	0.1110	3.1565

INVERSE OF INFORMATION MATRIX

0.0705	-0.0019	0.0277	-0.0049	-0.0014
-0.0019	0.0600	0.0051	0.0102	-0.0263
0.0277	0.0051	0.3698	0.0008	-0.1166
-0.0049	0.0102	0.0008	0.2524	-0.0137
-0.0014	-0.0263	-0.1166	-0.0137	0.3647

DATA		ESTIMATES		RESIDUALS	
1420.	470.	1419.3920	455.4515	0.6078	14.5485
1188.	476.	1191.7790	490.1515	-3.7791	-14.1515
1015.	539.	1021.0570	552.0391	-6.0567	-13.0391
830.	655.	835.8889	662.8408	-5.8889	-7.8408
660.	825.	663.1567	827.6081	-3.1567	-2.6081
543.	1041.	531.0313	1035.3420	11.9687	5.6577
468.	1268.	455.4884	1265.5690	12.5116	2.4308
459.	1528.	441.1519	1529.4960	17.8481	-1.4961
510.	1804.	506.2181	1805.5060	3.7819	-1.5061
628.	2063.	646.4303	2048.4960	-18.4303	14.5044
795.	2221.	804.9326	2208.6670	-9.9326	12.3329
1040.	2345.	1038.0070	2349.5790	1.9934	-4.5788
1303.	2417.	1301.8300	2424.9300	1.1703	-7.9303
1452.	2431.	1451.9830	2436.1840	0.0166	-5.1842
1738.	2411.	1734.5620	2398.5040	3.4379	12.4955
1901.	2318.	1908.4610	2333.5910	-7.4607	-15.5907
2091.	2222.	2090.8450	2221.7980	0.1550	0.2022
2230.	2117.	2218.0730	2105.9520	11.9267	11.0476
2311.	1984.	2313.4760	1985.6700	-2.4755	-1.6704
2385.	1837.	2394.2520	1841.1940	-9.2518	-4.1943
2451.	1630.	2461.8330	1632.1880	-10.8328	-2.1882
2467.	1462.	2480.6950	1462.2970	-13.6950	-0.2967
2472.	1263.	2464.4650	1264.4130	7.5355	-1.4126
2446.	1112.	2425.3450	1119.3370	20.6547	-7.3367
2387.	963.	2361.4770	977.0116	25.5227	-14.0116
2255.	796.	2242.8230	806.5399	12.1768	-10.5398
2109.	696.	2117.7400	685.2596	-8.7397	10.7405
1929.	597.	1942.6510	570.5976	-13.6507	26.4024
1846.	556.	1856.1900	530.8438	-10.1901	25.1563
1620.	486.	1622.9630	466.7079	-2.9625	19.2921
1418.	437.	1418.7830	455.4772	-0.7826	-18.4772
1259.	453.	1263.0220	473.7592	-4.0221	-20.7591

```

C      .. ULCC Toolpack/1 2.1
C      SUBROUTINE initial(ns, m, emax, x, hx, hpx, lb, xlb, ub, xub,
*          ifault, iwv, rwv)
C
C      ALGORITHM AS 287.1 APPL.STATIST. (1993), VOL.42, NO.4
C
C      This subroutine takes as input the number of starting values M
C      and the starting points x(i), hx(i), hpx(i) i=1, m. As output
C      we have pointer ipt along with ilow and ihigh and the lower
C      and upper hulls defined by z, hz, scum, cu, hulb, huub stored
C      in working vectors iwv and rwv
C
C      INTEGER ns, m, ifault, iwv( * )
C      LOGICAL lb, ub
C      REAL emax, x( * ), hx( * ), hpx( * ), xlb, xub, rwv( * )
C
C      INTEGER i, ihigh, ihpx, ihuz, ihx, ipt, ilow, iscum, ix, iz, nn
C      LOGICAL HORIZ
C      REAL a, b, alcu, cu, eps, expon, hulb, huub, huzmax, zlog, zmax
C
C      zlog(a) = alog(a)
C      zmax(a, b) = amax1(a, b)
C      eps = expon(-emax, emax)
C
C      ifault = 0
C      ilow = 1
C      ihigh = 1
C      nn = ns + 1
C
C      at least one starting point
C
C      IF (m .LT. 1) ifault = 1
C
C      huzmax = hx(1)
C
C      IF ( .NOT. ub) xub = 0.0
C      IF ( .NOT. lb) xlb = 0.0
C
C      hulb = (xlb - x(1)) * hpx(1) + hx(1)
C      huub = (xub - x(1)) * hpx(1) + hx(1)
C
C      if bounded on both sides
C
C      IF ((ub) .AND. (lb)) THEN
C          huzmax = zmax(huub, hulb)
C          horiz = (abs(hpx(1)) .LT. eps)
C          IF (horiz) THEN
C              cu = expon((huub + hulb) * 0.5 - huzmax, emax) * (xub - xlb)
C          ELSE
C              cu = expon(huub - huzmax, emax) *
*              (1 - expon(hulb - huub, emax)) / hpx(1)
C          END IF
C      ELSE IF ((ub) .AND. ( .NOT. lb)) THEN
C
C          if bounded on the right and unbounded on the left
C
C          huzmax = huub
C          cu = 1.0 / hpx(1)
C      ELSE IF (( .NOT. ub) .AND. (lb)) THEN
C
C          if bounded on the left and unbounded on the right

```

```
C
    huzmax = hulb
    cu = -1.0 / hpx(1)
C
C    if unbounded at least 2 starting points
C
ELSE
    cu = 0.0
    IF (m .LT. 2) ifault = 1
END IF
C
IF (cu .GT. 0.0) alcu = zlog(cu)
C
C    set pointers
C
    iipt = 6
    iz = 9
    ihuz = nn + iz
    iscum = nn + ihuz
    ix = nn + iscum
    ihx = nn + ix
    ihpx = nn + ihx
C
C    store values in working vectors
C
    iwv(1) = ilow
    iwv(2) = ihigh
    iwv(3) = ns
    iwv(4) = 1
C
    IF (lb) THEN
        iwv(5) = 1
    ELSE
        iwv(5) = 0
    END IF
C
    IF (ub) THEN
        iwv(6) = 1
    ELSE
        iwv(6) = 0
    END IF
C
    IF (ns .LT. m) ifault = 2
C
    iwv(iipt + 1) = 0
    rwv(1) = hulb
    rwv(2) = huub
    rwv(3) = emax
    rwv(4) = eps
    rwv(5) = cu
    rwv(6) = alcu
    rwv(7) = huzmax
    rwv(8) = xlb
    rwv(9) = xub
    rwv(iscum + 1) = 1.0
    DO 10 i = 1, m
        rwv(ix + i) = x(i)
        rwv(ihx + i) = hx(i)
        rwv(ihpx + i) = hpx(i)
10 CONTINUE
C
```

```

C      create lower and upper hulls
C
      i = 1
20  IF (i .LT. m) THEN
      CALL update(iwv(4), iwv(1), iwv(2), iwv(iipt + 1),
*           rwv(iscum + 1), rwv(5), rwv(ix + 1), rwv(ihx + 1),
*           rwv(ihpx + 1), rwv(iz + 1), rwv(ihuz + 1), rwv(7),
*           rwv(3), lb, rwv(8), rwv(1), ub, rwv(9), rwv(2),
*           ifault, rwv(4), rwv(6))
      i = iwv(4)
      IF (ifault .NE. 0) RETURN
      GO TO 20
END IF

C
C      test for wrong starting points
C
      IF ((.NOT. lb) .AND. (hpx(iwv(1)) .LT. eps)) ifault = 3
      IF ((.NOT. ub) .AND. (hpx(iwv(2)) .GT. -eps)) ifault = 4

C
      RETURN
      END
      SUBROUTINE sample(iwv, rwv, eval, beta, ifault)

C
C      ALGORITHM AS 287.2 APPL.STATIST. (1993), VOL.42, NO.4
C
      INTEGER iwv( * ), ifault
      REAL rwv( * ), beta

C
      INTEGER ihpx, ihuz, ihx, ipt, iscum, ix, iz, nn, ns
      LOGICAL lb, ub
      EXTERNAL EVAL

C
C      set pointers
C
      ipt = 6
      iz = 9
      ns = iwv(3)
      nn = ns + 1
      ihuz = nn + iz
      iscum = nn + ihuz
      ix = nn + iscum
      ihx = nn + ix
      ihpx = nn + ihx
      lb = .FALSE.
      ub = .FALSE.

C
      IF (iwv(5) .EQ. 1) lb = .TRUE.
      IF (iwv(6) .EQ. 1) ub = .TRUE.

C
C      call sampling subroutine
C
      CALL spl1(ns, iwv(4), iwv(1), iwv(2), iwv(iipt + 1),
*           rwv(iscum + 1), rwv(5), rwv(ix + 1), rwv(ihx + 1),
*           rwv(ihpx + 1), rwv(iz + 1), rwv(ihuz + 1), rwv(7), lb,
*           rwv(8), rwv(1), ub, rwv(9), rwv(2), eval, beta, ifault,
*           rwv(3), rwv(4), rwv(6))

C
      RETURN
      END
      SUBROUTINE spl1(ns, n, ilow, ihigh, ipt, scum, cu, x, hx, hpx, z,
*           huz, huzmax, lb, xlb, hulb, ub, xub, huub, eval,

```



```

      *                beta, ifault, emax, eps, alcu)
C
C      ALGORITHM AS 287.3 APPL.STATIST. (1993), VOL.42, NO.4
C
C      this subroutine performs the adaptive rejection sampling, it
C      calls subroutine splhull to sample from the upper hull, if the
C      sampling involves a function evaluation it calls the updating
C      subroutine
C
      INTEGER ns, n, ilow, ihigh, ipt( * ), ifault
      LOGICAL lb, ub
      REAL scum( * ), cu, x( * ), hx( * ), hpx( * ), z( * ), huz( * ),
      *      huzmax, xlb, hulb, xub, huub, beta, emax, eps, alcu
C
      INTEGER i, j, l, n1
      LOGICAL sampld
      REAL a, alhl, alhu, alul, fx, random, u1, u2, zlog
      EXTERNAL eval
C
      zlog(a) = alog(a)
C
      sampld = .FALSE.
10  IF ( .NOT. sampld) THEN
      u2 = random(L)
C
      test for zero random number
C
      IF (u2 .EQ. 0.0) THEN
      ifault = 6
      RETURN
      END IF
      CALL splhull(u2, ipt, ilow, lb, xlb, hulb, huzmax, alcu, x, hx,
      *      hpx, z, huz, scum, eps, emax, beta, i, j)
C
      sample u1 to compute rejection
C
      u1 = random(l)
      IF (u1 .EQ. 0.0) ifault = 6
      alul = zlog(u1)
C
      compute alhu: upper hull at point u1
C
      alhu = hpx(i) * (beta - x(i)) + hx(i) - huzmax
      IF ((beta .GT. x(ilow)) .AND. (beta .LT. x(ihigh))) THEN
C
      compute alhl: value of the lower hull at point u1
C
      IF (beta .GT. x(i)) THEN
      j = i
      i = ipt(i)
      END IF
      alhl = hx(i) + (beta - x(i)) * (hx(i) - hx(j)) /
      *      (x(i) - x(j)) - huzmax
C
      squeezing test
C
      IF ((alhl - alhu) .GT. alul) THEN
      sampld = .TRUE.
      END IF
      END IF
C

```

```

C      if not sampled evaluate the function, do the rejection test
C      and update
C
C      IF ( .NOT. sampld) THEN
C          n1 = n + 1
C          x(n1) = beta
C          CALL eval(x(n1), hx(n1), hpx(n1))
C          fx = hx(n1) - huzmax
C          IF (alul .LT. (fx - alhu)) sampld = .TRUE.
C
C      update while the number of points defining the hulls is lower
C      than ns
C
C          IF (n .LT. ns) THEN
C              CALL update(n, ilow, ihigh, ipt, scum, cu, x, hx, hpx, z,
*                  huz, huzmax, emax, lb, xlb, hulb, ub, xub,
*                  huub, ifault, eps, alcu)
C              END IF
C              IF (ifault .NE. 0) RETURN
C          END IF
C          GO TO 10
C      END IF
C
C      RETURN
C      END
C      SUBROUTINE splhull(u2, ipt, ilow, lb, xlb, hulb, huzmax, alcu, x,
*          hx, hpx, z, huz, scum, eps, emax, beta, i, j)
C
C      ALGORITHM AS 287.4 APPL.STATIST. (1993), VOL.42, NO.4
C
C      this subroutine samples beta from the normalised upper hull
C
C      REAL u2, xlb, hulb, huzmax, alcu, x( * ), hx( * ), hpx( * ),
*          z( * ), huz( * ), scum( * ), eps, emax, beta
C      INTEGER ipt( * ), ilow, i, j
C      LOGICAL lb
C
C      REAL a, eh, expon, logdu, logtg, sign, zlog
C      LOGICAL horiz
C
C      zlog(a) = alog(a)
C      i = ilow
C
C      find from which exponential piece you sample
C
C 10 IF (u2 .GT. scum(i)) THEN
C      j = i
C      i = ipt(i)
C      GO TO 10
C  END IF
C
C      IF (i .EQ. ilow) THEN
C
C          sample below z(ilow), depending on the existence of a lower
C          bound
C
C          IF (lb) THEN
C              eh = hulb - huzmax - alcu
C              horiz = (abs(hpx(ilow)) .LT. eps)
C              IF (horiz) THEN
C                  beta = xlb + u2 * expon(-eh, emax)

```

```

        ELSE
            sign = abs(hpx(i)) / hpx(i)
            logtg = zlog(abs(hpx(i)))
            logdu = zlog(u2)
            eh = logdu + logtg - eh
            IF (eh .LT. emax) THEN
                beta = xlb + zlog(1.0 + sign * expon(eh, emax)) /
*                hpx(i)
            ELSE
                beta = xlb + eh / hpx(i)
            END IF
        END IF
    ELSE
C
C      hpx(i) must be positive, x(ilow) is left of the mode
C
        beta = (zlog(hpx(i) * u2) + alcu - hx(i) + x(i) * hpx(i) +
*        huzmax) / hpx(i)
    END IF
ELSE
C
C      sample above (j)
C
    eh = huz(j) - huzmax - alcu
    horiz = (abs(hpx(i)) .LT. eps)
    IF (horiz) THEN
        beta = z(j) + (u2 - scum(j)) * expon(-eh, emax)
    ELSE
        sign = abs(hpx(i)) / hpx(i)
        logtg = zlog(abs(hpx(i)))
        logdu = zlog(u2 - scum(j))
        eh = logdu + logtg - eh
        IF (eh .LT. emax) THEN
            beta = z(j) + (zlog(1.0 + sign * expon(eh, emax))) /
*            hpx(i)
        ELSE
            beta = z(j) + eh / hpx(i)
        END IF
    END IF
END IF
END IF
C
RETURN
END
SUBROUTINE intersection(x1, y1, yp1, x2, y2, yp2, z1, hz1, eps,
*                        ifault)
C
C      ALGORITHM AS 287.5 APPL.STATIST. (1993), VOL.42, NO.4
C
C      computes the intersection (z1,hz1) between 2 tangents defined
C      by x1, y1, yp1 and x2, y2, yp2
C
REAL x1, y1, yp1, x2, y2, yp2, z1, hz1, eps
INTEGER ifault
C
REAL y12, dh
C
C      first test for non-concavity
C
y12 = y1 + yp1 * (x2 - x1)
y21 = y2 + yp2 * (x1 - x2)
IF ((y21 .LT. y1) .OR. (y12 .LT. y2)) THEN

```

```

        ifault = 5
        RETURN
    END IF
C
    dh = yp2 - yp1
C
    IF the lines are nearly parallel,
    the intersection is taken at the mid-point
C
    IF (abs(dh) .LE. eps) THEN
        z1 = 0.5 * (x1 + x2)
        hz1 = 0.5 * (y1 + y2)
C
    Else compute from the left or the right for greater
    numerical precision
C
    ELSE IF (abs(yp1) .LT. abs(yp2)) THEN
        z1 = x2 + (y1 - y2 + yp1 * (x2 - x1)) / dh
        hz1 = yp1 * (z1 - x1) + y1
    ELSE
        z1 = x1 + (y1 - y2 + yp2 * (x2 - x1)) / dh
        hz1 = yp2 * (z1 - x2) + y2
    END IF
C
    test for misbehaviour due to numerical imprecision
C
    IF ((z1 .LT. x1) .OR. (z1 .GT. x2)) ifault = 7
C
    RETURN
    END
    SUBROUTINE update(n, ilow, ihigh, ipt, scum, cu, x, hx, hpx, z,
*          huz, HUZMAX, EMAX, lb, xlb, hulb, ub, xub, huub,
*          ifault, eps, alcu)
C
    ALGORITHM AS 287.6 APPL.STATIST. (1993), VOL.42, NO.4
C
    this subroutine increments n and updates all the parameters
    which define the lower and the upper hull
C
    INTEGER n, ilow, ihigh, ipt( * ), ifault
    LOGICAL lb, ub
    REAL scum( * ), cu, x( * ), hx( * ), hpx( * ), z( * ), huz( * ),
*    huzmax, emax, xlb, hulb, xub, huub, eps, alcu
C
    INTEGER i, j
    LOGICAL horiz
    REAL a, b, dh, expon, u, zlog, zmax
    EXTERNAL eval
C
    zlog(a) = alog(a)
    zmax(a, b) = amax1(a, b)
C
    n = n + 1
C
    update z, huz and ipt
C
    IF (x(n) .LT. x(ilow)) THEN
C
    insert x(n) below x(ilow), test for non-concavity
C
    IF (hpx(ilow) .GT. hpx(n)) ifault = 5

```

```

C
    ipt(n) = ilow
    CALL intersection(x(n), hx(n), hpx(n), x(ilow), hx(ilow),
*                   hpx(ilow), z(n), huz(n), eps, ifault)
C
    IF (ifault .NE. 0) RETURN
    IF (lb) hulb = hpx(n) * (xlb - x(n)) + hx(n)
C
    ilow = n
ELSE
    i = ilow
    j = i
C
    find where to insert x(n)
C
    10  IF ((x(n) .GE. x(i)) .AND. (ipt(i) .NE. 0)) THEN
        j = i
        i = ipt(i)
        GO TO 10
    END IF
C
    IF (x(n) .GE. x(i)) THEN
C
    insert above x(ihigh), test for non-concavity
C
        IF (hpx(i) .LT. hpx(n)) ifault = 5
C
        ihigh = n
        ipt(i) = n
        ipt(n) = 0
        CALL intersection(x(i), hx(i), hpx(i), x(n), hx(n), hpx(n),
*                   z(i), huz(i), eps, ifault)
C
        IF (ifault .NE. 0) RETURN
C
        huub = hpx(n) * (xub - x(n)) + hx(n)
        z(n) = 0.0
        huz(n) = 0.0
    ELSE
C
    insert x(n) between x(j) and x(i), test for non-concavity
C
        IF ((hpx(j) .LT. hpx(n)) .OR.
*         (hpx(i) .GT. hpx(n))) ifault = 5
C
        ipt(j) = n
        ipt(n) = i
C
    insert z(j) between x(j) and x(n)
C
        CALL intersection(x(j), hx(j), hpx(j), x(n), hx(n), hpx(n),
*                   z(j), huz(j), eps, ifault)
C
        IF (ifault .NE. 0) RETURN
C
    insert z(n) between x(n) and x(i)
C
        CALL intersection(x(n), hx(n), hpx(n), x(i), hx(i), hpx(i),
*                   z(n), huz(n), eps, ifault)
C
        IF (ifault .NE. 0) RETURN

```

```

C
    END IF
END IF

C
C    update huzmax
C
    j = ilow
    i = ipt(j)
    huzmax = huz(j)

C
20 IF ((huz(j) .LT. huz(i)) .AND. (ipt(i) .NE. 0)) THEN
    j = i
    i = ipt(i)
    huzmax = zmax(huzmax, huz(j))
    GO TO 20
END IF

C
IF (lb) huzmax = zmax(huzmax, hulb)
IF (ub) huzmax = zmax(huzmax, huub)

C
C    update cu, scum receives area below exponentiated upper hull
C    left of z(i)
C
    i = ilow
    horiz = (abs(hpx(ilow)) .LT. eps)
    IF ((.NOT. lb) .AND. (.NOT. horiz)) THEN
        cu = expon(huz(i) - huzmax, emax) / hpx(i)
    ELSE IF (lb .AND. horiz) THEN
        cu = (z(ilow) - xlb) * expon(hulb - huzmax, emax)
    ELSE IF (lb .AND. (.NOT. horiz)) THEN
        dh = hulb - huz(i)
        IF (dh .GT. emax) THEN
            cu = -expon(hulb - huzmax, emax) / hpx(i)
        ELSE
            cu = expon(huz(i) - huzmax, emax) * (1 - expon(dh, emax)) /
*           hpx(i)
        END IF
    ELSE
        cu = 0
    END IF
    scum(i) = cu
    j = i
    i = ipt(i)

C
30 IF (ipt(i) .NE. 0) THEN
    dh = huz(j) - huz(i)
    horiz = (abs(hpx(i)) .LT. eps)
    IF (horiz) THEN
        cu = cu + (z(i) - z(j)) * expon((huz(i) + huz(j)) * 0.5 -
*           huzmax, emax)
    ELSE
        IF (dh .LT. emax) THEN
            cu = cu + expon(huz(i) - huzmax, emax) *
*           (1 - expon(dh, emax)) / hpx(i)
        ELSE
            cu = cu - expon(huz(j) - huzmax, emax) / hpx(i)
        END IF
    END IF
    j = i
    i = ipt(i)
    scum(j) = cu

```

```

        GO TO 30
    END IF
C
    horiz = (abs(hpx(i)) .LT. eps)
C
    if the derivative is very small the tangent is nearly
C    horizontal
C
    IF ( .NOT. (ub .OR. horiz)) THEN
        cu = cu - expon(huz(j) - huzmax, emax) / hpx(i)
    ELSE IF (ub .AND. horiz) THEN
        cu = cu + (xub - x(i)) * expon((huub + hx(i)) * 0.5 - huzmax,
*        emax)
    ELSE IF (ub .AND. ( .NOT. horiz)) THEN
        dh = huz(j) - huub
        IF (dh .GT. emax) THEN
            cu = cu - expon(huz(j) - huzmax, emax) / hpx(i)
        ELSE
*        cu = cu + expon(huub - huzmax, emax) *
            (1 - expon(dh, emax)) / hpx(i)
        END IF
    END IF
C
    END IF
C
    scum(i) = cu
    IF (cu .GT. 0) alcu = zlog(cu)
C
    normalize scum to obtain a cumulative probability while
C    excluding unnecessary points
C
    i = ilow
    u = (cu - scum(i)) / cu
C
    IF ((u .EQ. 1.0) .AND. (hpx(ipt(i)) .GT. 0)) THEN
        ilow = ipt(i)
        scum(i) = 0.0
    ELSE
        scum(i) = 1.0 - u
    END IF
C
    j = i
    i = ipt(i)
C
40 IF (ipt(i) .NE. 0) THEN
    j = i
    i = ipt(i)
    u = (cu - scum(j)) / cu
    IF ((u .EQ. 1.0) .AND. (hpx(i) .GT. 0)) THEN
        ilow = i
    ELSE
        scum(j) = 1.0 - u
    END IF
    GO TO 40
END IF
C
    scum(i) = 1.0
    IF (ub) huub = hpx(ihigh) * (xub - x(ihigh)) + hx(ihigh)
    IF (lb) hulb = hpx(ilow) * (xlb - x(ilow)) + hx(ilow)
C
    RETURN
    END
    REAL FUNCTION expon(x, emax)

```

```
C
C      ALGORITHM AS 287.7 APPL.STATIST. (1993), VOL.42, NO.4
C
C      performs an exponential without underflow
C
C      REAL x, emax
C
C      REAL ZEXP
C
C      zexp(x) = exp(x)
C
C      IF (x .LT. -emax) THEN
C          expon = 0.0
C      ELSE
C          expon = zexp(x)
C      END IF
C
C      RETURN
C      END
```



```
      SUBROUTINE GSMIRN (NX, NY, KIND, M, DSTAT, P, Q, IFAULT)
C
C ALGORITHM AS 288 APPL.STATIST. (1994), VOL.43, NO.1
C
C P-value calculation for the generalized two-sample
C Smirnov tests.
C The tests are conditional on ties in the pooled sample.
C
      DIMENSION P(*), M(*)
      REAL P, DSTAT, Q, SLOPE, DELTA, DEVIAT, DL, ONE, ZERO, EPS, FLO
*, SMALL, SCL, SMALLN, T, FL, ALN2, CHKNUM
      LOGICAL NEWRCT
      DATA ONE /1.0/ ZERO /0.0/ EPS /1E-6/
      DATA SMALL /1E-35/ SMALLN /-80.5904782547916/
      DATA ALN2 /0.69314718056/ CHKNUM /1E32/ ITERUP /116/
      FLO(L) = FLOAT(L)
C
      N = NX + NY
      IFAULT = 1
      IF (NX .LE. 0 .OR. NY .LE. 0) RETURN
      IFAULT = 2
      IF (KIND .LT. 1 .OR. KIND .GT. 3) RETURN
      IFAULT = 4
      ICAT = 0
      L = 0
1  L = L + 1
      IF (M(L) .LE. 0) RETURN
      ICAT = ICAT + M(L)
      IF (ICAT - N) 1, 3, 2
2  RETURN
C
3  IFAULT = 0
      Q = ONE
      DELTA = DSTAT - EPS
      IF (DELTA .LE. ZERO) RETURN
      P(1) = ONE
C
C Parameters to define a set for trajectories to lie within it
C
      SLOPE = NX / FLO(N)
      DEVIAT = SLOPE * DELTA * NY
C*  DELTA = DEVIAT
      NEWRCT = .TRUE.
      ICAT = 1
      NTIES = M(1)
      ILE = 0
      IRI = 0
C
C Variables to prevent from overflows in P
C
      IC = ITERUP
      NOFDIV = 0
      SCL = ONE
C
      DO 100 L = 1, N - 1
          IF (NTIES .EQ. 1) THEN
C
C Calculate boundaries for current L (if Lth value in the
C pooled sample is unique or `last' in a series of tied values)
C
          DL = L * SLOPE
```

```
C*      T = FLOAT (L) / N
C*      DEVIAT = DELTA * SQRT (T * (ONE - T))
      IRI = MIN0 (INT (DL + DEVIAT), L, NX)
      ILE = MAX0 (INT (DL - DEVIAT + ONE), L - NY, 0)
      ICAT = ICAT + 1
      NTIES = M(ICAT)
      NEWRCT = .TRUE.
ELSE
C
C      Calculations for tied observations
C
      NTIES = NTIES - 1
C
C      If we have the first observation with the new value (that
C      is not unique), then determine the ICATth `rectangle'
C
      IF (NEWRCT) THEN
        NEWRCT = .FALSE.
        L2 = L + NTIES
C*      IF (L2 .EQ. N) THEN
C*          IRI2 = NX
C*          ILE2 = NX
C*      ELSE
        DL = L2 * SLOPE
C*      T = FLOAT (L2) / N
C*      DEVIAT = DELTA * SQRT (T * (ONE - T))
C
C      X axis boundaries of the subset of `line' L(l+1) within
C      ICATth rectangle
C
        IRI2 = MIN0 (INT (DL + DEVIAT), L2, NX)
        ILE2 = MAX0 (INT (DL - DEVIAT + ONE), L2 - NY, 0)
C*      ENDIF
C
C      Four sides of the rectangle on the X and Y axes
C
        ILEFT = ILE
        IRIGHT = IRI2
        JUPP = L2 - ILE2
        JLOW = L - IRI - 1
      ENDIF
C
C      Calculate boundaries for current L (Lth value is tied)
C
        ILE = MAX0 (ILEFT, L - JUPP)
        IRI = MIN0 (IRIGHT, L - JLOW)
      ENDIF
C
C      Set the left (right) boundary for the one-sided test
C
      GOTO (30, 20, 10) KIND
10    IRI = MIN0 (NX, L)
      GOTO 30
20    ILE = MAX0 (0, L - NY)
C
C      Calculate the number of trajectories p(i,j) for current L
C
30    ILES = MAX0 (1, ILE)
      IRIS = MIN0 (L - 1, IRI)

      DO 50 I = IRIS, ILES, - 1
```

```
50    P(I + 1) = P(I + 1) + P(I)
C
C Check whether elements of P are large enough to multiply
C them by SMALL
C
      IC = IC - 1
      IF (IC .LE. 0) THEN
        DL = ZERO
        DO 60 I = ILES + 1, IRIS + 1
60     DL = MAX (P(I), DL)
        IF (DL .EQ. ZERO) RETURN
        IF (DL .GT. CHKNUM) THEN
          DO 65 I = ILES + 1, IRIS + 1
65     P(I) = P(I) * SMALL
          IC = ITERUP
          NOFDIV = NOFDIV + 1
          SCL = SCL * SMALL
        ELSE
C
C Estimate the number of iterations for DL=Pmax to become
C of order 1/SMALL
C
          IC = (- SMALLN - LOG (DL)) / ALN2
          END IF
        END IF
C
C Define, whether boundaries lie on the left and lower sides
C of the rectangle R and define boundary values for the next
C iterations
C
      IF (ILE .EQ. 0) THEN
        P(ILES) = SCL
      ELSE
        P(ILES) = ZERO
      ENDIF

      IF (IRI .EQ. L) THEN
        P(IRIS + 2) = SCL
      ELSE
        P(IRIS + 2) = ZERO
      ENDIF
C
100 CONTINUE
C
      DL = P(NX + 1) + P(NX)
      IF (DL .EQ. ZERO) RETURN
C
C The P-value
C
      Q= ONE - EXP (FL(NX) + FL(NY) + LOG(DL) - NOFDIV * SMALLN - FL(N))
C
C Q=1 is allowable, Q<=0 is not (accuracy loss due to
C rounding errors)
C
      IF (Q .LE. ZERO) IFAULT = 3
      END
```

```

SUBROUTINE CNV2X2(IK, MXS, MXZ, MXD, LGE, ITAB, HYP, DS, II, K1,
*                K2, IERR)
C
C   ALGORITHM AS 289.1 APPL.STATIST. (1994), VOL.43, NO.1
C
C   Convolves hypergeometric distributions generated by
C   several 2x2 tables
C
C   INTEGER IK, MXS, MXZ, MXD, ITAB(IK,4), II, K1, K2, IERR
C   REAL LGE, HYP(0:MXZ), DS(0:1,0:MXD)
C
C   INTEGER I, IAM, IH1, IH2, ILS, IL1, IL2, IMM, INN, IR, ITT, IXX,
*       J, JJ, JR, KK
C   REAL AM, DD1, DD2, DSMX, EL, HYMAX, ONE, SUMLG, X, ZERO, ZEXP,
*       ZLOG
C
C   DATA ONE, ZERO / 1.0E + 00, 0.0E + 00 /
C
C   EXTERNAL SUMLG
C
C   ZEXP(X) = EXP(X)
C   ZLOG(X) = LOG(X)
C
C   IERR = 0
C
C       Check input parameters
C
C   IF (IK .GT. MXS) IERR = 1
C   K1 = 0
C   DO 10 I = 1, IK
C       IMM = ITAB(I, 1) + ITAB(I, 2)
C       INN = ITAB(I, 3) + ITAB(I, 4)
C       ITT = ITAB(I, 1) + ITAB(I, 3)
C
C       Lower and upper limits for stratum distribution
C
C       IF (ITT .GT. INN) THEN
C           IL1 = ITT - INN
C       ELSE
C           IL1 = 0
C       ENDIF
C       IF (ITT .LT. IMM) THEN
C           IL2 = ITT
C       ELSE
C           IL2 = IMM
C       ENDIF
C       ITT = IL2 - IL1
C       IF (ITT .GT. MXZ) IERR = 2
C       K1 = K1 + IL1
C   10 CONTINUE
C   IF (IERR .GT. 0) RETURN
C
C   DD1 = 10 * ONE
C   EL = LGE * ZLOG(DD1)
C
C       Initialize and set log-scale indicator
C
C   II = 0
C   JJ = 1
C   IR = 0
C   DS(0, 0) = ONE / ZEXP(EL)

```

```

      DSMX = ZERO - EL
      ILS = 0
C
C      For strata = 1, ..., IK, compute hypergeometric distribution
C      and perform convolution in a recursive fashion
C
DO 130 I = 1, IK
  IMM = ITAB(I, 1) + ITAB(I, 2)
  INN = ITAB(I, 3) + ITAB(I, 4)
  ITT = ITAB(I, 1) + ITAB(I, 3)
C
C      Lower and upper limits for convolution
C
  IF (ITT .GT. INN) THEN
    IL1 = ITT - INN
  ELSE
    IL1 = 0
  ENDIF
  IF (ITT .LT. IMM) THEN
    IL2 = ITT
  ELSE
    IL2 = IMM
  ENDIF
  IL2 = IL2 - IL1
  K2 = IR + IL2
  IF (K2 .GT. MXD) THEN
    IERR = 3
    RETURN
  ENDIF
C
C      Compute stratum distribution on log-scale
C
  HYP(0) = ZERO
  DO 20 J = 1, IL2
    DD1 = (FLOAT(IMM-J-IL1+1)) * (FLOAT(ITT-J-IL1+1))
    DD2 = (FLOAT(J+IL1)) * (FLOAT(INN-ITT+J+IL1))
    HYP(J) = HYP(J - 1) + ZLOG(DD1 / DD2)
20  CONTINUE
  IF (ILS .EQ. 1) GOTO 90
C
C      Get maximum hypergeometric coefficient on log-scale and
C      check for potential overflow in stratum distribution
C
  AM = (1.0 + FLOAT(ITT)) / (1.0 + FLOAT(INN + 1)/FLOAT(IMM + 1))
  IAM = IFIX(AM) - IL1
  IF (HYP(0) .GT. HYP(IL2)) THEN
    DO 30 J = 0, IL2
      HYP(J) = HYP(J) - HYP(IL2)
30  CONTINUE
  ENDIF
  HYMAX = HYP(IAM)
  IF (HYMAX .GT. EL) THEN
    ILS = 1
    GOTO 70
  ENDIF
C
C      Check for potential overflow in the ith convolution
C
  IF (IL2 .LT. IR) THEN
    IXX = IL2 + 1
  ELSE

```

```
        IXX = IR + 1
    ENDIF
    DD1 = IXX
    DD1 = ZLOG(DD1)
    DSMX = DSMX + HYMAX + DD1
    IF (DSMX .GE. (EL - ONE)) THEN
        ILS = 1
        GOTO 70
    ENDIF
C
C      Convert stratum distribution to natural scale
C
    DO 40 J = 0, IL2
        HYP(J) = ZEXP(HYP(J))
40    CONTINUE
C
C      Perform convolution on natural scale
C
    DSMX = ZERO - EL
    DO 60 J = 0, K2
        IF (J .GT. IL2) THEN
            IH1 = J - IL2
        ELSE
            IH1 = 0
        ENDIF
        IF (J .LT. IR) THEN
            IH2 = J
        ELSE
            IH2 = IR
        ENDIF
        DS(JJ, J) = DS(II, IH1) * HYP(J - IH1)
        DO 50 JR = IH1 + 1, IH2
            DD1 = DS(II, JR) * HYP(J - JR)
            DS(JJ, J) = DS(JJ, J) + DD1
50    CONTINUE
        DD1 = ZLOG(DS(JJ, J))
        IF (DD1 .GT. DSMX) DSMX = DD1
60    CONTINUE
        GOTO 120
70    CONTINUE
C
C      Convert (i-1)th convolved distribution to log-scale
C
    DO 80 KK = 0, IR
        DS(II, KK) = EL + ZLOG(DS(II, KK))
80    CONTINUE
C
C      Perform convolution on logarithmic scale
C
90    CONTINUE
    DO 110 J = 0, K2
        IF (J .GT. IL2) THEN
            IH1 = J - IL2
        ELSE
            IH1 = 0
        ENDIF
        IF (J .LT. IR) THEN
            IH2 = J
        ELSE
            IH2 = IR
        ENDIF
```

```
        DS(JJ, J) = DS(II, IH1) + HYP(J - IH1)
        DO 100 JR = IH1 + 1, IH2
            DD1 = DS(II, JR) + HYP(J - JR)
            DD2 = DS(JJ, J)
            DS(JJ, J) = SUMLG(DD1, DD2)
100     CONTINUE
110     CONTINUE
C
C     Reset for next step
C
120     II = JJ
        JJ = 1 - II
        IR = K2
C
130 CONTINUE
C
C     Normalize final distribution
C
        IF (ILS .NE. 1) THEN
            DO 140 I = 0, K2
                DS(II, I) = ZLOG(DS(II, I))
140     CONTINUE
            ENDIF
            DSMX = DS(II, 0)
            DO 150 I = 1, K2
                DD1 = DS(II, I)
                DD2 = SUMLG(DSMX, DD1)
                DSMX = DD2
150 CONTINUE
            DO 160 I=0, K2
                DS(II, I) = DS(II, I) - DSMX
160 CONTINUE
            K2 = K1 + K2
            RETURN
        END
C
        REAL FUNCTION SUMLG(DD1, DD2)
C
C     ALGORITHM AS 289.2 APPL.STATIST. (1994), VOL.43, NO.1
C
C     Adds two logarithmic scale numbers
C
        REAL DD1, DD2
C
        REAL DDD, X, ZEXP, ZLOG
C
        ZEXP(X) = EXP(X)
        ZLOG(X) = LOG(X)
C
        DDD = DD1
        IF (DD2 .GT. DD1) DDD = DD2
        DD1 = ZEXP(DD1 - DDD)
        DD2 = ZEXP(DD2 - DDD)
        DDD = ZLOG(DD1 + DD2) + DDD
        SUMLG = DDD
        RETURN
    END
```

```
      SUBROUTINE HALPRN(PARAM, NP, NCOLS, NOBS, NP1, NP2, P1LO, P1HI,  
+          P2LO, P2HI, CONF, NCONF, F, GRID, DIM1, NGRID1, NGRID2,  
+          DERIV, WK, DIMWK, LINDEP, IFAULT)
```

```
C  
C ALGORITHM AS290 APPL. STATIST. (1994) VOL. 43, NO. 1
```

```
C  
C Generate a rectangular 2-D grid of variance ratios from which  
C to plot confidence regions for two parameters using Halperin's  
C method. If the model is linear in all parameters other than  
C the two selected, the confidence regions are exact; otherwise  
C they are approximate and the user should test the sensitivity of  
C the confidence regions to variation in the other parameters.
```

```
C  
C Auxiliary routines required: CLEAR, INCLUD, SS, TOLSET and SING,  
C from AS 274 and a routine DERIV supplied by the user to calculate  
C first derivatives.
```

```
C Arguments:
```

```
C PARAM(NP) Parameter values  
C NP Number of parameters  
C NCOLS Number of first derivatives, usually the same as NP  
C NOBS Number of observations (needed to calculate deg. of freedom  
C NP1, NP2 The numbers (positions) of the two parameters for which  
C the confidence regions are needed  
C P1LO, P1HI Upper and lower limits for parameter number NP1  
C P2LO, P2HI Same for the other parameter  
C CONF(NCONF) The confidence levels in percent  
C NCONF The number of confidence levels  
C F (Output) F ratios corresponding to the confidence levels  
C GRID(DIM1, NGRID2) (Output) 2-D array of variance ratios on a regular  
C grid of values of the two parameters  
C DIM1 1st dimension of array GRID in the calling program  
C NGRID1, NGRID2 The numbers of grid points required  
C DERIV The name of the user's routine to calculate 1st derivatives  
C WK(DIMWK) Workspace  
C DIMWK Must be at least NCOLS(NCOLS + 9)/2  
C LINDEP(NCOLS) (Output) Logical array. LINDEP(I) = .TRUE. if the Ith  
C column of derivatives is linearly related to previous columns  
C IFAULT (Output) Error indicator  
C = 0 if no errors detected  
C = 1 if NCOLS < 2  
C = 2 if NOBS < NCOLS  
C = 4 if NP1 outside the range 1 to NP  
C = 8 ditto for NP2  
C = 16 if NP1 = NP2  
C = 32 if NGRID1 < 2 or NGRID2 < 2 or NGRID1 > DIM1  
C = 64 if DIMWK is too small  
C = -I if the Ith confidence level is not between 0 and 100  
C N.B. IFAULT may equal a sum of some of the above values if there is more  
C than one error.
```

```
C  
C INTEGER NP, NCOLS, NOBS, NP1, NP2, NCONF, DIM1, NGRID1, NGRID2,  
+ DIMWK, IFAULT  
C REAL PARAM(NP), P1LO, P1HI, P2LO, P2HI, CONF(*), F(NCONF),  
+ GRID(DIM1, NGRID2), WK(DIMWK)  
C LOGICAL LINDEP(NCOLS)  
C EXTERNAL DERIV
```

```
C  
C Local variables
```

```
C  
C INTEGER I, NDF, NRBAR, XPTR, DPTR, THPTR, RSSPTR, TOLPTR, I1, I2,
```



```
+      IOBS
REAL ZERO, ONE, HUNDRD, HALF, TWO, Q, RESID, SSERR, STEP1, STEP2,
+      WT, P1SAVE, P2SAVE, SSQ1
DATA ZERO/0.0/, ONE/1.0/, HUNDRD/100.0/, HALF/0.5/, TWO/2.0/,
+      WT/1.0/
C
C      Some checks
C
      IFAULT = 0
      IF (NCOLS .LT. 2) IFAULT = 1
      IF (NOBS .LE. NCOLS) IFAULT = IFAULT + 2
      IF (NP1 .LT. 1 .OR. NP1 .GT. NP) IFAULT = IFAULT + 4
      IF (NP2 .LT. 1 .OR. NP2 .GT. NP) IFAULT = IFAULT + 8
      IF (NP1 .EQ. NP2) IFAULT = IFAULT + 16
      IF (NGRID1 .LT. 2 .OR. NGRID2 .LT. 2 .OR. NGRID1 .GT. DIM1)
+      IFAULT = IFAULT + 32
      IF (IFAULT .GT. 0) RETURN
C
C      Set up pointers to the workspace.
C
      NRBAR = NCOLS * (NCOLS - 1) / 2
      XPTR = NRBAR + 1
      DPTR = XPTR + NCOLS
      THPTR = DPTR + NCOLS
      RSSPTR = THPTR + NCOLS
      TOLPTR = RSSPTR + NCOLS
      IF (TOLPTR + NCOLS - 1 .GT. DIMWK) THEN
          IFAULT = 64
          RETURN
      END IF
C
C      Calculate step sizes.
C
      STEP1 = (P1HI - P1LO) / (NGRID1 - 1)
      STEP2 = (P2HI - P2LO) / (NGRID2 - 1)
      P1SAVE = PARAM(NP1)
      P2SAVE = PARAM(NP2)
C-----
C
C      Start of cycle through the grid.
C
      PARAM(NP1) = P1LO
      DO 30 I1 = 1, NGRID1
          PARAM(NP2) = P2LO
          DO 20 I2 = 1, NGRID2
C
C      Initialize orthogonal reduction.
C
          CALL CLEAR(NCOLS, NRBAR, WK(DPTR), WK, WK(THPTR), SSERR,
*              IFAULT)
          DO 10 IOBS = 1, NOBS
              CALL DERIV(PARAM, NP, NCOLS, IOBS, WK(XPTR), RESID, WT)
C
C      Re-order the derivatives so that those for parameters NP1 & NP2
C      are at the end.
C
          IF (NP1 .LT. NCOLS-1) THEN
              IF (NP2 .NE. NCOLS-1) THEN
                  Q = WK(XPTR + NCOLS - 2)
                  WK(XPTR + NCOLS - 2) = WK(XPTR + NP1 - 1)
                  WK(XPTR + NP1 - 1) = Q
```

```

        ELSE
          Q = WK(XPTR + NCOLS - 1)
          WK(XPTR + NCOLS - 1) = WK(XPTR + NP1 - 1)
          WK(XPTR + NP1 - 1) = Q
        END IF
      END IF
    IF (NP2 .LT. NCOLS-1) THEN
      Q = WK(XPTR + NCOLS - 1)
      WK(XPTR + NCOLS - 1) = WK(XPTR + NP2 - 1)
      WK(XPTR + NP2 - 1) = Q
    END IF
  C
  C   Update QR factorization.
  C
  C           CALL INCLUD(NCOLS, NRBAR, WT, WK(XPTR), RESID, WK(DPTR), WK,
+           WK(THPTR), SSERR, IFAULT)
  10   CONTINUE
  C
  C-----
  C
  C   Test for singularities
  C
  C   CALL TOLSET(NCOLS, NRBAR, WK(DPTR), WK, WK(TOLPTR), WK(XPTR),
+   IFAULT)
  C   CALL SING(NCOLS, NRBAR, WK(DPTR), WK, WK(THPTR), SSERR,
+   WK(TOLPTR), LINDEP, WK(XPTR), IFAULT)
  C
  C   If IFAULT < 0, it contains the rank deficiency.
  C
  C   NDF = NOBS - NCOLS - IFAULT
  C
  C   Calculate variance ratio.
  C
  C           CALL SS(NCOLS, WK(DPTR), WK(THPTR), SSERR, WK(RSSPTR), IFAULT)
  C           IF (NCOLS .GT. 2) THEN
  C             SSQ1 = WK(RSSPTR + NCOLS - 3)
  C           ELSE
  C             SSQ1 = WK(RSSPTR) + WK(DPTR)*WK(THPTR)**2
  C           END IF
  C           GRID(I1, I2) = HALF * (SSQ1 - SSERR) / (SSERR / NDF)
  C           PARAM(NP2) = PARAM(NP2) + STEP2
  20   CONTINUE
  C           PARAM(NP1) = PARAM(NP1) + STEP1
  30   CONTINUE
  C
  C           PARAM(NP1) = P1SAVE
  C           PARAM(NP2) = P2SAVE
  C
  C   Convert confidence levels in % to F-values, if NCONF > 0.
  C
  C   DO 40 I = 1, NCONF
  C     Q = ONE - CONF(I) / HUNDRD
  C     IF (Q .LE. ZERO .OR. Q .GT. ONE) THEN
  C       IFAULT = -I
  C       RETURN
  C     END IF
  C     F(I) = HALF * NDF * (Q**(-TWO/NDF) - ONE)
  40   CONTINUE
  C
  C   RETURN
  C   END

```

```

SUBROUTINE OCCALC(SSEQ, L, MAXL, OC)
C
C   ALGORITHM AS 291.1 APPL.STATIST. (1994), VOL.43, NO.2
C
C   Calculates overlap capability of subsequence SSEQ of length L
C   OC(I) = 1 if SSEQ can overlap its own last I letters
C           (I = 1, ... , L)
C           = 0 otherwise
C
C   INTEGER L, MAXL, OC(MAXL), SSEQ(MAXL)
C
C   INTEGER I, INDEX, LM1, LMI
C
C   OC(L) = 1
C   LM1 = L - 1
C   DO 20 I = 1, LM1
C       LMI = L - I
C       OC(I) = 0
C       DO 10 INDEX = 1, I
C           IF (SSEQ(INDEX) .EQ. SSEQ(INDEX + LMI)) GO TO 10
C       GO TO 20
10  CONTINUE
C       OC(I) = 1
20  CONTINUE
C   RETURN
C   END

SUBROUTINE EXPVAR(M, L, MAXL, OC, P, EXPECT, VARIAN, IFAULT)
C
C   ALGORITHM AS 291.2 APPL.STATIST. (1994), VOL.43, NO.2
C
C   Compute expected value and variance of frequency of
C   occurrence
C
C   INTEGER M, L, MAXL, OC(MAXL), IFAULT
C   REAL P(MAXL), EXPECT, VARIAN
C
C   INTEGER I, INDEX, LM1, NN
C   REAL TERM
C
C   IFAULT = 1
C   IF (M .LT. L .OR. L .LT. 2 .OR. L .GT. MAXL) RETURN
C   IFAULT = 0
C   NN = M - L + 1
C   EXPECT = NN * P(L)
C   VARIAN = EXPECT * (1.0 - EXPECT)
C   IF ((NN - L) .GT. 0) VARIAN = VARIAN +
*   ((P(L) ** 2) * (NN - L) * (NN - L + 1))
C   TERM = 0.0
C   LM1 = L - 1
C   DO 10 I = 1, LM1
C       IF ((NN - I) .LE. 0) GO TO 10
C       INDEX = L - I
C       IF (OC(INDEX) .EQ. 0) GO TO 10
C       TERM = TERM + OC(INDEX) * (NN - I) * P(I)
10  CONTINUE
C   TERM = 2.0 * P(L) * TERM
C   VARIAN = VARIAN + TERM
C   RETURN
C   END

```

```
      SUBROUTINE PROW(M, N, MAXNP1, L, MAXL, OC, INDPP, C, POWER, PP,  
*          ROWNEW, IFAULT)  
C  
C      ALGORITHM AS 291.3 APPL.STATIST. (1994), VOL.43, NO.2  
C  
C      Calculate prob(J occurrences of a subsequence of length L  
C          within a sequence of length M) for J = 0, ... , N.  
C      Prob(J occurrences) is stored in ROWNEW(J + 1)  
C  
C      INTEGER M, N, MAXNP1, L, MAXL, OC(MAXL), INDPP(MAXL), IFAULT  
C      REAL C(MAXL, 2), POWER(MAXL), PP(MAXL, MAXNP1),  
*          ROWNEW(MAXNP1)  
C  
C      INTEGER I, INDOLD, IP1, JP1, LM1, NP1, SEQLEN  
C  
C      Calculate IFAULT  
C  
C      IFAULT = 0  
C      NP1 = N + 1  
C      IF (M .GE. L .AND. N .GE. 0 .AND. N .LE. M - L + 1  
* .AND. NP1 .LE. MAXNP1 .AND. L .GE. 2 .AND. L .LE. MAXL) GO TO 10  
C      IFAULT = 1  
C      GO TO 80  
C  
C      Initialize PP using boundary conditions  
C      (PP = previous L rows of probabilities needed to calculate  
C          ROWNEW recursively)  
C  
10 DO 30 IP1 = 1, L  
C      PP(IP1, 1) = 1.0  
C      IF (N .LT. 1) GO TO 30  
C      DO 20 JP1 = 2, NP1  
C          PP(IP1, JP1) = 0.0  
20 CONTINUE  
30 CONTINUE  
C  
C      Initialize INDPP  
C      (INDPP = address in PP of rows 1 to L of P)  
C  
C      DO 40 I = 1, L  
C          INDPP(I) = I  
40 CONTINUE  
C  
C      Loop to generate new rows of PP recursively  
C  
C      DO 70 SEQLEN = L, M  
C  
C      Generate next row of probabilities  
C  
C      CALL ROWGEN(N, L, MAXL, OC, MAXNP1, PP, INDPP, C,  
*          POWER, ROWNEW)  
C      IF (SEQLEN .EQ. M) GO TO 80  
C  
C      Shift rows of PP up one, overwriting first row  
C      (effectively, using indirect addresses)  
C  
C      LM1 = L - 1  
C      INDOLD = INDPP(1)  
C      DO 50 I = 1, LM1  
C          INDPP(I) = INDPP(I + 1)  
50 CONTINUE
```

```

        INDPP(L) = INDOLD
C
C      Move ROWNEW into bottom row of PP
C      (effectively, using indirect addresses)
C
        DO 60 JP1 = 1, NP1
            PP(INDOLD, JP1) = ROWNEW(JP1)
60     CONTINUE
70     CONTINUE
80     RETURN
        END
C
        SUBROUTINE ROWGEN (N, L, MAXL, OC, MAXNP1, PP,
*           INDPP, C, POWER, ROWNEW)
C
C      ALGORITHM AS 291.4 APPL.STATIST. (1994), VOL.43, NO.2
C
C      Used by SUBROUTINE PROW to calculate one row of values:
C      prob(J occurrences of subsequence of length L)
C      for J = 0, ... , N.
C      Prob(J occurrences) is stored in ROWNEW(J + 1)
C
        INTEGER N, L, MAXL, OC(MAXL), MAXNP1, INDPP(MAXL)
        REAL PP(MAXL, MAXNP1), C(MAXL, 2), POWER(MAXL),
*          ROWNEW(MAXNP1)
C
        INTEGER I, INDEX, J, JNDEX, JP1, K, LIMJ, LM1, LM2, NP1
        REAL Q, Q1
C
        NP1 = N + 1
        LM1 = L - 1
        LM2 = L - 2
        DO 10 I = 1, NP1
            ROWNEW(I) = 0.0
10     CONTINUE
C
        Define C and POWER:
C      - C is coefficients in recursive formula;
C      - POWER is powers in recursive formula
C
        DO 20 I = 1, L
            POWER(I) = 4 ** I
20     CONTINUE
        Q = OC(L - 1)
        C(1, 1) = (4.0 - Q) / POWER(1)
        C(1, 2) = Q / POWER(1)
        Q = OC(1)
        C(L, 1) = (4.0 * Q - 1.0) / POWER(L)
        C(L, 2) = -C(L, 1)
        IF (L .EQ. 2) GO TO 40
        DO 30 K = 1, LM2
            Q = OC(K)
            Q1 = OC(K + 1)
            C(L - K, 1) = ( - Q + 4.0 * Q1) / POWER(L - K)
            C(L - K, 2) = -C(L - K, 1)
30     CONTINUE
C
        Compute new probabilities from old ones
C
40     DO 70 JP1 = 1, NP1
            ROWNEW(JP1) = 0.0

```

```
LIMJ = 2
IF (JP1 .EQ. 1) LIMJ = 1
DO 60 J = 1, LIMJ
  DO 50 I = 1, L
    INDEX = INDPP(L - I + 1)
    JINDEX = JP1 - J + 1
    ROWNEW(JP1) = ROWNEW(JP1) + C(I, J) * PP(INDEX, JINDEX)
50  CONTINUE
60  CONTINUE
70  CONTINUE
RETURN
END
```

```
      SUBROUTINE LSINF(IDIST, ITYPE, ZL, ZR, F11, F12, F22, IFAULT)
C
C      ALGORITHM AS 292.1 APPL.STATIST. (1994), VOL.43, NO.3
C
C      Computes Fisher information matrix elements for time (type I)
C      or failure (type II) censored units from the smallest extreme
C      value (sev), largest extreme value (lev), normal or logistic
C      distribution
C
      INTEGER IDIST, ITYPE, IFAULT
      REAL ZL, ZR, F11, F12, F22
C
      INTEGER NDIST
C
      PARAMETER (NDIST = 4)
C
      REAL BIG, BOUNDS(2, NDIST), CDF, DEN, ETA, PDF, SUR, THET0L,
*      THET1L, THET2L, THET0R, THET1R, THET2R, ZERO, ZMAX, ZMIN,
*      ZU
C
      DATA BOUNDS / 3.6E + 00, -34.0E + 00,
*      34.0E + 00, -3.6E + 00,
*      8.0E + 00, -8.0E + 00,
*      34.0E + 00, -34.0E + 00 /
C
      PARAMETER (BIG = 1.0E + 10, ZERO = 0.0E + 00)
C
      EXTERNAL LSINT
C
      Check for illegal idist
C
      IFAULT = 1
      IF (IDIST .LT. 1 .OR. IDIST .GT. NDIST) RETURN
C
      Check for illegal itype
C
      IFAULT = 2
      IF (ITYPE .LT. 1 .OR. ITYPE .GT. 4) RETURN
C
      Check for illegal arguments
C
      IFAULT = 3
      IF (ITYPE .EQ. 4 .AND. ZL .GT. ZR) RETURN
      IFAULT = 0
      ZMAX = BOUNDS(1, IDIST)
      ZMIN = BOUNDS(2, IDIST)
C
      Identify the censoring type
C
      GOTO (10, 20, 30, 40), ITYPE
C
      Uncensored case
C
      10 CALL LSINT(IDIST, ZMIN, ZMAX, BIG, F11, F12, F22, IFAULT)
      RETURN
C
      Right censored at zr
C
      20 CALL LSINT(IDIST, ZMIN, ZMAX, ZR, F11, F12, F22, IFAULT)
      RETURN
C
```

```
C      Left censored at z1
C
30 ZU = BIG
C
C      Left and right censored data
C
40 IF (ITYPE .EQ. 4) ZU = ZR
   CALL LSINT(IDIST, ZMIN, ZMAX, ZU, THET0R, THET1R, THET2R, IFAULT)
   IF (IFAUULT .EQ. 4 .OR. IFAUULT .EQ. 5) RETURN
   CALL LSINT(IDIST, ZMIN, ZMAX, ZL, THET0L, THET1L, THET2L, IFAULT)
   IF (IFAUULT .EQ. 4 .OR. IFAUULT .EQ. 5) RETURN
C
   ETA = ZERO
   IF (ZL .GT. ZMIN .AND. ZL .LT. ZMAX) THEN
     CALL PCSFUN(IDIST, ZL, PDF, CDF, SUR)
     DEN = CDF * SUR
     IF (DEN .GT. ZERO) ETA = PDF * PDF / DEN
   ENDIF
C
C      Left or left and right censored data - Fisher matrix elements
C
F11 = THET0R - THET0L + ETA
F12 = THET1R - THET1L + ZL * ETA
F22 = THET2R - THET2L + ZL * ZL * ETA
RETURN
END
C
SUBROUTINE LSINT(IDIST, ZMIN, ZMAX, Z, THETA0, THETA1, THETA2,
*                IFAULT)
C
C      ALGORITHM AS 292.2 APPL.STATIST. (1994), VOL.43, NO.3
C
C      Computes theta0, theta1, theta2 for the sev, lev, normal and
C      logistic distributions
C
INTEGER IDIST, IFAULT
REAL ZMIN, ZMAX, Z, THETA0, THETA1, THETA2
C
INTEGER NDIST
PARAMETER (NDIST = 4)
C
INTEGER IDISEV, J, JMAXLO, JTERM, N
REAL ASYM(3, NDIST), ANUZ, CDF, CONST0, DEN, DUM, EMABSZ, ETASEV,
*   HALF, ONE, PDF, SUR, S3, S3OLD, THREE, TMP0, TMP1, TOL, TWO,
*   T0SEV, T1SEV, T2SEV, WKSP(40), X1, X2, X3, X4, ZERO, ZSEV
C
DATA ASYM /
* 1.0E + 00, 0.4227843350984671E + 00, 0.1823680660852879E + 01,
* 1.0E + 00, -0.4227843350984671E + 00, 0.1823680660852879E + 01,
* 1.0E + 00, 0.0E + 00, 2.0E + 00,
* 0.3333333333333333E + 00, 0.0E + 00, 0.14299560445654842E + 01 /
C
PARAMETER (CONST0 = 0.1644934066848226E + 01, HALF = 0.5E + 00,
*          IDISEV = 1, JMAXLO = 40, ONE = 1.0E + 00,
*          THREE = 3.0E + 00, TOL = 1.0E - 11, TWO = 2.0E + 00,
*          ZERO = 0.0E + 00)
C
EXTERNAL INTEGR, PCSFUN
C
IFAUULT = 0
C
```



```
C      Routing computations
C
C      IF (Z .LE. ZMIN) THEN
C
C      Integrals are negligible
C
C      THETA0 = ZERO
C      THETA1 = ZERO
C      THETA2 = ZERO
C      ELSE IF (Z .GE. ZMAX) THEN
C
C      Integrals take limiting values
C
C      THETA0 = ASYM(1, IDIST)
C      THETA1 = ASYM(2, IDIST)
C      THETA2 = ASYM(3, IDIST)
C      ELSE
C
C      Computed integrals - z is in interval (zmin, zmax)
C      First select the distribution
C
C      GOTO (10, 20, 30, 40), IDIST
C
C      Smallest extreme value (sev) distribution
C
C      10  CALL INTEGR(Z, THETA0, THETA1, THETA2, IFAULT)
C         IF (IFAULT .NE. 0) IFAULT = 4
C         RETURN
C
C      Largest extreme value (lev) distribution
C      First compute thetas and eta for the sev at -z
C
C      20  ZSEV = -Z
C         CALL INTEGR(ZSEV, T0SEV, T1SEV, T2SEV, IFAULT)
C         IF (IFAULT .NE. 0) THEN
C           IFAULT = 4
C           RETURN
C         ENDIF
C         ETASEV = ZERO
C         CALL PCSFUN(IDISEV, ZSEV, PDF, CDF, SUR)
C         DEN = CDF * SUR
C         IF (DEN .GT. ZERO) ETASEV = PDF * PDF / DEN
C
C      Compute thetas for the lev
C
C      THETA0 = ONE - T0SEV + ETASEV
C      THETA1 = ASYM(2, IDIST) + T1SEV + Z * ETASEV
C      THETA2 = ASYM(3, IDIST) - T2SEV + Z * Z * ETASEV
C      RETURN
C
C      Normal distribution
C
C      30  CALL PCSFUN(IDIST, Z, PDF, CDF, SUR)
C         THETA0 = CDF - Z * PDF
C         IF (SUR .GT. ZERO) THETA0 = THETA0 + PDF * PDF / SUR
C         THETA1 = Z * THETA0 - Z * CDF - PDF
C         THETA2 = Z * THETA1 + TWO * CDF
C         RETURN
C
C      Logistic distribution
C
C
```

```

40    CALL PCSFUN(IDIST, Z, PDF, CDF, SUR)
      THETA0 = (ONE - SUR ** 3) / THREE
      TMP0 = LOG(ONE + EXP(Z))
      THETA1 = Z * THETA0 + (PDF - TMP0) / THREE
C
C    Compute theta2 for the logistic
C    S3 is computed using a power series expansion with
C    accelerated convergence using Euler transformation
C
      EMABSZ = EXP(-ABS(Z))
      X1 = EMABSZ
      S3 = ZERO
C
C    Euler partial sum based on the first term
C
      N = 1
      WKSP(1) = X1
      S3 = HALF * X1
      S3OLD = S3
      DO 60 JTERM = 2, JMAXLO
        X2 = REAL(JTERM) ** 2
        X3 = REAL(JTERM - 1) ** 2
        X1 = -X1 * EMABSZ * X3 / X2
C
C    Euler partial sum based on two or more terms
C
      TMP1 = WKSP(1)
      WKSP(1) = X1
      DO 50 J = 1, N
        IF (J .LT. N) DUM = WKSP(J + 1)
        WKSP(J + 1) = HALF * (WKSP(J) + TMP1)
        IF (J .LT. N) TMP1 = DUM
50    CONTINUE
C
C    Euler improved partial sums
C
      IF (ABS(WKSP(N + 1)) .GT. ABS(WKSP(N))) THEN
        S3 = S3 + WKSP(N + 1)
      ELSE
        S3 = S3 + HALF * WKSP(N + 1)
        N = N + 1
      ENDIF
C
C    Tests for convergence of the series - a fault is declared if
C    convergence is not reached in a maximum of jmaxlo terms
C
      X4 = ABS(S3OLD - S3)
      S3OLD = S3
      IF (X4 .LT. TOL) THEN
C
C    Add terms to obtain the integral
C
        ANUZ = S3
        IF (Z .GT. ZERO) ANUZ = CONST0 + Z * Z / TWO - S3
        THETA2 = Z * THETA1
        *      + (CDF - Z * TMP0 + Z * PDF + TWO * ANUZ) / THREE
        RETURN
      ENDIF
60    CONTINUE
      IFAULT = 5
      ENDIF

```

```
      RETURN
      END
C
      SUBROUTINE PCSFUN(IDIST, Z, PDF, CDF, SUR)
C
C      ALGORITHM AS 292.3 APPL.STATIST. (1994), VOL.43, NO.3
C
C      Computes the p.d.f., c.d.f. and survival functions for the
C      sev, lev, normal and logistic distributions
C
      INTEGER IDIST
      REAL Z, PDF, CDF, SUR
C
      REAL ALNORM, CVAL, ENZ, EPZ, HALF, ONE
C
      PARAMETER (CVAL = 0.3989422804014326E + 00, HALF = 0.5E + 00,
*              ONE = 1.0E + 00)
C
      EXTERNAL ALNORM
C
      Select the distribution
C
      GOTO (10, 20, 30, 40), IDIST
C
      sev
C
10  EPZ = EXP(Z)
      PDF = EXP(Z - EPZ)
      CDF = ONE - EXP(-EPZ)
      SUR = EXP(-EPZ)
      RETURN
C
      lev
C
20  ENZ = EXP(-Z)
      PDF = EXP(-Z - ENZ)
      CDF = EXP(-ENZ)
      SUR = ONE - EXP(-ENZ)
      RETURN
C
      Normal
C
30  PDF = CVAL * EXP(-HALF * Z * Z)
      CDF = ALNORM(Z, .FALSE.)
      SUR = ALNORM(Z, .TRUE.)
      RETURN
C
      Logistic
C
40  ENZ = EXP(-Z)
      CDF = ONE / (ONE + ENZ)
      SUR = ENZ / (ONE + ENZ)
      PDF = CDF * SUR
      RETURN
C
      END
```

```

SUBROUTINE CNV2XK(IK, K, MC, MXC, MXR, MS, MZ, MD, LGE, ITAB, ISC,
*          LBUF, CBUF, X, DS, LFACT, II, K1, K2, IERR)
C
C      ALGORITHM AS 293.1 APPL.STATIST. (1994), VOL.43, NO.3
C
C      Convolves conditional distributions generated by
C      several 2xK tables
C
C      INTEGER IK, K, MC, MXC, MXR, MS, MZ, MD, ITAB(MS, 2, MC), ISC,
*          LBUF(0:1, 0:MXR, 2), X(MC, 0:2), II, K1, K2, IERR
REAL LGE, CBUF(0:1, 0:MZ), DS(0:1, 0:MD), LFACT(MXC+1)
C
C      INTEGER I, IAA, IH1, IH2, IKK, ILS, IMC, IMM, IMR, IXX, IZ1, IZ2,
*          J, JJ, JR, KK
REAL DD1, DD2, DSMX, EL, HYMAX, ONE, SUMLG, Y, ZERO, ZEXP, ZLOG
C
C      DATA ONE, ZERO / 1.0E + 00, 0.0E + 00 /
C
C      EXTERNAL SUMLG
C
C      ZEXP(Y) = EXP(Y)
C      ZLOG(Y) = ALOG(Y)
C
C      IERR = 0
C
C      Check input parameters
C
C      IF (IK .GT. MS) IERR = 1
C      IF (K .GT. MC) IERR = 2
C      IAA = 0
C      DO 20 I = 1, IK
C          IMM = 0
C          IMR = 0
C          DO 10 J = 1, K
C              IMM = IMM + ITAB(I, 1, J) + ITAB(I, 2, J)
C              IMR = IMR + ITAB(I, 2, J)
C              IMC = ITAB(I, 1, J) + ITAB(I, 2, J)
C              IF (IMC .GT. MXC) IERR = 3
C              IAA = MAX0(IAA, IMC)
10      CONTINUE
C          IF (IMR .GT. MXR) IERR = 4
20      CONTINUE
C      IF (IERR .GT. 0) RETURN
C
C      DD1 = 10 * ONE
C      EL = LGE * ZLOG(DD1)
C
C      Compute log-factorials:
C          LFACT(I) = LOG( (I - 1)! )
C
C      LFACT(1) = ZERO
C      DO 30 I = 2, IAA + 1
C          DD1 = I - 1
C          LFACT(I) = LFACT(I - 1) + ZLOG(DD1)
30      CONTINUE
C
C      Initialize and set scale indicator
C
C      II = 0
C      JJ = 1
C      IR = 0

```

```

      K1 = 0
      DS(0, 0) = ONE / ZEXP(EL)
      DSMX = ZERO - EL
      ILS = 0
C
C      For strata = 1, ..., IK, compute sub-distributions and
C      perform convolution in a recursive fashion
C
      DO 160 I = 1, IK
C
C      Extract the ith stratum
C
      IAA = 0
      IKK = 0
      DO 40 J = 1, K
          X(J, 0) = ITAB(I, 1, J)
          X(J, 1) = ITAB(I, 2, J)
          IKK = IKK + X(J, 1)
          IAA = IKK + X(J, 0)
40      CONTINUE
C
C      Log-scale check
C
      IF (ILS .EQ. 1) GOTO 110
C
C      Check for overflow in ith conditional distribution
C
      HYMAX = LFACT(IAA + 1) - LFACT(IKK + 1)
      HYMAX = HYMAX - LFACT(IAA - IKK + 1)
      IF (HYMAX .GT. EL) ILS = 1
      CALL EX2XK(K, MC, MXC, MXR, MZ, ILS, EL, X, CBUF, LBUF, LFACT,
*           IP, ISC, IZ1, IZ2, IERR)
      IF (IERR .GT. 0) RETURN
C
C      Lower and upper limits for convolution
C
      K1 = K1 + IZ1
      IZ2 = IZ2 - IZ1
      K2 = IR + IZ2
      IF (K2 .GT. MD) THEN
          IERR = 5
          RETURN
      ENDIF
      IF (ILS .EQ. 1) GOTO 90
C
C      Check for potential overflow in ith convolution
C
      IF (IZ2 .LT. IR) THEN
          IXX = IZ2 + 1
      ELSE
          IXX = IR + 1
      ENDIF
      DD1 = IXX
      DD1 = ZLOG(DD1)
      DSMX = DSMX + HYMAX + DD1
      IF (DSMX .GE. (EL - ONE)) THEN
          ILS = 1
          GOTO 70
      ENDIF
C
C      Perform convolution on natural scale

```

```

C
DSMX = ZERO - EL
DO 60 J = 0, K2
  IF (J .GT. IZ2) THEN
    IH1 = J - IZ2
  ELSE
    IH1 = 0
  ENDIF
  IF (J .LT. IR) THEN
    IH2 = J
  ELSE
    IH2 = IR
  ENDIF
  DS(JJ, J) = DS(II, IH1) * CBUF(IP, J - IH1)
  DO 50 JR = IH1 + 1, IH2
    DD1 = DS(II, JR) * CBUF(IP, J - JR)
    DS(JJ, J) = DS(JJ, J) + DD1
50  CONTINUE
  IF (DS(JJ, J) .GT. ZEXP(-EL)) THEN
    DD1 = ZLOG(DS(JJ, J))
  ELSE
    DD1 = -EL
  ENDIF
  IF (DD1 .GT. DSMX) DSMX = DD1
60  CONTINUE
  GOTO 150
C
C      Convert ith stratum distribution to log-scale
C
70  CONTINUE
DO 80 KK = 0, IR
  CBUF(IP, KK) = ZLOG(CBUF(IP, KK))
80  CONTINUE
C
C      Convert (i-1)th cumulated distribution to log-scale
C
90  CONTINUE
DO 100 KK = 0, IR
  DS(II, KK) = EL + ZLOG(DS(II, KK))
100 CONTINUE
DSMX = EL + DSMX
GOTO 120
C
C      Perform convolution on logarithmic scale
C
110 CONTINUE
CALL EX2XK(K, MC, MXC, MXR, MZ, ILS, EL, X, CBUF, LBUF, LFACT,
*      IP, ISC, IZ1, IZ2, IERR)
IF (IERR .GT. 0) RETURN
K1 = K1 + IZ1
IZ2 = IZ2 - IZ1
K2 = IR + IZ2
IF (K2 .GT. MD) THEN
  IERR = 5
  RETURN
ENDIF
120 CONTINUE
DO 140 J = 0, K2
  IF (J .GT. IZ2) THEN
    IH1 = J - IZ2
  ELSE

```

```

        IH1 = 0
    ENDIF
    IF (J .LT. IR) THEN
        IH2 = J
    ELSE
        IH2 = IR
    ENDIF
    DS(JJ, J) = DS(II, IH1) + CBUF(IP, J - IH1)
    DO 130 JR = IH1 + 1, IH2
        DD1 = DS(II, JR) + CBUF(IP, J - JR)
        DD2 = DS(JJ, J)
        DS(JJ, J) = SUMLG(DD1, DD2)
130    CONTINUE
140    CONTINUE
C
C    Reset for next step
C
150    II = JJ
        JJ = 1 - II
        IR = K2
160    CONTINUE
C
C    Normalize final distribution
C
    IF (ILS .NE. 1) THEN
        DO 170 I = 0, K2
            IF (DS(II, I) .EQ. ZERO) THEN
                DS(II, I) = -EL
            ELSE
                DS(II, I) = EL + ZLOG(DS(II, I))
            ENDIF
170    CONTINUE
        ENDIF
        DSMX = DS(II, 0)
        DO 180 I = 1, K2
            DD1 = DS(II, I)
            IF (DD1 .EQ. -EL) GOTO 180
            DD2 = SUMLG(DSMX, DD1)
            DSMX = DD2
180    CONTINUE
        DO 190 I = 0, K2
            IF (DS(II, I) .EQ. -EL) GOTO 190
            DS(II, I) = DS(II, I) - DSMX
190    CONTINUE
        K2 = K1 + K2
        RETURN
    END
C
    SUBROUTINE EX2XK(K, MC, MXC, MXR, MZ, ILS, EL, X, CBUF, LBUF,
*                   LFACT, IP, ISC, IZ1, IZ2, IERR)
C
C    ALGORITHM AS 293.2 APPL.STATIST. (1994), VOL.43, NO.3
C
C    Recursively generates the exact distribution for a single
C    ordered 2xK table using a bivariate shift algorithm
C
    INTEGER K, MC, MXC, MXR, MZ, ILS, X(MC, 0:2),
*         LBUF(0:1, 0:MXR, 2), IP, ISC, IZ1, IZ2, IERR
    REAL EL, CBUF(0:1, 0:MZ), LFACT(MXC + 1)
C
    INTEGER I, IJ, ILL, ILT(0:1), IMI, IMN, IS, ISS, IS1, IS2,

```

```

*          IST(0:1), IT, ITT, IT1, IT2, IXT, J, JP, LADR, LLL, NI,
*          TO(0:1)
REAL ADD, BNM, CCC, ONE, SL, SUM, SUMLG, Y, ZERO, ZEXP
C
DATA ONE, ZERO / 1.0E + 00, 0.0E + 00 /
C
EXTERNAL BNM, LADR, SUMLG
C
ZEXP(Y) = EXP(Y)
C
SL = ZERO - EL
C
C      Construct the data matrix ordered scores set in x(i,2)
C
DO 10 I = 1, K
  X(I, 0) = X(I, 0) + X(I, 1)
  IF (ISC .EQ. 1) X(I, 2) = I - 1
  IF (ISC .EQ. 2) X(I, 2) = (I - 1) * (I - 1)
  IF (ISC .EQ. 3) X(I, 2) = 2 ** (I - 1)
10 CONTINUE
C
C      to(j) : observed value of sufficient statistics
C
DO 20 J = 0, 1
  TO(J) = 0
20 CONTINUE
DO 30 I = 1, K
  TO(0) = TO(0) + X(I, 1)
  TO(1) = TO(1) + X(I, 1) * X(I, 2)
30 CONTINUE
C
C      Scale factor: ils
C      Set record for initial stage
C      jp - current record indicator
C      ip - past record indicator
C
DO 40 J=0, MZ
  IF (ILS .EQ. 0) THEN
    CBUF(0, J) = ZERO
  ELSE
    CBUF(0, J) = SL
  ENDIF
40 CONTINUE
DO 50 J=0, MXR
  LBUF(0, J, 1) = 0
  LBUF(0, J, 2) = 0
  LBUF(1, J, 1) = 0
  LBUF(1, J, 2) = 0
50 CONTINUE
C
IMN = 0
DO 60 I=1, K
  IMN = IMN + X(I, 0)
60 CONTINUE
IMI = 0
C
C      ij - current stage (ij <= k)
C      ip - previous stage indicator
C      jp - current stage indicator
C
IJ = 0

```



```
      IP = 0
      JP = 1 - IP
      IS = 0
      IST(IP) = 0
      ILT(IP) = 0
C
C      Smallest t for s=is
C      Address of largest t with s=is
C
      LBUF(IP, IS, 1) = 0
      LBUF(IP, IS, 2) = 0
C
C      Store the initial distribution
C
      LLL = 0
      IF (ILS .EQ. 0) THEN
        CBUF(IP, LLL) = ONE
      ELSE
        CBUF(IP, LLL) = ZERO
      ENDIF
C
C      Perform the recursions for obtaining the conditional
C      distribution
C
70 IJ = IJ + 1
C
C      Compute lower and upper bounds for s
C
      IMI = IMI + X(IJ, 0)
      IS1 = MAX0(0, IMI + TO(0) - IMN)
      IS2 = MIN0(TO(0), IMI)
C
C      ist(jp) - smallest value of s for current stage
C      ilt(jp) - largest value of s for current stage
C
      IST(JP) = IS1
      ILT(JP) = IS2
      DO 100 IS = IS1, IS2
C
C      Compute minimum (it1) and maximum (it2) of t given s and
C      set buffer limits for this stage
C
      CALL OPT(MC, IJ, IS, X, IT1, IT2)
      LBUF(JP, IS, 1) = IT1
      IXT = IT2 - IT1
      IF (IS .EQ. IS1) THEN
        LBUF(JP, IS, 2) = IXT
      ELSE
        LBUF(JP, IS, 2) = LBUF(JP, IS - 1, 2) + IXT + 1
      ENDIF
C
C      Perform recursion
C
      NI = X(IJ, 0)
      IZ1 = MAX0(0, IS - ILT(IP))
      IZ2 = MIN0(NI, IS - IST(IP))
      DO 90 IT = IT1, IT2
        IF (ILS .EQ. 0) THEN
          SUM = ZERO
        ELSE
          SUM = SL
```

```

        ENDIF
        DO 80 KK = IZ1, IZ2
            ISS = IS - KK
            ITT = IT - KK * X(IJ, 2)
            ILL = LBUF(IP, ISS, 1)
            IF (ITT .LT. ILL) GOTO 80
            ILL = ILL + LBUF(IP, ISS, 2)
            IF (ISS .GT. IST(IP)) THEN
                ILL = ILL - LBUF(IP, ISS - 1, 2) - 1
            ENDIF
            IF (ITT .GT. ILL) GOTO 80
            LLL = LADR(ISS, ITT, IP, LBUF, IST, MXR)
            CCC = CBUF(IP, LLL)
            IF (ILS .EQ. 0) THEN
                IF (CCC .EQ. ZERO) GOTO 80
            ELSE
                IF (CCC .EQ. SL) GOTO 80
            ENDIF
            ADD = BNM(KK, NI, LFACT, MXC)
            IF (ILS .EQ. 0) THEN
                ADD = ZEXP(ADD)
                ADD = ADD * CCC
                SUM = SUM + ADD
            ELSE
                ADD = ADD + CCC
                SUM = SUMLG(SUM, ADD)
            ENDIF
80      CONTINUE
            LLL = LADR(IS, IT, JP, LBUF, IST, MXR)
            IF (LLL .GE. MZ) THEN
                IERR = 6
                RETURN
            ENDIF
            CBUF(JP, LLL) = SUM
90      CONTINUE
100     CONTINUE
C
C       Check if final stage is reached
C
        IF (IJ .GE. K) GOTO 110
C
C       Change parity and continue
C
        IP = JP
        JP = 1 - JP
        GOTO 70
110     CONTINUE
C
C       Lower and upper support of stratum distribution
C
        IZ1 = LBUF(JP, TO(0), 1)
        IZ2 = IZ1 + LBUF(JP, TO(0), 2)
        IP = JP
        RETURN
        END
C
        SUBROUTINE OPT(MC, IJ, IS, X, IT1, IT2)
C
C       ALGORITHM AS 293.3 APPL.STATIST. (1994), VOL.43, NO.3
C
C       Computes optimum values for t given s

```

```
C
      INTEGER MC, IJ, IS, X(MC, 0:2), IT1, IT2
C
      INTEGER I, IX, MM
C
      Compute minimum
C
      IT1 = 0
      IX = IS
      DO 10 I = 1, IJ
        MM = MIN0(IX, X(I, 0))
        IT1 = IT1 + MM * X(I, 2)
        IF (IX .LE. X(I, 0)) THEN
          GOTO 20
        ELSE
          IX = IX - X(I, 0)
        ENDIF
10 CONTINUE
20 CONTINUE
      IT2 = 0
      IX = IS
      DO 30 I = IJ, 1, -1
        MM = MIN0(IX, X(I, 0))
        IT2 = IT2 + MM * X(I, 2)
        IF (IX .LE. X(I, 0)) THEN
          RETURN
        ELSE
          IX = IX - X(I, 0)
        ENDIF
30 CONTINUE
      RETURN
      END

C
      INTEGER FUNCTION LADR(IS, IT, KP, LBUF, IST, MXR)
C
      ALGORITHM AS 293.4 APPL.STATIST. (1994), VOL.43, NO.3
C
      Determines an address for (s,t) in the linear array cbuf
C
      INTEGER IS, IT, KP, LBUF(0:1, 0:MXR, 2), IST(0:1), MXR
C
      INTEGER IXT
C
      IXT = IT - LBUF(KP, IS, 1)
      IF (IS .EQ. IST(KP)) THEN
        LADR = IXT
      ELSE
        LADR = LBUF(KP, IS - 1, 2) + IXT + 1
      ENDIF
      RETURN
      END

C
      REAL FUNCTION BNM(K, N, LFACT, MXC)
C
      ALGORITHM AS 293.5 APPL.STATIST. (1994), VOL.43, NO.3
C
      Computes binomial coefficient on log-scale
C
      INTEGER K, N, MXC
      REAL LFACT(MXC + 1)
C
```

```
      INTEGER L
      REAL DD
C
      L = N - K
      DD = LFACT(N + 1)
      DD = DD - LFACT(L + 1)
      DD = DD - LFACT(K + 1)
      BNM = DD
      RETURN
      END
C
      REAL FUNCTION SUMLG(D1, D2)
C
      ALGORITHM AS 293.6 APPL.STATIST. (1994), VOL.43, NO.3
C
      Adds two logarithmic scale numbers
C
      REAL D1, D2
C
      REAL DD, X, ZEXP, ZLOG
C
      ZEXP(X) = EXP(X)
      ZLOG(X) = ALOG(X)
C
      DD = D1
      IF (D2 .GT. D1) DD = D2
      D1 = ZEXP(D1 - DD)
      D2 = ZEXP(D2 - DD)
      DD = ZLOG(D1 + D2) + DD
      SUMLG = DD
      RETURN
      END
```

```
PROCEDURE Error(VAR Size: IntGC; MaxSize: IntGC; ErrorNumber: NonnegInt;  
                AnotherError: Boolean; VAR Fault: NonnegInt);
```

```
{ALGORITHM AS 294.1 APPL.STATIST. (1994) VOL.43, NO.3}
```

```
BEGIN IF (Size>MaxSize) OR AnotherError THEN  
    BEGIN Fault:=ErrorNumber; Size:=MaxSize  
    END  
END; {of Error}
```

```
PROCEDURE Reduce(VAR NumNumerSet, NumDenomSet: IntGC;  
                VAR NumeratorSet, NumerSetOC, DenominatorSet, DenomSetOC: SetArr;  
                AnObsConfig: IntSet);
```

```
{ALGORITHM AS 294.2 APPL.STATIST. (1994) VOL.43, NO.3}
```

```
{Reduce the fraction: NumeratorSet/DenominatorSet}
```

```
VAR i,j,k,m: IntGC; Reducible: Boolean;  
BEGIN k:=0;  
FOR i:=1 TO NumNumerSet DO  
    BEGIN  
        IF AnObsConfig>=NumeratorSet[i] THEN  
            BEGIN j:=1;  
                WHILE (j<=NumDenomSet) AND (NOT(AnObsConfig>=DenominatorSet[j]) OR  
                    (NumerSetOC[i]<>DenomSetOC[j]) OR  
                    (NumeratorSet[i]<>DenominatorSet[j])) DO j:=j+1;  
                Reducible:= j <= NumDenomSet;  
                IF Reducible THEN  
                    BEGIN  
                        FOR m:=j+1 TO NumDenomSet DO  
                            BEGIN DenominatorSet[m-1]:=DenominatorSet[m];  
                                DenomSetOC[m-1]:=DenomSetOC[m]  
                            END;  
                        NumDenomSet:=NumDenomSet-1  
                    END  
                END;  
            IF NOT Reducible OR NOT(AnObsConfig>=NumeratorSet[i]) THEN  
                BEGIN k:=k+1; NumeratorSet[k]:=NumeratorSet[i];  
                    NumerSetOC[k]:=NumerSetOC[i]  
                END  
            END; {of FOR i}  
    NumNumerSet:=k  
END; {of Reduce}
```

```
PROCEDURE MissMLE (SizeGeClass, NumObsConfig: IntGC;  
                  GeClass, ObsConfig: SetArr;  
                  VAR NumNumer, NumDenom, NumSubGC: IntGC;  
                  VAR Numerator, Denominator, NumerOC, DenomOC, SGClassOC: SetArr;  
                  VAR SubGeClass: SetArr2;  
                  VAR SizeSubGC: IntArr;  
                  VAR VarSetModel: IntSet;  
                  VAR Fault: NonnegInt);
```

```
{ALGORITHM AS 294.3 APPL.STATIST. (1994) VOL.43, NO.3}
```

```
{Find the factor formula of MLEs}
```

```
VAR i,j,k,m,OrigNumNumer: IntGC; Incomplete: Boolean;  
    Variables, NumerConfig, DenomConfig, OCInModel, Block, BlockOC: IntSet;
```

```

PROCEDURE Nest(Block: IntSet; VAR BlockOC: IntSet);

{Factorizing by nested pattern of observations}

VAR j,m: NonnegInt; OCj,OCUnion,Union,Intersect: IntSet;
    Unchange,Separa: Boolean;
BEGIN
  IF BlockOC<>[] THEN
{Find the union of inside observing configurations, OCUnion}
  BEGIN Intersect:=Block; Union:=[]; OCUnion:=[];
  REPEAT Unchange:=True;
  FOR j:=1 TO NumObsConfig DO
  IF j IN BlockOC THEN
  BEGIN OCj:=ObsConfig[j]*Block;
  IF Intersect>=OCj THEN
  BEGIN Intersect:=OCj; OCUnion:=OCj; Union:=[j]
  END
  ELSE
  BEGIN Intersect:=Intersect*OCj;
  IF NOT(j IN Union) AND (NOT(OCj>=OCUnion) OR (OCj=OCUnion)) THEN
  BEGIN OCUnion:=OCUnion+OCj; Union:=Union+[j]; Unchange:=false
  END
  END
  UNTIL Unchange;
  IF NOT (OCUnion>=Block) THEN
  BEGIN
{Check whether OCUnion is contained in a generator}
  IF i<=OrigNumNumer THEN Separa:=True
  ELSE
  BEGIN m:=i-OrigNumNumer; j:=0;
  REPEAT j:=j+1; Separa:=OCUnion<=SubGeClass[m,j]
  UNTIL Separa OR (j>=SizeSubGC[m])
  END;
  IF Separa THEN
{Factorize the MLEs by nested pattern}
  BEGIN NumNumer:=NumNumer+1;
  Error(NumNumer,MaxGenerator,3,false,Fault);
  Numerator[NumNumer]:=OCUnion; NumerOC[NumNumer]:=BlockOC;
  NumDenom:=NumDenom+1; Error(NumDenom,MaxGenerator,4,false,Fault);
  Denominator[NumDenom]:=OCUnion; DenomOC[NumDenom]:=BlockOC-Union;
  BlockOC:=BlockOC-Union; Nest(Block,BlockOC)
  END
  END {of IF NOT (OCUnion>=Block) THEN}
  END {of IF BlockOC<>[] THEN}
  END; {of Nest}

{Check Whether the block A is separable}
FUNCTION Separable(OtherConditionHolds:Boolean;
  VarsInA,Generator: IntSet; VAR Bound,OCInModel: IntSet): Boolean;
VAR k: NonnegInt; Unchange, Separa: Boolean;
BEGIN
  IF NOT OtherConditionHolds THEN Separable:=false
  ELSE
  IF Bound=[] THEN
{For the cases that the blocks A and B do not intersect:}
  BEGIN Separable:=True; NumerConfig:=OCInModel;
  FOR k:=1 TO NumObsConfig DO
  IF k IN OCInModel THEN
  BEGIN IF ObsConfig[k]*(Variables-VarsInA)=[]
  THEN OCInModel:=OCInModel-[k];

```

```

        IF ObsConfig[k]*VarsInA=[] THEN NumerConfig:=NumerConfig-[k]
    END
END
ELSE
{For the cases that the blocks A and B intersect:}
    BEGIN
{Adjust the Bound according to the observing configurations}
    REPEAT  Unchange:=true;
    FOR k:=1 TO NumObsConfig DO
        IF k IN OCInModel THEN
            IF (ObsConfig[k]*(VarsInA-Bound)<>[]) AND
                (ObsConfig[k]*(Variables-VarsInA)<>[]) AND
                NOT (ObsConfig[k]>=Bound) THEN
                BEGIN  Bound:=Bound+ObsConfig[k]*VarsInA; Unchange:=false
                END
            UNTIL  Unchange;
            IF NOT (Generator>=Bound) OR (VarsInA-Bound=[]) THEN
                Separable:=false
            ELSE
                BEGIN
{Check whether the block A is separable as a submodel}
                k:=0; NumerConfig:=[]; Separa:=true;
                REPEAT  k:=k+1;
                IF k IN OCInModel THEN
                    BEGIN  Separa:=ObsConfig[k]*(VarsInA-Bound)=[];
                    IF NOT Separa THEN
                        BEGIN  Separa:= Bound<=ObsConfig[k];
                        IF Separa THEN NumerConfig:=NumerConfig+[k]
                        END
                    END
                UNTIL (k>=NumObsConfig) OR NOT Separa;
                IF Separa THEN DenomConfig:=NumerConfig
                ELSE
{Check whether the block A is separable as a main model}
                BEGIN  k:=0; Separa:=true;
                REPEAT  k:=k+1;
                IF k IN OCInModel THEN
                    Separa:= (VarsInA>=ObsConfig[k]*Variables)
                        OR (Bound<=ObsConfig[k])
                UNTIL (k>=NumObsConfig) OR NOT Separa;
                IF Separa THEN
{Find sets of observing configurations of blocks A, B and denominator}
                BEGIN NumerConfig:=OCInModel; DenomConfig:=OCInModel;
                FOR k:=1 TO NumObsConfig DO
                    IF (k IN OCInModel) AND(VarsInA>=ObsConfig[k]*Variables) THEN
                        DenomConfig:=DenomConfig-[k];
                        OCInModel:=DenomConfig
                    END
                END; {of IF Separa ... ELSE}
                Separable:=Separa
            END {of IF NOT (Generator>=Bound)...ELSE}
        END {of IF Bound=[]...ELSE}
    END; {of Separable}

{Check whether the generating class is decomposable or not}
PROCEDURE Deco(VAR SizeGeClass: IntGC; VAR GeClass: SetArr;
    VAR OCInModel: IntSet);
VAR i, j: IntGC; Bound, OneClass: IntSet;
    GeClassUnchange, GeneratorUnchange, NoSubGenerator: Boolean;
BEGIN {of Deco}
    REPEAT  GeClassUnchange:=true;

```

```

{Delete variables which exist in only a single generator}
REPEAT  GeneratorUnchange:=true;
FOR i:=1 TO SizeGeClass DO
  BEGIN  OneClass:=GeClass[i];
  FOR j:=1 TO SizeGeClass DO
    IF i<>j THEN OneClass:=OneClass-GeClass[j];
  Bound:=GeClass[i]-OneClass;
  IF Separable(OneClass<>[],GeClass[i],GeClass[i],Bound,OCInModel)
  THEN
    BEGIN Variables:=Variables-GeClass[i]+Bound;
    NumNumer:=NumNumer+1; Error(NumNumer,MaxGenerator,3,false,Fault);
    Numerator[NumNumer]:=GeClass[i]; NumerOC[NumNumer]:=NumerConfig;
    IF Bound<>[] THEN
      BEGIN NumDenom:=NumDenom+1;
      Error(NumDenom,MaxGenerator,4,false,Fault);
      Denominator[NumDenom]:=Bound; DenomOC[NumDenom]:=DenomConfig
      END;
    GeClass[i]:=Bound;  GeneratorUnchange:=false
  END
  END
UNTIL GeneratorUnchange;
{Delete generators which are contained in others}
REPEAT  NoSubGenerator:=true;
FOR i:=1 TO SizeGeClass DO
  FOR j:=1 TO SizeGeClass DO
    IF (i<>j) AND (GeClass[i]<=GeClass[j]) AND (GeClass[i]<>[]) THEN
      BEGIN GeClass[i]:=[];NoSubGenerator:=false;GeClassUnchange:=false
      END;
{Delete the null generators}
j:=0;
FOR i:=1 TO SizeGeClass DO
  IF GeClass[i]<>[] THEN
    BEGIN j:=j+1;  GeClass[j]:=GeClass[i]
    END;
  SizeGeClass:=j
UNTIL NoSubGenerator OR (SizeGeClass=0)
UNTIL GeClassUnchange OR (SizeGeClass=0)
END; {of Deco}

{Decompose generating class}
PROCEDURE DecompGC(VAR SizeGeClass: IntGC; VAR GeClass: SetArr;
  OCInModel: IntSet);
VAR i,j,k,m,InAGeneratorsNum,InBGeneratorsNum: IntGC; GeClassA: SetArr;
  BoundaryOfAB,Bound,VarInA,VarInB,T: IntSet;
  Researched: ARRAY [1..MaxGenerator] OF Boolean;
  DecomposedOrCannotDecompose,NoVarAddedInA: Boolean;
BEGIN  Variables:=[];
  FOR i:=1 TO SizeGeClass DO Variables:=Variables+GeClass[i];
  Deco(SizeGeClass,GeClass,OCInModel);
  IF SizeGeClass<>0 THEN
    BEGIN i:=0;  DecomposedOrCannotDecompose:=false;
    REPEAT
{Set [] or GeClass[i] as the separator, BoundaryOfAB}
    IF i=0 THEN BoundaryOfAB:=[] ELSE BoundaryOfAB:=GeClass[i];  m:=0;
    REPEAT  m:=m+1;
      IF (m<>i) AND NOT ((i=0) AND (m<>1)) THEN
        BEGIN  InAGeneratorsNum:=1; GeClassA[1]:=GeClass[m];
          Researched[m]:=true; VarInA:=GeClassA[1];
          FOR j:=1 TO SizeGeClass DO IF j<>m THEN Researched[j]:=false;
{Find the set of variables in A, VarInA}
          REPEAT  NoVarAddedInA:=true;

```



```

FOR j:=1 TO SizeGeClass DO
  IF (i<>j) AND NOT Researched[j] AND
    (VarInA*GeClass[j]-BoundaryOfAB<>[]) THEN
    BEGIN NoVarAddedInA:=false; VarInA:=VarInA+GeClass[j];
      Researched[j]:=true; InAGeneratorsNum:=InAGeneratorsNum+1;
      GeClassA[InAGeneratorsNum]:=GeClass[j]
    END
  UNTIL NoVarAddedInA;
  IF i<>0 THEN InBGeneratorsNum:=SizeGeClass-InAGeneratorsNum-1
  ELSE InBGeneratorsNum:=SizeGeClass-InAGeneratorsNum;
  VarInA:=VarInA+BoundaryOfAB; VarInB:=[];
{Find the set of variables in B, VarInB}
  FOR k:=1 TO SizeGeClass DO
    IF (k<>i) AND NOT Researched[k] THEN VarInB:=VarInB+GeClass[k];
    Bound:=VarInA*VarInB;
    IF Separable(InBGeneratorsNum<>0,VarInA,BoundaryOfAB,
      Bound,OCInModel) THEN
{The generating class can be decomposed by GeClass[i]}
    BEGIN j:=0; DecomposedOrCannotDecompose:=true;
      FOR k:=1 TO SizeGeClass DO
        IF (k<>i) AND NOT Researched[k] THEN
          BEGIN j:=j+1; GeClass[j]:=GeClass[k]
          END;
        IF i<>0 THEN
          BEGIN InAGeneratorsNum:=InAGeneratorsNum+1;
            GeClassA[InAGeneratorsNum]:=BoundaryOfAB;
            InBGeneratorsNum:=InBGeneratorsNum+1;
            GeClass[InBGeneratorsNum]:=Bound;
            NumDenom:=NumDenom+1;
            Error(NumDenom,MaxGenerator,4,false,Fault);
            Denominator[NumDenom]:=GeClass[InBGeneratorsNum];
            DenomOC[NumDenom]:=DenomConfig
          END;
        {Decompose recursively A and B}
        DecompGC(InAGeneratorsNum,GeClassA,NumerConfig);
        DecompGC(InBGeneratorsNum,GeClass,OCInModel)
      END {of IF Separable(...) THEN}
    END {of IF (m<>i) AND NOT ((i=0) AND (m<>1)) THEN}
  UNTIL (m>=SizeGeClass) OR DecomposedOrCannotDecompose;
  IF NOT DecomposedOrCannotDecompose THEN
    BEGIN
{The generating class cannot be decomposed by GeClass[i]}
    IF i=SizeGeClass THEN
{The generating class cannot be decomposed by any generator}
    BEGIN DecomposedOrCannotDecompose:=true; NumSubGC:=NumSubGC+1;
      Error(NumSubGC,MaxGenerator,5,false,Fault);
      SGClassOC[NumSubGC]:=OCInModel;SizeSubGC[NumSubGC]:=SizeGeClass;
      FOR k:=1 TO SizeGeClass DO SubGeClass[NumSubGC,k]:=GeClass[k]
      END
    ELSE i:=i+1
    END {of IF NOT Decomp... THEN}
  UNTIL DecomposedOrCannotDecompose
  END {of IF SizeGeClass<>0 THEN}
END; {of DecompGC}
BEGIN {of MissMLE} Fault:=0;
  Error(SizeGeClass,MaxGenerator,1,SizeGeClass<1,Fault); VarSetModel:=[];
  IF (NumObsConfig<=0) OR (NumObsConfig>MaxGenerator) THEN Fault:=6;
  IF Fault=0 THEN
    FOR i:=1 TO SizeGeClass DO
      BEGIN
        IF NOT([1..MaxVar]>=GeClass[i]) OR (GeClass[i]=[]) THEN Fault:=2;

```

```

    VarSetModel:=VarSetModel+GeClass[i]
  END;
IF Fault=0 THEN
  FOR i:=1 TO NumObsConfig DO
    IF NOT([1..MaxVar]>=ObsConfig[i])OR(ObsConfig[i]=[]) THEN Fault:=7;
  NumNumer:=0; NumDenom:=0; NumSubGC:=0;
  IF Fault=0 THEN
    BEGIN OCInModel:=[1..NumObsConfig];
    DecompGC(SizeGeClass,GeClass,OCInModel); OrigNumNumer:=NumNumer;
    {Factorize MLEs according to nested pattern}
    FOR i:=1 TO OrigNumNumer+NumSubGC DO
      BEGIN IF i<=OrigNumNumer THEN
        BEGIN Block:=Numerator[i]; Nest(Block,NumOC[i])
        END
      ELSE
        BEGIN m:=i-OrigNumNumer; Block:=[];
        FOR j:=1 TO SizeSubGC[m] DO Block:=Block+SubGeClass[m,j];
        Nest(Block,SGClassOC[m])
        END
      END;
    Reduce(NumNumer,NumDenom,Numerator,NumOC,Denominator,DenomOC,
      VarSetModel);
    {Change the incomplete Numerator into SubGeClass}
    k:=0;
    FOR i:=1 TO NumNumer DO
      BEGIN j:=1;
      Incomplete:=(j IN NumOC[i]) AND NOT(ObsConfig[j]>=Numerator[i]);
      WHILE (j<=NumObsConfig) AND NOT Incomplete DO
        BEGIN Incomplete:=(j IN NumOC[i]) AND
          NOT(ObsConfig[j]>=Numerator[i]); j:=j+1
        END;
      IF Incomplete THEN
        BEGIN NumSubGC:=NumSubGC+1;
        Error(NumSubGC,MaxGenerator,5,false,Fault);
        SGClassOC[NumSubGC]:=Numerator[i]; SizeSubGC[NumSubGC]:=1;
        SubGeClass[NumSubGC,1]:=Numerator[i]
        END
      ELSE
        BEGIN k:=k+1;
        Numerator[k]:=Numerator[i]; NumOC[k]:=NumOC[i]
        END
      END; {of FOR i}
    NumNumer:=k
  END {of IF Fault=0 THEN}
END; {of MissMLE}

```

```

PROCEDURE MissHiMod(NumModels:                               NonnegInt;
  M1SizeGeClass,M2SizeGeClass,NumObsConfig:                 IntGC;
  M1GeClass,M2GeClass,ObsConfig:                             SetArr;
  VAR LRNNumer,LRNNumDenom,LRNNumGeClass,
  LRDNumer,LRDNumDenom,LRDNumGeClass:                       IntArr;
  VAR LRNSizeGeClass,LRDSizeGeClass:                         IntArr2;
  VAR LRNNumer,LRNDenom,LRDNumer,LRDDenom,LRNOCNumer,LRNOCDenom,
  LRNOCGeClass,LRDOCNumer,LRDOCDenom,LRDOCGeClass:          SetArr2;
  VAR LRNGeClass,LRDGeClass:                                  SetArr3;
  VAR VariableSet:                                           IntSet;
  VAR Fault:                                                  NonnegInt);

```

{ALGORITHM AS 294.4 APPL.STATIST. (1994) VOL.43, NO.3}

{Find the reduced formula of LR statistic}

```

VAR i,j,k,m,n,p: NonnegInt;      VarSetModel,UnionN,Union:  IntSet;
  Reducible:    Boolean;          M1SubGeClass,M2SubGeClass: SetArr2;
  M1NumNumer,M2NumNumer,M1NumDenom,M2NumDenom,
  M1NumSubGC,M2NumSubGC,NNumNumer,DNumNumer:  IntGC;
  M1SizeSubGC,M2SizeSubGC,NNumerInd,DNumerInd: IntArr;
  M1Numerator,M2Numerator,M1Denominator,M2Denominator,
  M1NumerOC,M2NumerOC,M1DenomOC,M2DenomOC,M1SGClassOC,
  M2SGClassOC,NNumer,DNumer,NOCNumer,DOCNumer: SetArr;
{Check whether the sub-generating classes in models 1 and 2 are same}
FUNCTION ClassesNotSame(h, i, j: NonnegInt): Boolean;
VAR k: IntGC; m: NonnegInt; NotSame: Boolean;
BEGIN k:=0; NotSame:=LRNSizeGeClass[h,i]<>LRDSizeGeClass[h,j];
  WHILE NOT NotSame AND (k<LRNSizeGeClass[h,i]) DO
    BEGIN k:=k+1; m:=1;
      WHILE (m<=LRDSizeGeClass[h,j]) AND
        (LRNGeClass[h,i,k]<>LRDGeClass[h,j,m]) DO m:=m+1;
      NotSame:=NotSame OR (m>LRDSizeGeClass[h,j])
    END;
  ClassesNotSame:=NotSame
END; {of ClassesNotSame}

{Find the union of generators}
PROCEDURE UnionSet(NumSet: IntGC; Sets: SetArr; VAR Union: IntSet);
VAR i: NonnegInt;
BEGIN Union:=[]; FOR i:=1 TO NumSet DO Union:=Union+Sets[i]
END;

{Set summed numerator and summed denominator of LR}
PROCEDURE Sum(ObsConfig: IntSet; LRNumNumer,LRNumGeClass: IntGC;
  VAR NumNumer: IntGC; VAR LRNumer,LROCNumer,LROCGeClass,Numer,OCNumer:
  SetArr; VAR LRSizeGeClass,NumerInd: IntArr; VAR LRGeClass: SetArr2);
VAR p: IntGC; j,k,m: NonnegInt; Union,Unionj,UnionOther: IntSet;
BEGIN UnionOther:=[];
  FOR k:=1 TO LRNumGeClass DO
    FOR m:=1 TO LRSizeGeClass[k] DO UnionOther:=UnionOther+LRGeClass[k,m];
  p:=0;
  FOR j:=1 TO LRNumNumer DO
    BEGIN Union:=UnionOther;
      FOR k:=1 TO LRNumNumer DO IF k<>j THEN Union:=Union+LRNumer[k];
      IF LRNumer[j]*Union <= ObsConfig THEN
        BEGIN p:=p+1; Numer[p]:=LRNumer[j]*ObsConfig;
          OCNumer[p]:=LROCNumer[j]; NumerInd[p]:=j
        END
      END; {of FOR j}
    UnionOther:=[];
    FOR k:=1 TO LRNumNumer DO UnionOther:=UnionOther+LRNumer[k];
    FOR j:=1 TO LRNumGeClass DO
      BEGIN Union:=UnionOther; Unionj:=[];
        FOR k:=1 TO LRNumGeClass DO
          FOR m:=1 TO LRSizeGeClass[k] DO
            IF k=j THEN Unionj:=Unionj+LRGeClass[j,m]
            ELSE Union :=Union +LRGeClass[k,m];
          IF Unionj*Union <= ObsConfig THEN
            BEGIN m:=1; Unionj:=Unionj*ObsConfig;
              WHILE (m<=LRSizeGeClass[j]) AND NOT(LRGeClass[j,m]>=Unionj) DO
                m:=m+1;
              IF m<=LRSizeGeClass[j] THEN
                BEGIN p:=p+1; Error(p,MaxGenerator,8,false,Fault);
                  OCNumer[p]:=LROCGeClass[j]; Numer[p]:=Unionj;
                    NumerInd[p]:=LRNumNumer+j
                END
              END
            END
          END
        END
      END
    END
  END

```

```

        END
    END
    END; {of FOR j}
    NumNumer:=p
END; {of Sum}

{Delete null numerator}
PROCEDURE Delete(VAR LRNumNumer,LRNumGeClass: IntGC;
    VAR LRNumer,LROCNumer,LROCGeClass: SetArr; VAR LRSizeGeClass: IntArr;
    VAR LRGeClass: SetArr2);
VAR j,k,m: NonnegInt;
BEGIN k:=0;
    FOR j:=1 TO LRNumNumer DO IF LRNumer[j] <> [] THEN
        BEGIN k:=k+1; LRNumer[k]:=LRNumer[j]; LROCNumer[k]:=LROCNumer[j]
        END;
    LRNumNumer:=k; k:=0;
    FOR j:=1 TO LRNumGeClass DO IF LRSizeGeClass[j]<>0 THEN
        BEGIN k:=k+1; LRSizeGeClass[k]:=LRSizeGeClass[j];
        LROCGeClass[k]:=LROCGeClass[j];
        FOR m:=1 TO LRSizeGeClass[j] DO LRGeClass[k,m]:=LRGeClass[j,m]
        END;
    LRNumGeClass:=k
END; {of Delete}
BEGIN {of MissHiMod}
M1NumNumer:=0; M1NumDenom:=0; M1NumSubGC:=0; VariableSet:=[];
M2NumNumer:=0; M2NumDenom:=0; M2NumSubGC:=0; Fault:=0;
IF NumModels <> 2 THEN Fault:=9
ELSE
    BEGIN
        MissMLE(M1SizeGeClass,NumObsConfig,M1GeClass,ObsConfig,M1NumNumer,
            M1NumDenom,M1NumSubGC,M1Numerator,M1Denominator,M1NumerOC,
            M1DenomOC,M1SGClassOC,M1SubGeClass,M1SizeSubGC,VarSetModel,Fault);
        VariableSet:=VarSetModel;
        IF Fault=0 THEN
            BEGIN
                MissMLE(M2SizeGeClass,NumObsConfig,M2GeClass,ObsConfig,M2NumNumer,
                    M2NumDenom,M2NumSubGC,M2Numerator,M2Denominator,M2NumerOC,
                    M2DenomOC,M2SGClassOC,M2SubGeClass,M2SizeSubGC,VarSetModel,Fault);
                IF VariableSet<>VarSetModel THEN Fault:=10;
                IF Fault=0 THEN
                    {Find the likelihood ratio: M1/M2}
                    FOR i:=1 TO NumObsConfig DO
                        BEGIN k:=0;
                            {Set the numerator of LR}
                            FOR j:=1 TO M1NumNumer DO
                                IF i IN M1NumerOC[j] THEN
                                    BEGIN k:=k+1; LRNNumer[i,k]:=M1Numerator[j];
                                        LRNOCNumer[i,k]:=M1NumerOC[j]
                                    END;
                                LRNNumer[i]:=k; k:=0;
                                FOR j:=1 TO M1NumDenom DO
                                    IF i IN M1DenomOC[j] THEN
                                        BEGIN k:=k+1; LRNDenom[i,k]:=M1Denominator[j];
                                            LRNOCDenom[i,k]:=M1DenomOC[j]
                                        END;
                                    LRNNumDenom[i]:=k; k:=0;
                                    FOR j:=1 TO M1NumSubGC DO
                                        IF i IN M1SGClassOC[j] THEN
                                            BEGIN k:=k+1; LRNSizeGeClass[i,k]:=M1SizeSubGC[j];
                                                LRNOCGeClass[i,k]:=M1SGClassOC[j];
                                                FOR m:=1 TO M1SizeSubGC[j] DO

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        LRNGeClass[i,k,m]:=M1SubGeClass[j,m]
    END;
    LRNNumGeClass[i]:=k; k:=0;
{Set the denominator of LR}
    FOR j:=1 TO M2NumNumer DO
    IF i IN M2NumerOC[j] THEN
        BEGIN k:=k+1; LRDNummer[i,k]:=M2Numerator[j];
            LRDOCNummer[i,k]:=M2NumerOC[j]
        END;
    LRDNumNumer[i]:=k; k:=0;
    FOR j:=1 TO M2NumDenom DO
    IF i IN M2DenomOC[j] THEN
        BEGIN k:=k+1; LRDDenom[i,k]:=M2Denominator[j];
            LRDOCDenom[i,k]:=M2DenomOC[j]
        END;
    LRDNumDenom[i]:=k; k:=0;
    FOR j:=1 TO M2NumSubGC DO
    IF i IN M2SGClassOC[j] THEN
        BEGIN k:=k+1; LRDSIZEGeClass[i,k]:=M2SizeSubGC[j];
            LRDOCGeClass[i,k]:=M2SGClassOC[j];
            FOR m:=1 TO M2SizeSubGC[j] DO
                LRDSIZEGeClass[i,k,m]:=M2SubGeClass[j,m]
            END;
    LRDNumGeClass[i]:=k;
{Reduce the numerator and denominator contained in ObsConfig[i]}
    Reduce(LRNNumNumer[i],LRDNumNumer[i],LRNNummer[i],LRNOCNummer[i],
        LRDSIZEGeClass[i,k],LRDOCNummer[i],ObsConfig[i]);
    Reduce(LRNNumDenom[i],LRDNumDenom[i],LRNNDenom[i],LRNOCDenom[i],
        LRDDenom[i],LRDOCDenom[i],ObsConfig[i]);
{Reduce sub-generating classes contained in ObsConfig[i]}
    k:=0;
    FOR m:=1 TO LRNNumGeClass[i] DO
        BEGIN j:=1;
            UnionSet(LRNSizeGeClass[i,m],LRNGeClass[i,m],UnionN);
            IF ObsConfig[i] >= UnionN THEN
                BEGIN UnionSet(LRDSIZEGeClass[i,j],LRDSIZEGeClass[i,j],Union);
                    WHILE (j<=LRDNumGeClass[i]) AND (NOT(ObsConfig[i]>=Union) OR
                        (LRDOCGeClass[i,j]<>LRNOCGeClass[i,m]) OR
                        ClassesNotSame(i,m,j)) DO
                        BEGIN j:=j+1;
                            IF j<=LRDNumGeClass[i] THEN
                                UnionSet(LRDSIZEGeClass[i,j],LRDSIZEGeClass[i,j],Union)
                            END;
                        Reducible:= j <= LRDNumGeClass[i];
                        IF Reducible THEN
                            BEGIN
                                FOR p:=j+1 TO LRDNumGeClass[i] DO
                                    BEGIN LRDSIZEGeClass[i,p-1]:=LRDSIZEGeClass[i,p];
                                        LRDOCGeClass[i,p-1]:=LRDOCGeClass[i,p];
                                        FOR n:=1 TO LRDSIZEGeClass[i,p-1] DO
                                            LRDSIZEGeClass[i,p-1,n]:=LRDSIZEGeClass[i,p,n]
                                        END;
                                    LRDNumGeClass[i]:=LRDNumGeClass[i]-1
                                END
                            END;
                        IF NOT Reducible OR NOT(ObsConfig[i] >= UnionN) THEN
                            BEGIN k:=k+1; LRNSIZEGeClass[i,k]:=LRNSIZEGeClass[i,m];
                                LRNOCGeClass[i,k]:=LRNOCGeClass[i,m];
                                FOR n:=1 TO LRNSIZEGeClass[i,k] DO
                                    LRNGeClass[i,k,n]:=LRNGeClass[i,m,n]
                                END
                            END
                END;
            END;
        END;
    END;
    IF NOT Reducible OR NOT(ObsConfig[i] >= UnionN) THEN
        BEGIN k:=k+1; LRNSIZEGeClass[i,k]:=LRNSIZEGeClass[i,m];
            LRNOCGeClass[i,k]:=LRNOCGeClass[i,m];
            FOR n:=1 TO LRNSIZEGeClass[i,k] DO
                LRNGeClass[i,k,n]:=LRNGeClass[i,m,n]
            END
        END
    END

```

```

        END; {of FOR m}
        LRNNumGeClass[i]:=k;
{Reduce summed numerator and denominator of LR}
        Sum(ObsConfig[i],LRNNumNumer[i],LRNNumGeClass[i],NNumNumer,
            LRNNumer[i],LRNOCNumer[i],LRNOCGeClass[i],NNumNumer,NOCNumer,
            LRNSizeGeClass[i],NNumNumerInd,LRNGeClass[i]);
        Sum(ObsConfig[i],LRDNumNumer[i],LRDNumGeClass[i],DNumNumer,
            LRDNumer[i],LRDOCNumer[i],LRDOCGeClass[i],DNumNumer,DOCNumer,
            LRDSizeGeClass[i],DNumNumerInd,LRDGeClass[i]);
        FOR p:=1 TO NNumNumer DO
        BEGIN   j:=1;
        WHILE (j<=DNumNumer) AND ((NOCNumer[p]<>DOCNumer[j]) OR
            (NNumNumer[p]<>DNumNumer[j])) DO j:=j+1;
        IF j<=DNumNumer THEN
        BEGIN n:=NNumNumerInd[p];
            IF n<=LRNNumNumer[i] THEN LRNNumer[i,n]:=[]
            ELSE LRNSizeGeClass[i,n-LRNNumNumer[i]]:=0;
            n:=DNumNumerInd[j];
            IF n<=LRDNumNumer[i] THEN LRDNumer[i,n]:=[]
            ELSE LRDSizeGeClass[i,n-LRDNumNumer[i]]:=0
        END
        END; {of FOR p}
        Delete(LRNNumNumer[i],LRNNumGeClass[i],LRNNumer[i],
            LRNOCNumer[i],LRNOCGeClass[i],LRNSizeGeClass[i],LRNGeClass[i]);
        Delete(LRDNumNumer[i],LRDNumGeClass[i],LRDNumer[i],
            LRDOCNumer[i],LRDOCGeClass[i],LRDSizeGeClass[i],LRDGeClass[i]);
{Reduce the whole LR if numerator is the same as denominator}
        Reducible:= (LRNNumNumer[i]=LRDNumNumer[i]) AND
            (LRNNumDenom[i]=LRDNumDenom[i]) AND
            (LRNNumGeClass[i]=LRDNumGeClass[i]);
        IF Reducible THEN
        BEGIN   j:=1;
        WHILE Reducible AND (j<=LRNNumNumer[i]) DO
            BEGIN   Reducible:=Reducible AND (LRNNumer[i,j]=LRDNumer[i,j])
                AND (LRNOCNumer[i,j]=LRDOCNumer[i,j]);   j:=j+1
            END;
            j:=1;
        WHILE Reducible AND (j<=LRNNumDenom[i]) DO
            BEGIN   Reducible:=Reducible AND (LRNDenom[i,j]=LRDDenom[i,j])
                AND (LRNOCDenom[i,j]=LRDOCDenom[i,j]);   j:=j+1
            END;
            j:=1;
        WHILE Reducible AND (j<=LRNNumGeClass[i]) DO
            BEGIN   Reducible:= Reducible
                AND (LRNOCGeClass[i,j]=LRDOCGeClass[i,j]);   k:=1;
                WHILE ClassesNotSame(i,j,k) AND (k<=LRDNumGeClass[i]) DO
                    k:=k+1;
                    Reducible:=Reducible AND (k<=LRDNumGeClass[i]);   j:=j+1
                END;
            IF Reducible THEN
            BEGIN LRNNumNumer[i]:=0;LRDNumNumer[i]:=0;LRNNumDenom[i]:=0;
                LRDNumDenom[i]:=0; LRNNumGeClass[i]:=0; LRDNumGeClass[i]:=0
            END
        END {IF Reducible THEN}
        END {of FOR i}
    END
END
END
END; {of MissHiMod}

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SUBROUTINE DOPT(X, DIM1, NCAND, KIN, N, NBLOCK, IN, BLKSIZ, K,
*   RSTART, NRBAR, D, RBAR, PICKED, LNDET, XX, TOL, ZPZ, WK,
*   IFAULT)
C
C   ALGORITHM AS295.1 APPL. STATIST. (1994) VOL.43, NO.4
C
C   Heuristic algorithm to pick N rows of X out of NCAND to
C   maximize the determinant of X'X, using the Fedorov exchange
C   algorithm.
C
C   INTEGER DIM1, NCAND, KIN, N, NBLOCK, IN(*), BLKSIZ(*), K, NRBAR,
*   PICKED(N), IFAULT
C   REAL X(DIM1, KIN), D(K), RBAR(NRBAR), LNDET, XX(K),
*   TOL(K), ZPZ(NCAND, *), WK(K)
C   LOGICAL RSTART
C
C   INTEGER I, J, NIN, POINT, CASE, NB, BLOCK, L, POS, BEST, FIRST,
*   LAST, CAND, LASTIN, LSTOUT, DROP, REMPOS, BL, RPOS, LAST1,
*   LAST2, FIRST1, FIRST2, POS1, POS2, BLOCK1, BLOCK2, CASE1,
*   CASE2, POSI, POSJ, BESTB1, BESTB2, BESTP1, BESTP2, RANK,
*   MXRANK, INC
C   REAL ONE, ZERO, MINUS1, TEMP, EPS, DETMAX, ABOVE1,
*   SUM, SMALL, HUNDRD
C   LOGICAL CHANGE
C
C   REAL DELTA, RAND
C   EXTERNAL BKSUB1, BKSUB2, CLEAR, DELTA, GETX, MODTRI, MODTR2,
*   RAND, REGCF, SINGM
C
C   DATA ONE /1.0E + 00/, ZERO /0.0E + 00/, ABOVE1 /1.0001E + 00/,
*   EPS /1.0E - 06/, MINUS1 /-1.0E + 00/, SMALL /1.0E - 04/,
*   HUNDRD /100.0E + 00/
C
C   IFAULT = 0
C   IF (DIM1 .LT. NCAND) IFAULT = 1
C   IF (K .GT. N) IFAULT = IFAULT + 2
C   IF (NRBAR .LT. K*(K-1)/2) IFAULT = IFAULT + 4
C   IF (K .NE. KIN+NBLOCK) IFAULT = IFAULT + 8
C   IF (NBLOCK .GT. 1) THEN
C     L = 0
C     DO 10 BLOCK = 1, NBLOCK
C       L = L + BLKSIZ(BLOCK)
10    CONTINUE
C     IF (N .NE. L) IFAULT = IFAULT + 16
C   ELSE
C     IF (N .NE. BLKSIZ(1)) IFAULT = IFAULT + 16
C   END IF
C
C   NB = max(1, NBLOCK) so that we can force it to go through
C   DO-loops once. NIN = no. of design points forced into the
C   design.
C
C   NB = MAX(1, NBLOCK)
C   NIN = 0
C   DO 20 I = 1, NB
C     IF (IN(I) .LT. 0) GO TO 30
C     IF (IN(I) .GT. 0) THEN
C       IF (IN(I) .GT. BLKSIZ(I)) GO TO 30
C       NIN = NIN + IN(I)
C     END IF
20  CONTINUE

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      IF (NIN .LE. N) GO TO 40
30  IFAULT = IFAULT + 32
40  CONTINUE
      IF (IFAUULT .NE. 0) RETURN
      CALL CLEAR(K, NRBAR, D, RBAR, IFAULT)
C
C      Set up an array of tolerances
C
      DO 50 I = 1, K
          TOL(I) = ZERO
50  CONTINUE
      BLOCK = 1
      DO 70 CASE = 1, NCAND
          CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, CASE)
          DO 60 I = 1, K
              TOL(I) = TOL(I) + ABS(XX(I))
60  CONTINUE
70  CONTINUE
      TEMP = FLOAT(N) * EPS / NCAND
      DO 80 I = 1, K
          IF (I .LE. NBLOCK) THEN
              TOL(I) = EPS
          ELSE
              TOL(I) = TOL(I) * TEMP
          END IF
80  CONTINUE
C
C      Form initial Cholesky factorization
C
      POS = 1
      DO 120 BLOCK = 1, NB
          IF (RSTART) THEN
              LAST1 = (IN(BLOCK) + BLKSIZ(BLOCK))/2
              INC = SQRT(FLOAT(NCAND) + SMALL)
          END IF
          DO 110 I = 1, BLKSIZ(BLOCK)
              IF (RSTART .AND. I .GT. IN(BLOCK)) THEN
                  POINT = 1 + NCAND * RAND()
C
C      If I <= LAST1, use a random point, otherwise find the
C      candidate which maximizes the rank, and then maximizes the
C      subspace determinant for that rank.
C
                  IF (I .GT. LAST1) THEN
                      MXRANK = 0
                      LNDET = -HUNDRD
                      DO 100 CAND = 1, NCAND, INC
                          CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, POINT)
                          CALL MODTR2(K, NRBAR, XX, D, RBAR, TOL, RANK, SUM)
                          IF (RANK .LT. MXRANK) GO TO 90
                          IF (RANK .EQ. MXRANK .AND. SUM .LT. LNDET) GO TO 90
                          BEST = POINT
                          MXRANK = RANK
                          LNDET = SUM * ABOVE1
90  POINT = POINT + INC
                          IF (POINT .GT. NCAND) POINT = POINT - NCAND
100  CONTINUE
                          POINT = BEST
                      END IF
                      PICKED(POS) = POINT
                  ELSE

```



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C
C      Case in which a full design has been input, or points are
C      to be forced into the design.
C
C          POINT = PICKED(POS)
C          END IF
C
C      Augment the Cholesky factorization
C
C          CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, POINT)
C          CALL MODTRI(K, NRBAR, ONE, XX, D, RBAR, TOL)
C          POS = POS + 1
110     CONTINUE
120 CONTINUE
C
C      Adjust factorization in case of singular matrix
C
C      CALL SINGM(K, NRBAR, D, RBAR, TOL, WK, IFAULT)
C
C      If rank of input design < K, try replacing points.
C
C      IF (IFAULT .EQ. 0) GO TO 280
C
C      Find first row of Cholesky factorization with a zero
C      multiplier
C
180 DO 190 POS = 1, K
C          IF (D(POS) .LT. TOL(POS)) GO TO 200
190 CONTINUE
C      GO TO 280
C
C      Find linear relationship between variable in position POS
C      and the previous variables
C
200 L = POS - 1
C      DO 210 I = 1, POS - 1
C          WK(I) = RBAR(L)
C          L = L + K - I - 1
210 CONTINUE
C      CALL REGCF(K, NRBAR, D, RBAR, WK, TOL, WK, POS-1, IFAULT)
C
C      Find a candidate point which does not satisfy this linear
C      relationship. Use a random start.
C
C      BL = 1
C      CASE = 1 + NCAND * RAND()
C      DO 230 CAND = 1, NCAND
C          CALL GETX(X, DIM1, KIN, NBLOCK, K, BL, XX, CASE)
C          SUM = XX(POS)
C          DO 220 I = 1, POS - 1
C              SUM = SUM - WK(I) * XX(I)
220     CONTINUE
C          IF (ABS(SUM) .GT. HUNDRD * TOL(POS)) GO TO 240
C          CASE = CASE + 1
C          IF (CASE .GT. NCAND) CASE = 1
230 CONTINUE
C
C      Failed to find any candidate point which would make the design
C      of higher rank
C
C      IFAULT = -1
```

```

      RETURN
C
C   Before adding the point, find one which it can replace without
C   lowering the rank.
C
240  BL = 0
      TEMP = ONE - SMALL
      POS = IN(1) + 1
      DO 270 BLOCK = 1, NB
          DO 260 J = IN(BLOCK) + 1, BLKSIZ(BLOCK)
              L = PICKED(POS)
              CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, L)
              CALL BKSUB2(RBAR, NRBAR, K, XX, WK)
              SUM = ZERO
              DO 250 I = 1, K
                  IF (D(I) .GT. TOL(I)) SUM = SUM + WK(I)**2 / D(I)
250          CONTINUE
              IF (SUM .LT. TEMP) THEN
                  TEMP = SUM
                  REMPOS = POS
                  BL = BLOCK
              END IF
              POS = POS + 1
260          CONTINUE
              IF (BLOCK .LT. NBLOCK) POS = POS + IN(BLOCK+1)
270  CONTINUE
C
C   If BL = 0 it means that any point removed from the existing
C   design would reduce the rank
C
      IF (BL .EQ. 0) THEN
          IFAULT = -1
          RETURN
      END IF
C
C   Add candidate CASE in block BL, then delete the design point
C   already in that position.
C
      CALL GETX(X, DIM1, KIN, NBLOCK, K, BL, XX, CASE)
      CALL MODTRI(K, NRBAR, ONE, XX, D, RBAR, TOL)
      L = PICKED(REMPOS)
      CALL GETX(X, DIM1, KIN, NBLOCK, K, BL, XX, L)
      CALL MODTRI(K, NRBAR, MINUS1, XX, D, RBAR, TOL)
      PICKED(REMPOS) = CASE
      GO TO 180
C
C   Design is now of full rank. Calculate z'z for all candidate
C   points. z is the solution of R'z = x, so that
C   z'z = x'.inv(X'X).x. WK holds sqrt(D) times vector z on
C   return from BKSUB2.
C
280  DO 310 BLOCK = 1, NB
          DO 300 CASE = 1, NCAND
              CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, CASE)
              CALL BKSUB2(RBAR, NRBAR, K, XX, WK)
              TEMP = ZERO
              DO 290 I = 1, K
                  TEMP = TEMP + WK(I)**2 / D(I)
290          CONTINUE
              ZPZ(CASE, BLOCK) = TEMP
300          CONTINUE
310  CONTINUE

```

```

310 CONTINUE
C
C   Start of Fedorov exchange algorithm
C
      LASTIN = 0
      LSTOUT = 0
320 CHANGE = .FALSE.
      LAST = 0
      DO 420 BLOCK = 1, NB
          FIRST = LAST + 1 + IN(BLOCK)
          LAST = LAST + BLKSIZ(BLOCK)
          DETMAX = SMALL
          BEST = 0
C
C   Start at a random position within the block.
C   I = no. of point being considered for deletion.
C
          POS = FIRST + (BLKSIZ(BLOCK) - IN(BLOCK)) * RAND()
          DO 350 CASE = IN(BLOCK)+1, BLKSIZ(BLOCK)
              POS = POS + 1
              IF (POS .GT. LAST) POS = FIRST
              I = PICKED(POS)
              IF (I .EQ. LASTIN) GO TO 350
              CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, I)
              CALL BKSUB2(RBAR, NRBAR, K, XX, WK)
              CALL BKSUB1(RBAR, NRBAR, K, WK, WK, TOL, D)
C
C   Cycle through the candidates for exchange, using a random
C   start. J = no. of point being considered for addition.
C
              J = 1 + NCAND * RAND()
              DO 340 CAND = 1, NCAND
                  J = J + 1
                  IF (J .GT. NCAND) J = 1
                  IF (J .EQ. I .OR. J .EQ. LSTOUT) GO TO 340
C
C   The Cauchy-Schwarz test
C
                  TEMP = ZPZ(J,BLOCK) - ZPZ(I,BLOCK)
                  IF (TEMP .LT. DETMAX) GO TO 340
C
                  CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, J)
                  SUM = ZERO
                  DO 330 L = 1, K
                      SUM = SUM + XX(L) * WK(L)
330          CONTINUE
                  TEMP = TEMP + SUM**2 - ZPZ(I,BLOCK) * ZPZ(J,BLOCK)
                  IF (TEMP .GT. DETMAX) THEN
                      DETMAX = TEMP * ABOVE1
                      BEST = J
                      REMPOS = POS
                      DROP = I
                  END IF
340          CONTINUE
350          CONTINUE
C
C   Exchange points BEST and DROP in position REMPOS, if the
C   determinant is increased.
C
          IF (BEST .NE. 0) THEN
              CHANGE = .TRUE.

```

```

        IF (NB .EQ. 1) THEN
            LASTIN = BEST
            LSTOUT = DROP
        END IF
C
C   Add the new point, BEST, first to avoid ill-conditioning.
C   Update z'z.
C
        CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, BEST)
        CALL BKSUB2(RBAR, NRBAR, K, XX, WK)
        CALL BKSUB1(RBAR, NRBAR, K, WK, WK, TOL, D)
        CALL MODTRI(K, NRBAR, ONE, XX, D, RBAR, TOL)
        TEMP = ONE + ZPZ(BEST,BLOCK)
        DO 360 BL = 1, NB
            DO 380 CASE = 1, NCAND
                CALL GETX(X, DIM1, KIN, NBLOCK, K, BL, XX, CASE)
                SUM = ZERO
                DO 370 L = 1, K
                    SUM = SUM + XX(L) * WK(L)
370                CONTINUE
                ZPZ(CASE,BL) = ZPZ(CASE,BL) - SUM**2 / TEMP
380                CONTINUE
360            CONTINUE
C
C   Remove the point DROP, and update z'z.
C
        CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, DROP)
        CALL BKSUB2(RBAR, NRBAR, K, XX, WK)
        CALL BKSUB1(RBAR, NRBAR, K, WK, WK, TOL, D)
        CALL MODTRI(K, NRBAR, MINUS1, XX, D, RBAR, TOL)
        TEMP = ONE - ZPZ(DROP,BLOCK)
        DO 390 BL = 1, NB
            DO 410 CASE = 1, NCAND
                CALL GETX(X, DIM1, KIN, NBLOCK, K, BL, XX, CASE)
                SUM = ZERO
                DO 400 L = 1, K
                    SUM = SUM + XX(L)*WK(L)
400                CONTINUE
                ZPZ(CASE,BL) = ZPZ(CASE,BL) + SUM**2 / TEMP
410                CONTINUE
390            CONTINUE
C
        PICKED(REMPOS) = BEST
        END IF
420 CONTINUE
C
C   Repeat until there is no further improvement
C
        IF (CHANGE) GO TO 320
C
C   If there is more than one block, try swapping treatments
C   between blocks. This is the Cook & Nachtsheim(1989) algorithm.
C
        IF (NBLOCK .LE. 1) GO TO 500
C
C   RPOS is the position of the first element in RBAR after the
C   rows for the block constants
C
        RPOS = NBLOCK * K - NBLOCK * (NBLOCK + 1)/2 + 1
C
430 LAST1 = 0

```

```

C
C   POS1 and POS2 will hold the positions of the start of the means
C   of the X-variables in the two blocks being considered in RBAR
C
   POS1 = NBLOCK
   DETMAX = SMALL
   CHANGE = .FALSE.
   DO 490 BLOCK1 = 1, NBLOCK - 1
     FIRST1 = LAST1 + 1 + IN(BLOCK1)
     LAST1 = LAST1 + BLKSIZ(BLOCK1)
     LAST2 = LAST1
     POS2 = POS1 + K - 1 - BLOCK1
     DO 480 BLOCK2 = BLOCK1+1, NBLOCK
       FIRST2 = LAST2 + 1 + IN(BLOCK2)
       LAST2 = LAST2 + BLKSIZ(BLOCK2)
       DO 470 CASE1 = IN(BLOCK1)+1, BLKSIZ(BLOCK1)
         POSI = FIRST1 - 1 + CASE1
         I = PICKED(POSI)
         CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, I)
         DO 440 L = 1, KIN
           ZPZ(L,1) = XX(L+NBLOCK)
440        CONTINUE
         DO 460 CASE2 = IN(BLOCK2) + 1, BLKSIZ(BLOCK2)
           POSJ = FIRST2 - 1 + CASE2
           J = PICKED(POSJ)
           IF (I .EQ. J) GO TO 460
           CALL GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, J)
           DO 450 L = 1, KIN
             ZPZ(L,2) = XX(L+NBLOCK)
450          CONTINUE
C
C   Pass the orthogonal factorization to DELTA with the top NBLOCK
C   rows removed, i.e. without that part relating to the blocks.
C
           TEMP = DELTA(KIN, ZPZ(1,1), ZPZ(1,2), RBAR(POS1),
*           RBAR(POS2), BLKSIZ(BLOCK1), BLKSIZ(BLOCK2), NRBAR,
*           D(NBLOCK+1), RBAR(RPOS), ZPZ(1,3), WK, XX, ZPZ(1,2))
           IF (TEMP .GT. DETMAX) THEN
             DETMAX = TEMP * ABOVE1
             BESTB1 = BLOCK1
             BESTB2 = BLOCK2
             BESTP1 = POSI
             BESTP2 = POSJ
             CHANGE = .TRUE.
           END IF
460          CONTINUE
470          CONTINUE
           POS2 = POS2 + K - 1 - BLOCK2
480          CONTINUE
           POS1 = POS1 + K - 1 - BLOCK1
490          CONTINUE
C
C   If CHANGE=.TRUE. then make the swap, otherwise the search ends.
C
   IF (CHANGE) THEN
     I = PICKED(BESTP1)
     J = PICKED(BESTP2)
     CALL GETX(X, DIM1, KIN, NBLOCK, K, BESTB2, XX, I)
     CALL MODTRI(K, NRBAR, ONE, XX, D, RBAR, TOL)
     CALL GETX(X, DIM1, KIN, NBLOCK, K, BESTB1, XX, J)
     CALL MODTRI(K, NRBAR, ONE, XX, D, RBAR, TOL)

```

```
        CALL GETX(X, DIM1, KIN, NBLOCK, K, BESTB1, XX, I)
        CALL MODTRI(K, NRBAR, MINUS1, XX, D, RBAR, TOL)
        CALL GETX(X, DIM1, KIN, NBLOCK, K, BESTB2, XX, J)
        CALL MODTRI(K, NRBAR, MINUS1, XX, D, RBAR, TOL)
        PICKED(BESTP1) = J
        PICKED(BESTP2) = I
        GO TO 430
    END IF
C
C   Calculate log of determinant
C
500  LNDET = ZERO
      DO 510 I = 1, K
          LNDET = LNDET + LOG(D(I))
510  CONTINUE
      RETURN
      END
C
      SUBROUTINE MODTRI(NP, NRBAR, WEIGHT, XROW, D, RBAR, TOL)
C
C   ALGORITHM AS295.2 APPL. STATIST. (1994) VOL.43, NO.4
C
C   Modify a triangular (Cholesky) decomposition. Calling this
C   routine updates D and RBAR by adding another design point with
C   weight = WEIGHT, which may be negative. Algorithm based on
C   AS75.1 with modifications.
C   *** WARNING: Array XROW is overwritten ***
C
      INTEGER NP, NRBAR
      REAL WEIGHT, XROW(NP), D(NP), RBAR(*), TOL(NP)
C
      INTEGER I, K, NEXTR
      REAL CBAR, DI, DPI, SBAR, W, WXI, XI, XK, ZERO
C
      DATA ZERO /0.0E + 00/
C
      W = WEIGHT
      NEXTR = 1
      DO 30 I = 1, NP
C
C   Skip unnecessary transformations. Test on exact zeroes must
C   be used or stability can be destroyed.
C
          IF (W .EQ. ZERO) RETURN
C
          XI = XROW(I)
          IF (ABS(XI) .LT. TOL(I)) THEN
              NEXTR = NEXTR + NP - I
              GO TO 30
          END IF
C
          DI = D(I)
          WXI = W*XI
          DPI = DI + WXI * XI
C
C   Test for new singularity
C
          IF (DPI .LT. TOL(I)) THEN
              DPI = ZERO
              CBAR = ZERO
              SBAR = ZERO
```

```

        W = ZERO
    ELSE
        CBAR = DI/DPI
        SBAR = WXI/DPI
        W = CBAR*W
    END IF
C
    D(I) = DPI
    DO 20 K = I + 1, NP
        XK = XROW(K)
        XROW(K) = XK - XI*RBAR(NEXTR)
        RBAR(NEXTR) = CBAR*RBAR(NEXTR) + SBAR*XK
        NEXTR = NEXTR + 1
20    CONTINUE
30    CONTINUE
    RETURN
    END

C
SUBROUTINE MODTR2(NP, NRBAR, XROW, D, RBAR, TOL, RANK, LNDET)
C
C    ALGORITHM AS295.3 APPL. STATIST. (1994) VOL.43, NO.4
C
C    Calculate the effect of an update of a QR factorization
C    upon the rank and determinant, without changing D or
C    RBAR. Algorithm based on AS75.1 with modifications.
C    *** WARNING: Array XROW is overwritten ***
C
    INTEGER NP, NRBAR, RANK
    REAL XROW(NP), D(NP), RBAR(*), TOL(NP), LNDET
C
    INTEGER I, J, K, NEXTR
    REAL CBAR, DI, DPI, ONE, W, WXI, XI, XK, ZERO
C
    DATA ZERO /0.0E + 00/, ONE /1.0E + 00/
C
    W = ONE
    RANK = 0
    LNDET = ZERO
    NEXTR = 1
    DO 30 I = 1, NP
C
C    Skip unnecessary transformations. Test on exact zeroes must be
C    used or stability can be destroyed.
C
        IF (W .EQ. ZERO) THEN
            DO 10 J = I, NP
                IF (D(J) .GT. TOL(J)) THEN
                    RANK = RANK + 1
                    LNDET = LNDET + LOG(D(J))
                END IF
10            CONTINUE
            RETURN
        END IF
C
        XI = XROW(I)
        IF (ABS(XI) .LT. TOL(I)) THEN
            IF (D(I) .GT. TOL(I)) THEN
                RANK = RANK + 1
                LNDET = LNDET + LOG(D(I))
            END IF
            NEXTR = NEXTR + NP - I

```

```
        GO TO 30
        END IF
C
        DI = D(I)
        WXI = W * XI
        DPI = DI + WXI * XI
C
C      Test for new singularity
C
        IF (DPI .LT. TOL(I)) THEN
            DPI = ZERO
            CBAR = ZERO
            W = ZERO
        ELSE
            CBAR = DI / DPI
            W = CBAR * W
            LNDET = LNDET + LOG(DPI)
            RANK = RANK + 1
        END IF
C
        DO 20 K = I + 1, NP
            XK = XROW(K)
            XROW(K) = XK - XI * RBAR(NEXTR)
            NEXTR = NEXTR + 1
20      CONTINUE
30      CONTINUE
        RETURN
        END
C
SUBROUTINE GETX(X, DIM1, KIN, NBLOCK, K, BLOCK, XX, CASE)
C
C      ALGORITHM AS295.4 APPL. STATIST. (1994) VOL.43, NO.4
C
C      Copy one case from X to XX
C
        INTEGER DIM1, KIN, NBLOCK, K, BLOCK, CASE
        REAL X(DIM1, KIN), XX(K)
C
        INTEGER I, J
        REAL ONE, ZERO
C
        DATA ZERO /0.0E + 00/, ONE /1.0E + 00/
C
        DO 10 I = 1, NBLOCK
            IF (I .NE. BLOCK) THEN
                XX(I) = ZERO
            ELSE
                XX(I) = ONE
            END IF
10      CONTINUE
        J = NBLOCK + 1
        DO 20 I = 1, KIN
            XX(J) = X(CASE, I)
            J = J + 1
20      CONTINUE
        RETURN
        END
C
SUBROUTINE BKSUB1(RBAR, NRBAR, K, RHS, SOLN, TOL, D)
C
C      ALGORITHM AS295.5 APPL. STATIST. (1994) VOL.43, NO.4
```



```
C
C   Solves  $DRy = z$  for  $y$  (SOLN), where  $z = RHS$ .
C   RBAR is an upper-triangular matrix with implicit 1's on it's
C   diagonal, stored by rows.
C
C   INTEGER NRBAR, K
C   REAL RBAR(NRBAR), RHS(K), SOLN(K), TOL(K), D(K)
C
C   INTEGER COL, POS, ROW
C   REAL TEMP, ZERO
C
C   DATA ZERO /0.0E + 00/
C
C   POS = K * (K - 1) / 2
C   DO 20 ROW = K, 1, -1
C       IF (D(ROW) .GT. TOL(ROW)) THEN
C           TEMP = RHS(ROW) / D(ROW)
C           DO 10 COL = K, ROW + 1, -1
C               TEMP = TEMP - RBAR(POS) * SOLN(COL)
C               POS = POS - 1
10      CONTINUE
C           SOLN(ROW) = TEMP
C       ELSE
C           POS = POS - K + ROW
C           SOLN(ROW) = ZERO
C       END IF
20 CONTINUE
C   RETURN
C   END
C
C   SUBROUTINE BKSUB2(RBAR, NRBAR, K, RHS, SOLN)
C
C   ALGORITHM AS295.6 APPL. STATIST. (1994) VOL.43, NO.4
C
C   Solves  $R'(\sqrt{D}).z = x$  where  $(\sqrt{D}).z = SOLN$  and  $x = RHS$ .
C   RBAR is an upper-triangular matrix with implicit 1's on it's
C   diagonal, stored by rows.
C
C   INTEGER NRBAR, K
C   REAL RBAR(NRBAR), RHS(K), SOLN(K)
C
C   INTEGER COL, POS, ROW
C   REAL TEMP
C
C   SOLN(1) = RHS(1)
C   DO 20 ROW = 2, K
C       TEMP = RHS(ROW)
C       POS = ROW - 1
C       DO 10 COL = 1, ROW - 1
C           TEMP = TEMP - RBAR(POS) * SOLN(COL)
C           POS = POS + K - COL - 1
10      CONTINUE
C       SOLN(ROW) = TEMP
20 CONTINUE
C   RETURN
C   END
C
C   REAL FUNCTION DELTA(K, XJ, XL, XBARI, XBARK, NI, NK,
*           NRBAR, D, RBAR, Z, A, B, DIFF)
C
C   ALGORITHM AS295.7 APPL. STATIST. (1994) VOL.43, NO.4
```

```

C
C   Calculate the delta function for the swap of case J in block I
C   with case L in block K. Uses the method of Cook & Nachtsheim.
C
C   INTEGER K, NI, NK, NRBAR
C   REAL XJ(K), XL(K), XBARI(K), XBARK(K), D(K),
*     RBAR(NRBAR), Z(K,3), A(K), B(K), DIFF(K)
C
C   INTEGER I
C   REAL CONST, E11, E12, E21, E22, ONE, TEMP, TWO
C
C   REAL DOTPRD
C   EXTERNAL BKSUB2, DOTPRD
C
C   DATA ONE /1.0E + 00/, TWO /2.0E + 00/
C
C   Calculate vectors DIFF, A and B
C
C   CONST = TWO - ONE/NI - ONE/NK
C   DO 10 I = 1, K
C     TEMP = XJ(I) - XL(I)
C     DIFF(I) = -TEMP
C     A(I) = TEMP - XBARI(I) + XBARK(I)
C     B(I) = A(I) - CONST * TEMP
10 CONTINUE
C
C   Calculate the z-vectors by back-substitution. Z1 for A, Z2
C   for B and Z3 for DIFF. The solutions returned from
C   BKSUB2 have the I-th element multiplied by sqrt(D(I)).
C
C   CALL BKSUB2(RBAR, NRBAR, K, A, Z(1,1))
C   CALL BKSUB2(RBAR, NRBAR, K, B, Z(1,2))
C   CALL BKSUB2(RBAR, NRBAR, K, DIFF, Z(1,3))
C
C   Calculate the elements E11, E12, E21 and E22 as dot-products
C   of the appropriate z-vectors
C
C   E11 = DOTPRD(K, Z(1,3), Z(1,1), D)
C   E12 = DOTPRD(K, Z(1,3), Z(1,3), D)
C   E21 = DOTPRD(K, Z(1,2), Z(1,1), D)
C   E22 = DOTPRD(K, Z(1,2), Z(1,3), D)
C
C   Return the determinant of the matrix:
C
C   E11+1   E12
C   E21     E22+1
C
C   minus 1
C
C   DELTA = (E11+ONE) * (E22+ONE) - E12 * E21 - ONE
C   RETURN
C   END
C
C   REAL FUNCTION DOTPRD(K, X, Y, D)
C
C   ALGORITHM AS295.8 APPL. STATIST. (1994) VOL.43, NO.4
C
C   Dot-product scaled by vector D
C
C   INTEGER K
C   REAL X(K), Y(K), D(K)
C
C   INTEGER I
C   REAL ZERO

```

```
C
  DATA ZERO /0.0E + 00/
C
  DOTPRD = ZERO
  DO 10 I = 1, K
    DOTPRD = DOTPRD + X(I) * Y(I) / D(I)
10 CONTINUE
  RETURN
  END
C
  SUBROUTINE SINGM(NP, NRBAR, D, RBAR, TOL, WORK, IFAULT)
C
  ALGORITHM AS295.9 APPL. STATIST. (1994) VOL.43, NO.4
C
  Checks for singularities, and adjusts orthogonal
  reductions produced by AS75.1. Modified from AS274.5
C
  INTEGER NP, NRBAR, IFAULT
  REAL D(NP), RBAR(NRBAR), TOL(NP), WORK(NP)
C
  INTEGER COL, J, NP2, POS, POS1, ROW
  REAL TEMP, ZERO
C
  EXTERNAL MODTRI
C
  DATA ZERO /0.0E + 00/
C
  Check input parameters
C
  IFAULT = 0
  IF (NP .LE. 0) IFAULT = 1
  IF (NRBAR .LT. NP * (NP - 1)/2) IFAULT = IFAULT + 2
  IF (IFAULT .NE. 0) RETURN
C
  DO 10 COL = 1, NP
    WORK(COL) = SQRT(D(COL))
10 CONTINUE
C
  DO 40 COL = 1, NP
C
  Set elements within RBAR to zero if they are less than TOL(COL)
  in absolute value after being scaled by the square root of
  their row multiplier
C
    TEMP = TOL(COL)
    POS = COL - 1
    DO 20 ROW = 1, COL - 1
      IF (ABS(RBAR(POS)) * WORK(ROW) .LT. TEMP) RBAR(POS) = ZERO
      POS = POS + NP - ROW - 1
20 CONTINUE
C
  If diagonal element is near zero, set it to zero, and use
  MODTRI to augment the projections in the lower rows of the
  factorization.
C
    IF (WORK(COL) .LE. TEMP) THEN
      IFAULT = IFAULT - 1
    IF (COL .LT. NP) THEN
      NP2 = NP - COL
      POS2 = POS + NP - COL + 1
      IF (NP2 .GT. 1) THEN
```

```
      CALL MODTRI(NP2, NP2*(NP2-1)/2, D(COL), RBAR(POS+1),
*          D(COL+1), RBAR(POS2), TOL)
      ELSE
      CALL MODTRI(1, 0, D(COL), RBAR(POS+1), D(COL+1),
*          RBAR(1), TOL)
      END IF
      DO 30 J = POS + 1, POS2 - 1
      RBAR(J) = ZERO
30    CONTINUE
      END IF
      D(COL) = ZERO
      END IF
40 CONTINUE
RETURN
END
```

```
C
SUBROUTINE XXTR(NP, NRBAR, D, RBAR, NREQ, TRACE, RINV)
C
C   ALGORITHM AS295.10 APPL. STATIST. (1994) VOL.43, NO.4
C
C   Calculate the trace of the inverse of X'X (= R'R)
C
C   INTEGER NP, NRBAR, NREQ
C   REAL D(NP), RBAR(NRBAR), TRACE, RINV(*)
C
C   INTEGER COL, POS, ROW
C   REAL ONE, ZERO
C
C   EXTERNAL INV
C   AS274.8, Appl.Statist.(1992), vol.41, no.2
C
C   DATA ONE /1.0E + 00/, ZERO /0.0E + 00/
C
C   Get the inverse of R
C
C   CALL INV(NP, RBAR, NREQ, RINV)
C
C   Trace = the sum of the diagonal elements
C   of RINV * (1/D) * (RINV)'
C
C   TRACE = ZERO
C   POS = 1
C   DO 20 ROW = 1, NREQ
C     TRACE = TRACE + ONE / D(ROW)
C     DO 10 COL = ROW + 1, NREQ
C       TRACE = TRACE + RINV(POS)**2 / D(COL)
C       POS = POS + 1
10    CONTINUE
20 CONTINUE
RETURN
END
```

```

SUBROUTINE SWILK (INIT, X, N, N1, N2, A, W, PW, IFAULT)
C
C   ALGORITHM AS R94 APPL. STATIST. (1995) VOL.44, NO.4
C
C   Calculates the Shapiro-Wilk W test and its significance level
C
INTEGER N, N1, N2, IFAULT
REAL X(*), A(*), PW, W
REAL C1(6), C2(6), C3(4), C4(4), C5(4), C6(3), C7(2)
REAL C8(2), C9(2), G(2)
REAL Z90, Z95, Z99, ZM, ZSS, BF1, XX90, XX95, ZERO, ONE, TWO
REAL THREE, SQRTH, QTR, TH, SMALL, PI6, STQR
REAL SUMM2, SSUMM2, FAC, RSN, AN, AN25, A1, A2, DELTA, RANGE
REAL SA, SX, SSX, SSA, SAX, ASA, XSX, SSASSX, W1, Y, XX, XI
REAL GAMMA, M, S, LD, BF, Z90F, Z95F, Z99F, ZFM, ZSD, ZBAR
C
C   Auxiliary routines
C
REAL PPND, ALNORM, POLY
C
INTEGER NCENS, NN2, I, I1, J
LOGICAL INIT, UPPER
C
DATA C1 /0.0E0, 0.221157E0, -0.147981E0, -0.207119E1,
*   0.4434685E1, -0.2706056E1/
DATA C2 /0.0E0, 0.42981E-1, -0.293762E0, -0.1752461E1,
*   0.5682633E1, -0.3582633E1/
DATA C3 /0.5440E0, -0.39978E0, 0.25054E-1, -0.6714E-3/
DATA C4 /0.13822E1, -0.77857E0, 0.62767E-1, -0.20322E-2/
DATA C5 /-0.15861E1, -0.31082E0, -0.83751E-1, 0.38915E-2/
DATA C6 /-0.4803E0, -0.82676E-1, 0.30302E-2/
DATA C7 /0.164E0, 0.533E0/
DATA C8 /0.1736E0, 0.315E0/
DATA C9 /0.256E0, -0.635E-2/
DATA G  /-0.2273E1, 0.459E0/
DATA Z90, Z95, Z99 /0.12816E1, 0.16449E1, 0.23263E1/
DATA ZM, ZSS /0.17509E1, 0.56268E0/
DATA BF1 /0.8378E0/, XX90, XX95 /0.556E0, 0.622E0/
DATA ZERO /0.0E0/, ONE/1.0E0/, TWO/2.0E0/, THREE/3.0E0/
DATA SQRTH /0.70711E0/, QTR/0.25E0/, TH/0.375E0/, SMALL/1E-19/
DATA PI6 /0.1909859E1/, STQR/0.1047198E1/, UPPER/.TRUE./
C
PW = ONE
IF (W .GE. ZERO) W = ONE
AN = N
IFAULT = 3
NN2 = N/2
IF (N2 .LT. NN2) RETURN
IFAULT = 1
IF (N .LT. 3) RETURN
C
C   If INIT is false, calculates coefficients for the test
C
IF (.NOT. INIT) THEN
  IF (N .EQ. 3) THEN
    A(1) = SQRTH
  ELSE
    AN25 = AN + QTR
    SUMM2 = ZERO
    DO 30 I = 1, N2
      A(I) = PPND((I - TH)/AN25)

```

```

        SUMM2 = SUMM2 + A(I) ** 2
30      CONTINUE
        SUMM2 = SUMM2 * TWO
        SSUMM2 = SQRT(SUMM2)
        RSN = ONE / SQRT(AN)
        A1 = POLY(C1, 6, RSN) - A(1) / SSUMM2
C
C      Normalize coefficients
C
        IF (N .GT. 5) THEN
            I1 = 3
            A2 = -A(2)/SSUMM2 + POLY(C2,6,RSN)
            FAC = SQRT((SUMM2 - TWO * A(1) ** 2 - TWO *
*             A(2) ** 2)/(ONE - TWO * A1 ** 2 - TWO * A2 ** 2))
            A(1) = A1
            A(2) = A2
        ELSE
            I1 = 2
            FAC = SQRT((SUMM2 - TWO * A(1) ** 2)/
*             (ONE - TWO * A1 ** 2))
            A(1) = A1
        END IF
        DO 40 I = I1, NN2
            A(I) = -A(I)/FAC
40      CONTINUE
        END IF
        INIT = .TRUE.
    END IF
    IF (N1 .LT. 3) RETURN
    NCENS = N - N1
    IFAULT = 4
    IF (NCENS .LT. 0 .OR. (NCENS .GT. 0 .AND. N .LT. 20)) RETURN
    IFAULT = 5
    DELTA = FLOAT(NCENS)/AN
    IF (DELTA .GT. 0.8) RETURN
C
C      If W input as negative, calculate significance level of -W
C
    IF (W .LT. ZERO) THEN
        W1 = ONE + W
        IFAULT = 0
        GOTO 70
    END IF
C
C      Check for zero range
C
    IFAULT = 6
    RANGE = X(N1) - X(1)
    IF (RANGE .LT. SMALL) RETURN
C
C      Check for correct sort order on range - scaled X
C
    IFAULT = 7
    XX = X(1)/RANGE
    SX = XX
    SA = -A(1)
    J = N - 1
    DO 50 I = 2, N1
        XI = X(I)/RANGE
        IF (XX-XI .GT. SMALL) PRINT *, ' ANYTHING '
        SX = SX + XI

```

```

        IF (I .NE. J) SA = SA + SIGN(1, I - J) * A(MIN(I, J))
        XX = XI
        J = J - 1
50    CONTINUE
        IFAULT = 0
        IF (N .GT. 5000) IFAULT = 2
C
C        Calculate W statistic as squared correlation
C        between data and coefficients
C
        SA = SA/N1
        SX = SX/N1
        SSA = ZERO
        SSX = ZERO
        SAX = ZERO
        J = N
        DO 60 I = 1, N1
            IF (I .NE. J) THEN
                ASA = SIGN(1, I - J) * A(MIN(I, J)) - SA
            ELSE
                ASA = -SA
            END IF
            XSX = X(I)/RANGE - SX
            SSA = SSA + ASA * ASA
            SSX = SSX + XSX * XSX
            SAX = SAX + ASA * XSX
            J = J - 1
60    CONTINUE
C
C        W1 equals (1-W) claculated to avoid excessive rounding error
C        for W very near 1 (a potential problem in very large samples)
C
        SSASSX = SQRT(SSA * SSX)
        W1 = (SSASSX - SAX) * (SSASSX + SAX)/(SSA * SSX)
70    W = ONE - W1
C
C        Calculate significance level for W (exact for N=3)
C
        IF (N .EQ. 3) THEN
            PW = PI6 * (ASIN(SQRT(W)) - STQR)
            RETURN
        END IF
        Y = LOG(W1)
        XX = LOG(AN)
        M = ZERO
        S = ONE
        IF (N .LE. 11) THEN
            GAMMA = POLY(G, 2, AN)
            IF (Y .GE. GAMMA) THEN
                PW = SMALL
                RETURN
            END IF
            Y = -LOG(GAMMA - Y)
            M = POLY(C3, 4, AN)
            S = EXP(POLY(C4, 4, AN))
        ELSE
            M = POLY(C5, 4, XX)
            S = EXP(POLY(C6, 3, XX))
        END IF
        IF (NCENS .GT. 0) THEN

```

```
C      Censoring by proportion NCENS/N. Calculate mean and sd
C      of normal equivalent deviate of W.
C
      LD = -LOG(DELTA)
      BF = ONE + XX * BF1
      Z90F = Z90 + BF * POLY(C7, 2, XX90 ** XX) ** LD
      Z95F = Z95 + BF * POLY(C8, 2, XX95 ** XX) ** LD
      Z99F = Z99 + BF * POLY(C9, 2, XX) ** LD
C
C      Regress Z90F,...,Z99F on normal deviates Z90,...,Z99 to get
C      pseudo-mean and pseudo-sd of z as the slope and intercept
C
      ZFM = (Z90F + Z95F + Z99F)/THREE
      ZSD = (Z90*(Z90F-ZFM)+Z95*(Z95F-ZFM)+Z99*(Z99F-ZFM))/ZSS
      ZBAR = ZFM - ZSD * ZM
      M = M + ZBAR * S
      S = S * ZSD
END IF
PW = ALNORM((Y - M)/S, UPPER)
C
RETURN
END
```



```
subroutine wext(x, n, ssq, a, n2, eps, w, pw, ifault)
c
c   Algorithm AS 181   Appl. Statist. (1982) Vol. 31, No. 2
c
c   Calculates Shapiro and Wilk's W statistic and its sig. level
c
c   Auxiliary routines required: ALNORM = algorithm AS 66 and NSCOR2
c   from AS 177.
c
c   real x(n), a(n2), lamda, wa(3), wb(4), wc(4), wd(6), we(6), wf(7),
*   c1(5, 3), c2(5, 3), c(5), un1(3), unh(3)
c   integer ncl(3), nc2(3)
c   logical upper
c   data wa(1), wa(2), wa(3)
*   /0.118898, 0.133414, 0.327907/,
*   wb(1), wb(2), wb(3), wb(4)
*   /-0.37542, -0.492145, -1.124332, -0.199422/,
*   wc(1), wc(2), wc(3), wc(4)
*   /-3.15805, 0.729399, 3.01855, 1.558776/,
*   wd(1), wd(2), wd(3), wd(4), wd(5), wd(6)
*   /0.480385, 0.318828, 0.0, -0.0241665, 0.00879701, 0.002989646/,
*   we(1), we(2), we(3), we(4), we(5), we(6)
*   /-1.91487, -1.37888, -0.04183209, 0.1066339, -0.03513666,
*   -0.01504614/,
*   wf(1), wf(2), wf(3), wf(4), wf(5), wf(6), wf(7)
*   /-3.73538, -1.015807, -0.331885, 0.1773538, -0.01638782,
*   -0.03215018, 0.003852646/
c   data c1(1,1), c1(2,1), c1(3,1), c1(4,1), c1(5,1),
*   c1(1,2), c1(2,2), c1(3,2), c1(4,2), c1(5,2),
*   c1(1,3), c1(2,3), c1(3,3), c1(4,3), c1(5,3) /
*   -1.26233, 1.87969, 0.0649583, -0.0475604, -0.0139682,
*   -2.28135, 2.26186, 0.0, 0.0, -0.00865763,
*   -3.30623, 2.76287, -0.83484, 1.20857, -0.507590/
c   data c2(1,1), c2(2,1), c2(3,1), c2(4,1), c2(5,1),
*   c2(1,2), c2(2,2), c2(3,2), c2(4,2), c2(5,2),
*   c2(1,3), c2(2,3), c2(3,3), c2(4,3), c2(5,3) /
*   -0.287696, 1.78953, -0.180114, 0.0, 0.0,
*   -1.63638, 5.60924, -3.63738, 1.08439, 0.0,
*   -5.991908, 21.04575, -24.58061, 13.78661, -2.835295/
c   data un1(1), un1(2), un1(3) /-3.8, -3.0, -1.0/,
*   unh(1), unh(2), unh(3) / 8.6, 5.8, 5.4/
c   data ncl(1), ncl(2), ncl(3) /5, 5, 5/,
*   nc2(1), nc2(2), nc2(3) /3, 4, 5/
c   data pi6 /1.90985932/, stqr /1.04719755/, upper /.true./,
*   zero/0.0/, tqr /0.75/, one /1.0/, onept4 /1.4/, three/3.0/,
*   five/5.0/
c
c   ifault = 1
c   pw = one
c   w = one
c   if(n.le.2) return
c   ifault = 3
c   if(n/2 .ne. n2) return
c   ifault = 2
c   if(n.gt.2000) return
c
c   Calculate W
c
c   ifault = 0
c   w = zero
c   an = n
```

```
      i = n
      do 10 j = 1,n2
        w = w+a(j) * (x(i)-x(j))
        i = i-1
10 continue
      w = w * w / ssq
      if (w .lt. one) goto 20
      w = one
      return
c
c      Get significance level of W
c
c      20 if (n .le. 6) goto 100
c
c      N between 7 and 2000 ... Transform W to Y, get mean and sd,
c      standardize and get significance level
c
      if(n.gt.20) goto 30
      al = log(an) - three
      lamda = poly(wa,3,al)
      ybar = exp(poly(wb,4,al))
      sdy = exp(poly(wc,4,al))
      goto 40
30 al = log(an) - five
      lamda = poly(wd,6,al)
      ybar = exp(poly(we,6,al))
      sdy = exp(poly(wf,7,al))
40 y = (one-w) ** lamda
      z = (y - ybar) / sdy
      pw = alnorm(z,upper)
      return
c
c      Deal with N less than 7 (Exact significance level for N = 3).
c
c      100 if(w .le. eps) goto 160
      ww = w
      if(n.eq.3) goto 150
      un = log((w-eps)/(one-w))
      n3 = n-3
      if(un .lt. unl(n3)) goto 160
      if (un .ge. onept4) goto 120
      nc = ncl(n3)
      do 110 i = 1,nc
110 c(i) = c1(i,n3)
      eu3 = exp(poly(c,nc,un))
      goto 140
120 if (un .gt. unh(n3)) return
      nc = nc2(n3)
      do 130 i = 1,nc
130 c(i) = c2(i,n3)
      un = log(un)
      eu3 = exp(exp(poly(c,nc,un)))
140 ww = (eu3+stqr)/(one+eu3)
150 pw = pi6 *(atan(sqrt(ww/(one-ww)))-stqr)
      return
160 pw = zero
      return
      end
c
c      subroutine wcoef(a, n, n2, eps, ifault)
```

```
c
c      Algorithm AS 181.1  Appl. Statist.  (1982) Vol. 31, No. 2
c
c      Obtain array A of weights for calculating W
c
      real a(n2), c4(2), c5(2), c6(3)
      data c4(1), c4(2) /0.6869, 0.1678/, c5(1), c5(2) /0.6647, 0.2412/,
*   c6(1), c6(2), c6(3) /0.6431, 0.2806, 0.0875/
      data rsqrt2 /0.70710678/, zero/0.0/, half/0.5/, one/1.0/,
*   two/2.0/, six/6.0/, seven/7.0/, eight/8.0/, thirt /13.0/
      ifault = 1
      if(n.le.2) return
      ifault = 3
      if(n/2 .ne. n2) return
      ifault = 2
      if(n.gt.2000) return
      ifault = 0
      if(n .le. 6) goto 30
c
c      N .GT. 6  Calculate rankits using approximate routine nscor2
c                (AS177)
c
      call nscor2(a, n, n2, ifault)
      sastar = zero
      do 10 j = 2,n2
10  sastar = sastar+a(j)*a(j)
      sastar = sastar*eight
      nn = n
      if (n .le. 20) nn = nn-1
      an = nn
      alsq = exp(log(six*an+seven)-log(six*an+thirt)
*   +half*(one+(an-two)*log(an+one)-(an-one)
*   *log(an+two)))
      alstar = sastar/(one/alsq-two)
      sastar = sqrt(sastar+two*alstar)
      a(1) = sqrt(alstar)/sastar
      do 20 j = 2,n2
20  a(j) = two*a(j)/sastar
      goto 70
c
c      n.le.6  Use exact values for weiughts
c
30  a(1) = rsqrt2
      if(n.eq.3) goto 70
      n3 = n-3
      goto (40,50,60), n3
40  do 45 j = 1,2
45  a(j) = c4(j)
      goto 70
50  do 55 j = 1,2
55  a(j) = c5(j)
      goto 70
60  do 65 j = 1,3
65  a(j) = c6(j)
c
c      Calculate the minimum possible value of W
c
70  eps = a(1)*a(1)/(one-one/float(n))
      return
      end
c
```

```
c
function poly(c, nord, x)
c
c
c   Algorithm AS 181.2   Appl. Statist.   (1982) Vol. 31, No. 2
c
c   Calculates the algebraic polynomial of order nored-1 with
c   array of coefficients c. Zero order coefficient is c(1)
c
real c(nord)
poly = c(1)
if(nord.eq.1) return
p = x*c(nord)
if(nord.eq.2) goto 20
n2 = nord-2
j = n2+1
do 10 i = 1,n2
p = (p+c(j))*x
j = j-1
10 continue
20 poly = poly+p
return
end

c
c
c
subroutine wgp(x, n, ssq, gp, h, a, n2, eps, w, u, p, ifault)
c
c   AS R63 Appl. Statist. (1986) Vol. 35, No.2
c
c   A remark on AS 181
c
c   Calculates Sheppard corrected version of W test.
c
c   Auxiliary functions required: ALNORM = algorithm AS 66, and
c   PPN7 = algorithm AS 111 (or PPN7 from AS 241).
c
real x(n), a(n2)
data twelve /1.2e01/, ten/1.0e1/, five/5.0e0/, one/1.0e0/,
*   zero/0.0e0/
c
zbar = zero
zsd = one
ifault = 1
if (n.lt.7) return
c
c   No correction applied if gp=0.
c
if (gp .le. zero) goto 10
an1 = float(n-1)
c
c   correct ssq and find standardized grouping interval (h)
c
ssq = ssq - an1 * gp * gp / twelve
h = gp / sqrt(ssq / an1)
ifault = 4
if (h .gt. 1.5) return
10 call wext(x, n, ssq, a, n2, eps, w, p, ifault)
if (ifault .ne. 0) return
if (p .gt. zero .and. p .lt. one) goto 20
u = five - ten * p
```

```
    return
20  if (gp .le. zero) goto 30
c
c      correct u for grouping interval (n .le. 100 and n .gt. 100
c      separately)
c
    hh = sqrt(h)
    if (n .gt. 100) goto 25
    zbar = -h*(1.07457 + hh*(-2.8185 + hh*1.8898))
    zsd = one + h*(0.50933 + hh*(-0.98305 + hh*0.7408))
    goto 30
25  zbar = -h*(0.96436 + hh*(-2.1300 + hh*1.3196))
    zsd = one + h*(0.2579 + h*0.15225)
c
c      ppnd is AS 111 (Beasley and Springer, 1977)
c
30  u = (-ppnd(p, ifppnd) - zbar) / zsd
c
c      alnorm is AS 66 (Hill, 1973)
c
    p = alnorm(u, .true.)
    return
end
```

```
      SUBROUTINE INTBD(G, N, E, ET, DELTA, ITAIL)
C
C      ALGORITHM AS R96 APPL. STATIST. (1996) VOL.45, NO.2
C
C      Interval for trapezoidal rule integration to limit error to
C      E using moment generating function bound for weighted sum of
C      chi-squared(1) random variables
C
      INTEGER N, ITAIL
      REAL DELTA, G(N), E, ET
C
      INTEGER I
      REAL ZERO, TWO, POINT1, POINT5, TWOPI, ULM, PSI, DPSI, D2PSI,
*      HB, U, U1, U2, ELOG, EPS, HM, HSD, SGN, ZABS, ZEXP, ZFLOAT,
*      ZLOG, ZMAX1, ZMIN1, ZSQRT
C
      EXTERNAL LMGFEV
C
      DATA ZERO, TWO, POINT1, POINT5 /0.0E0, 2.0E0, 0.1E0, 0.5E0/
      DATA TWOPI /6.28318530717959E0/
      DATA EPS /0.09531E0/
C
      ZABS(U) = ABS(U)
      ZEXP(U) = EXP(U)
      ZFLOAT(I) = FLOAT(I)
      ZLOG(U) = ALOG(U)
      ZMAX1(U, U1) = AMAX1(U, U1)
      ZMIN1(U, U1) = AMIN1(U, U1)
      ZSQRT(U) = SQRT(U)
C
      Tail check
C
      SGN = ZFLOAT(ITAIL)
      IF (ITAIL .EQ. 1) THEN
        IF (G(N) .LE. ZERO) RETURN
        ULM = POINT5 / G(N)
      ELSE
        IF (G(1) .GE. ZERO) RETURN
        ULM = POINT5 / G(1)
      ENDIF
      HM = ZERO
      HSD = ZERO
      DO 10 I = 1, N
        HM = HM + G(I)
        HSD = HSD + G(I) ** 2
10 CONTINUE
C
      Newton search for zero log(m.g.f.) derivative
C
      HSD = ZSQRT(HSD)
      U1 = ZERO
      U2 = ZERO
      IF (SGN * HM .LT. ZERO .AND. -SGN * HM / HSD .GT. TWO) THEN
        DPSI = HM
20      IF (DPSI * SGN .LT. ZERO) THEN
          U1 = U2
          U2 = POINT5 * (U2 + ULM)
          CALL LMGFEV (U2, G, N, PSI, DPSI, D2PSI)
          GOTO 20
        ENDIF
25      IF (DPSI ** 2 .GE. POINT1 * D2PSI) THEN
```

```
        U2 = U2 - DPSI / D2PSI
        CALL LMGFEV(U2, G, N, PSI, DPSI, D2PSI)
    ENDIF
    IF (ZEXP(PSI) .LE. E) RETURN
ENDIF
C
C      Bound equality
C
    ELOG = - ZLOG(ET)
    CALL LMGFEV(U2, G, N, PSI, DPSI, D2PSI)
    HB = PSI - U2 * DPSI + ELOG
30 IF (HB .GT. ZERO) THEN
    U1 = U2
    U2 = POINT5 * (U2 + ULIM)
    CALL LMGFEV(U2, G, N, PSI, DPSI, D2PSI)
    HB = PSI - U2 * DPSI + ELOG
    GOTO 30
ENDIF
C
C      Newton/binary search solution
C
    U = U2
40 IF (ZABS(HB) .GE. EPS) THEN
    U = U + HB / (U * D2PSI)
    IF (U .LE. ZMIN1(U1, U2) .OR. U .GT. ZMAX1(U1, U2))
*      U = POINT5 * (U1 + U2)
    CALL LMGFEV(U, G, N, PSI, DPSI, D2PSI)
    HB = PSI - U * DPSI + ELOG
    IF (HB .GT. ZERO) THEN
        U1 = U
    ELSE
        U2 = U
    ENDIF
    GOTO 40
ENDIF
IF (ITAIL .EQ. 1 .AND. DPSI .GT. ZERO) THEN
    DELTA = TWOPI / DPSI
    ITAIL = 0
ELSEIF (ITAIL .EQ. -1 .AND. DPSI .LT. ZERO) THEN
    DELTA = - TWOPI / DPSI
    ITAIL = 0
ENDIF
C
RETURN
END
```

```
      SUBROUTINE ULTRA (BW,M,MORD,MUE,N,NUE,OPTIO1,OPTIO2,OPTIO3,
*                   XIN,XOU,YIN,IWKAR,WKAR,IFAU,LT,W2,YOU)
C
C      ALGORITHM AS297.1 APPL. STATIST. (1995) VOL.44, NO.2
C
C      Nonparametric regression using ultraspherical
C      polynomials
C
      INTEGER I0, I1, I2, I3, I4, I5, I6, I7, I8, I9, I10, I11, I12,
*          I13, I11, I12, IFLG, IFLG1, IL, ILB, IR, IRB, IZ, M,
*          IWKAR(2*M), MORD, N, IFAULT, NUE, OPTIO1, OPTIO2, OPTIO3
      DOUBLE PRECISION BW, PHIJU, SUMW2, XA, XAMB, XAMBN, XAPB, XB, XC,
*          XX, XIN(N), XOU(M), W2(M),YIN(N), YOU(M), YOUT,
*          YOUT1, WKAR(60*N+2000)
C
      EXTERNAL BOUND, ERROR, INIT, PHIJ, SAVE, WEIGHT
C
C      Error checks
C
      CALL ERROR (BW,M,MORD,MUE,N,NUE,OPTIO1,OPTIO2,XIN,XOU,IFAU,LT)
      IF (IFAU,LT.EQ.0.OR.IFAU,LT.EQ.7) GO TO 5
      GO TO 200
C
C      Convert XIN(N) and XOU(M) to interval [-1,1]
C
5  XA = XIN(1)-(XIN(2)-XIN(1))/2.0D0
   XB = XIN(N)+(XIN(N)-XIN(N-1))/2.0D0
   XAMB = XB-XA
   XAPB = XA+XB
   DO 10 I=1, N
       XIN(I) = 2.0D0*XIN(I)/XAMB-XAPB/XAMB
10 CONTINUE
   DO 15 I=1, M
       XOU(I) = 2.0D0*XOU(I)/XAMB-XAPB/XAMB
15 CONTINUE
C
C      Store boundaries of windows and corresponding indices
C
      I0 = 1
      I1 = I0+N
      I2 = I1+2*M
      CALL BOUND (BW,M,N,OPTIO1,OPTIO2,XIN,XOU,IWKAR(I0),
*              ILB,IRB,WKAR(I1),WKAR(I2))
C
C      Calculate the initial values
C
      I3 = I2+N+1
      I4 = I3+MUE+1
      I5 = I4+(MUE+1)*(MUE+1)
      I6 = I5+(MORD+1)*(MORD+1)
      I7 = I6+MORD+1
      CALL INIT(WKAR(I3),BW,MORD,MUE,WKAR(I4),WKAR(I5),WKAR(I6),
*            WKAR(I7))
      I8 = I7+MUE+1
      I9 = I8+N+1
      I10 = I9+MORD+1
      I11 = I10+(N+1)*(MORD+2*MUE+1)
      I12 = I11+MORD+1
      I13 = I12+N*(MORD+1)
C
C      Calculations for the:
```



```

C          1 - left boundary (III = 1)
C          2 - right boundary (III = 2)
C          3 - interior (III = 3)
C
DO 120 III=1, 3
  IF (III.EQ.1.AND.ILB.LE.0) GO TO 120
  IF (III.EQ.2.AND.IRB.LE.0) GO TO 120
  IF (III.EQ.3.AND.ILB.GT.IRB-2) GO TO 120
  IF (III.EQ.3) GO TO 30
  IL = IWKAR(1+(M-1)*(III-1))
  IR = IWKAR(M+1+(M-1)*(III-1))
  IZ = IR-IL
  IF (IZ.LE.0) GO TO 120
  DO 20 I=IL, IR
    WKAR(I8-IL+I) = WKAR(I2+I-1)
20  CONTINUE
  WKAR(I8) = WKAR(N+1+(M-1)*(III-1))
  WKAR(I8+IZ) = WKAR(N+M+1+(M-1)*(III-1))
  IF (III.EQ.2) GO TO 25
  II1 = 1
  II2 = ILB
  IFLG = 0
  IFLG1 = 0
  XC = WKAR(N+1)+BW
  GO TO 40
25  IF (ILB.EQ.IRB) IRB = IRB +1
  II1 = IRB
  II2 = M
  IFLG = 0
  IFLG1 = 0
  XC = WKAR(N+2*M)-BW
  GO TO 40
30  IF ((ILB+1).EQ.IRB) GO TO 120
  II1 = ILB+1
  II2 = IRB -1
40  DO 110 II=II1, II2
  XX = XOU(II)
  IF (III.NE.3) GO TO 55
  XC = XX
  IL = IWKAR(II)
  IR = IWKAR(M+II)
  IZ = IR-IL
  IF (IZ.LE.0) GO TO 110
  DO 50 I=IL, IR
    WKAR(I8-IL+I) = WKAR(I2+I-1)
50  CONTINUE
  WKAR(I8) = WKAR(N+II)
  WKAR(I8+IZ) = WKAR(N+M+II)
  GO TO 60
55  IF (IFLG.EQ.1) GO TO 65
60  CALL SAVE (BW,WKAR(I5),WKAR(I6),IZ,MORD,MUE,WKAR(I7),
*          N,WKAR(I8),XC,WKAR(I10),WKAR(I12))
  IFLG = 1
C
C          Calculate array PHIAR(MORD+1)
C
65  DO 70 JJ=0, MORD
  CALL PHIJ (BW,WKAR(I5),JJ,WKAR(I6),MORD,NUE,XC,XX,
*          WKAR(I9),PHIJU)
  WKAR(I11+JJ) = PHIJU
70  CONTINUE

```

```

        YOUT = 0.0D0
        IF (III.EQ.3.AND.OPTIO1.EQ.1) GO TO 130
        IF (OPTIO3.EQ.0) GO TO 80
C
C      Sum of squared weights is requested (OPTIO3 = 1)
C
        CALL WEIGHT (IZ,MORD,N,NUE,WKAR(I11),WKAR(I12),SUMW2,
*          WKAR(I0))
        DO 75 I=1, IZ
          YOUT = YOUT+WKAR(I0+I-1)*YIN(IL+I-1)
75      CONTINUE
        YOU(II) = YOUT
        W2(II) = SUMW2
        GO TO 110
C
C      Sum of squared weights not requested (OPTIO3 = 0)
C
80      IF (IFLG1.EQ.1.AND.III.EQ.1) GO TO 100
        IF (IFLG1.EQ.1.AND.III.EQ.2) GO TO 100
        DO 95 J=NUE, MORD
          YOUT1 = 0.0D0
          DO 90 I=1, IZ
            YOUT1 = YOUT1+YIN(IL+I-1)*WKAR(I12+I-1+N*J)
90          CONTINUE
          WKAR(I13+J) = YOUT1
95          CONTINUE
        IFLG1 = 1
100     DO 105 J=NUE, MORD
          YOUT = YOUT+WKAR(I13+J)*WKAR(I11+J)
105     CONTINUE
        YOU(II) = YOUT
110     CONTINUE
120     CONTINUE
        GO TO 160
C
C      Calculation for the interior in the equidistant case
C
130     CALL WEIGHT (IZ,MORD,N,NUE,WKAR(I11),WKAR(I12),SUMW2,
*          WKAR(I0))
        DO 150 II=III1, II2
          YOUT = 0.0D0
          IL = IWKAR(II)
          DO 140 I=1, IZ
            YOUT = YOUT+WKAR(I0+I-1)*YIN(IL+I-1)
140         CONTINUE
          YOU(II) = YOUT
          W2(II) = SUMW2
150     CONTINUE
C
C      Convert XIN(N), XOUM(M) and YOU(M) to the original scales
C
160     CONTINUE
        DO 170 I=1, N
          XIN(I) = (XAMB*XIN(I)+XAPB)/2.0D0
170     CONTINUE
        XAMBN = 1.0D0
        IF (NUE.EQ.0) GO TO 185
        DO 180 I=1, NUE
          XAMBN = (2.0D0/XAMB)*XAMBN
180     CONTINUE
185     DO 190 I=1, M

```

```

        XOU(I) = (XAMB*XOU(I)+XAPB)/2.0D0
        YOU(I) = XAMBN*YOU(I)
190 CONTINUE
200 CONTINUE
    RETURN
    END
C
    SUBROUTINE ERROR (BW,M,MORD,MUE,N,NUE,OPTIO1,OPTIO2,XIN,
*                   XOU,IFAUULT)
C
C     ALGORITHM AS297.2 APPL. STATIST. (1995) VOL.44, NO.2
C
C     Error checking
C
    INTEGER M, MO, MORD, MUE, N, IFAUULT, NU, NUE, OPTIO1, OPTIO2
    DOUBLE PRECISION BW, ERR, X1, X2, XIN(N), XOU(M)
C
    IFAUULT = 0
C
C     Error code messages
C
    IF (N.GE.4.AND.M.GE.1) GO TO 10
    IFAUULT = 1
10 IF (MORD.LE.30.AND.MUE.LE.10.AND.NUE.LE.3.AND.NUE.LE.MORD)
*   GO TO 20
    IFAUULT = 2
20 DO 30 I=1, N-1
    IF (XIN(I).LE.XIN(I+1)) GO TO 30
    IFAUULT = 3
30 CONTINUE
    DO 40 I=1, M-1
    IF (XOU(I).LE.XOU(I+1)) GO TO 40
    IFAUULT = 4
40 CONTINUE
    IF (BW.LE.0.AND.OPTIO2.NE.1) IFAUULT=5
    IF (OPTIO1.NE.1) GO TO 70
    ERR = 0.00001D0
    DO 50 I=1, N
    IF (DABS(XOU(I)-XIN(I)).LT.ERR) GO TO 50
    IFAUULT = 6
50 CONTINUE
    DO 60 I=1, N-2
    X1 = XIN(I+1)-XIN(I)
    X2 = XIN(I+2)-XIN(I+1)
    IF (DABS(X1-X2).LT.ERR) GO TO 60
    IFAUULT = 6
60 CONTINUE
70 IF (IFAUULT.NE.0) GO TO 80
C
C     Warning message (error code 7)
C
    MO = (MORD/2)*2
    NU = (NUE/2)*2
    IF (MO.EQ.MORD.AND.NU.EQ.NUE.OR.MO.NE.MORD.AND.NU.NE.NUE)
*   GO TO 80
    IFAUULT = 7
80 CONTINUE
    RETURN
    END
C
    SUBROUTINE BOUND (BW,M,N,OPTIO1,OPTIO2,XIN,XOU,IBND,ILB,

```

```

*                IRB,BND,S)
C
C      ALGORITHM AS297.3 APPL. STATIST. (1995) VOL.44, NO.2
C
C      Calculate left and right boundaries and indices of windows
C      midpoints
C
C      INTEGER IL, IR, IZ, ILB, IRB, M,
*          IBND(M,2), N, OPTIO1, OPTIO2
C      DOUBLE PRECISION B1, B11, B2, B22, BND(M,2), BW, S(N+1),
*          XIN(N), XOU(M)
C
C      S(1) = XIN(1)-(XIN(2)-XIN(1))/2.0D0
C      S(N+1) = XIN(N)+(XIN(N)-XIN(N-1))/2.0D0
C      DO 10 I=1, N-1
C          S(I+1) = (XIN(I+1)+XIN(I))/2.0D0
10 CONTINUE
C      IF (OPTIO2.EQ.1) BW = (S(N+1)-S(1))/2.0D0
C      B1 = S(1)+BW
C      B11 = B1+BW
C      B2 = S(N+1)-BW
C      B22 = B2-BW
C
C      Find the indices of the boundaries for the output points
C
C      IF (OPTIO1.EQ.0) GO TO 15
C
C      Equidistant case
C
C      IZ = BW/(XIN(2)-XIN(1))
C      ILB = 1+IZ
C      IRB = N-IZ
C      GO TO 25
C
C      Non-equidistant case
C
15 DO 20 I=1, M
C      IF (XOU(I).LE.B1) ILB = I
C      IF (XOU(M-I+1).GE.B2) IRB = M-I+1
20 CONTINUE
C
C      Find the indices of the boundaries for the input points
C
C      IF (OPTIO1.EQ.0) GO TO 30
C
C      Equidistant case
C
25 IZ = INT(2*BW/(XIN(2)-XIN(1)))
C      IL = 1+IZ
C      IR = N+1-IZ
C      GO TO 40
C
C      Non-equidistant case
C
30 DO 35 I=1, N
C      IF (S(I).LT.B11) IL = I
C      IF (S(N-I+2).GT.B22) IR = N-I+2
35 CONTINUE
C      IL = IL+1
C      IF (IR.GT.1) IR = IR-1
C      IZ = IR-IL

```

```
C
C      Record the boundaries and boundary indices
C
40 IF (XOU(1).GT.B1) GO TO 45
   IBND(1,1) = 1
   IBND(1,2) = IL
   BND(1,1) = S(1)
   BND(1,2) = B11
45 IF (XOU(M).LT.B2) GO TO 50
   IBND(M,1) = IR
   IBND(M,2) = N+1
   BND(1,1) = S(1)
   BND(1,2) = B11
   BND(M,1) = B22
   BND(M,2) = S(N+1)
50 IF (OPTIO2.EQ.1) GO TO 110
   IF (B1.EQ.B2) GO TO 100
   IF (XOU(M).LT.B2) IRB = M+1
   IF (ILB.GT.IRB-2) GOTO 110
   DO 90 I=ILB+1, IRB-1
     XL = XOU(I)-BW
     XR = XOU(I)+BW
C
C      Computation of relevant indices
C
   IF (OPTIO1.EQ.0) GO TO 55
C
C      Equidistant case
C
   IZ = INT(BW/(XIN(2)-XIN(1)))
   IL = I-IZ
   IR = I+IZ+1
   GO TO 85
C
C      Non-equidistant case
C
55   IL = 1
60   IR = IL
   IF (S(IL).GT.XL) GO TO 65
   IL = IL+1
   GO TO 60
65   IR = IL-1
70   IR = IR+1
   IF (IR.EQ.N+1) GO TO 80
   IF (S(IR).LT.XR) GO TO 70
80   IF (IL.GT.1) IL = IL-1
   IZ = IR-IL
C
C      Record the indices
C
85   IBND(I,1) = IL
   IBND(I,2) = IR
   BND(I,1) = XL
   BND(I,2) = XR
90 CONTINUE
   GO TO 110
100 OPTIO2 = 1
110 RETURN
   END
C
SUBROUTINE INIT (BIN,BW,MORD,MUE,WKM1,COEF,HJAR,M1BIN)
```

```
C
C      ALGORITHM AS297.4 APPL. STATIST. (1995) VOL.44, NO.2
C
C      Computes necessary constants
C
      INTEGER JM, MORD, MUE
      DOUBLE PRECISION AA, BB, BCD, BIN(MUE+1), BW, CC,
*          COEF(MORD+1,MORD+1), DD, EE, FF, HJAR(MORD+1),
*          HJMU, M1BIN(MUE+1), MUP1, POW2, RR,
*          WKM1(MUE+1,MUE+1)
C
      Calculate multiple of binomial coefficients
C
      EXTERNAL BINOM, HJ, RGAMMA
      INTRINSIC DSQRT
C
      CALL BINOM (MUE,WKM1,BIN)
      DO 5 K=0, MUE
          M1BIN(K+1) = ((-1)**K)*BIN(K+1)
5  CONTINUE
C
      Calculate HJAR(MORD+1)
C
      MUP1 = (1.0D0)*MUE+1.0D0
      POW2 = 1.0D0
      DO 10 I=1,2*MUE+1
          POW2 = 2.0D0*POW2
10  CONTINUE
      POW2 = DSQRT(POW2)
      CALL RGAMMA (2*MUP1-1,MUP1,RR)
      DO 15 JJ=0, MORD
          CALL HJ (JJ,MUE,HJMU)
          HJAR(JJ+1) = HJMU*RR/POW2
15  CONTINUE
C
      Calculate COEF(MORD+1,MORD+1)
C
      DO 80 JJ=0, MORD
          DO 70 MM=0, JJ/2
              JM = JJ-2*MM
              IF (JJ.GE.3) GO TO 85
              BB = 1.0D0
              IF (MM.EQ.0) GO TO 30
              DO 20 I=1, MM
                  BB = BB*(2.0D0*I-1)/(2.0D0*I)
20  CONTINUE
30  CC = 1.0D0
              DO 40 UU=1, MUE
                  CC = CC*(2*MM+2*UU-1.0D0)/(2*UU-1.0D0)
40  CONTINUE
              DD = 1.0D0
              IF (JM.EQ.0) GO TO 60
              DO 50 K=1, JM
                  DD = DD*(2*MM+2*MUE+2*K-1.0D0)/FLOAT(K)
50  CONTINUE
60  DD = ((-1.0D0)**MM)*DD
              BCD = BB*CC*DD
              AA = 1.0D0
              COEF(JJ+1,MM+1) = AA*BCD*DSQRT(BW)
70  CONTINUE
80  CONTINUE
```

```

85 IF (MORD.LT.3) GO TO 130
DO 120 JJ=3, MORD
DO 110 MM=0, JJ/2
JM = JJ-2*MM
EE = COEF(JJ,MM+1)
IF (MM.EQ.0) GO TO 90
FF = COEF(JJ-1,MM)
GO TO 100
90 FF = 0.0D0
100 BCD = 2*((JJ+MUE-0.5D0)/FLOAT(JJ))*EE
*      -((JJ+2*MUE-1.0D0)/FLOAT(JJ))*FF
COEF (JJ+1,MM+1) = BCD
110 CONTINUE
120 CONTINUE
130 RETURN
END

```

```

C
SUBROUTINE SAVE (BW,COEF,HJAR,IZ,MORD,MUE,M1BIN,N,S1,
*              XC,WKM2,RINT)
C
C      ALGORITHM AS297.5 APPL. STATIST. (1995) VOL.44, NO.2
C
C      Saves integrals for the boundaries given in array S1(IZ)
C
INTEGER IZ, JMK1, N, MORD, MO2, MUE
DOUBLE PRECISION AA, BB, BW, CC, COEF(MORD+1,MORD+1),
*              HJAR(MORD+1), M1BIN(MUE+1), RINT(N,MORD+1),
*              S1(N+1), SUM, XC, WKM2(N+1,MORD+2*MUE+1)
C
C      Calculate the powers
C
MO2 = MORD+2*MUE+1
DO 30 I=1, IZ+1
WKM2(I,1) = (S1(I)-XC)/BW
IF (WKM2(I,1).GT.1.0D0) WKM2(I,1) = 1.0D0
IF (WKM2(I,1).LT.-1.0D0) WKM2(I,1) = -1.0D0
DO 20 J=2, MO2
WKM2(I,J) = WKM2(I,1)*WKM2(I,J-1)
20 CONTINUE
30 CONTINUE
C
C      Calculate the integral
C
DO 70 II=1, IZ
DO 60 JJ=0, MORD
AA = HJAR(JJ+1)
SUM = 0.0D0
DO 50 MM=0, JJ/2
BB = COEF(JJ+1,MM+1)
CC = 0.0D0
DO 40 K=0, MUE
JMK1 = JJ-2*MM+2*K+1
CC = CC+(M1BIN(K+1)*(WKM2(II+1,JMK1)
*      -WKM2(II,JMK1)))/FLOAT(JMK1)
40 CONTINUE
SUM = SUM +BB*CC
50 CONTINUE
RINT(II,JJ+1) = AA*SUM
60 CONTINUE
70 CONTINUE
RETURN

```

```

      END
C
      SUBROUTINE WEIGHT (IZ,MORD,N,NUE,PHIAR,RINT,SUMW2,W)
C
C      ALGORITHM AS297.6 APPL. STATIST. (1995) VOL.44, NO.2
C
C      Calculate weights W(N) corresponding to estimating NUE-th
C      derivative at point XX using ultraspherical polynomial of
C      order MORD on the interval [XX-BW,XX+BW]
C
      INTEGER IZ, MORD, N, NUE
      DOUBLE PRECISION PHIAR(MORD+1), RINT(N,MORD+1), SUM,
*          SUMW2, W(N)
C
      SUMW2 = 0
      DO 10 I=1, N
          W(I) = 0
10  CONTINUE
      DO 30 I=1, IZ
          SUM = 0.0D0
          DO 20 J=NUE, MORD
              SUM = SUM +PHIAR(J+1)*RINT(I,J+1)
20  CONTINUE
          W(I) = SUM
          SUMW2 = SUMW2+SUM*SUM
30  CONTINUE
      RETURN
      END
C
      SUBROUTINE PHIJ (BW,COEF,JJ,HJAR,MORD,NUE,XC,XX,WKAR1,PHIJU)
C
C      ALGORITHM AS297.7 APPL. STATIST. (1995) VOL.44, NO.2
C
C      Calculate NUE-th derivative of the JJ-th ultraspherical
C      polynomial with degree of smoothness MUE, on the interval
C      [XC-BW,XC+BW], evaluated at point XX
C
      INTEGER JJ, JM, MORD, MM, NUE
      DOUBLE PRECISION AA, BB, BW, BWN, CC, CENX, COEF(MORD+1,MORD+1),
*          HJAR(MORD+1), HJMU, PHIJU, SUM, XC, XX,
*          WKAR1(MORD+1)
C
      CENX = (XX-XC)/BW
      WKAR1(1) = 1.0D0
      DO 10 I=2, JJ+1
          WKAR1(I) = CENX*WKAR1(I-1)
10  CONTINUE
      BWN = 1.0D0
      DO 20 I=0, NUE
          BWN = BW*BWN
20  CONTINUE
      SUM = 0.0D0
      DO 50 MM=0, (JJ-NUE)/2
          JM = JJ-2*MM
          BB = COEF(JJ+1,MM+1)
          IF (NUE.EQ.0) GO TO 40
          DO 30 KK=1, NUE
              BB = BB*(JM-KK+1)
30  CONTINUE
40  CC = WKAR1(JM-NUE+1)
      AA = BB*CC

```



```
        SUM = SUM+AA
50 CONTINUE
    HJMU = HJAR(JJ+1)
    PHIJU = HJMU*SUM/BWN
    RETURN
    END

C
    SUBROUTINE HJ(JJ,MUE,HJMU)

C
C    ALGORITHM AS297.8 APPL. STATIST. (1995) VOL.44, NO.2
C
C    Calculates part of the normalizing constant for
C    ultraspherical polynomials of order JJ, constant for
C    JJ-th polynomial
C
    INTEGER JJ, MUE
    DOUBLE PRECISION AA, BB, JJP1, JP1MU, HJMU

C
    EXTERNAL RGAMMA
    INTRINSIC DSQRT

C
    JJP1 = FLOAT(JJ+1)
    JP1MU = JJP1+2*MUE
    CALL RGAMMA (JJP1,JP1MU,BB)
    AA = JJ+JP1MU
    HJMU = DSQRT(AA*BB)
    RETURN
    END

C
    SUBROUTINE GAMMA (NN,GM)

C
C    ALGORITHM AS297.9 APPL. STATIST. (1995) VOL.44, NO.2
C
C    Calculate gamma function at argument which is an
C    integer or integer + 0.5
C
    INTEGER N
    DOUBLE PRECISION ABSN, GM, PI, NN

C
    INTRINSIC DABS, DASIN, DSQRT

C
    PI = 2.0D0*DASIN(1.0D0)
    GM = 1.0D0
    IF (NN.EQ.0.5D0) GO TO 20
    N = NINT(NN+0.00001D0)
    DO 10 I=1, N-1
        GM = GM*(NN-I)
10 CONTINUE
    ABSN = DABS(N-NN)
    IF (ABSN.GT.0.1D0) GO TO 20
    GO TO 30
20 GM = GM*DSQRT(PI)
30 RETURN
    END

C
    SUBROUTINE RGAMMA (MM,NN,RGM)

C
C    ALGORITHM AS297.10 APPL. STATIST. (1995) VOL.44, NO.2
C
C    Calculate the ratio of two gamma functions
C
```

```
      DOUBLE PRECISION MM, NN, RGM
C
      RGM = 1.0D0
      IF (MM.EQ.NN) GO TO 40
      IF (MM.LT.NN) GO TO 20
      DO 10 I=1, NINT(MM-NN)
         RGM = RGM*(MM-I)
10  CONTINUE
      GO TO 40
20  DO 30 I=1, NINT(NN-MM)
         RGM = RGM*(NN-I)
30  CONTINUE
      RGM = 1.0D0/RGM
40  RETURN
      END

C
      SUBROUTINE BINOM (P,WKM1,BIN)
C
C      ALGORITHM AS297.11 APPL. STATIST. (1995) VOL.44, NO.2
C
C      Binomial coefficients for power P using the method of
C      Pascal triangle
C
      INTEGER P, P1
      DOUBLE PRECISION BIN(P+1), WKM1(P+1,P+1)
C
      P1 = P+1
      DO 20 I=1, P1
         DO 10 J=1, P1
            WKM1(I,J) = 1.0D0
10      CONTINUE
20     CONTINUE
      IF (P.LT.2) GO TO 50
      DO 40 I=3, P1
         DO 30 J=2, I-1
            WKM1(I,J) = WKM1(I-1,J-1)+WKM1(I-1,J)
30      CONTINUE
40     CONTINUE
50  DO 60 J=1, P1
         BIN(J) = WKM1(P1,J)
60  CONTINUE
      RETURN
      END
```

```
      SUBROUTINE HYBRID(NPARAM,PARAM,N,T0,RHO,NT,BL,BU,NP,POINTS,LOW,
+          IFAULT)
C      .. Scalar Arguments ..
      DOUBLE PRECISION RHO,T0
      INTEGER IFAULT,N,NP,NPARAM,NT
C      ..
C      .. Array Arguments ..
      DOUBLE PRECISION BL(NPARAM),BU(NPARAM),LOW(NPARAM+1),
+          PARAM(NPARAM),POINTS(NPARAM,N)
C      ..
C      .. Local Scalars ..
      DOUBLE PRECISION BST,DIFF,NEWOBJ,OBJF,ONE,P,T,U,ZERO
      INTEGER I,I1,I2
C      ..
C      .. External Functions ..
      DOUBLE PRECISION RANDOM
      EXTERNAL RANDOM
C      ..
C      .. External Subroutines ..
      EXTERNAL FUNCT1,TRADNL
C      ..
C      .. Intrinsic Functions ..
      INTRINSIC DEXP
C
C      Define the constants ZERO and ONE and set
C      initial values for BST and IFAULT
C
C      .. Data statements ..
      DATA ZERO,ONE,BST/0.0D0,1.0D0,1.0D+10/
C      ..
      IFAULT = 0
C
C      *****
C      *** Start of Annealing component to      ***
C      *** generate a set of starting points. ***
C      *****
C
C      Initialise the temperature
C
      T = T0
C
C      Choose an initial point
C
      DO 10 I = 1,NPARAM
          PARAM(I) = RANDOM(BL(I),BU(I))
10 CONTINUE
C
C      Calculate the function value for the initial point
C
      CALL FUNCT1(NPARAM,PARAM,OBJF)
C
C      Begin the loop over I1 until Nt Temp. reductions.
C
      DO 90 I1 = 1,NT
C
C          Set the counter for the No of points accepted to one
C
          NP = 1
C
C          Begin the loop over I2 until N points have been considered.
```

```

      DO 80 I2 = 1,N
C
C      Record the present point
C
      DO 20 I = 1,NPARAM
        POINTS(I,NP+1) = PARAM(I)
20      CONTINUE
C
C      Select a new point
C
      DO 30 I = 1,NPARAM
        PARAM(I) = RANDOM(BL(I),BU(I))
30      CONTINUE
C
C      Calculate the function value of this new point
C
      CALL FUNCT1(NPARAM,PARAM,NEWOBJ)
C
C      Calculate the difference
C
      DIFF = (NEWOBJ-OBJF)
C
C      If the new point is better than the old one then increase the
C      Np counter, and record it as a possible starting point. Move
C      to this new point.
C
      IF (DIFF.LT.ZERO) THEN
        NP = NP + 1
        DO 40 I = 1,NPARAM
          POINTS(I,NP) = PARAM(I)
40      CONTINUE
        OBJF = NEWOBJ
        IF (NEWOBJ.LT.BST) THEN
          BST = NEWOBJ
          DO 50 I = 1,NPARAM
            POINTS(I,1) = PARAM(I)
50      CONTINUE
          END IF
C
C      Otherwise use the Metropolis Criterion
C
      ELSE
C
C      P is the comparison statistic. U is a standard Uniform variate.
C
        P = DEXP(-DIFF/T)
        U = RANDOM(ZERO,ONE)
C
C      If U < P then accept this point. Increase the Np counter,
C      Record this point as a possible starting point, and move
C      to this new point.
C
        IF (U.LT.P) THEN
          NP = NP + 1
          OBJF = NEWOBJ
          DO 60 I = 1,NPARAM
            POINTS(I,NP) = PARAM(I)
60      CONTINUE
C
C      If U >= P then reject this point and return to the old point.
C

```

```

        ELSE
          DO 70 I = 1,NPARAM
            PARAM(I) = POINTS(I,NP+1)
70          CONTINUE
          END IF

C
C   Both alternatives for the comparison of the new and old point
C   Have been considered.
C
C         END IF

C
C   Continue with the loop until N new points have been considered
C
80    CONTINUE

C
C   Set the error indicator to 1 if the algorithm appears to have
C   converged.
C
C         IF (NP.EQ.1) THEN
C           IFAULT = I1
C         END IF

C
C   Once N points have been considered, lower the Temperature.
C
C         T = T*RHO

C
C   Continue with the loop until the Temp. has been reduced Nt times
C
90 CONTINUE

C
C   *****
C   *** End of Annealing component, NP      ***
C   *** starting points are now stored in ***
C   *** the array POINTS.                  ***
C   *****

C
C   Set an initially high value of LOW(NPARAM+1)

LOW(NPARAM+1) = 1.0D+10

C
C   *****
C   *** Start of the traditional component, ***
C   *** which loops over the NP starting   ***
C   *** points calling the traditional     ***
C   *** minimisation routine for each.    ***
C   *****

C
C   Begin the loop over the Np starting points.

DO 130 I1 = 1,NP

C
C   Set the PARAM array to be the values of the I1st start point
C
C         DO 110 I2 = 1,NPARAM
C           PARAM(I2) = POINTS(I2,I1)
110    CONTINUE

C
C   Call traditional minimisation routine
C
C         CALL TRADNL(NPARAM,PARAM,BL,BU,OBJF)

C

```

```
C      Check to see if this starting point gives the
C      lowest function value to date
C
C      IF (OBJF.LT.LOW(NPARAM+1)) THEN
C          DO 120 I = 1,NPARAM
C              LOW(I) = PARAM(I)
120      CONTINUE
C          LOW(NPARAM+1) = OBJF
C      END IF
C
C      End the Np loop
C
130 CONTINUE
C
C      *****
C      *** End of the second, traditional ***
C      *** component. ***
C      *****
C
C      Return to calling routine
C
RETURN
C
C      End of subroutine HYBRID
C
END
```

```

SUBROUTINE SPP (DI, NIN, SPEC, LARGE, NOUT, XSTORE, XOUT, ISEED,
*           RANNUM, IFAULT)
C
C   ALGORITHM AS 300.1 APPL. STATIST. (1996), VOL.45, NO.1
C
C   Efficient algorithm for determining a simulated percentile
C   point with a fixed degree of accuracy
C
INTEGER DI, NIN(4), NOUT(3), ISEED, IFAULT
REAL SPEC(4), XSTORE(DI), XOUT(3), RANNUM,
LOGICAL LARGE
C
INTEGER HIGH, LOW, N, N1, N2, NBND, NCHK, NDEX1, NDEX2, NSTORE
REAL AN, ANP, C1, C2, D, ERR, HALF, MAXERR, ONE, P, PQ, TWO,
*   THREE, XNEW, ZERO
C
PARAMETER (ONE = 1.0E0, TWO = 2.0E0, THREE = 3.0E0, HALF = 0.5,
*   ZERO = 0.0E0)
C
EXTERNAL INSERT, RANNUM
C
C   Initialise local variables and check for input failures
C
IFAULT = 0
N1 = NIN(1)
IF (N1 .LE. 2) IFAULT = IFAULT + 1
N2 = NIN(2)
IF (N2 .LE. N1) IFAULT = IFAULT + 2
NCHK = NIN(3)
IF (NCHK .LE. N2) IFAULT = IFAULT + 4
NBND = NIN(4)
IF (NBND .LE. NCHK) IFAULT = IFAULT + 8
C1 = SPEC(1)
IF (C1 .LE. ZERO) IFAULT = IFAULT + 16
C2 = SPEC(2)
IF (C2 .LE. C1) IFAULT = IFAULT + 32
MAXERR = SPEC(3)
IF (MAXERR .LE. ZERO) IFAULT = IFAULT + 64
P = SPEC(4)
IF (P .LE. ZERO .OR. P .GT. HALF) IFAULT = IFAULT + 128
IF (DI .LT. TWO * C2 * SQRT(NBND * P * (ONE - P)) + THREE)
*   IFAULT = IFAULT + 256
IF (IFAULT .NE. 0) RETURN
PQ = P * (ONE - P)
NDEX1= 1
NDEX2 = MAX0(2, N1)
C
C   Start iterating simulated values
C
DO 50 N = 1, NBND
XNEW = RANNUM(ISEED)
IF (N .EQ. 1) THEN
XSTORE(1) = XNEW
ELSE IF (N .EQ. 2) THEN
XSTORE(2) = XNEW
NSTORE = 2
IF (XNEW .GT. XSTORE(1) .EQV. LARGE) THEN
XSTORE(2) = XSTORE(1)
XSTORE(1) = XNEW
ENDIF

```

```
C      Stage 1: sort and store all of the first N1 simulated values
C
      ELSE IF (N .LE. N1) THEN
          CALL INSERT (NSTORE, DI, XNEW, XSTORE, 0, LARGE)
C
C      Stage 2: sort and store only N1 of the first N2 simulated
C      values
C
      ELSE IF (N .LE. N2) THEN
          IF (XNEW .GT. XSTORE(NDEX2) .EQV. LARGE) THEN
              CALL INSERT (NSTORE, DI, XNEW, XSTORE, 2, LARGE)
          ENDIF
C
C      Stage 3: sort and store only a probabilistically determined
C      number of simulated values
C      3.1: do not store simulated value but change index
C      numbers
C
      ELSE IF (XNEW .GT. XSTORE(1) .EQV. LARGE) THEN
          NDEX1 = NDEX1 + 1
          NDEX2 = NDEX2 + 1
C
C      3.2: sort and store the simulated value
C
      ELSE IF (XNEW .GT. XSTORE(NSTORE) .EQV. LARGE) THEN
          AN = N
          ANP = AN * P
          D = C2 * SQRT(AN * PQ)
          LOW = ANP - D
C
C      3.2.1: delete the simulated value that had been in the first
C      storage location
C
          IF (NDEX1 .LT. LOW) THEN
              CALL INSERT (NSTORE, DI, XNEW, XSTORE, 1, LARGE)
              NDEX1 = NDEX1 + 1
              NDEX2 = NDEX2 + 1
C
C      3.2.2: no previously stored simulated value is to be
C      deleted
C
          ELSE
              HIGH = ANP + D + 1
              IF (NDEX2 .LT. HIGH) THEN
                  NDEX2 = NDEX2 + 1
                  CALL INSERT (NSTORE, DI, XNEW, XSTORE, 0, LARGE)
C
C      3.2.3: delete the simulated value that had been in the last
C      storage location
C
          ELSE
              CALL INSERT (NSTORE, DI, XNEW, XSTORE, 2, LARGE)
          ENDIF
      ENDIF
C
      3.3: do not store simulated value and do not change index
C      numbers
C
      ENDIF
C
      Stage 4: check to see if the desired precision has been
```



```
C          achieved at the end of each NCHK iterations
C
C          IF (N .EQ. (N / NCHK) * NCHK .OR. N .EQ. NBND) THEN
C              AN = N
C              ANP = AN * P
C              D = C1* SQRT(AN * PQ)
C              LOW = ANP - D + HALF
C              HIGH = ANP + D + ONE + HALF
C
C              4.1: the desired order statistics are not in storage
C                  (abnormal termination)
C
C              IF (NDEX1 .GT. LOW .OR. NDEX2 .LT. HIGH) THEN
C                  IFAULT = 999
C                  GOTO 100
C              ENDIF
C
C              4.2: the desired order statistics are in storage
C
C              LOW = LOW - NDEX1 + 1
C              HIGH = HIGH - NDEX1 + 1
C              IF (LARGE) THEN
C                  XOUT(3) = XSTORE(LOW)
C                  XOUT(2) = XSTORE(HIGH)
C              ELSE
C                  XOUT(3) = XSTORE(HIGH)
C                  XOUT(2) = XSTORE(LOW)
C              ENDIF
C              ERR = (XOUT(3) - XOUT(2)) / TWO
C              LOW = ANP - NDEX1 + 1
C              XOUT(1) = XSTORE(LOW)
C
C              4.3: the desired precision has been achieved when ERR is
C                  less than MAXERR
C
C              IF (ERR .LT. MAXERR) GOTO 100
C          ENDIF
C      50 CONTINUE
C
C          4.4: the desired precision is not achieved within the
C              fixed number of iterations
C
C          N = N - 1
C      100 NOUT(1) = N
C          NOUT(2) = NSTORE
C          NOUT(3) = NDEX1
C
C          RETURN
C          END
C
C          SUBROUTINE INSERT (NSTORE, DI, XNEW, XSTORE, CONTRL, LARGE)
C
C              ALGORITHM AS 300.2 APPL. STATIST. (1996), VOL.45, NO.1
C
C              Divide and conquer algorithm to sort and store a new value
C              (XNEW) among a set of previously sorted and stored values
C
C              INTEGER NSTORE, DI, CONTRL
C              REAL XNEW, XSTORE(DI)
C              LOGICAL LARGE
C
```

```
      INTEGER I, IBND1, IBND2, ITRY
      REAL XHOLD
C
C      Initialise local variables
C
      IBND1 = 0
      IBND2 = NSTORE + 1
C
C      Find the appropriate position to insert XNEW into the
C      sorted set
C
50  ITRY = (IBND1 + IBND2) / 2
      IF (ITRY.LT.0 .OR. ITRY.GT.NSTORE) RETURN
      IF (ITRY.EQ.IBND1) GOTO 100
      IF (XSTORE(ITRY) .GT. XNEW .EQV. LARGE) THEN
          IBND1 = ITRY
      ELSE
          IBND2 = ITRY
      ENDIF
      GOTO 50
100 IF (CONTRL .NE. 1) THEN
C
C      If CONTRL equals 0, add XNEW to the list
C
      IF (CONTRL .EQ. 0) NSTORE = NSTORE + 1
C
C      If CONTRL equals 2, add XNEW to the list and delete the value
C      in the last storage location
C
      DO 150 I = IBND2, NSTORE
          XHOLD = XSTORE(I)
          XSTORE(I) = XNEW
          XNEW = XHOLD
150  CONTINUE
C
C      If CONTRL equals 1, add XNEW to the list and delete the
C      first storage location
C
      ELSE
          DO 200 I = IBND1, 1, -1
              XHOLD = XSTORE(I)
              XSTORE(I) = XNEW
              XNEW = XHOLD
200  CONTINUE
      ENDIF
C
      RETURN
      END
```

```

SUBROUTINE LOGF1(CELL, DELTA, EPS, INQCOL, INQROW, LQ, R, RS,
*   S, UQ, COL, IFAULT, LFCELL, LFCOL, LFROW, LOGEF1, LOGPH,
*   LOGPHP, MU1, N, QCELL, QCOL, QROW, ROW)
C
C   ALGORITHM AS 301.1 APPL. STATIST. (1996), VOL.45, NO.2
C
C   Computes the logarithms of F1, P(H) and P(H')
C
INTEGER R, RS, S, CELL(RS), COL(S), IFAULT, N, ROW(R)
REAL DELTA, EPS, INQCOL(S), INQROW(R), LQ, UQ, LOGEF1, LOGPH,
*   LOGPHP, MU1, QCELL(RS), QCOL(S), QROW(R)
DOUBLE PRECISION LFCELL(RS), LFCOL(S), LFROW(R)
C
INTEGER I, J, K
DOUBLE PRECISION LFM
REAL C1, C2, INTOFG, LGPHI1, LGPHI2, LGPHI3, LOGFY,
*   MLOGG, RPI, XMAX
C
EXTERNAL MRGINS, KAPPA0, PARRHO, LIMITS, MXLOGG
C
IFAULT = 0
CALL MRGINS(CELL, INQCOL, INQROW, R, RS, S, COL, IFAULT,
*   LFCELL, LFCOL, LFM, LFROW, N, ROW)
IF (IFAULT .EQ. 0) THEN
  CALL KAPPA0(N, DELTA, EPS, LFM, LFROW,
*   ROW, INQROW, R, IFAULT, QROW)
  CALL KAPPA0(N, DELTA, EPS, LFM, LFCOL,
*   COL, INQCOL, S, IFAULT, QCOL)
  CALL PARRHO(LQ, UQ, IFAULT, MU1, RPI)
  IF (IFAULT .NE. 1) THEN
C
C   Compute log(Fisher-Yates probability) and the cell
C   probabilities
C
      LOGFY = -SNGL(LFM)
      K = 0
      DO 10 I = 1, R
        LOGFY = LOGFY + SNGL(LFROW(I))
        DO 5 J = 1, S
          K = K + 1
          QCELL(K) = QROW(I)*QCOL(J)
          LOGFY = LOGFY - SNGL(LFCELL(K))
5          CONTINUE
10         CONTINUE
        DO 15 J = 1, S
15         LOGFY = LOGFY + SNGL(LFCOL(J))
C
C   Compute log PHI1 = log INTOFG((N(I, J)), EXP(X)(Q(I.)Q(.J)))
C
      CALL LIMITS(N, LFM, LFCELL, CELL, QCELL, RS, C1, C2)
      CALL MXLOGG(N, C1, C2, LFM, LFCELL, CELL,
*   QCELL, RS, 1, 1, MLOGG, XMAX)
      LGPHI1 = ALOG(RPI*INTOFG(N, C1, C2, DELTA, EPS, LFM, LFCELL,
*   CELL, MLOGG, QCELL, RS, 1, XMAX, IFAULT)) + MLOGG
C
C   Compute log PHI2 = log INTOFG((N(I.)), EXP(X)(Q(I.)))
C
      CALL LIMITS(N, LFM, LFROW, ROW, QROW, R, C1, C2)
      CALL MXLOGG(N, C1, C2, LFM, LFROW, ROW,
*   QROW, R, 1, 1, MLOGG, XMAX)
      LGPHI2 = ALOG(RPI*INTOFG(N, C1, C2, DELTA, EPS, LFM,

```

```

*          LFCOL, COL, MLOGG, QCOL, S, 1, XMAX, IFAULT)) + MLOGG
C
C          Compute log PHI3 = log INTOFG((N(.J)), EXP(X)(Q(.J)))
C
C          CALL LIMITS(N, LFM, LFCOL, COL, QCOL, S,      C1, C2)
C          CALL MXLOGG(N, C1, C2, LFM, LFCOL, COL,
*              QCOL, S, 1, 1, MLOGG, XMAX)
C          LGPHI3 = ALOG(RPI*INTOFG(N, C1, C2, DELTA, EPS, LFM,
*              LFCOL, COL, MLOGG, QCOL, S, 1, XMAX, IFAULT)) + MLOGG
C
C          Compute the logarithms of F1, P(H) and P(H')
C
C          LOGEF1 = LGPHI1 - (LOGFY + LGPHI2 + LGPHI3)
C          LOGPH  = LOGFY + LGPHI3
C          LOGPHP = LGPHI1 - LGPHI2
C          ENDIF
C          ENDIF
C
C          RETURN
C          END
C
C          SUBROUTINE MRGINS(CELL, INQCOL, INQROW, R, RS, S, COL, IFAULT,
*              LFCOL, LFCOL, LFM, LFROW, N, ROW)
C
C          ALGORITHM AS 301.2 APPL. STATIST. (1996), VOL.45, NO.2
C
C          Computes the table total N, the row and column totals, N(I.)
C          and N(.J), log N(I.)!, log N(.J)!, and checks whether (Q(I.))
C          and (Q(.J)) sum to 1, CELL(I) < 0 and N < 1 or N > 10E+09
C
C          INTEGER R, RS, S, CELL(RS), COL(S), IFAULT, N, ROW(R)
C          REAL INQCOL(S), INQROW(R)
C          DOUBLE PRECISION LFCOL(RS), LFCOL(S), LFM, LFROW(R)
C
C          DOUBLE PRECISION LFACT
C          REAL APPONE, NINES, SUMQ, ZERO
C          INTEGER I, J, K, L
C
C          DATA APPONE, NINES, ZERO /1.000001, 0.999999, 0.0/
C
C          DO 5 I = 1, RS
C              IF (CELL(I) .LT. 0) IFAULT = 2
C          5 CONTINUE
C          IF (IFAULT .NE. 2) THEN
C              SUMQ = ZERO
C              N = 0
C              DO 15 I = 1, R
C                  SUMQ = SUMQ + INQROW(I)
C                  ROW(I) = 0
C                  L = (I - 1)*S
C                  DO 10 J = 1, S
C                      K = L + J
C                      ROW(I) = ROW(I) + CELL(K)
C                      LFCOL(K) = LFACT(CELL(K))
C          10 CONTINUE
C                  LFROW(I) = LFACT(ROW(I))
C                  N = N + ROW(I)
C          15 CONTINUE
C              IF (N .GE. 1 .AND. N .LE. 1000000000) THEN
C                  IF (SUMQ .LE. NINES .OR. SUMQ .GE. APPONE) THEN
C                      IFAULT = 3

```



```

      INTEGER I
C
      DATA FIFTY, TEN, ZERO /50.0, 10.0, 0.0/
C
      EXTERNAL PARRHO, LIMITS, MXLOGG
C
      CALL PARRHO(TEN, FIFTY, IFAULT, DUMMY1, DUMMY2)
      CALL LIMITS(BIGM, LFM, LOGFAC, M, PRQ, T, C1, C2)
      CALL MXLOGG(BIGM, ZERO, C2, LFM, LOGFAC, M,
*              PRQ, T, 2, 2, MLOGG, XMAX)
      LGNUM = ALOG(INTOFG(BIGM, ZERO, C2, DELTA, EPS, LFM,
*              LOGFAC, M, MLOGG, PRQ, T, 2, XMAX, IFAULT)) + MLOGG
      CALL MXLOGG(BIGM, C1/BIGM, ZERO, LFM, LOGFAC, M,
*              PRQ, T, 3, 3, MLOGG, XMAX)
      LGDNOM = ALOG(INTOFG(BIGM, C1/BIGM, ZERO, DELTA, EPS, LFM,
*              LOGFAC, M, MLOGG, PRQ, T, 3, XMAX, IFAULT)) + MLOGG
      K0 = EXP(LGNUM - LGDNOM)
      DO 5 I = 1, T
          Q(I) = (FLOAT(M(I)) + PRQ(I)*K0)/(BIGM + K0)
5 CONTINUE
C
      RETURN
      END
C
      SUBROUTINE LIMITS(BIGM, LFM, LOGFAC, M, Q, T, C1, C2)
C
      ALGORITHM AS 301.5 APPL. STATIST. (1996), VOL.45, NO.2
C
      Computes the logarithms of the limits C1 and C2
C
      INTEGER BIGM, T, M(T)
      DOUBLE PRECISION LFM, LOGFAC(T)
      REAL Q(T), C1, C2
C
      DOUBLE PRECISION DPC2
      REAL ZERO
      INTEGER I
C
      DATA ZERO /0.0/
C
      C1 = ZERO
      DPC2 = LFM
      DO 5 I = 1, T
          DPC2 = DPC2 + DBLE(M(I))*DLOG(DBLE(Q(I))) - LOGFAC(I)
          IF (M(I) .EQ. BIGM) C1 = ALOG(Q(I))
5 CONTINUE
      C2 = SNGL(DPC2)
C
      RETURN
      END
C
      SUBROUTINE MXLOGG(BIGM, C1, C2, LFM, LOGFAC, M,
*              Q, T, TAU, ZETA, MLOGG, XMAX)
C
      ALGORITHM AS 301.6 APPL. STATIST. (1996), VOL.45, NO.2
C
      Finds the approximate maximum of  $\log G(X)$ ,
       $\log G(X)/(1 + M/EXP(X))$  or  $\log G(X)/(M + EXP(X))$  where
      M denotes BIGM.
C
      INTEGER BIGM, T, M(T), TAU, ZETA

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```

REAL C1, C2, Q(T), MLOGG, XMAX
DOUBLE PRECISION LFM, LOGFAC(T)
C
DOUBLE PRECISION D1, D2, DPZERO, EPS, LOGDM
REAL CONDTN, KMAX, LMB, LMB2, LMU1, LXLMU1, ONE,
*   ONED2, RHO, RLMB, SAVEK, THRTY2, U, Y, ZERO
INTEGER I
C
COMMON /RHOPAR/ LMB, LMB2, LMU1, RLMB
C
DATA DPZERO, ONE, ONED2, EPS, THRTY2, ZERO
*   /0.0D0, 1.0, 0.5, 0.001D0, 32.0, 0.0/
C
RHO(U) = LMB/(LMB2 + (U - LMU1)**2)
LXLMU1 = SNGL(LOGDM(BIGM, LFM, LOGFAC, M, Q, T, TAU, LMU1)) +
*   ALOG(RHO(LMU1))
IF (C1 .NE. ZERO) THEN
  IF (C1 + ALOG(RHO(-THRTY2)) .LT. LXLMU1) THEN
    XMAX = LMU1
    MLOGG = LXLMU1
  ELSE
    XMAX = -THRTY2
    MLOGG = C1 + ALOG(RHO(-THRTY2))
  ENDIF
ELSE
  CONDTN = ONE
  DO 5 I = 1, T
    Y = Q(I)*BIGM
    CONDTN = CONDTN + ((FLOAT(M(I)) - Y)**2 - FLOAT(M(I)))/Y
5  CONTINUE
  IF (CONDTN .LE. ZERO .AND. C2 .NE. ZERO) THEN
    IF (C2 + ALOG(RHO(THRTY2)) .LT. LXLMU1) THEN
      XMAX = LMU1
      MLOGG = LXLMU1
    ELSE
      XMAX = THRTY2
      MLOGG = C2 + ALOG(RHO(THRTY2))
    ENDIF
  ELSE
C
C   Find the zero of  $d(\log F(X))/dx$ ,
C    $d(\log F(X)/(1 + M/EXP(X)))/dx$  or  $d(\log F(X)/(M + EXP(X)))/dx$ 
C   by Newton-Raphson's method where M denotes BIGM.
C
    KMAX = ONE
    SAVEK = KMAX
    CALL DERIV(BIGM, M, Q, T, KMAX, ZETA, D1, D2)
10  IF (DABS(D1) .LT. EPS .OR. ABS(ALOG(KMAX)) .GT. THRTY2)
*   GO TO 15
    IF (D2 .LT. DPZERO) THEN
      KMAX = KMAX - D1/D2
      IF (KMAX .LT. ZERO) THEN
        SAVEK = ONED2*SAVEK
        KMAX = SAVEK
      ENDIF
    ELSE
      SAVEK = ONED2*SAVEK
      KMAX = SAVEK
    ENDIF
    CALL DERIV(BIGM, M, Q, T, KMAX, ZETA, D1, D2)
    GO TO 10

```

```

15      XMAX = ALOG(KMAX)
      IF (XMAX .GT. THRTY2) XMAX = THRTY2
      MLOGG = SNGL(LOGDM(BIGM, LFM, LOGFAC, M, Q, T, TAU, XMAX))
*          + ALOG(RHO(XMAX))
      IF (MLOGG .LT. LXLMU1) THEN
          XMAX = LMU1
          MLOGG = LXLMU1
      ENDIF
      IF (TAU .LT. 3 .AND. MLOGG .LT. C2 + ALOG(RHO(THRTY2))) THEN
          XMAX = THRTY2
          MLOGG = C2 + ALOG(RHO(THRTY2))
      ENDIF
      ENDIF
      ENDIF
      ENDIF
C
      RETURN
      END
C
      SUBROUTINE DERIV(BIGM, M, Q, T, K, ZETA, D1, D2)
C
C      ALGORITHM AS 301.7 APPL. STATIST. (1996), VOL.45, NO.2
C
C      Computes the derivatives of  $d(\log F(X))/dx$ ,
C       $d(\log F(X)/(1 + M/EXP(X)))/dx$  or  $d(\log F(X)/(M + EXP(X)))/dx$ 
C      where M denotes BIGM.
C
      INTEGER BIGM, T, M(T), ZETA
      REAL Q(T), K
      DOUBLE PRECISION D1, D2
C
      INTEGER ALPHA, I
      DOUBLE PRECISION C1, C2, ONE, ONED2, PSIAPP, PSIPAP,
*          TEN, TWO, U, Z, ZERO
C
      DATA C1, C2 /0.08333333333333333D0, 0.16666666666666667D0/,
* ONE, ONED2, TEN, TWO, ZERO /1.0D0, 0.5D0, 10.0D0, 2.0D0, 0.0D0/
C
      PSIAPP(U) = DLOG(U) - ONED2/U - C1*(ONE/U)**2
      PSIPAP(U) = ONE/U + ONED2*(ONE/U)**2 + C2*(ONE/U)**3
      D1 = ZERO
      D2 = ZERO
      DO 15 ALPHA = 1, T
          IF (M(ALPHA) .GT. 0) THEN
              Z = DBLE(Q(ALPHA)*K)
              I = 0
          5      IF (I + Z .GT. TEN .OR. I .EQ. M(ALPHA)) GO TO 10
              D1 = D1 + Q(ALPHA)/(I + Z)
              D2 = D2 - (Q(ALPHA)/(I + Z))**2
              I = I + 1
              GO TO 5
          10     IF (I .LT. M(ALPHA)) THEN
              D1 = D1 + Q(ALPHA)*(PSIAPP(M(ALPHA) + Z) - PSIAPP(I + Z))
              D2 = D2 + Q(ALPHA)**2*(PSIPAP(M(ALPHA) + Z) -
*          PSIPAP(I + Z))
          *
          ENDIF
          ENDIF
      15 CONTINUE
      I = 0
      20 IF (DBLE(I + K) .GT. TEN .OR. I .EQ. BIGM) GO TO 25
          D1 = D1 - ONE/(I + K)
          D2 = D2 + (ONE/(I + K))**2

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        I = I + 1
        GO TO 20
25 IF (I .LT. BIGM) THEN
        D1 = D1 - PSIAPP(DBLE(BIGM + K)) + PSIAPP(DBLE(I + K))
        D2 = D2 - PSIPAP(DBLE(BIGM + K)) + PSIPAP(DBLE(I + K))
    ENDIF
    IF (ZETA .EQ. 2) THEN
        D1 = D1 + ONE/(K*(ONE + K/BIGM))
        D2 = D2 - (ONE + TWO*K/BIGM)*(ONE/(K*(ONE + K/BIGM)))**2
    ELSE IF (ZETA .EQ. 3) THEN
        D1 = D1 - ONE/(BIGM + K)
        D2 = D2 + (ONE/(BIGM + K))**2
    ENDIF
C
    RETURN
    END
C
    REAL FUNCTION INTOFG(BIGM, C1, C2, DELTA, EPS, LFM, LGF,
*
        M, MLOGG, Q, T, TAU, XMAX, IFAULT)
C
        ALGORITHM AS 301.8 APPL. STATIST. (1996), VOL.45, NO.2
C
        Computes the integral of G(X), G(X)/(1 + M/EXP(X)) or
C
        G(X)/(M + EXP(X)) where M denotes BIGM.
C
        INTEGER BIGM, T, M(T), TAU, IFAULT
        REAL C1, C2, DELTA, EPS, MLOGG, Q(T), XMAX
        DOUBLE PRECISION LFM, LGF(T)
C
        REAL C, CONST, ONE,
*
        QG8, THRTY2, XLIMIT, YL, YU, ZERO
        INTEGER CVERG, I
C
        DATA CONST, ONE, THRTY2, ZERO /-23.0, 1.0, 32.0, 0.0/
C
        EXTERNAL CHKCVG
C
        INTOFG = ZERO
C
        Integrate to the left from XMAX and then to the right
C
        from XMAX
C
        XLIMIT = -THRTY2
        C = C1
        YL = -(ONE - ONE/DELTA)
        YU = ZERO
        DO 15 I = 1, 2
            CVERG = 0
            IF (XMAX .EQ. XLIMIT) CALL CHKCVG(BIGM, C, MLOGG + CONST,
*
                DELTA, EPS, LFM, LGF, M, MLOGG, Q, I, T, TAU, XMAX, CVERG,
*
                IFAULT, INTOFG, ZERO, ZERO)
5          IF (CVERG .EQ. 1) GO TO 10
            INTOFG = INTOFG + QG8(BIGM, LFM, LGF, M, MLOGG, Q, T,
*
                TAU, XMAX + YL, XMAX + YU)
            IF (YL .LT. ZERO) THEN
                CALL CHKCVG(BIGM, C, MLOGG + CONST, DELTA, EPS, LFM, LGF,
*
                    M, MLOGG, Q, I, T, TAU, XMAX, CVERG, IFAULT, INTOFG,
*
                    YU, YL)
            ELSE
                CALL CHKCVG(BIGM, C, MLOGG + CONST, DELTA, EPS, LFM, LGF,
*
                    M, MLOGG, Q, I, T, TAU, XMAX, CVERG, IFAULT, INTOFG,

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*          YL, YU)
      ENDIF
      GO TO 5
10     XLIMIT = THRTY2
      C = C2
      YL = ZERO
      YU = ONE - ONE/DELTA
15 CONTINUE
C
      RETURN
      END
C
      SUBROUTINE CHKCVG(BIGM, C, CRITER, DELTA, EPS, LFM, LOGFAC, M,
*     MLOGG, Q, SIDE, T, TAU, XMAX, CVERG, IFAULT, INTOFG, YL, YU)
C
C     ALGORITHM AS 301.9 APPL. STATIST. (1996), VOL.45, NO.2
C
C     Checks for the convergence to the limit C and updates the
C     end-points of the integration intervals
C
      INTEGER BIGM, T, M(T), SIDE, TAU, CVERG, IFAULT
      REAL C, CRITER, DELTA, EPS, MLOGG, Q(T), XMAX, INTOFG, YL, YU
      DOUBLE PRECISION LFM, LOGFAC(T)
C
      DOUBLE PRECISION LOGDM
      REAL LDIRMT, LMB, LMB2,
*     LMU1, LTERM, ONE, PID2, RHO, RLMB,
*     THRTY2, U, V, ZERO
C
      COMMON /RHOPAR/ LMB, LMB2, LMU1, RLMB
C
      DATA ONE, PID2, THRTY2, ZERO /1.0, 1.5707963, 32.0, 0.0/
C
      RHO(U) = LMB/(LMB2 + (U - LMU1)**2)
      LDIRMT = SNGL(LOGDM(BIGM, LFM, LOGFAC, M, Q, T, TAU, XMAX + YU))
      IF (C .EQ. ZERO) THEN
          IF (LDIRMT + ALOG(RHO(XMAX + YU)) .LT. CRITER) CVERG = 1
      ELSE
          IF (ABS(LDIRMT - C) .LT. ALOG(ONE + EPS)) CVERG = 1
      ENDIF
      IF (CVERG .EQ. 0) THEN
          IF (ABS(XMAX + DELTA*YU) .GE. THRTY2) THEN
              CVERG = 1
              IF (TAU .EQ. 1) IFAULT = 5
          ELSE
              YL = YU
              YU = DELTA*YU
          ENDIF
      ENDIF
      IF (CVERG .EQ. 1) THEN
          IF (C .NE. ZERO) THEN
C
C     LTERM is assigned the value of the integral of DX
C
              V = ATAN((XMAX + YU - LMU1)*RLMB)
              LTERM = ZERO
              IF (SIDE .EQ. 1) THEN
                  IF (V + PID2 .GT. ZERO) LTERM = V + PID2
              ELSE
                  IF (PID2 - V .GT. ZERO) LTERM = PID2 - V
              ENDIF
          ENDIF
      ENDIF

```

```

        IF (LTERM .GT. ZERO) INTOFG = INTOFG +
*                               EXP(C + ALOG(LTERM) - MLOGG)
        ENDIF
    ENDIF
C
    RETURN
    END
C
    REAL FUNCTION QG8(BIGM, LFM, LOGFAC, M, MLOGG, Q, T, TAU, XL, XU)
C
C     ALGORITHM AS 301.10 APPL. STATIST. (1996), VOL.45, NO.2
C
C     Integrates from XL to XU by eight-point Gaussian quadrature
C
    INTEGER BIGM, T, M(T), TAU
    DOUBLE PRECISION LFM, LOGFAC(T)
    REAL MLOGG, Q(T), XL, XU
C
    DOUBLE PRECISION LOGDM
    REAL C(8), CONST, G, LMB, LMB2, LMU1, ONED2, RHO, RLMB, U, X,
*     Y, Z, ZERO
    INTEGER I, J
C
    COMMON /RHOPAR/ LMB, LMB2, LMU1, RLMB
C
    DATA C /0.48014493, 0.050614268, 0.39833324, 0.11119052,
*     0.26276620, 0.15685332, 0.091717321, 0.18134189/,
*     CONST, ONED2, ZERO /-23.0, 0.5, 0.0/
C
    RHO(U) = LMB/(LMB2 + (U - LMU1)**2)
    Y = ONED2*(XL + XU)
    QG8 = ZERO
    DO 10 I = 2, 8, 2
        Z = C(I - 1)*(XU - XL)
        X = Y - Z
        DO 5 J = 1, 2
            G = SNGL(LOGDM(BIGM, LFM, LOGFAC, M, Q, T, TAU, X))
*             + ALOG(RHO(X)) - MLOGG
            IF (G .GT. CONST) QG8 = QG8 + C(I)*EXP(G)
            X = Y + Z
        5     CONTINUE
    10 CONTINUE
    QG8 = (XU - XL)*QG8
C
    RETURN
    END
C
    DOUBLE PRECISION FUNCTION LOGDM(BIGM, LFM, LOGFAC, M, Q, T,
*     TAU, X)
C
C     ALGORITHM AS 301.11 APPL. STATIST. (1996), VOL.45, NO.2
C
C     Computes log F(X), log F(X)/(1 + M/EXP(X)) or
C     log F(X)/(M + EXP(X)) where M denotes BIGM.
C
    INTEGER BIGM, T, M(T), TAU, X
    DOUBLE PRECISION LFM, LOGFAC(T)
    REAL Q(T)
C
    DOUBLE PRECISION C, K, LGAPP, L2PID2, ONE, ONED2, TEN,
*     U, Z

```

```

      INTEGER ALPHA, I
C
      DATA C /0.08333333333333333333333333333333D0/, L2PID2, ONE, ONED2, TEN
* /0.9189385332046728D0, 1.0D0, 0.5D0, 10.0D0/
C
      LGAPP(U) = (U - ONED2)*DLOG(U) - U + L2PID2 + C/U
      K = DEXP(DBLE(X))
      LOGDM = LFM
      DO 15 ALPHA = 1, T
        IF (M(ALPHA) .GT. 0) THEN
          LOGDM = LOGDM - LOGFAC(ALPHA)
          Z = Q(ALPHA)*K
          I = 0
5          IF (I + Z .GT. TEN .OR. I .EQ. M(ALPHA)) GO TO 10
            LOGDM = LOGDM + DLOG(I + Z)
            I = I + 1
            GO TO 5
10         IF (I .LT. M(ALPHA)) LOGDM = LOGDM +
*           LGAPP(M(ALPHA) + Z) - LGAPP(I + Z)
          ENDIF
15 CONTINUE
      I = 0
20 IF (I + K .GT. TEN .OR. I .EQ. BIGM) GO TO 25
      LOGDM = LOGDM - DLOG(I + K)
      I = I + 1
      GO TO 20
25 IF (I .LT. BIGM) LOGDM = LOGDM - LGAPP(BIGM + K) + LGAPP(I + K)
      IF (TAU .EQ. 2) THEN
        LOGDM = LOGDM - DLOG(ONE + BIGM/K)
      ELSE IF (TAU .EQ. 3) THEN
        LOGDM = LOGDM - DLOG(BIGM + K)
      ENDIF
C
      RETURN
      END
C
      SUBROUTINE PARRHO(LQ, UQ, IFAULT, MU1, RPI)
C
C       ALGORITHM AS 301.12 APPL. STATIST. (1996), VOL.45, NO.2
C
C       Computes the parameter values of the log-Cauchy density
C
      REAL LQ, UQ, MU1, RPI
      INTEGER IFAULT
C
      REAL LMB, LMB2, LMU1, ONE, PI, RLMB, TENE9, TWO, ZERO
C
      COMMON /RHOPAR/ LMB, LMB2, LMU1, RLMB
C
      DATA ONE, PI, TENE9, TWO, ZERO
* /1.0, 3.1415927, 1.0E+09, 2.0, 0.0/
C
      IF (LQ .LE. ZERO .OR. LQ .GE. UQ .OR. UQ .GE. TENE9) THEN
        IFAULT = 1
      ELSE
        MU1 = SQRT(LQ*UQ)
        LMU1 = ALOG(MU1)
        LMB = ALOG(UQ/LQ)/TWO
        LMB2 = LMB**2
        RLMB = ONE/LMB
        RPI = ONE/PI

```

ENDIF

C

RETURN

END

```

      SUBROUTINE MISRE(K, IP, IPP, NH, INV, COV, X, EPS, ITMAX,
*           IB, COVINV, XA, Y, Z, AII, A, W, WK, IT, SITA,
*           STAT, IFAULT)
C
C     ALGORITHM AS 302.1 APPL. STATIST. (1996), VOL.45, NO.2
C
C     Subroutine to compute a multiple isotonic regression
C     for umbrella ordering with known peak
C
      INTEGER I, IFAULT, II, I1, INC, IP, IP1, IPP, IT, ITMAX, J,
*           J1, K, L, NULLTY
      REAL DET, EPS, RABS, RMAX, STAT
      REAL A(IP), AII(K), COV(IPP, K), COVINV(IPP, K), SITA(IP, K),
*           W(IP), WK(K, 6), X(IP, K), XA(K), Y(K), Z(K)
      INTEGER IB(IP), NH(IP)
C
      EXTERNAL ISRE, SUBINV
C
      IFAULT = 0
      IF (IP .LE. 1) IFAULT = 1
      IF (IPP .NE. IP * (IP + 1) / 2) IFAULT = 6
      IF (IFAULT .NE. 0) RETURN
C
      Find inversions of covariances
C
      IF (INV .EQ. 1) THEN
        DO 10 I = 1, IP
          IB(I) = I
10       CONTINUE
        DO 20 I = 1, K
          CALL SUBINV(COV(1, I), IP, IB, IP, COVINV(1, I), W, NULLTY,
*           IFAULT, IPP, DET)
          IF (IFAULT .NE. 0) RETURN
20       CONTINUE
        INV = 0
      ENDIF
C
      IT = 1
      IP1 = IP - 1
      DO 40 I = 2, IP
        DO 30 J = 1, K
          SITA(I, J) = X(I, J)
30       CONTINUE
40      CONTINUE
C
      Find multivariate isotonic regression iteratively
C
50     RMAX = 0.0
      DO 120 I = 1, IP
        II = I * (1 + I) / 2
C
C     For the i-th univariate isotonic regression
C
      DO 100 L = 1, K
        AII(L) = COVINV(II, L)
C
C     Set A(1), ..., A(IP - 1) to the elements of A21
C
      IF (I .GT. 1) THEN
        I1 = II - I
        DO 60 J = 1, I - 1

```

```

        III1 = III1 + 1
        A(J) = COVINV(III1, L)
60      CONTINUE
      ENDIF
      IF (I .LT. IP) THEN
        III1 = II + I
        INC = I + 1
        DO 70 J = I, IP1
          A(J) = COVINV(III1, L)
          III1 = III1 + INC
          INC = INC + 1
70      CONTINUE
      ENDIF
C
C      Prepare the input data Z(1),...,Z(IP - 1) for
C      univariate isotonic regression
C
        J1 = 1
        DO 80 J = 1, IP
          IF (J .NE. I) THEN
            Y(J1) = X(J, L) - SITA(J, L)
            J1 = J1 + 1
          ENDIF
80      CONTINUE
        Z(L) = X(I, L)
        DO 90 J = 1, IP1
          Z(L) = Z(L) + Y(J) * A(J) / AII(L)
90      CONTINUE
100     CONTINUE
C
C      Find a univariate isotonic regression
C
        CALL ISRE(K, NH(I), Z, AII, WK(1, 1), WK(1, 2), WK(1, 3),
*         WK(1, 4), WK(1, 5), WK(1, 6), XA, IFAULT)
        IF (IFAULT .NE. 0) THEN
          IFAULT = IFAULT + 2
          RETURN
        ENDIF
        DO 110 J = 1, K
          IF (IT .NE. 1) THEN
            RABS = ABS(XA(J) - SITA(I,J))
            IF (RABS .GT. RMAX) RMAX = RABS
          ENDIF
          SITA(I, J) = XA(J)
110     CONTINUE
120     CONTINUE
        IT = IT + 1
        IF (IT .EQ. 2 .OR. RMAX .GT. EPS .AND. IT .LE. ITMAX) GOTO 50
        IF (RMAX .GT. EPS .AND. IT .GT. ITMAX) IFAULT = 7
C
C      Calculate likelihood ratio statistics
C
        STAT = 0.0
        DO 150 L = 1, K
          DO 140 I = 1, IP
            II = I * (1 + I) / 2
            STAT = STAT + COVINV(II, L) * (X(I, L) - SITA(I, L)) ** 2
            IF (I .GT. 1) THEN
              III1 = II - I
              DO 130 J = 1, I - 1
                STAT = STAT + 2.0 * COVINV(III1+J,L) * (X(I,L) - SITA(I,L))

```

```

* (X(J, L) - SITA(J, L))
130     CONTINUE
      ENDIF
140     CONTINUE
150     CONTINUE
C
      RETURN
      END
C
      SUBROUTINE MISREU(K, IP, IPP, KP, NH, COV, X, EPS, ITMAX, IB,
*                   COVINV, XA, Y, Z, AII, A, W, WK, ITM, SITA,
*                   SITAMIN, STATMIN, NHMIN, STATMAT, IFAULT)
C
      ALGORITHM AS 302.2 APPL. STATIST. (1996), VOL.45, NO.2
C
      Subroutine to compute a multiple isotonic regression
      for umbrella ordering with unknown peak
C
      INTEGER I, IFAULT, II, I1, INC, INV, IP, IP1, IPP, IT, ITM,
*          ITMAX, J, J1, K, KP, L, NULLTY
      REAL DET, EPS, RABS, RMAX, STAT, STATMIN
      REAL A(IP), AII(K), COV(IPP, K), COVINV(IPP, K), SITA(IP, K),
*          SITAMIN(IP,K), STATMAT(KP), W(IP), WK(K, 6), X(IP, K),
*          XA(K), Y(K), Z(K)
      INTEGER IB(IP), NH(IP), NHMIN(IP)
C
      EXTERNAL MISRE
C
      IF (KP .LT. K ** IP) THEN
          IFAULT = 8
          RETURN
      ENDIF
C
      INV = 1
      ITM = 0
      STATMIN = 0.99E10
      NUM = 1
      DO 10 I = 1, IP
          NH(I) = 1
10     CONTINUE
C
      Calculate multiple isotonic regression for all possible
      peaks
C
20     CALL MISRE(K, IP, IPP, NH, INV, COV, X, EPS, ITMAX,
*             IB, COVINV, XA, Y, Z, AII, A, W, WK, IT, SITA, STAT,
*             IFAULT)
      IF (IFAULT .NE. 0) RETURN
      STATMAT(NUM) = STAT
      NUM = NUM + 1
      IF (IT .GT. ITM) ITM = IT
C
      Save the best regression and peak vector
C
      IF (STAT .LE. STATMIN) THEN
          STATMIN = STAT
          DO 40 I = 1, IP
              DO 30 J = 1, K
                  SITAMIN(I, J) = SITA(I, J)
30             CONTINUE
              NHMIN(I) = NH(I)

```



```
      40    CONTINUE
        ENDDIF
C
C      Set the next peak
C
      DO 50 I = 1, IP
        NH(I) = NH(I) + 1
        IF (NH(I) .LE. K) GOTO 20
        NH(I) = 1
50 CONTINUE
C
      RETURN
      END
```

```
      SUBROUTINE OPART(N, K, NI, MCOUNT, IFAULT)
C
C      ALGORITHM AS 303.1 APPL.STATIST. (1996), VOL.45, NO.3
C
C      Generation of ordered multinomial frequencies.  Given integers
C      N (N >= 0) and K (K >= 1), generates all possible integer arrays
C      NI of size K, whose elements are non-negative, non-decreasing
C      and sum to N.
C
      INTEGER N, K, NI(K), MCOUNT, IFAULT
C
      INTEGER I, IO, I1, J, K1, KSUM, NSUM
C
      EXTERNAL JOB
C
      Perform domain checks.  Initialize MCOUNT, NI, K1 and KSUM.
      Set NI(IO) = 0; for IO = 1 to K-1.
C
      IFAULT = 1
      MCOUNT = 0
      IF(K .LT. 1) RETURN
      IF(N .LT. 0) RETURN
      IFAULT = 0
      K1 = K - 1
      IF(K .EQ. 1) K1 = 1
      KSUM = 0
C
      DO 10 I = 1, K1
         NI(I) = 0
10 CONTINUE
C
      Begin with pivot element in position K-1 of array NI
C
      IO = K1
20 IF(IO .EQ. K1) GO TO 40
C
      Set NI(J); for J = IO+1 to K-1, equal to pivot cell
      frequency.  Update KSUM.
C
      I1 = IO + 1
C
      DO 30 J = I1, K1
         NI(J) = NI(IO)
         KSUM = KSUM + NI(IO)
30 CONTINUE
C
      Assign NI(K)
C
40 MCOUNT = MCOUNT + 1
      NSUM = NI(K1)
      NI(K) = N - KSUM
C
      CALL JOB(K, NI, MCOUNT)
C
      Reset pivot cell to K-1 and update NSUM.  Check upper limit
      for NI(IO).
C
      IO = K1
      NSUM = NSUM + NI(K)
50 IF( NI(IO) .LT. NSUM / (K - IO + 1) ) GO TO 60
C
```

```
C      Move pivot I0 to next lower cell.  Update KSUM and NSUM.
C
      I0 = I0 - 1
      IF(I0 .LE. 0) RETURN
      KSUM = KSUM - NI(I0+1)
      NSUM = NSUM + NI(I0)
      GO TO 50
C
      Increment NI(I0) by 1 and update KSUM.
C
60  NI(I0) = NI(I0) + 1
      KSUM = KSUM + 1
      GO TO 20
      END
C
      SUBROUTINE JOB(K, NI, MCOUNT)
C
      ALGORITHM AS 303.2 APPL.STATIST. (1996), VOL.45, NO.3
C
      Evaluates C(X) for X = NI and writes out ordered K-tuple
C
      INTEGER K, NI(K), MCOUNT
C
      REAL SIZE, TIES
      INTEGER J, K1, KTEMP, NTEMP, RK
C
      K1 = K-1
      NTEMP = NI(1)
      SIZE = K
      KTEMP = K
      TIES = 1.0D0
C
      DO 30 J = 1, K1
          KTEMP = KTEMP - 1
          RK = KTEMP
          IF(NI(J + 1) .EQ. NTEMP) GO TO 10
          NTEMP = NI(J + 1)
          TIES = 1.0D0
          GO TO 20
10     TIES = TIES + 1.0D0
20     SIZE = SIZE * RK / TIES
30 CONTINUE
C
      WRITE(*, 40) MCOUNT, SIZE, (NI(J), J = 1, K)
40  FORMAT(1X,I5,1X,F15.0,7X,10I4/
*        1X,21X,10I4)
      RETURN
      END
```

```

SUBROUTINE FISHER (X, M, Y, N, TOTAL, POSSIB, P, IFAULT)
C
C   ALGORITHM AS 304.1 APPL.STATIST. (1996), VOL.45, NO.3
C
C   Fisher's non-parametric randomization test for two small
C   independent random samples
C
INTEGER M, N, TOTAL, POSSIB, IFAULT
REAL X(*), Y(*), P
C
INTEGER MAXSAM, MAXSIZ
PARAMETER (MAXSAM = 14, MAXSIZ = 3432)
C
C   Important : set MAXSIZ >= COMB(MAXSAM, MAXSAM / 2)
C
INTEGER K, SIZE1, SIZE2, WS3(MAXSAM), COUNT
REAL SUMX, SUMY, WS1(MAXSIZ), WS2(MAXSIZ), SUMM
C
INTEGER COMB, TRADES
REAL MEAN, SUM
EXTERNAL COMB, SUM, TRADES
C
EXTERNAL CMLPMT, EXCHNG, KTRADE
C
MEAN(SUMM, COUNT) = SUMM / REAL(COUNT)
C
IF (COMB(MAXSAM, MAXSAM/2) .GT. MAXSIZ) THEN
  IFAULT = 1
ELSE IF (M .GT. MAXSAM .OR. N .GT. MAXSAM) THEN
  IFAULT = 2
ELSE
  IFAULT = 0
  SUMX = SUM(X, M)
  SUMY = SUM(Y, N)
  IF (MEAN(SUMX, M) .GT. MEAN(SUMY, N)) THEN
    CALL EXCHNG(X, M, Y, N, SUMX, SUMY)
  END IF
  TOTAL = 0
  IF (M .EQ. N) THEN
    DO 10 K = 1, (M-1)/2
      CALL KTRADE(X, M, WS1, SIZE1, WS3, K)
      CALL KTRADE(Y, N, WS2, SIZE2, WS3, K)
      TOTAL = TOTAL + TRADES(WS1, SIZE1, WS2, SIZE2)
      CALL CMLPMT(WS1, SIZE1, SUMX)
      CALL CMLPMT(WS2, SIZE2, SUMY)
      TOTAL = TOTAL + TRADES(WS1, SIZE1, WS2, SIZE2)
10    CONTINUE
    IF (MOD(M, 2) .EQ. 0) THEN
      CALL KTRADE(X, M, WS1, SIZE1, WS3, K)
      CALL KTRADE(Y, N, WS2, SIZE2, WS3, K)
      TOTAL = TOTAL + TRADES(WS1, SIZE1, WS2, SIZE2)
    END IF
  ELSE
    DO 20 K = 1, MIN(M, N)
      CALL KTRADE(X, M, WS1, SIZE1, WS3, K)
      CALL KTRADE(Y, N, WS2, SIZE2, WS3, K)
      TOTAL = TOTAL + TRADES(WS1, SIZE1, WS2, SIZE2)
20    CONTINUE
  END IF
  POSSIB = COMB(M+N, M)
  P = REAL(TOTAL + 1) / REAL(POSSIB)

```

```
      END IF
C
      RETURN
      END
C
      SUBROUTINE EXCHNG (X, M, Y, N, SX, SY)
C
C      ALGORITHM AS 304.2 APPL.STATIST. (1996), VOL.45, NO.3
C
C      Exchanges the sample data. Assumes both X and Y have been
C      previously dimensioned to at least max(M, N) elements
C
      INTEGER M, N
      REAL X(*), Y(*), SX, SY
C
      INTEGER C, K
      REAL TEMP
C
      TEMP = SX
      SX = SY
      SY = TEMP
C
      C = MIN(M, N)
      DO 10 K = 1, C
          TEMP = X(K)
          X(K) = Y(K)
          Y(K) = TEMP
10  CONTINUE
      IF (M .GT. N) THEN
          DO 20 K = C+1, M
              Y(K) = X(K)
20  CONTINUE
          N = M
          M = C
      ELSE IF (M .LT. N) THEN
          DO 30 K = C+1, N
              X(K) = Y(K)
30  CONTINUE
          M = N
          N = C
      END IF
C
      RETURN
      END
C
      SUBROUTINE KTRADE (W, K, WPRIME, KPRIME, WS, R)
C
C      ALGORITHM AS 304.3 APPL.STATIST. (1996), VOL.45, NO.3
C
C      Generates and sorts the sums of the R-combinations of the
C      elements of W
C
      INTEGER K, KPRIME, WS(*), R
      REAL W(*), WPRIME(*)
C
      INTEGER COMB
      REAL SUM
      EXTERNAL COMB, SUM
C
      EXTERNAL CMPLMT, GENER, SORT
C
```

```
KPRIME = COMB(K, R)
IF (R .LE. K - R .OR. R .EQ. K) THEN
  CALL GENER(W, K, WPRIME, KPRIME, WS, R)
  CALL SORT(WPRIME, KPRIME)
ELSE
  CALL GENER(W, K, WPRIME, KPRIME, WS, K - R)
  CALL SORT(WPRIME, KPRIME)
  CALL CMPLMT(WPRIME, KPRIME, SUM(W, K))
ENDIF
C
RETURN
END
C
INTEGER FUNCTION TRADES (XPRIME, MPRIME, YPRIME, NPRIME)
C
C   ALGORITHM AS 304.4 APPL.STATIST. (1996), VOL.45, NO.3
C
C   Returns the number of 1-for-1 trades that refutes the null
C   hypothesis. Assumes that XPRIME has the smaller mean and
C   that both arrays are sorted in ascending order.
C
C   INTEGER MPRIME, NPRIME
C   REAL XPRIME(*), YPRIME(*)
C
C   INTEGER I, J
C
C   TRADES = 0
C   I = 1
C   J = 1
10 IF (J .GT. NPRIME) GOTO 40
20 IF (XPRIME(I) .GE. YPRIME(J)) GOTO 30
  I = I + 1
  IF (I .LE. MPRIME) GOTO 20
30 TRADES = TRADES + (MPRIME - I + 1)
  J = J + 1
  IF (I .LE. MPRIME) GOTO 10
C
40 RETURN
END
C
SUBROUTINE CMPLMT (WPRIME, KPRIME, SUM)
C
C   ALGORITHM AS 304.5 APPL.STATIST. (1996), VOL.45, NO.3
C
C   Reverse and complement the data in WPRIME
C
C   INTEGER KPRIME
C   REAL WPRIME(*), SUM
C
C   INTEGER I, J
C   REAL TEMP
C
C   J = KPRIME
C   DO 10 I = 1, KPRIME / 2 + MOD(KPRIME, 2)
C     TEMP = WPRIME(I)
C     WPRIME(I) = REAL(DBLE(SUM) - DBLE(WPRIME(J)))
C     WPRIME(J) = REAL(DBLE(SUM) - DBLE(TEMP))
C     J = J - 1
10 CONTINUE
C
RETURN
```

```
END
C
SUBROUTINE GENER (W, N, WPRIME, NPRIME, INDEX, R)
C
C   ALGORITHM AS 304.6 APPL.STATIST. (1996), VOL.45, NO.3
C
C   Computes an array of sums of the various R-combinations of
C   the elements of W
C
INTEGER N, NPRIME, R, INDEX(R)
REAL W(N), WPRIME(NPRIME)
C
INTEGER I, J
DOUBLE PRECISION SUM
LOGICAL INIT
C
EXTERNAL NEXT
C
INIT = .TRUE.
C
DO 20 I = 1, NPRIME
  CALL NEXT(INDEX, R, N, INIT)
  SUM = 0.0D0
  DO 10 J = 1, R
    SUM = SUM + DBLE(W(INDEX(J)))
10  CONTINUE
  WPRIME(I) = REAL(SUM)
20 CONTINUE
C
RETURN
END
C
SUBROUTINE NEXT (RCOMBO, R, N, INIT)
C
C   ALGORITHM AS 304.7 APPL.STATIST. (1996), VOL.45, NO.3
C
C   Accepts some R-combination of the first N integers and then
C   computes the next R-combination in the lexicographic
C   ordering of the  $N! / (R! * (N - R)!)$  such R-combinations.
C   Returns the first R-combination if the initialization
C   indicator is .true. and then resets the indicator.
C
INTEGER R, N, RCOMBO(R)
LOGICAL INIT
C
INTEGER I, J, D
C
IF (INIT) THEN
  DO 10 I = 1, R
    RCOMBO(I) = I
10  CONTINUE
  INIT = .FALSE.
ELSE
  D = N - R
  J = R
C
C   The counter J is not prevented from going out of bounds
C   which will happen if there is no next R-combination
C
20  IF (RCOMBO(J) .LT. D + J) GOTO 30
    J = J - 1
```

```
        GOTO 20
30     RCOMBO(J) = RCOMBO(J) + 1
        DO 40 I = J + 1, R
            RCOMBO(I) = RCOMBO(I - 1) + 1
40     CONTINUE
    END IF
C
    RETURN
    END
C
C     General purpose subroutines
C
    SUBROUTINE SORT (X, N)
C
C     ALGORITHM AS 304.8 APPL.STATIST. (1996), VOL.45, NO.3
C
C     Sorts the N values stored in array X in ascending order
C
    INTEGER N
    REAL X(N)
C
    INTEGER I, J, INCR
    REAL TEMP
C
    INCR = 1
C
C     Loop : calculate the increment
C
10    INCR = 3 * INCR + 1
    IF (INCR .LE. N) GOTO 10
C
C     Loop : Shell-Metzner sort
C
20    INCR = INCR / 3
    I = INCR + 1
30    IF (I .GT. N) GOTO 60
    TEMP = X(I)
    J = I
40    IF (X(J - INCR) .LT. TEMP) GOTO 50
    X(J) = X(J - INCR)
    J = J - INCR
    IF (J .GT. INCR) GOTO 40
50    X(J) = TEMP
    I = I + 1
    GOTO 30
60    IF (INCR .GT. 1) GOTO 20
C
    RETURN
    END
C
    INTEGER FUNCTION COMB (N, K)
C
C     ALGORITHM AS 304.9 APPL.STATIST. (1996), VOL.45, NO.3
C
C     Returns the number of combinations of N things taken K at a
C     time or 0 if the parameters are incompatible
C
    INTEGER N, K
C
    INTEGER M, I
```



```
REAL NUMER, DENOM, FACT
EXTERNAL FACT
C
IF (K .LT. 0 .OR. K .GT. N) THEN
  COMB = 0
ELSE
  M = N - K
  NUMER = 1.0
  DO 10 I = N, 1 + MAX(K, M), -1
    NUMER = NUMER * REAL(I)
10  CONTINUE
  DENOM = FACT(MIN(K, M))
  COMB = NINT(NUMER / DENOM)
END IF
C
RETURN
END
C
REAL FUNCTION FACT (N)
C
C   ALGORITHM AS 304.10 APPL.STATIST. (1996), VOL.45, NO.3
C
C   Returns the factorial of N or 0.0 if the parameter is
C   negative
C
INTEGER N
C
INTEGER I
C
IF (N .LT. 0) THEN
  FACT = 0.0
ELSE
  FACT = 1.0
  DO 10 I = 2, N
    FACT = FACT * REAL(I)
10  CONTINUE
END IF
C
RETURN
END
C
REAL FUNCTION SUM (X, N)
C
C   ALGORITHM AS 304.11 APPL.STATIST. (1996), VOL.45, NO.3
C
C   Returns the sum of the values stored in X
C
INTEGER N
REAL X(N)
C
INTEGER I
DOUBLE PRECISION ACCUM
C
ACCUM = 0.0D0
DO 10 I = 1, N
  ACCUM = ACCUM + DBLE(X(I))
10 CONTINUE
SUM = REAL(ACCUM)
C
RETURN
END
```

```
      SUBROUTINE ARLM(K,H,U,DELTA,ARL,IFAULT)
C
C      ALGORITHM AS 305.1 APPL. STATIST. (1996), VOL.45, NO.4
C
C      Compute the ARL of a CUSUM mean chart with linear drift
C
      DOUBLE PRECISION K,H,U,DELTA,ARL
      INTEGER IFAULT
C
      DOUBLE PRECISION SIGMA
      INTEGER NN, NSIDE, NTYPE
C
      EXTERNAL COMARL
C
      NTYPE=1
      NSIDE=1
      CALL COMARL(NTYPE,NSIDE,NN,K,H,U,DELTA,SIGMA,ARL,IFAULT)
C
      RETURN
      END
C
      SUBROUTINE ARLV(NSIDE,NN,K,H,U,SIGMA,ARL,IFAULT)
C
C      ALGORITHM AS 305.2 APPL. STATIST. (1996), VOL.45, NO.4
C
C      Compute the ARL of a CUSUM variance chart
C
      INTEGER NSIDE, NN, IFAULT
      DOUBLE PRECISION K,H,U,SIGMA,ARL
C
      INTEGER NTYPE
      DOUBLE PRECISION DELTA
C
      EXTERNAL COMARL
C
      NTYPE=2
      CALL COMARL(NTYPE,NSIDE,NN,K,H,U,DELTA,SIGMA,ARL,IFAULT)
C
      RETURN
      END
C
      SUBROUTINE COMARL(NTYPE,NSIDE,NN,K,H,U,DELTA,SIGMA,ARL,IFAULT)
C
C      ALGORITHM AS 305.3 APPL. STATIST. (1996), VOL.45, NO.4
C
C      Compute the ARL of a CUSUM chart or a CUSUM variance chart
C
      INTEGER NTYPE, NSIDE, NN, IFAULT
      DOUBLE PRECISION K,H,U,DELTA,SIGMA,ARL
C
      INTEGER I, IA, IB, IP1, IFLAG, IPIVOT(25), J, JJ, JP1, JP2,
*      MMM, MP1, ND2, NPTS, NQM1, NQUAD, NSIDE2
      DOUBLE PRECISION A(25, 25), ALPHA, B(25), BETA, DMEAN(3000),
*      P(25), SIDE, SK, SS, W(25), WK(25), X(25),
*      XOLD(25)
C
      DOUBLE PRECISION CDFLG, PDFLG, PDFN
      REAL ALNORM, DNORM
C
      EXTERNAL FACTOR, SUBST, SETUP
```

```
C
C      Gaussian quadrature abscissas
C
```

```
P(1)=0.9951872199970213D0
P(2)=0.9747285559713095D0
P(3)=0.9382745520027327D0
P(4)=0.8864155270044010D0
P(5)=0.8200019859739029D0
P(6)=0.7401241915785543D0
P(7)=0.6480936519369755D0
P(8)=0.5454214713888395D0
P(9)=0.4337935076260451D0
P(10)=0.3150426796961634D0
P(11)=0.1911188674736163D0
P(12)=0.0640568928626056D0
```

```
C
C      Gaussian quadrature weights
C
```

```
W(1)=0.0123412297999872D0
W(2)=0.0285313886289337D0
W(3)=0.0442774388174198D0
W(4)=0.0592985849154368D0
W(5)=0.0733464814110803D0
W(6)=0.0861901615319533D0
W(7)=0.0976186521041139D0
W(8)=0.1074442701159656D0
W(9)=0.1155056680537256D0
W(10)=0.1216704729278034D0
W(11)=0.1258374563468283D0
W(12)=0.1279381953467521D0
```

```
C
C      Initialise variables
C
```

```
NPTS=25
NQUAD=NPTS-1
ND2=NQUAD/2
SIDE=NSIDE
SS=NN
ALPHA=(SS-1.0D0)/2.0D0
BETA=(SIGMA*SIGMA)/ALPHA
SK=SIDE*K
```

```
C
C      Set IFAULT to be 0, 1, 2, 3, 4, 5, 6
C
```

```
IFAULT=0
IF(NTYPE.EQ.1.AND.(DELTA.GE.0.0D0.AND.
*DELTA.LT.0.0001D0)) IFAULT=1
IF(NTYPE.EQ.1.AND.DELTA.LT.0.0D0) IFAULT=2
NSIDE2=NSIDE*NSIDE
IF(NTYPE.EQ.2.AND.NSIDE2.NE.1) IFAULT=3
IF(NTYPE.EQ.2.AND.SIGMA.LE.0.0D0) IFAULT=4
IF(NTYPE.EQ.1.AND.(U.LT.0.0D0.OR.U.GT.H)) IFAULT=5
IF(NTYPE.EQ.2.AND.NSIDE.EQ.1.AND.
*(U.LT.0.0D0.OR.U.GT.H)) IFAULT=5
IF(NTYPE.EQ.2.AND.NSIDE.EQ.-1.AND.
*(U.LT.-H.OR.U.GT.0.0D0)) IFAULT=5
IF(NTYPE.EQ.2.AND.NN.LE.1) IFAULT=6
IF(IFAULT.GE.2) RETURN
```

```
C
C      Obtain the full Gaussian abscissas and weights
C
```

```

      DO 2 I=1,ND2
        P(NPTS-I)=-P(I)
        W(NPTS-I)=W(I)
2     CONTINUE
C
C       Transform the Gaussian abscissas and weights
C       from the interval (-1,1) to (0,h) or (-h,0)
C
      DO 3 I=1,NQUAD
        W(I)=H*W(I)/2.0D0
        P(I)=H*P(I)/2.0D0 + SIDE*H/2.0D0
3     CONTINUE
C
C       Compute the ARL of a CUSUM variance chart under step shift
C
      IF(NTYPE.EQ.2) THEN
C
C       Replace the integral equation by a system of linear
C       equations AX=B
C
      B(NPTS)=-1.D0
      A(1,1)=-1.0D0+CDFLG(SK,ALPHA,BETA)
      IF(NSIDE.EQ.-1) A(1,1)=-1.0D0-A(1,1)
      DO 4 I=1,NQUAD
        A(1,I+1)=W(I)*PDFLG(SK+P(I),ALPHA,BETA)
        B(I)=-1.D0
4     CONTINUE
      DO 5 I=1,NQUAD
        IP1=I+1
        A(IP1,1)=CDFLG(SK-P(I),ALPHA,BETA)
        IF(NSIDE.EQ.-1) A(IP1,1)=1.0D0-A(IP1,1)
5     CONTINUE
      DO 7 I=1,NQUAD
        DO 6 J=1,NQUAD
          IP1=I+1
          JP1=J+1
          IF(I.EQ.J) THEN
            A(IP1,JP1)=W(I)*PDFLG(SK,ALPHA,BETA)-1.0D0
          ELSE
            A(IP1,JP1)=W(J)*PDFLG(P(J)-P(I)+SK,
*           ALPHA,BETA)
          ENDIF
6     CONTINUE
7     CONTINUE
C
C       Call the subroutines FACTOR and SUBST to solve the system
C       of equations for X. Set IFAULT to be 7 if matrix A is
C       singular.
C
      CALL FACTOR(A,NPTS,WK,IPIVOT,IFLAG)
      IF(IFLAG.EQ.0) THEN
        IFAULT=7
        RETURN
      ENDIF
      CALL SUBST(A,IPIVOT,B,NPTS,X)
C
C       Compute L(u) of a CUSUM variance chart
C
      ARL=CDFLG(SK-U,ALPHA,BETA)
      IF(NSIDE.EQ.-1) ARL=1.0D0-ARL
      ARL=1.D0+X(1)*ARL+W(1)*X(2)*PDFLG(P(1)+SK-U,

```

```

      * ALPHA, BETA)
      NQM1=NQUAD-1
      DO 8 J=1, NQM1
        JP1=J+1
        JP2=J+2
        ARL=ARL+W(JP1)*X(JP2)*PDFLG(P(JP1)+SK-U,
      * ALPHA, BETA)
8      CONTINUE

C
C      Compute the ARL of a CUSUM mean chart under linear drift
C
      ELSE

C
C      Compute the process mean mu_0, mu_1, ..., mu_m
C
      CALL SETUP(DELTA, DMEAN, MP1)

C
C      Replace the integral equation by a system of linear
C      equations AX=B
C
      DO 20 I=1, NPTS
        B(I)=-1.0D0
        DO 10 J=1, NPTS
          IF(I.LE.NQUAD.AND.J.EQ.I) THEN
            A(I, J)=W(J)*PDFN(P(J)+K-P(I),
      *      DMEAN(MP1), 1.0D0)-1.0D0
          ELSEIF(I.LE.NQUAD.AND.J.LE.NQUAD) THEN
            A(I, J)=W(J)*PDFN(P(J)+K-P(I),
      *      DMEAN(MP1), 1.0D0)
          ELSEIF(I.LE.NQUAD.AND.J.EQ.NPTS) THEN
            DNORM=K-P(I)-DMEAN(MP1)
            A(I, J)=ALNORM(DNORM, .FALSE.)
          ELSEIF(I.EQ.NPTS.AND.J.LT.I) THEN
            A(I, J)=W(J)*PDFN(P(J)+K,
      *      DMEAN(MP1), 1.0D0)
          ELSE
            DNORM=K-DMEAN(MP1)
            A(I, J)=ALNORM(DNORM, .FALSE.)-1.0D0
          ENDIF
        10 CONTINUE
      20 CONTINUE

C
C      Call the subroutines FACTOR and SUBST to solve the system
C      of equations for X. Set IFAULT to be 7 if matrix A is
C      singular.
C
      CALL FACTOR(A, NPTS, WK, IPIVOT, IFLAG)
      IF(IFLAG.EQ.0) THEN
        IFAULT=7
        RETURN
      ENDIF
      CALL SUBST(A, IPIVOT, B, NPTS, X)

C
C      Compute intermediate ARL functions
C
      MMM=MP1-1
      DO 80 J=2, MMM
        JJ=MP1-J+1
        DO 60 I=1, NPTS
          XOLD(I)=X(I)
          X(I)=1.0D0

```

```

60      CONTINUE
      DO 75 IA=1,NPTS
        IF(IA.EQ.NPTS) THEN
          DNORM = K-DMEAN(JJ)
        ELSE
          DNORM = K-P(IA)-DMEAN(JJ)
        ENDIF
        X(IA) = X(IA)+ALNORM(DNORM,.FALSE.)*XOLD(NPTS)
        DO 70 IB=1,NQUAD
          IF(IA.EQ.NPTS) THEN
            X(IA) = X(IA)+W(IB)*XOLD(IB)*
*          PDFN(P(IB)+K,DMEAN(JJ),1.0D0)
          ELSE
            X(IA) = X(IA)+W(IB)*XOLD(IB)*
*          PDFN(P(IB)+K-P(IA),DMEAN(JJ),1.0D0)
          ENDIF
70      CONTINUE
75      CONTINUE
80      CONTINUE
C
C      Compute L_0(u,0)
C
      ARL=1.0D0
      DNORM = K-U-DMEAN(1)
      ARL = ARL+ALNORM(DNORM,.FALSE.)*X(NPTS)
      DO 90 J=1,NQUAD
        ARL=ARL+W(J)*PDFN(P(J)+K-U,DMEAN(1),1.0D0)*X(J)
90      CONTINUE
      ENDIF
C
      RETURN
      END
C
      SUBROUTINE SETUP(DELTA,DMEAN,MP1)
C
C      ALGORITHM AS 305.4 APPL. STATIST. (1996), VOL.45, NO.4
C
C      Determine MP1 and DMEAN where
C      DMEAN(j) = process mean at (j-1)th sample;
C                for j=1, 2, ...,MP1
C
      DOUBLE PRECISION DELTA, DMEAN(3000)
      INTEGER MP1
C
      INTEGER J, JM1
C
      IF(DELTA.LT.0.0001) THEN
        MP1=1
      ELSEIF(DELTA.LE.0.001) THEN
        MP1=3000
      ELSEIF(DELTA.LE.0.002) THEN
        MP1=2000
      ELSEIF(DELTA.LE.0.005) THEN
        MP1=1000
      ELSEIF(DELTA.LE.0.010) THEN
        MP1=500
      ELSEIF(DELTA.LE.0.015) THEN
        MP1=300
      ELSEIF(DELTA.LE.0.020) THEN
        MP1=200

```

```
ELSEIF(DELTA.LE.0.025) THEN
  MP1=150
ELSEIF(DELTA.LE.0.040) THEN
  MP1=100
ELSEIF(DELTA.LE.0.050) THEN
  MP1=70
ELSEIF(DELTA.LE.0.080) THEN
  MP1=60
ELSEIF(DELTA.LE.0.150) THEN
  MP1=40
ELSEIF(DELTA.LE.0.200) THEN
  MP1=30
ELSEIF(DELTA.LE.0.400) THEN
  MP1=20
ELSEIF(DELTA.LE.1.000) THEN
  MP1=15
ELSE
  MP1=10
ENDIF
DMEAN(1)=0.0D0
IF(MP1.GE.2) THEN
  DO 10 J=2,MP1
    JM1=J-1
    DMEAN(J)=DMEAN(JM1)+DELTA
10  CONTINUE
ENDIF
```

```
C
RETURN
END

C
DOUBLE PRECISION FUNCTION PDFN(X,XMU,SIGMA)
C
C   ALGORITHM AS 305.5 APPL. STATIST. (1996), VOL.45, NO.4
C
C   Compute the normal density function at X where XMU is the
C   mean and SIGMA is the sandard deviation
C
DOUBLE PRECISION X, XMU, SIGMA
C
DOUBLE PRECISION ARG
C
ARG=-0.5D0*(X-XMU)*(X-XMU)/(SIGMA*SIGMA)
PDFN=(3.989422804014327D-1/SIGMA)*DEXP(ARG)
C
RETURN
END
```

```
      SUBROUTINE BIB(AMAT,A,B,BMAT,C,D,NEWMAT,FLAG)
C
C      ALGORITHM AS 306 APPL.STATIST. (1996), VOL.45, NO.4
C
C      Calculation of a BIB product operation on any two matrices
C
      INTEGER A, B, C, D
      REAL AMAT(A,B), BMAT(C,D), NEWMAT(A,B*D)
      LOGICAL FLAG
C
      INTEGER CT, I, J, K, PT
C
C      This block of code sets the logical variable FLAG to F and exits
C      the subroutine if the number of non-zero elements in each column
C      of A does not equal the number of rows of B
C
      DO 20 I = 1, B
         CT=0
         DO 10 J=1, A
            IF (AMAT(J,I).NE.0.0) CT = CT + 1
10        CONTINUE
         FLAG=CT.EQ.C
         IF(.NOT.FLAG) GOTO 70
20      CONTINUE
C
C      This block of code computes the BIB product
C
      DO 60 I = 1, B
         PT = 1
         DO 50 J = 1, A
            IF(AMAT(J,I).EQ.0.0) THEN
               DO 30 K = 1, D
                  NEWMAT(J,(I*D)-D+K)=0.0
30              CONTINUE
            ELSE
               DO 40 K = 1, D
                  NEWMAT(J,(I*D)-D+K)=AMAT(J,I)*BMAT(PT,K)
40              CONTINUE
               PT=PT+1
            END IF
50          CONTINUE
60        CONTINUE
70      RETURN
      END
```



```

SUBROUTINE DEPTH(U, V, N, X, Y, ALPHA, F, SDEP, HDEP)
C
C     ALGORITHM AS 307.1 APPL.STATIST. (1996), VOL.45, NO.4
C
C     Calculation of the simplicial depth and the halfspace
C     depth
C
C     INTEGER N, F(N)
C     REAL U, V, X(N), Y(N), ALPHA(N), SDEP, HDEP
C
C     INTEGER GI, I, J, JA, JB, KI, NBAD, NF, NN, NN2, NT, NU, NUMH,
*     NUMS
C     REAL ALPHK, ANGLE, BETAK, D, EPS, P, P2, XU, YU
C
C     EXTERNAL K, SORT
C
C     NUMS = 0
C     NUMH = 0
C     SDEP = 0.0
C     HDEP = 0.0
C
C     IF (N.LT.1) RETURN
C
C     P = ACOS(-1.0)
C     P2 = P * 2.0
C     EPS = 0.000001
C     NT = 0
C
C     Construct the array ALPHA
C
DO 10 I = 1, N
    D = SQRT((X(I)-U) * (X(I)-U) + (Y(I)-V) * (Y(I)-V))
    IF (D.LE.EPS) THEN
        NT = NT + 1
    ELSE
        XU = (X(I) - U) / D
        YU = (Y(I) - V) / D
        IF (ABS(XU).GT.ABS(YU)) THEN
            IF (X(I).GE.U) THEN
                ALPHA(I-NT) = ASIN(YU)
                IF (ALPHA(I-NT).LT.0.0) THEN
                    ALPHA(I-NT) = P2 + ALPHA(I-NT)
                ENDIF
            ELSE
                ALPHA(I-NT) = P - ASIN(YU)
            ENDIF
        ELSE
            IF (Y(I).GE.V) THEN
                ALPHA(I-NT) = ACOS(XU)
            ELSE
                ALPHA(I-NT) = P2 - ACOS(XU)
            ENDIF
        ENDIF
        IF (ALPHA(I-NT).GE.(P2 - EPS)) ALPHA(I-NT) = 0.0
    ENDIF
10 CONTINUE
    NN = N - NT
    IF (NN.LE.1) GOTO 60
C
C     Sort the array ALPHA
C

```

```

      CALL SORT(ALPHA, NN)
C
C      Check whether theta=(U,V) lies outside the data cloud
C
      ANGLE = ALPHA(1) - ALPHA(NN) + P2
      DO 20 I = 2, NN
        ANGLE = AMAX1(ANGLE, (ALPHA(I) - ALPHA(I-1)))
20    CONTINUE
      IF (ANGLE.GT.(P + EPS)) GOTO 60
C
C      Make smallest alpha equal to zero, and
C      compute NU = number of alpha < pi
C
      ANGLE = ALPHA(1)
      NU = 0
      DO 30 I = 1, NN
        ALPHA(I) = ALPHA(I) - ANGLE
        IF (ALPHA(I).LT.(P - EPS)) NU = NU + 1
30    CONTINUE
      IF (NU.GE.NN) GOTO 60
C
C      Mergesort the alpha with their antipodal angles beta, and
C      at the same time update I, F(I), and NBAD
C
      JA = 1
      JB = 1
      ALPHK = ALPHA(1)
      BETAK = ALPHA(NU+1) - P
      NN2 = NN * 2
      NBAD = 0
      I = NU
      NF = NN
      DO 40 J = 1, NN2
        IF ((ALPHK + EPS).LT.BETAK) THEN
          NF = NF + 1
          IF (JA.LT.NN) THEN
            JA = JA + 1
            ALPHK = ALPHA(JA)
          ELSE
            ALPHK = P2 + 1.0
          ENDIF
        ELSE
          I = I + 1
          IF (I.EQ.(NN + 1)) THEN
            I = 1
            NF = NF - NN
          ENDIF
          F(I) = NF
          NBAD = NBAD + K((NF-I), 2)
          IF (JB.LT.NN) THEN
            JB = JB + 1
            IF ((JB + NU).LE.NN) THEN
              BETAK = ALPHA(JB+NU) - P
            ELSE
              BETAK = ALPHA(JB+NU-NN) + P
            ENDIF
          ELSE
            BETAK = P2 + 1.0
          ENDIF
        ENDIF
      40 CONTINUE

```

```
NUMS = K(NN, 3) - NBAD
C
C      Computation of NUMH for halfspace depth
C
GI = 0
JA = 1
ANGLE = ALPHA(1)
NUMH = MIN0(F(1), (NN - F(1)))
DO 50 I = 2, NN
  IF(ALPHA(I).LE.(ANGLE + EPS)) THEN
    JA = JA + 1
  ELSE
    GI = GI + JA
    JA = 1
    ANGLE = ALPHA(I)
  ENDIF
  KI = F(I) - GI
  NUMH = MIN0(NUMH, MIN0(KI, (NN-KI)))
50 CONTINUE
C
C      Adjust for the number NT of data points equal to theta
C
60 NUMS = NUMS + K(NT, 1)*K(NN, 2) + K(NT, 2)*K(NN, 1) + K(NT, 3)
  IF (N.GE.3) SDEP = (NUMS + 0.0) / (K(N, 3) + 0.0)
  NUMH = NUMH + NT
  HDEP = (NUMH + 0.0) / (N + 0.0)
C
RETURN
END
C
INTEGER FUNCTION K(M, J)
C
C      ALGORITHM AS 307.2 APPL.STATIST. (1996), VOL.45, NO.4
C
C      Returns the value zero if M < J; otherwise computes the
C      number of combinations of J out of M
C
INTEGER M, J
C
IF (M.LT.J) THEN
  K = 0
ELSE
  IF (J.EQ.1) K = M
  IF (J.EQ.2) K = (M * (M - 1)) / 2
  IF (J.EQ.3) K = (M * (M - 1) * (M - 2)) / 6
ENDIF
C
RETURN
END
```

```
      REAL FUNCTION NCBETA (A, B, LAMBDA, X, ERRMAX, IFAULT)
C
C      ALGORITHM AS 310 APPL. STATIST. (1997), VOL. 46, NO. 1
C
C      Computes the cumulative distribution function of a
C      non-central beta random variable
C
      REAL A, B, LAMBDA, X, ERRMAX
      INTEGER IFAULT
C
      INTEGER XJ, M, I, J, ITER1, ITER2, ITERLO, ITERHI
C
      Local variable XJ gives the number of iterations taken
C
      REAL FX, GX, TEMP, FTEMP, EBD, ERRBD,
*      Q, R, S, T, S0, S1, T0, T1, SUM, PSUM,
*      C, HALF, ONE, ZERO, FIVE, BETA,
*      ALNGAM, BETAIN, BETANC, GAMMAD
C
      EXTERNAL ALNGAM, BETAIN, BETANC, GAMMAD
C
      DATA ZERO, HALF, ONE, FIVE /
*      0.0E+00, 0.5E+00, 1.0E+00, 5.0E+00 /
C
      NCBETA = X
C
      Check for admissibility of parameters
C
      IFAULT = 3
      IF (LAMBDA .LE. ZERO .OR. A .LE. ZERO .OR. B .LE. ZERO) RETURN
      IFAULT = 2
      IF (X .LT. ZERO .OR. X .GT. ONE) RETURN
      IFAULT = 1
      IF (X .EQ. ZERO .OR. X .EQ. ONE) RETURN
      IFAULT = 0
C
      C = LAMBDA * HALF
      XJ = ZERO
C
      IF (LAMBDA .LT. 54.0) THEN
C
      AS 226 as it stands is sufficient in this situation
C
      NCBETA = BETANC(X, A, B, LAMBDA, IFAULT)
      RETURN
      ELSE
      M = INT(C + HALF)
      ITERLO = M - FIVE * SQRT(M)
      ITERHI = M + FIVE * SQRT(M)
      T = - C + M * ALOG(C) - ALNGAM(M + ONE)
      Q = EXP(T)
      R = Q
      PSUM = Q
C
      BETA = ALNGAM(A+ M) + ALNGAM(B) - ALNGAM(A+ M +B)
      S1 = (A + M) * ALOG(X) + B * ALOG(ONE - X) - ALOG(A + M) - BETA
      GX = EXP(S1)
      FX = GX
      TEMP = BETAIN(X, A + M, B, BETA, IFAULT)
      FTEMP= TEMP
      XJ = XJ + ONE
```

```
SUM = Q - TEMP
ITER1= M
```

```
C
C The first set of iterations starts from M and goes downwards
C
```

```
20 IF (ITER1 .LT. ITERLO) GO TO 30
   IF (Q .LT. ERRMAX) GO TO 30
   Q = Q - ITER1 / C
   XJ = XJ + ONE
   GX = (A + ITER1) / (X * (A + B + ITER1 - ONE)) * GX
   ITER1= ITER1- ONE
   TEMP =TEMP + GX
   PSUM = PSUM + Q
   SUM = SUM + Q * TEMP
   GO TO 20
30 T0 = ALNGAM(A + B) - ALNGAM(A + ONE) - ALNGAM(B)
   S0 = A * ALOG(X) + B * ALOG(ONE - X)
```

```
C
   DO 40 I=1, ITER1
     J = I - ONE
     S = S + EXP(T0 + S0 + J * ALOG(X))
     T1 = ALOG(A + B + J) - ALOG(A + ONE + J) + T0
     T0 = T1
40 CONTINUE
```

```
C
C Compute the first part of error bound
C
```

```
ERRBD=(ONE- GAMMAD(C,FLOAT(ITER1),IFAUULT))*(TEMP + S)
Q = R
TEMP = FTEMP
GX = FX
ITER2 = M
50 EBD = ERRBD + (ONE - PSUM) * TEMP
   IF (EBD .LT. ERRMAX .OR. ITER2 .GE. ITERHI) GO TO 60
   ITER2 = ITER2 + ONE
   XJ = XJ + ONE
   Q = Q * C / ITER2
   PSUM = PSUM + Q
   TEMP = TEMP - GX
   GX = X * (A + B + ITER2 - ONE) / (A + ITER2) * GX
   SUM = SUM + Q * TEMP
   GO TO 50
60 CONTINUE
```

```
END IF
70 NCBETA = SUM
C
RETURN
END
```

```
REAL FUNCTION BETANC(X, A, B, LAMBDA, IFAULT)
```

```
C
C ALGORITHM AS226 APPL. STATIST. (1987) VOL. 36, NO. 2
C Incorporates modification AS R84 from AS vol. 39, pp311-2, 1990
C
C Returns the cumulative probability of X for the non-central beta
C distribution with parameters A, B and non-centrality LAMBDA
C
C Auxiliary routines required: ALOGAM - log-gamma function (ACM
C 291 or AS 245), and BETAIN - incomplete-beta function (AS 63)
```

```
C
  REAL A, AX, B, BETA, C, ERRBD, ERRMAX, GX, HALF, LAMBDA, ONE, Q,
*   SUMQ, TEMP, X, XJ, ZERO
  REAL A0, X0, UALPHA

C
C   Change ERRMAX and ITRMAX if desired ...
C
  DATA ERRMAX, ITRMAX /1.0E-6, 100/, UALPHA /5.0/

C
  DATA ZERO, HALF, ONE /0.0, 0.5, 1.0/

C
  BETANC = X

C
  IFAULT = 2
  IF (LAMBDA .LT. ZERO .OR. A .LE. ZERO .OR. B .LE. ZERO) RETURN
  IFAULT = 3
  IF (X .LT. ZERO .OR. X .GT. ONE) RETURN
  IFAULT = 0
  IF (X .EQ. ZERO .OR. X .EQ. ONE) RETURN

C
  C = LAMBDA * HALF

C
C   Initialize the series ...
C
  X0 = INT( MAX(C - UALPHA*SQRT(C), ZERO) )
  A0 = A + X0
  BETA = ALOGAM(A0, IFAULT) + ALOGAM(B, IFAULT) -
*   ALOGAM(A0+B, IFAULT)
  TEMP = BETAIN(X, A0, B, BETA, IFAULT)
  GX = EXP(A0 * LOG(X) + B * LOG(ONE - X) - BETA - LOG(A0))
  IF (A0 .GT. A) THEN
    Q = EXP(-C + X0*LOG(C)) - ALOGAM(X0 + ONE, IFAULT)
  ELSE
    Q = EXP(-C)
  END IF
  XJ = ZERO
  AX = Q * TEMP
  SUMQ = ONE - Q
  BETANC = AX

C
C   Recur over subsequent terms until convergence is achieved...
C
10 XJ = XJ + ONE
  TEMP = TEMP - GX
  GX = X * (A + B + XJ - ONE) * GX / (A + XJ)
  Q = Q * C / XJ
  SUMQ = SUMQ - Q
  AX = TEMP * Q
  BETANC = BETANC + AX

C
C   Check for convergence and act accordingly...
C
  ERRBD = (TEMP - GX) * SUMQ
  IF ((INT(XJ) .LT. ITRMAX) .AND. (ERRBD .GT. ERRMAX)) GO TO 10
  IF (ERRBD .GT. ERRMAX) IFAULT = 1

C
  RETURN
  END
```

```

SUBROUTINE INVMOD(MAT,IMAT,RMOD,CMOD,IWK,NROW,IFAULT)
C
C   ALGORITHM AS 314.1 APPL. STATIST. (1997), VOL.46, NO.2
C
C   Inverts matrix with contents subject to modulo arithmetic
C
C   INTEGER   IFAULT,NROW
C   INTEGER   CMOD(NROW),IMAT(NROW*NROW),IWK(2*NROW),
*            MAT(NROW*NROW),RMOD(NROW)
C
C   INTEGER   I,IR,J,K,KIR,KJR,N
C
C   EXTERNAL  MSORT,MUSORT
C
C   INTRINSIC MOD
C
C   Check elements in 'mixed-moduli' positions are all zero
C
C   N=0
C   DO 26 I=1,NROW
C     DO 24 J=1,NROW
C       N=N+1
C       IF ((RMOD(I).NE.CMOD(J)).AND.(MAT(N).GT.0)) GO TO 1002
C       IF ((MAT(N).GT.RMOD(I)).OR.(MAT(N).LT.0)) GO TO 1001
C       IMAT(N)=0
C   24 CONTINUE
C   26 CONTINUE
C
C   Sort rows and columns into ascending order of moduli
C
C   CALL MSORT(MAT,IMAT,RMOD,CMOD,IWK,IWK(NROW+1),NROW)
C
C   Complete initialisation of inverse matrix
C
C   DO 28 N=1,NROW*NROW,NROW+1
C     IMAT(N)=1
C   28 CONTINUE
C
C   Invert the matrix
C
C   DO 190 IR=1,NROW
C     KIR=(IR-1)*NROW
C     IF (MAT(KIR+IR).EQ.0) THEN
C
C       Find a row JR below IR such that K(JR,IR)>0
C
C       DO 112 KJR=KIR+NROW+IR,NROW*NROW,NROW
C         IF (MAT(KJR).GT.0) GO TO 115
C   112 CONTINUE
C
C       Column IR contains all zeros in rows IR or below:
C       look for a row above with zeros to left of column IR
C       and K(JR,IR)>0
C
C       DO 114 KJR=IR,KIR,NROW
C         IF (MAT(KJR).GT.0) THEN
C           DO 113 I=KJR-IR+1,KJR-1
C             IF (MAT(I).GT.0) GO TO 1003
C   113 CONTINUE
C           GO TO 115
C         ENDIF

```

```
114      CONTINUE
C
C      Column IR contains all zeros
C
C      GO TO 190
C
C      Switch row JR with row IR
C
115      KJR=KJR-IR
        DO 116 I=1,NROW
            K=MAT(KIR+I)
            MAT(KIR+I)=MAT(KJR+I)
            MAT(KJR+I)=K
            K=IMAT(KIR+I)
            IMAT(KIR+I)=IMAT(KJR+I)
            IMAT(KJR+I)=K
116      CONTINUE
        END IF
C
C      Find multiplier N such that  $N \cdot \text{MAT}(\text{IR}, \text{IR}) = 1 \pmod{P\{\text{IR}\}}$ 
C
C      K=MAT(KIR+IR)
        DO 122 N=1,RMOD(IR)-1
            IF (MOD(N*K,RMOD(IR)).EQ.1) GO TO 125
122      CONTINUE
C
C      Multiply row IR by N
C
125      IF (N.GT.1) THEN
            DO 126 I=KIR+1,IR*NROW
                MAT(I)=MAT(I)*N
                IMAT(I)=IMAT(I)*N
126      CONTINUE
        END IF
C
C      Subtract  $\text{MAT}(\text{JR}, \text{IR}) * \text{row IR}$  from each row JR
C
C
        DO 136 KJR=0,NROW*NROW-1,NROW
            N=RMOD(IR)-MAT(KJR+IR)
            IF ((KJR.NE.KIR).AND.(N.NE.0)) THEN
                DO 132 I=1,NROW
                    MAT(KJR+I)=MOD(MAT(KJR+I)+N*MAT(KIR+I),CMOD(I))
                    IMAT(KJR+I)=MOD(IMAT(KJR+I)+N*IMAT(KIR+I),CMOD(I))
132      CONTINUE
                END IF
136      CONTINUE
190 CONTINUE
C
C      Check inversion was possible - that result has
C      non-zero elements only on diagonal
C
        IFAULT=0
        DO 202 N=1,NROW*NROW,NROW+1
C
C      Zero diagonal element => left inverse formed
C
            IF (MAT(N).EQ.0) IFAULT=-1
            MAT(N)=-MAT(N)
202 CONTINUE
        DO 204 N=1,NROW*NROW
            IF (MAT(N).GT.0) GO TO 1003
```



```
204 CONTINUE
    DO 206 N=1,NROW*NROW,NROW+1
        MAT(N)=-MAT(N)
206 CONTINUE
C
C     Sort rows and columns back into original order
C
    CALL MUSORT(MAT,IMAT,RMOD,CMOD,IWK,IWK(NROW+1),NROW)
C
    RETURN
C
C     Invalid entry (< 0 or > modulus)
C
1001 IFAULT=1
    RETURN
C
C     Non-zero entry in position where row mod does not
C     equal column mod
C
1002 IFAULT=2
    RETURN
C
C     Matrix cannot be inverted
C
1003 IFAULT=3
    RETURN
    END
C
SUBROUTINE MSORT(MAT,IMAT,RMOD,CMOD,RSORT,CSORT,NROW)
C
C     ALGORITHM AS 314.2 APPL. STATIST. (1997), VOL.46, NO.2
C
C     Sorts the matrix and associated information to put
C     rows and columns in ascending order of moduli
C
    INTEGER    NROW
    INTEGER    CMOD(NROW),CSORT(NROW),IMAT(*),MAT(*),RMOD(NROW),
*            RSORT(NROW)
C
    INTEGER    I,IRC,J,JRC,KIRC,KJRC,P
C
C     Initialise row and column addresses
C
    DO 22 I=1,NROW
        RSORT(I)=I
        CSORT(I)=I
22 CONTINUE
C
C     Sort rows
C
    DO 48 IRC=1,NROW
C
C     Find next row
C
        JRC=IRC
        P=RMOD(IRC)
        DO 42 I=IRC+1,NROW
            IF (RMOD(I).LT.P) THEN
                P=RMOD(I)
                JRC=I
            
```

```
      END IF
42  CONTINUE
      IF (IRC.NE.JRC) THEN
          I=RMOD(IRC)
          RMOD(IRC)=RMOD(JRC)
          RMOD(JRC)=I
          I=RSORT(IRC)
          RSORT(IRC)=RSORT(JRC)
          RSORT(JRC)=I
C
C      Switch rows
C
          KIRC=(IRC-1)*NROW
          KJRC=(JRC-1)*NROW
          DO 44 J=1,NROW
              I=MAT(KIRC+J)
              MAT(KIRC+J)=MAT(KJRC+J)
              MAT(KJRC+J)=I
44  CONTINUE
      END IF
48 CONTINUE
C
C      Sort columns
C
      DO 68 IRC=1,NROW
C
C      Find next column
C
          JRC=IRC
          P=CMOD(IRC)
          DO 62 I=IRC+1,NROW
              IF (CMOD(I).LT.P) THEN
                  P=CMOD(I)
                  JRC=I
              END IF
62  CONTINUE
          IF (IRC.NE.JRC) THEN
              I=CMOD(IRC)
              CMOD(IRC)=CMOD(JRC)
              CMOD(JRC)=I
              I=CSORT(IRC)
              CSORT(IRC)=CSORT(JRC)
              CSORT(JRC)=I
C
C      Switch columns
C
          DO 64 J=0,NROW*NROW-1,NROW
              I=MAT(IRC+J)
              MAT(IRC+J)=MAT(JRC+J)
              MAT(JRC+J)=I
64  CONTINUE
      END IF
68 CONTINUE
C
      RETURN
      END
C
      SUBROUTINE MUSORT(MAT,IMAT,RMOD,CMOD,RSORT,CSORT,NROW)
C
C      ALGORITHM AS 314.3 APPL. STATIST. (1997), VOL.46, NO.2
C
```

```
C      Sorts the inverse matrix and associated information into the
C      original order of rows and columns
C
C      INTEGER      NROW
C      INTEGER      CMOD(NROW),CSORT(NROW),IMAT(NROW*NROW),
*      MAT(NROW*NROW),RMOD(NROW),RSORT(NROW)
C
C      INTEGER      I,IRC,J,JRC,KIRC,KJRC
C
C      Sort rows of inverse (=columns of original)
C
C      DO 48 IRC=1,NROW
C
C      Find next row
C
C      IF (CSORT(IRC).NE.IRC) THEN
C      DO 42 JRC=IRC+1,NROW
C      IF (CSORT(JRC).EQ.IRC) GO TO 43
42  CONTINUE
43  I=CMOD(IRC)
C      CMOD(IRC)=CMOD(JRC)
C      CMOD(JRC)=I
C      I=CSORT(IRC)
C      CSORT(IRC)=CSORT(JRC)
C      CSORT(JRC)=I
C
C      Switch rows
C
C      KIRC=(IRC-1)*NROW
C      KJRC=(JRC-1)*NROW
C      DO 44 J=1,NROW
C      I=IMAT(KIRC+J)
C      IMAT(KIRC+J)=IMAT(KJRC+J)
C      IMAT(KJRC+J)=I
44  CONTINUE
C      END IF
48  CONTINUE
C
C      Sort columns of inverse (= rows of original)
C
C      DO 68 IRC=1,NROW
C
C      Find next column
C
C      IF (RSORT(IRC).NE.IRC) THEN
C      DO 62 JRC=IRC+1,NROW
C      IF (RSORT(JRC).EQ.IRC) GO TO 63
62  CONTINUE
63  I=RMOD(IRC)
C      RMOD(IRC)=RMOD(JRC)
C      RMOD(JRC)=I
C      I=RSORT(IRC)
C      RSORT(IRC)=RSORT(JRC)
C      RSORT(JRC)=I
C
C      Switch columns
C
C      DO 64 J=0,NROW*NROW-1,NROW
C      I=IMAT(IRC+J)
C      IMAT(IRC+J)=IMAT(JRC+J)
C      IMAT(JRC+J)=I
```

```
64      CONTINUE
C
C      Switch diagonal elements of MAT (others are zero)
C
      KIRC=(IRC-1)*NROW+IRC
      KJRC=(JRC-1)*NROW+JRC
      I=MAT(KIRC)
      MAT(KIRC)=MAT(KJRC)
      MAT(KJRC)=I
      END IF
68 CONTINUE
C
      RETURN
      END
```

Below are 2 versions of this algorithm, the first as submitted to the RSS in Fortran 77; the second is my Fortran 90 version. The author has given permission for his version to be submitted to the apstat collection.

As a `title' in the index I suggest:  
Unconstrained variable metric function minimization without derivatives.

The two versions are separated by a line of !!!!!!'s

Alan

P.S. I have tested the F90 version. As it was derived from the F77 version, that should work too!

C Algorithm AS 319 and test program

```

C-----
      PROGRAM VAR
C-----
C      A PROGRAM TO IMPLEMENT A QUASI-NEWTON METHOD.
C      USING NEW ALGORITHM VARMET    JULY 1994
C-----
C
      COMMON /FUNERR/LER
      COMMON /TEST/IG,IFN
      EXTERNAL FUN
      LOGICAL LER
C
      INTEGER N, NMAX
      PARAMETER (N=2, NMAX=50)
      INTEGER IG,IFN,GRADTL,MESS,MAXFN,IER
      PARAMETER (GRADTL = 12, MAXFN = 1000, MESS = 6)
      DOUBLE PRECISION X,XTMP,W,FP
      DIMENSION X(N),XTMP(N),W(225)
C
      WRITE(*,*)'  '
      WRITE(*,*) 'INPUT YOUR STARTING GUESS'
      DO 12 I=1,N
         READ(*,*) XTMP(I)
12 CONTINUE
      WRITE(*,*)'  '
      WRITE(*,*) 'INITIALIZATION COMPLETE.'
      WRITE(*,*) '*****'
C
      DO 24 J=1,N
24      X(J)=XTMP(J)
         IFN = 0
         CALL VARME(FUN,N,X,FP,W,GRADTL,MAXFN,MESS,IER)
C
      WRITE(*,*)'  '
      WRITE(*,*) 'THE NUMBER OF FUNCTION EVALUATIONS IS ',IFN
      WRITE(*,*)'  '
      WRITE(*,*) 'THE MINIMUM FOUND IS',(X(I),I=1,N)
      WRITE(*,*)'  '
      CALL FUN(N,X,FP)
      WRITE(*,*) 'THE FUNCTION VALUE IS: ',FP
      STOP
      END
C-----

```

SUBROUTINE FUN(NORD,BP,Q)

```

C-----
COMMON /FUNERR/LER
COMMON /TEST/IG,IFN
DIMENSION BP(*)
LOGICAL LER
DOUBLE PRECISION BP,Q
Q=100.*(BP(2)-BP(1)**2)**2+(BP(1)-1.)**2
IFN = IFN + 1
LER = .FALSE.
RETURN
END

```

SUBROUTINE VARME(FUN,NPAR,B,F0,W,NSIG,MAXFN,IOUT,IER)

```

C-----
C
C CALLING SUBROUTINE FOR SUBROUTINE VARMET
C
C ALLOWS FOR SETUP OF DEFAULT PARAMETERS
C AND EFFICIENT USE OF STORAGE
C AS WELL AS WRITING OF ERROR MESSAGES
C
C VERSION 0.1
C CODED BY JOHN J. KOVAL
C MARCH 1986
C
C VERSION 0.2
C CODED BY JOHN J. KOVAL
C JULY 1988
C
C VERSION 0.26
C CODED BY MURRAY ALEXANDER FOR JOHN J. KOVAL
C JULY 1989
C
C VERSION 0.27
C MODIFIED BY NAZIH HASSAN, JULY 1993
C
C VERSION 0.28
C MODIFIED BY JOHN KOVAL, JUNE 1996
C BECAUSE OF COMMENTS FROM REVIEWER FOR APPLIED STATISTICS
C CHANGES TO ORDER OF PARAMETERS IN GRAD
C
C PARAMETERS             MEANING             DEFAULT
C -----             -
C FUN                   NAME OF FUNCTION TO BE MINIMIZED
C
C NPAR                  ORDER OF PARAMETER VECTOR
C                      (NUMBER OF UNKNOWNNS)
C
C B                     ARRAY CONTAINING INITIAL ESTIMATES
C                      ON OUTPUT CONTAINING FINAL ESTIMATES
C
C F0                    VALUE OF FUNCTION AT MINIMUM
C
C W                     WORK ARRAY OF LENGTH FO (NPAR+5)*NPAR
C
C NSIG                  MACHINE ACCURACY AS NEGATIVE POWER      10 OR 5
C                      OF TEN
C
C MAXFN                 MAXIMUM NUMBER OF FUNCTION EVALUATIONS  1000

```

```

C          (DOES INCLUDE EVALUATIONS BY SUBROUTINE
C          GRAD WHICH CALCULATES APPROXIMATE GRADIENT)
C
C          IOUT          OUTPUT CHANNEL FOR ERROR MESSAGES          0
C          (IF 0, THEN MESSAGES NOT WRITTEN)
C
C          IER          ERROR INDICATOR          0
C          INTEGER
C
C-----
C          DOUBLE PRECISION W,B,F0,EPD,GRADTL
C          EXTERNAL FUN
C          DIMENSION B(*),W(*)
C          PARAMETER (MAXF = 1000, EPD = 1.0D-05, MSIG = 10)
C
C          INITIALIZE
C
C          IER=0
C
C          IF(NSIG.EQ.0) NSIG = MSIG
C          GRADTL = 1.0/(10.0**(NSIG))
C
C          IF(GRADTL.LT.0.0) THEN
C              IF(IOUT.GT.0) WRITE(IOUT,300) NSIG, GRADTL
300          FORMAT(' NSIG VALUE OF ',I3,' CREATES NEGATIVE VALUE OF',
1' GRADTL, NAMELY, ',G12.5)
C              GRADTL = 1.0/(10**(MSIG))
C              IF(IOUT.GT.0) WRITE(IOUT,310) MSIG, GRADTL
310          FORMAT(' PROGRAM SUBSTITUTES NSIG VALUE OF ',I3,' WHICH',
1' GIVES GRADTL VALUE OF ',G12.5)
C          ENDIF
C
C          IF(MAXFN.EQ.0) MAXFN = MAXF
C
C          NOW WE ARE READY TO CALL THE MINIMIZATION SUBROUTINE
C
C          I1 = NPAR*NPAP + 1
C          I2 = I1 + NPAR
C          I3 = I2 + NPAR
C          I4 = I3 + NPAR
C
C          CALL VARMET(FUN,NPAR,B,F0,W(I3),W,W(I1),W(I2),W(I4),
1 GRADTL,MAXFN,IER)
C
C          IF(IER.GT.0.AND.IOUT.GT.0)THEN
C              WRITE(IOUT,30) IER
30          FORMAT(/' SUBROUTINE VARMET ERROR NUMBER ',I3)
C              IF(IER.EQ.1) THEN
C                  WRITE(IOUT,40)
C              ELSE IF(IER.EQ.2) THEN
C                  WRITE(IOUT,60)
C              ELSE IF(IER.EQ.3) THEN
C                  WRITE(IOUT,70)
C              ELSE IF(IER.EQ.4) THEN
C                  WRITE(IOUT,80)
C              ENDIF
40          FORMAT(' FUNCTION UNDEFINED AT INITIAL VALUE          ')
60          FORMAT(' GRADIENT UNDEFINED IN TOO MANY DIMENSIONS  ')
70          FORMAT(' FUNCTON NOT MINIMIZED BUT '
1 /' UNABLE TO FIND MINIMUM IN DIRECTION OF SEARCH')
80          FORMAT(' TOO MANY FUNCTION EVALUATIONS REQUIRED          ')

```

```
C
      ENDIF
C
200 RETURN
      END

C-----
      SUBROUTINE VARMET(FUN,NPAR,B,F0,G,H,C,D,T,GRADTL,MAXFN,IFAU)
C
      ALGORITHM AS 319 APPL.STATIST. (1997), VOL.46, NO.4
C
      VARIABLE METRIC FUNCTION MINIMISATION
C
      EXTERNAL FUN
      COMMON/FUNERR/LER
      DIMENSION B(NPAR),G(NPAR),H(NPAR,NPAR),C(NPAR),D(NPAR),T(2*NPAR)
      DOUBLE PRECISION B,F0,G,H,C,D,T,GRADTL,W,TOLER,D1,S,CK,F1,D2
      INTEGER IFN,IG
      LOGICAL LER
      PARAMETER (ICMAX=20, TOLER=0.00001, W=0.2)
C
      IG = 0
      IFN = 0
      LER = .FALSE.
      IFAU = 0
      NP = NPAR + 1
C
      IF (MAXFN.EQ.0) MAXFN = 1000
      IF (GRADTL.EQ.0.0) GRADTL = 1.0D-10
C
      CALL FUN(NPAR,B,F0)
      IF(LER) THEN
          IFAU = 1
          RETURN
      ENDIF
      IFN = IFN + 1
C
      CALL GRAD(FUN,NPAR,B,F0,G,T(NP),GRADTL,IFAU)
      IF(IFAU.GT.0) RETURN
C
      IG = IG + 1
      IFN = IFN + NPAR
      IF(IFN.GT.MAXFN) THEN
          IFAU = 4
          RETURN
      ENDIF
C
10 DO 30 K = 1,NPAR
      DO 20 L = 1,NPAR
          H(K,L) = 0.0
20 CONTINUE
      H(K,K) = 1.00
30 CONTINUE
      ILAST = IG
C
40 DO 50 I = 1,NPAR
      D(I) = B(I)
      C(I) = G(I)
50 CONTINUE
C
      D1 = 0.0
```



```
      DO 70 I = 1, NPAR
        S = 0.0
        DO 60 J = 1, NPAR
          S = S - H(I, J) * G(J)
60      CONTINUE
        T(I) = S
        D1 = D1 - S * G(I)
70 CONTINUE
C
      IF(D1.LE.0.0) THEN
        IF(ILAST.EQ.IG) THEN
          RETURN
        ENDIF
        GO TO 10
      ELSE
        CK = 1.0
        IC = 0
90      ICOUNT = 0
        DO 100 I = 1, NPAR
          B(I) = D(I) + CK * T(I)
          IF(B(I).EQ.D(I)) THEN
            ICOUNT = ICOUNT + 1
          ENDIF
100     CONTINUE
C
        IF(ICOUNT.GE.NPAR) THEN
          IF(ILAST.EQ.IG) THEN
            RETURN
          ENDIF
          GO TO 10
        ELSE
          CALL FUN(NPAR, B, F1)
C
          IFN = IFN + 1
          IF(IFN.GT.MAXFN) THEN
            IFAULT = 4
            RETURN
          ELSE IF(LER) THEN
            CK = W * CK
            IC = IC + 1
            IF(IC.GT.ICMAX) THEN
              IFAULT = 3
              RETURN
            ENDIF
            GO TO 90
C
          ELSE IF(F1.GE.F0 - D1 * CK * TOLER) THEN
            CK = W * CK
            GO TO 90
          ELSE
            F0 = F1
            CALL GRAD(FUN, NPAR, B, F0, G, T(NP), GRADTL, IFAULT)
            IF(IFAULT.GT.0) THEN
              RETURN
            ENDIF
            IG = IG + 1
            IFN = IFN + NPAR
            IF(IFN.GT.MAXFN) THEN
              IFAULT = 4
              RETURN
            ENDIF
```

```

C
      D1 = 0.0
      DO 130 I = 1,NPAR
        T(I) = CK*T(I)
        C(I) = G(I) - C(I)
        D1 = D1 + T(I)*C(I)
130    CONTINUE
C
      IF(D1.LE.0.0) THEN
        GOTO 10
      ENDIF
C
      D2 = 0.0
      DO 150 I = 1,NPAR
        S = 0.0
        DO 140 J = 1,NPAR
          S = S + H(I,J)*C(J)
140    CONTINUE
        D(I) = S
        D2 = D2 + S*C(I)
150    CONTINUE
      D2 = 1.0 + D2/D1
C
      DO 170 I = 1,NPAR
        DO 170 J = 1,NPAR
          H(I,J) = H(I,J) - (T(I)*D(J) + D(I)*T(J) -
1      D2*T(I)*T(J))/D1
170    CONTINUE
      ENDIF
    ENDIF
  ENDIF
  GO TO 40
  END

SUBROUTINE GRAD(F,NPAR,B,F0,G,SA,ER,IFAU)
C
C  CALCULATE APPROXIMATE GRADIENT
C
  DIMENSION B(NPAR),G(NPAR),SA(NPAR)
  DOUBLE PRECISION B,F0,G,SA,ER,H,F1
  COMMON/FUNERR/LER
  LOGICAL LER
C
  JCMAX=NPAR-2
  JC = 0
C
  DO 20 I = 1,NPAR
    H =(DABS(B(I)) +DSQRT(ER)) *DSQRT(ER)
    SA(I) = B(I)
    B(I) = B(I) + H
    CALL F(NPAR,B,F1)
    B(I) = SA(I)
C
    IF(LER) THEN
      F1 = F0 + H
      JC = JC + 1
    ENDIF
C
    G(I) = (F1 -F0)/H
  20 CONTINUE
C

```

```

      IF(JC.GT.JCMAX) IFAULT = 2
      RETURN
      END

```

!!

```

! Algorithm AS 319 and test program
! Converted to Fortran 90 free-format style by Alan Miller
! e-mail: Alan.Miller @ vic.cmis.csiro.au
! URL: www.ozemail.com.au/~milleraj

```

```

MODULE as319
IMPLICIT NONE

```

```

! COMMON /funerr/ler
! COMMON /test/ig,ifn
LOGICAL, SAVE      :: ler
INTEGER, SAVE      :: ig, ifn

```

```

INTEGER, PARAMETER :: dp = SELECTED_REAL_KIND(14, 50)

```

```

END MODULE as319

```

!-----

```

SUBROUTINE varme(fun, npar, b, f0, nsig, maxfn, iout, ier)

```

!-----

```

!      CALLING SUBROUTINE FOR SUBROUTINE VARMET
!
!      ALLOWS FOR SETUP OF DEFAULT PARAMETERS
!      AND EFFICIENT USE OF STORAGE
!      AS WELL AS WRITING OF ERROR MESSAGES

```

```

!      VERSION 0.1
!      CODED BY JOHN J. KOVAL
!      MARCH 1986

```

```

!      VERSION 0.2
!      CODED BY JOHN J. KOVAL
!      JULY 1988

```

```

!      VERSION 0.26
!      CODED BY MURRAY ALEXANDER FOR JOHN J. KOVAL
!      JULY 1989

```

```

!      VERSION 0.27
!      MODIFIED BY NAZIH HASSAN, JULY 1993

```

```

!      VERSION 0.28
!      MODIFIED BY JOHN KOVAL, JUNE 1996
!      BECAUSE OF COMMENTS FROM REVIEWER FOR APPLIED STATISTICS
!      CHANGES TO ORDER OF PARAMETERS IN GRAD

```

```

!      PARAMETERS              MEANING              DEFAULT
!      -----              -

```

```

!      FUN              NAME OF FUNCTION TO BE MINIMIZED

```

```
!      NPAR      ORDER OF PARAMETER VECTOR
!                (NUMBER OF UNKNOWNNS)

!      B         ARRAY CONTAINING INITIAL ESTIMATES
!                ON OUTPUT CONTAINING FINAL ESTIMATES

!      F0        VALUE OF FUNCTION AT MINIMUM

!      NSIG      MACHINE ACCURACY AS NEGATIVE POWER      10 OR 5
!                OF TEN

!      MAXFN     MAXIMUM NUMBER OF FUNCTION EVALUATIONS  1000
!                (DOES INCLUDE EVALUATIONS BY SUBROUTINE
!                GRAD WHICH CALCULATES APPROXIMATE GRADIENT)

!      IOUT      OUTPUT CHANNEL FOR ERROR MESSAGES      0
!                (IF 0, THEN MESSAGES NOT WRITTEN)

!      IER       ERROR INDICATOR                        0
!                INTEGER

!-----
```

```
USE as319
IMPLICIT NONE
INTEGER, INTENT(IN)          :: npar
REAL (dp), INTENT(IN OUT)   :: b(:)
REAL (dp), INTENT(IN OUT)   :: f0
INTEGER, INTENT(IN OUT)     :: nsig
INTEGER, INTENT(IN OUT)     :: maxfn
INTEGER, INTENT(IN OUT)     :: iout
INTEGER, INTENT(OUT)        :: ier

INTERFACE
  SUBROUTINE fun(nord, bp, q)
    USE as319
    IMPLICIT NONE
    INTEGER, INTENT(IN)          :: nord
    REAL (dp), INTENT(IN)       :: bp(:)
    REAL (dp), INTENT(OUT)      :: q
  END SUBROUTINE fun
END INTERFACE

REAL (dp) :: gradtl

INTEGER, PARAMETER :: maxf = 1000, msig = 10

!      INITIALIZE

ier=0

IF(nsig == 0) nsig = msig
gradtl = 1.0 / (10.0**(nsig))

IF(gradtl < 0.0) THEN
  IF(iout > 0) WRITE(iout, 300) nsig, gradtl
  300   FORMAT(' NSIG VALUE OF ', i3, ' CREATES NEGATIVE VALUE OF', &
    ' GRADTL, NAMELY, ', g12.5)
  gradtl = 1.0/(10**(msig))
  IF(iout > 0) WRITE(iout, 310) msig, gradtl
  310   FORMAT(' PROGRAM SUBSTITUTES NSIG VALUE OF ', i3, ' WHICH', &
```

```

        ' GIVES GRADTL VALUE OF ', g12.5)
END IF

IF(maxfn == 0) maxfn = maxf

!      NOW WE ARE READY TO CALL THE MINIMIZATION SUBROUTINE

CALL varmet(fun, npar, b, f0, gradtl, maxfn, ier)

IF(ier > 0.AND.iout > 0)THEN
  WRITE(iout, 30) ier
  30  FORMAT('/' SUBROUTINE VARMET ERROR NUMBER ', i3)
  IF(ier == 1) THEN
    WRITE(iout, 40)
  ELSE IF(ier == 2) THEN
    WRITE(iout, 60)
  ELSE IF(ier == 3) THEN
    WRITE(iout, 70)
  ELSE IF(ier == 4) THEN
    WRITE(iout, 80)
  END IF
  40  FORMAT(' FUNCTION UNDEFINED AT INITIAL VALUE          ')
  60  FORMAT(' GRADIENT UNDEFINED IN TOO MANY DIMENSIONS    ')
  70  FORMAT(' FUNCTON NOT MINIMIZED BUT' &
    /' UNABLE TO FIND MINIMUM IN DIRECTION OF SEARCH')
  80  FORMAT(' TOO MANY FUNCTION EVALUATIONS REQUIRED        ')

```

END IF

RETURN

CONTAINS

!-----

```

SUBROUTINE varmet(fun, npar, b, f0, gradtl, maxfn, ifault)

```

! ALGORITHM AS 319 APPL.STATIST. (1997), VOL.46, NO.4

! VARIABLE METRIC FUNCTION MINIMISATION

```

INTEGER, INTENT(IN)           :: npar
REAL (dp), INTENT(IN OUT)    :: b(:)
REAL (dp), INTENT(OUT)       :: f0
REAL (dp), INTENT(OUT)       :: gradtl
INTEGER, INTENT(OUT)         :: maxfn
INTEGER, INTENT(OUT)         :: ifault

```

INTERFACE

```

  SUBROUTINE fun(nord, bp, q)
    USE as319
    IMPLICIT NONE
    INTEGER, INTENT(IN)       :: nord
    REAL (dp), INTENT(IN)    :: bp(:)
    REAL (dp), INTENT(OUT)   :: q
  END SUBROUTINE fun

```

END INTERFACE

```

REAL (dp)           :: d1, s, ck, f1, d2
INTEGER             :: i, ic, icount, ifn, ig, ilast, j, k, np

```

```
INTEGER, PARAMETER      :: icmax=20
REAL (dp), PARAMETER   :: toler=0.00001, w=0.2
REAL (dp)               :: g(npar), h(npar,npar), c(npar), d(npar), t(2*npar)

ig = 0
ifn = 0
ler = .false.
ifault = 0
np = npar + 1

IF (maxfn == 0) maxfn = 1000
IF (gradtl == 0.0) gradtl = 1.0D-10

CALL fun(npar, b, f0)
IF(ler) THEN
  ifault = 1
  RETURN
END IF
ifn = ifn + 1

CALL grad(fun, npar, b, f0, g, t(np:), gradtl, ifault)
IF(ifault > 0) RETURN

ig = ig + 1
ifn = ifn + npar
IF(ifn > maxfn) THEN
  ifault = 4
  RETURN
END IF

10 DO k = 1, npar
  h(k,1:npar) = 0.0
  h(k,k) = 1.00
END DO
ilast = ig

40 DO i = 1, npar
  d(i) = b(i)
  c(i) = g(i)
END DO

d1 = 0.0
DO i = 1, npar
  s = - DOT_PRODUCT( h(i,1:npar), g(1:npar) )
  t(i) = s
  d1 = d1 - s*g(i)
END DO

IF(d1 <= 0.0) THEN
  IF(ilast == ig) THEN
    RETURN
  END IF
  GO TO 10
ELSE
  ck = 1.0
  ic = 0
  90  icount = 0
  DO i = 1,npar
    b(i) = d(i) + ck*t(i)
    IF(b(i) == d(i)) THEN
      icount = icount + 1
    
```

```
END IF
END DO

IF(icount >= npar) THEN
  IF(ilast == ig) THEN
    RETURN
  END IF
  GO TO 10
ELSE
  CALL fun(npar, b, f1)

  ifn = ifn + 1
  IF(ifn > maxfn) THEN
    ifault = 4
    RETURN
  ELSE IF(ler) THEN
    ck = w * ck
    ic = ic+1
    IF(ic > icmax) THEN
      ifault = 3
      RETURN
    END IF
    GO TO 90

  ELSE IF(f1 >= f0 - d1*ck*toler) THEN
    ck = w * ck
    GO TO 90
  ELSE
    f0 = f1
    CALL grad(fun, npar, b, f0, g, t(np:), gradt1, ifault)
    IF(ifault > 0) THEN
      RETURN
    END IF
    ig = ig + 1
    ifn = ifn + npar
    IF(ifn > maxfn) THEN
      ifault = 4
      RETURN
    END IF

    d1 = 0.0
    DO i = 1, npar
      t(i) = ck*t(i)
      c(i) = g(i) - c(i)
      d1 = d1 + t(i)*c(i)
    END DO

    IF(d1 <= 0.0) THEN
      GO TO 10
    END IF

    d2 = 0.0
    DO i = 1, npar
      s = 0.0
      DO j = 1, npar
        s = s + h(i,j)*c(j)
      END DO
      d(i) = s
      d2 = d2 + s*c(i)
    END DO
    d2 = 1.0 + d2/d1
```

```
      DO i = 1, npar
        DO j = 1, npar
          h(i,j) = h(i,j) - (t(i)*d(j) + d(i)*t(j) - d2*t(i)*t(j))/d1
        END DO
      END DO
    END IF
  END IF
END IF
GO TO 40
END SUBROUTINE varmet
```

```
SUBROUTINE grad(f, npar, b, f0, g, sa, er, ifault)
```

```
!      CALCULATE APPROXIMATE GRADIENT
```

```
INTEGER, INTENT(IN)          :: npar
REAL (dp), INTENT(IN OUT)    :: b(:)
REAL (dp), INTENT(IN)        :: f0
REAL (dp), INTENT(OUT)       :: g(:)
REAL (dp), INTENT(OUT)       :: sa(:)
REAL (dp), INTENT(IN)        :: er
INTEGER, INTENT(OUT)         :: ifault
```

```
INTERFACE
```

```
  SUBROUTINE f(nord, bp, q)
    USE as319
    IMPLICIT NONE
    INTEGER, INTENT(IN)          :: nord
    REAL (dp), INTENT(IN)       :: bp(:)
    REAL (dp), INTENT(OUT)      :: q
  END SUBROUTINE f
END INTERFACE
```

```
REAL (dp) :: h, f1
INTEGER   :: i, jc, jcmax
```

```
jcmax=npar - 2
jc = 0
```

```
DO i = 1, npar
  h =(ABS(b(i)) + SQRT(er)) * SQRT(er)
  sa(i) = b(i)
  b(i) = b(i) + h
  CALL f(npar, b, f1)
  b(i) = sa(i)
```

```
  IF(1er) THEN
    f1 = f0 + h
    jc = jc + 1
  END IF
```

```
  g(i) = (f1 - f0)/h
END DO
```

```
IF(jc > jcmax) ifault = 2
RETURN
END SUBROUTINE grad
```

```
END SUBROUTINE varme
```



```

!-----
PROGRAM var
!-----
!       A PROGRAM TO IMPLEMENT A QUASI-NEWTON METHOD.
!       USING NEW ALGORITHM VARMET   JULY 1994
!-----

USE as319
IMPLICIT NONE
INTEGER, PARAMETER :: n=2
INTEGER             :: ier
INTEGER, SAVE      :: gradtl = 12, maxfn = 1000, mess = 6
REAL (dp)          :: x(n), xtmp(n), fp

INTERFACE
  SUBROUTINE fun(nord, bp, q)
    USE as319
    IMPLICIT NONE
    INTEGER, INTENT(IN)           :: nord
    REAL (dp), INTENT(IN)        :: bp(:)
    REAL (dp), INTENT(OUT)       :: q
  END SUBROUTINE fun

  SUBROUTINE varme(fun, npar, b, f0, nsig, maxfn, iout, ier)
    USE as319
    IMPLICIT NONE
    INTEGER, INTENT(IN)           :: npar
    REAL (dp), INTENT(IN OUT)     :: b(:)
    REAL (dp), INTENT(IN OUT)     :: f0
    INTEGER, INTENT(IN OUT)       :: nsig
    INTEGER, INTENT(IN OUT)       :: maxfn
    INTEGER, INTENT(IN OUT)       :: iout
    INTEGER, INTENT(OUT)          :: ier
  INTERFACE
    SUBROUTINE fun(nord, bp, q)
      USE as319
      IMPLICIT NONE
      INTEGER, INTENT(IN)           :: nord
      REAL (dp), INTENT(IN)        :: bp(:)
      REAL (dp), INTENT(OUT)       :: q
    END SUBROUTINE fun
  END INTERFACE
END SUBROUTINE varme
END INTERFACE

WRITE(*,*) ' '
WRITE(*,*) 'INPUT YOUR STARTING GUESS: '
READ(*,*) xtmp(1:n)
WRITE(*,*) ' '
WRITE(*,*) 'INITIALIZATION COMPLETE.'
WRITE(*,*) '*****'

x(1:n)=xtmp(1:n)
ifn = 0
CALL varme(fun, n, x, fp, gradtl, maxfn, mess, ier)

WRITE(*,*) ' '
IF (ier /= 0) WRITE(*, *) '** IER =', ier, ' **'

```

```
WRITE(*,*) ' THE NUMBER OF FUNCTION EVALUATIONS IS ', ifn
WRITE(*,*) ' '
WRITE(*,*) 'THE MINIMUM FOUND IS ', x(1:n)
WRITE(*,*) ' '
CALL fun(n, x, fp)
WRITE(*, *) 'THE FUNCTION VALUE IS: ', fp
STOP
END PROGRAM var
```

!-----

```
SUBROUTINE fun(nord, bp, q)
```

!-----

```
USE as319
```

```
IMPLICIT NONE
```

```
INTEGER, INTENT(IN) :: nord
```

```
REAL (dp), INTENT(IN) :: bp(:)
```

```
REAL (dp), INTENT(OUT) :: q
```

```
q=100.*(bp(2) - bp(1)**2)**2 + (bp(1) - 1.)**2
```

```
ifn = ifn + 1
```

```
ler = .false.
```

```
IF (nord < 1) WRITE(*, *) '*** NORD must be > 0, actual value =', nord
```

```
RETURN
```

```
END SUBROUTINE fun
```

# Pantelis Vlachos



Pantelis Vlachos ([vlachos@stat.cmu.edu](mailto:vlachos@stat.cmu.edu)) is a Research Scientist, in the Department of Statistics, at Carnegie Mellon University. He took over the [StatLib](#) service in June of 1998 from [Mike Meyer](#).

Mike started the StatLib, service in April of 1989. By 1995 StatLib had grown to a collection of about 150 Mbytes and the StatLib server was servicing about 60,000 transactions per month.

The people who really make StatLib a success are those who contribute software, datasets, and other information. Thanks to those who have already contributed, and keep those contributions coming.

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