5

NONLINEAR PROGRAMMING I: ONE-DIMENSIONAL MINIMIZATION METHODS

5.1 INTRODUCTION

In Chapter 2 we saw that if the expressions for the objective function and the constraints are fairly simple in terms of the design variables, the classical methods of optimization can be used to solve the problem. On the other hand, if the optimization problem involves the objective function and/or constraints that are not stated as explicit functions of the design variables or which are too complicated to manipulate, we cannot solve it by using the classical analytical methods. The following example is given to illustrate a case where the constraints cannot be stated as explicit functions of the design variables. Example 5.2 illustrates a case where the objective function is a complicated one for which the classical methods of optimization are difficult to apply.

Example 5.1 Formulate the problem of designing the planar truss shown in Fig. 5.1 for minimum weight subject to the constraint that the displacement of any node, either in the vertical or horizontal direction, should not exceed a value δ.

SOLUTION Let the density ρ and Young's modulus E of the material, the length of the members l, and the external loads Q, R, and S be known as design data. Let the member areas $A_1, A_2, \ldots, A_{11}$ be taken as the design variables $x_1, x_2, \ldots, x_{11}$, respectively. The equations of equilibrium can be derived in terms of the unknown nodal displacements $u_1, u_2, \ldots, u_{10}$ as[†] (the displace-

[†]According to the matrix methods of structural analysis, the equilibrium equations for the jth member are given by [5.1]

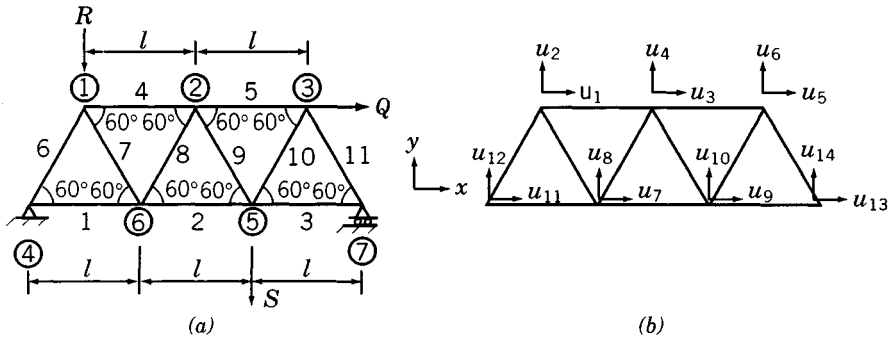


Figure 5.1 Planar truss: (*a*) nodal and member numbers; (*b*) nodal degrees of freedom.

ments u_{11}, u_{12}, u_{13}, and u_{14} are zero, as they correspond to the fixed nodes)

$$(4x_4 + x_6 + x_7)u_1 + \sqrt{3}(x_6 - x_7)u_2 - 4x_4u_3 - x_7u_7 + \sqrt{3}x_7u_8 = 0 \quad (E_1)$$

$$\sqrt{3}(x_6 - x_7)u_1 + 3(x_6 + x_7)u_2 + \sqrt{3}x_7u_7 - 3x_7u_8 = -\frac{4Rl}{E} \quad (E_2)$$

$$-4x_4u_1 + (4x_4 + 4x_5 + x_8 + x_9)u_3 + \sqrt{3}(x_8 - x_9)u_4 - 4x_5u_5 - x_8u_7 - \sqrt{3}x_8u_8 - x_9u_9 + \sqrt{3}x_9u_{10} = 0 \quad (E_3)$$

$$\sqrt{3}(x_8 - x_9)u_3 + 3(x_8 + x_9)u_4 - \sqrt{3}x_8u_7 - 3x_8u_8 + \sqrt{3}x_9u_9 - 3x_9u_{10} = 0 \quad (E_4)$$

$$-4x_5u_3 + (4x_5 + x_{10} + x_{11})u_5 + \sqrt{3}(x_{10} - x_{11})u_6 - x_{10}u_9 - \sqrt{3}x_{10}u_{10} = \frac{4Ql}{E} \quad (E_5)$$

$$\underset{4\times4}{[\mathbf{k}_j]}\ \underset{4\times1}{\mathbf{u}_j} = \underset{4\times1}{\mathbf{P}_j}$$

where the stiffness matrix can be expressed as

$$[\mathbf{k}_j] = \frac{A_jE_j}{l_j}\begin{bmatrix} \cos^2\theta_j & \cos\theta_j\sin\theta_j & -\cos^2\theta_j & -\cos\theta_j\sin\theta_j \\ \cos\theta_j\sin\theta_j & \sin^2\theta_j & -\cos\theta_j\sin\theta_j & -\sin^2\theta_j \\ -\cos^2\theta_j & -\cos\theta_j\sin\theta_j & \cos^2\theta_j & \cos\theta_j\sin\theta_j \\ -\cos\theta_j\sin\theta_j & -\sin^2\theta_j & \cos\theta_j\sin\theta_j & \sin^2\theta_j \end{bmatrix}$$

where θ_j is the inclination of the jth member with respect to the x axis, A_j the cross-sectional area of the jth member, l_j the length of the jth member, $\mathbf{u}_j$ the vector of displacements for the jth member, and $\mathbf{P}_j$ the vector of loads for the jth member. The formulation of the equilibrium equations for the complete truss follows fairly standard procedure [5.1].

$$\sqrt{3}(x_{10} - x_{11})u_5 + 3(x_{10} + x_{11})u_6 - \sqrt{3}x_{10}u_9 - 3x_{10}u_{10} = 0 \qquad (E_6)$$

$$-x_7u_1 + \sqrt{3}x_7u_2 - x_8u_3 - \sqrt{3}x_8u_4 + (4x_1 + 4x_2 + x_7 + x_8)u_7 - \sqrt{3}(x_7 - x_8)u_8 - 4x_2u_9 = 0 \qquad (E_7)$$

$$\sqrt{3}x_7u_1 - 3x_7u_2 - \sqrt{3}x_8u_3 - 3x_8u_4 - \sqrt{3}(x_7 - x_8)u_7 + 3(x_7 + x_8)u_8 = 0 \qquad (E_8)$$

$$-x_9u_3 + \sqrt{3}x_9u_4 - x_{10}u_5 - \sqrt{3}x_{10}u_6 - 4x_2u_7 + (4x_2 + 4x_3 + x_9 + x_{10})u_9 - \sqrt{3}(x_9 - x_{10})u_{10} = 0 \qquad (E_9)$$

$$\sqrt{3}x_9u_3 - 3x_9u_4 - \sqrt{3}x_{10}u_5 - 3x_{10}u_6 - \sqrt{3}(x_9 - x_{10})u_9 + 3(x_9 + x_{10})u_{10} = -\frac{4Sl}{E} \qquad (E_{10})$$

It is important to note that an explicit closed-form solution cannot be obtained for the displacements as the number of equations becomes large. However, given any vector $\mathbf{X}$, the system of Eqs. (E_1) to (E_{10}) can be solved numerically to find the nodal displacement $u_1, u_2, \ldots, u_{10}$.

The optimization problem can be stated as follows:

$$\text{Minimize } f(\mathbf{X}) = \sum_{i=1}^{11} \rho x_i l_i \qquad (E_{11})$$

subject to the constraints

$$g_j(\mathbf{X}) = |u_j(\mathbf{X})| - \delta \leq 0, \quad j = 1,2,\ldots,10 \qquad (E_{12})$$

$$x_i \geq 0, \quad i = 1,2,\ldots,11 \qquad (E_{13})$$

The objective function of this problem is a straightforward function of the design variables as given in Eq. (E_{11}). The constraints, although written by the abstract expressions $g_j(\mathbf{X})$, cannot easily be written as explicit functions of the components of $\mathbf{X}$. However, given any vector $\mathbf{X}$ we can calculate $g_j(\mathbf{X})$ numerically. Many engineering design problems possess this characteristic (i.e., the objective and/or the constraints cannot be written explicitly in terms of the design variables). In such cases we need to use the numerical methods of optimization for solution.

Example 5.2 The shear stress induced along the z-axis when two spheres are in contact with each other is given by

$$\frac{\tau_{zx}}{p_{\max}} = \frac{1}{2}\left[\frac{3}{2\left\{1 + \left(\frac{z}{a}\right)^2\right\}} - (1 + \nu)\left\{1 - \frac{z}{a}\tan^{-1}\left(\frac{1}{\frac{z}{a}}\right)\right\}\right] \qquad (E_1)$$

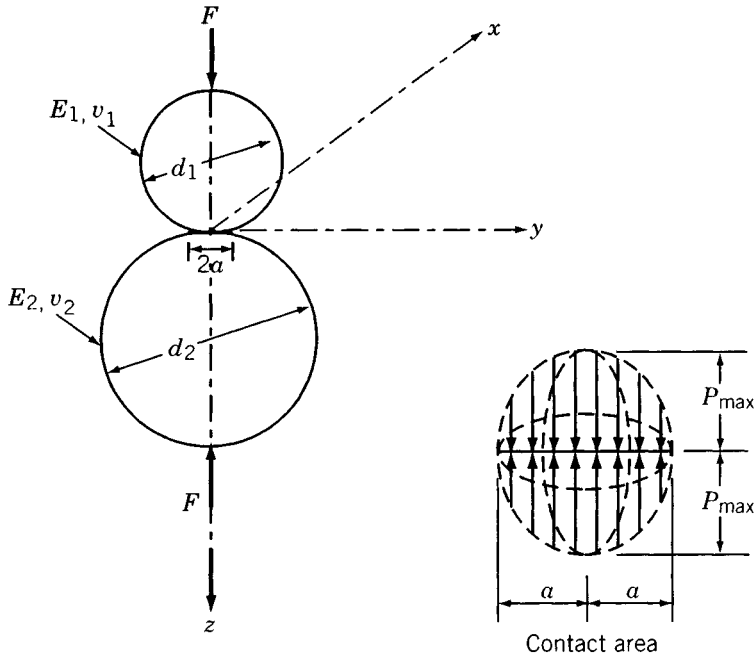


Figure 5.2 Contact stress between two spheres.

where a is the radius of the contact area and p_{max} is the maximum pressure developed at the center of the contact area (Fig. 5.2):

$$a = \left\{ \frac{3F}{8} \frac{\dfrac{1-\nu_1^2}{E_1} + \dfrac{1-\nu_2^2}{E_2}}{\dfrac{1}{d_1} + \dfrac{1}{d_2}} \right\}^{1/3} \tag{E_2}$$

$$p_{max} = \frac{3F}{2\pi a^2} \tag{E_3}$$

where F is the contact force, E_1 and E_2 are Young's moduli of the two spheres, ν_1 and ν_2 are Poisson's ratios of the two spheres, and d_1 and d_2 the diameters of the two spheres. In many practical applications such as ball bearings, when the contact load (F) is large, a crack originates at the point of maximum shear stress and propagates to the surface, leading to a fatigue failure. To locate the origin of a crack, it is necessary to find the point at which the shear stress attains its maximum value. Formulate the problem of finding the location of maximum shear stress for $\nu = \nu_1 = \nu_2 = 0.3$.

SOLUTION For $\nu_1 = \nu_2 = 0.3$, Eq. (E_1) reduces to

$$f(\lambda) = \frac{0.75}{1 + \lambda^2} + 0.65\lambda \tan^{-1}\frac{1}{\lambda} - 0.65 \qquad (E_4)$$

where $f = \tau_{zx}/p_{max}$ and $\lambda = z/a$. Since Eq. (E_4) is a nonlinear function of the distance, λ, the application of the necessary condition for the maximum of f, $df/d\lambda = 0$, gives rise to a nonlinear equation from which a closed-form solution for λ^* cannot easily be obtained.

The basic philosophy of most of the numerical methods of optimization is to produce a sequence of improved approximations to the optimum according to the following scheme.

1. Start with an initial trial point $\mathbf{X}_1$.
2. Find a suitable direction $\mathbf{S}_i$ ($i = 1$ to start with) which points in the general direction of the optimum.
3. Find an appropriate step length λ_i^* for movement along the direction $\mathbf{S}_i$.
4. Obtain the new approximation $\mathbf{X}_{i+1}$ as

$$\mathbf{X}_{i+1} = \mathbf{X}_i + \lambda_i^* \mathbf{S}_i \qquad (5.1)$$

5. Test whether $\mathbf{X}_{i+1}$ is optimum. If $\mathbf{X}_{i+1}$ is optimum, stop the procedure. Otherwise, set a new $i = i + 1$ and repeat step (2) onward.

The iterative procedure indicated by Eq. (5.1) is valid for unconstrained as well as constrained optimization problems. The procedure is represented graphically for a hypothetical two-variable problem in Fig. 5.3. Equation (5.1) indicates that the efficiency of an optimization method depends on the efficiency with which the quantities λ_i^* and $\mathbf{S}_i$ are determined. The methods of finding the step length λ_i^* are considered in this chapter and the methods of finding $\mathbf{S}_i$ are considered in Chapters 6 and 7.

If $f(\mathbf{X})$ is the objective function to be minimized, the problem of determining λ_i^* reduces to finding the value $\lambda_i = \lambda_i^*$ that minimizes $f(\mathbf{X}_{i+1}) = f(\mathbf{X}_i + \lambda_i \mathbf{S}_i) = f(\lambda_i)$ for fixed values of $\mathbf{X}_i$ and $\mathbf{S}_i$. Since f becomes a function of one variable λ_i only, the methods of finding λ_i^* in Eq. (5.1) are called *one-dimensional minimization methods.* Several methods are available for solving a one-dimensional minimization problem. These can be classified as shown in Table 5.1.

We saw in Chapter 2 that the differential calculus method of optimization is an analytical approach and is applicable to continuous, twice-differentiable functions. In this method, calculation of the numerical value of the objective function is virtually the last step of the process. The optimal value of the objective function is calculated after determining the optimal values of the decision variables. In the numerical methods of optimization, an opposite procedure is followed in that the values of the objective function are first found at

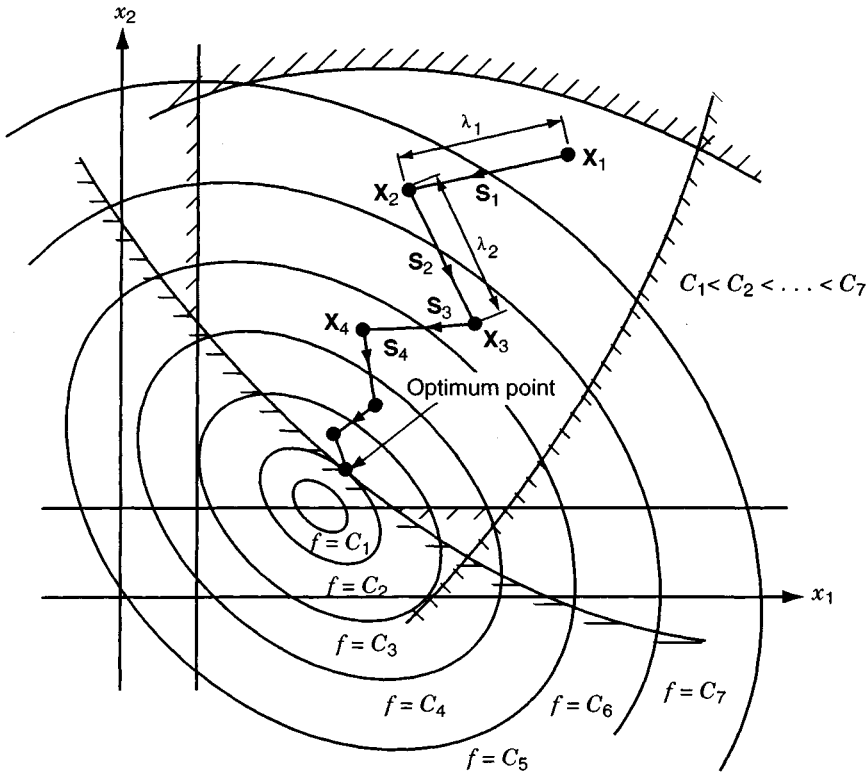


Figure 5.3 Iterative process of optimization.

TABLE 5.1 One-Dimensional Minimization Methods

Analytical methods (differential calculus methods)	Numerical methods		
	Elimination methods	Interpolation methods	
	Unrestricted search	Requiring no derivatives	Requiring derivatives
	Exhaustive search	(quadratic)	Cubic
	Dichotomous search		Direct root
	Fibonacci method		Newton
	Golden section method		Quasi-Newton
			Secant

various combinations of the decision variables and conclusions are then drawn regarding the optimal solution. The elimination methods can be used for the minimization of even discontinuous functions. The quadratic and cubic interpolation methods involve polynomial approximations to the given function. The direct root methods are root finding methods that can be considered to be equivalent to quadratic interpolation.

5.2 UNIMODAL FUNCTION

A *unimodal function* is one that has only one peak (maximum) or valley (minimum) in a given interval. Thus a function of one variable is said to be *unimodal* if, given that two values of the variable are on the same side of the optimum, the one nearer the optimum gives the better functional value (i.e., the smaller value in the case of a minimization problem). This can be stated mathematically as follows:

A function $f(x)$ is unimodal if (*i*) $x_1 < x_2 < x^*$ implies that $f(x_2) < f(x_1)$, and (ii) $x_2 > x_1 > x^*$ implies that $f(x_1) < f(x_2)$, where x^* is the minimum point.

Some examples of unimodal functions are shown in Fig. 5.4. Thus a unimodal function can be a nondifferentiable or even a discontinuous function. If a function is known to be unimodal in a given range, the interval in which the minimum lies can be narrowed down provided that the function values are known at two different points in the range.

For example, consider the normalized interval [0,1] and two function evaluations within the interval as shown in Fig. 5.5. There are three possible outcomes, namely, $f_1 < f_2$, or $f_1 > f_2$, or $f_1 = f_2$. If the outcome is that $f_1 < f_2$, the minimizing x cannot lie to the right of x_2. Thus that part of the interval $[x_2,1]$ can be discarded and a new smaller interval of uncertainty, $[0,x_2]$, results as shown in Fig. 5.5*a*. If $f(x_1) > f(x_2)$, the interval $[0,x_1]$ can be discarded to

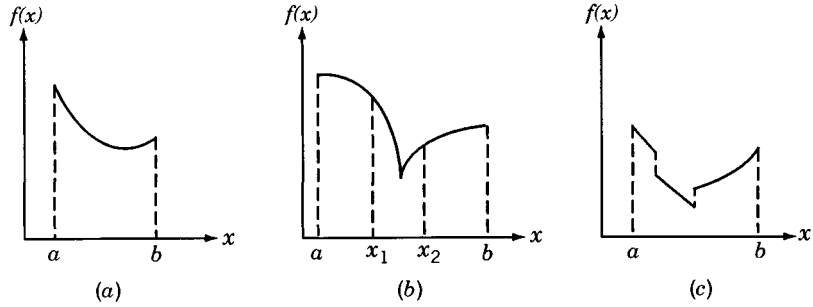


Figure 5.4 Unimodal function.

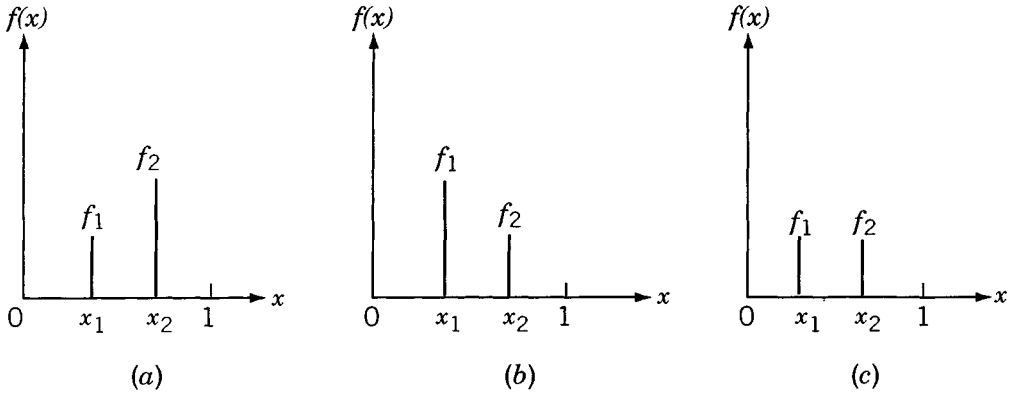


Figure 5.5 Outcome of first two experiments. (*a*) $f_1 < f_2$; (*b*) $f_1 > f_2$; (*c*) $f_1 = f_2$.

obtain a new smaller interval of uncertainty, $[x_1,1]$ (Fig. 5.5*b*), while if $f(x_1) = f(x_2)$, intervals $[0,x_1]$ and $[x_2,1]$ can both be discarded to obtain the new interval of uncertainty as $[x_1,x_2]$ (Fig. 5.5*c*). Further, if one of the original experiments[†] remains within the new interval, as will be the situation in Fig. 5.5*a* and *b*, only one other experiment need be placed within the new interval in order that the process be repeated. In situations such as Fig. 5.5*c*, two more experiments are to be placed in the new interval in order to find a reduced interval of uncertainty.

The assumption of unimodality is made in all the elimination techniques. If a function is known to be *multimodal* (i.e., having several valleys or peaks), the range of the function can be subdivided into several parts and the function treated as a unimodal function in each part.

ELIMINATION METHODS

5.3 UNRESTRICTED SEARCH

In most practical problems, the optimum solution is known to lie within restricted ranges of the design variables. In some cases this range is not known, and hence the search has to be made with no restrictions on the values of the variables.

5.3.1 Search with Fixed Step Size

The most elementary approach for such a problem is to use a fixed step size and move from an initial guess point in a favorable direction (positive or negative). The step size used must be small in relation to the final accuracy de-

[†]Each function evaluation is termed as an experiment or a trial in the elimination methods.

sired. Although this method is very simple to implement, it is not efficient in many cases. This method is described in the following steps.

1. Start with an initial guess point, say, x_1.
2. Find $f_1 = f(x_1)$.
3. Assuming a step size s, find $x_2 = x_1 + s$.
4. Find $f_2 = f(x_2)$.
5. If $f_2 < f_1$, and if the problem is one of minimization, the assumption of unimodality indicates that the desired minimum cannot lie at $x < x_1$. Hence the search can be continued further along points $x_3, x_4, \ldots$ using the unimodality assumption while testing each pair of experiments. This procedure is continued until a point, $x_i = x_1 + (i - 1)s$, shows an increase in the function value.
6. The search is terminated at x_i, and either x_{i-1} or x_i can be taken as the optimum point.
7. Originally, if $f_2 > f_1$, the search should be carried in the reverse direction at points $x_{-2}, x_{-3}, \ldots$, where $x_{-j} = x_1 - (j - 1)s$.
8. If $f_2 = f_1$, the desired minimum lies in between x_1 and x_2, and the minimum point can be taken as either x_1 or x_2.
9. If it happens that both f_2 and f_{-2} are greater than f_1, it implies that the desired minimum will lie in the double interval $x_{-2} < x < x_2$.

5.3.2 Search with Accelerated Step Size

Although the search with a fixed step size appears to be very simple, its major limitation comes because of the unrestricted nature of the region in which the minimum can lie. For example, if the minimum point for a particular function happens to be $x_{opt} = 50{,}000$ and, in the absence of knowledge about the location of the minimum, if x_1 and s are chosen as 0.0 and 0.1, respectively, we have to evaluate the function 5,000,001 times to find the minimum point. This involves a large amount of computational work. An obvious improvement can be achieved by increasing the step size gradually until the minimum point is bracketed. A simple method consists of doubling the step size as long as the move results in an improvement of the objective function. Several other improvements of this method can be developed. One possibility is to reduce the step length after bracketing the optimum in (x_{i-1}, x_i). By starting either from x_{i-1} or x_i, the basic procedure can be applied with a reduced step size. This procedure can be repeated until the bracketed interval becomes sufficiently small. The following example illustrates the search method with accelerated step size.

Example 5.3 Find the minimum of $f = x(x - 1.5)$ by starting from 0.0 with an initial step size of 0.05.

SOLUTION The function value at x_1 is $f_1 = 0.0$. If we try to start moving in the negative x direction, we find that $x_{-2} = -0.05$ and $f_{-2} = 0.0775$. Since $f_{-2} > f_1$, the assumption of unimodality indicates that the minimum cannot lie toward the left of x_{-2}. Thus we start moving in the positive x direction and obtain the following results:

i	Value of s	$x_i = x_1 + s$	$f_i = f(x_i)$	Is $f_i > f_{i-1}$?
1	—	0.0	0.0	—
2	0.05	0.05	−0.0725	No
3	0.10	0.10	−0.140	No
4	0.20	0.20	−0.260	No
5	0.40	0.40	−0.440	No
6	0.80	0.80	−0.560	No
7	1.60	1.60	+0.160	Yes

From these results, the optimum point can be seen to be $x_{\text{opt}} \approx x_6 = 0.8$. In this case, the points x_6 and x_7 do not really bracket the minimum point but provide information about it. If a better approximation to the minimum is desired, the procedure can be restarted from x_5 with a smaller step size.

5.4 EXHAUSTIVE SEARCH

The exhaustive search method can be used to solve problems where the interval in which the optimum is known to lie is finite. Let x_s and x_f denote, respectively, the starting and final points of the interval of uncertainty.[†] The *exhaustive search method* consists of evaluating the objective function at a predetermined number of equally spaced points in the interval (x_s,x_f), and reducing the interval of uncertainty using the assumption of unimodality. Suppose that a function is defined on the interval (x_s,x_f) and let it be evaluated at eight equally spaced interior points x_1 to x_8. Assuming that the function values appear as shown in Fig. 5.6, the minimum point must lie, according to the assumption of unimodality, between points x_5 and x_7. Thus the interval (x_5,x_7) can be considered as the final interval of uncertainty.

In general, if the function is evaluated at n equally spaced points in the original interval of uncertainty of length $L_0 = x_f - x_s$, and if the optimum value of the function (among the n function values) turns out to be at point x_j, the final interval of uncertainty is given by

$$L_n = x_{j+1} - x_{j-1} = \frac{2}{n+1} L_0 \tag{5.2}$$

[†]Since the interval (x_s,x_f), but not the exact location of the optimum in this interval, is known to us, the interval (x_s,x_f) is called the *interval of uncertainty*.

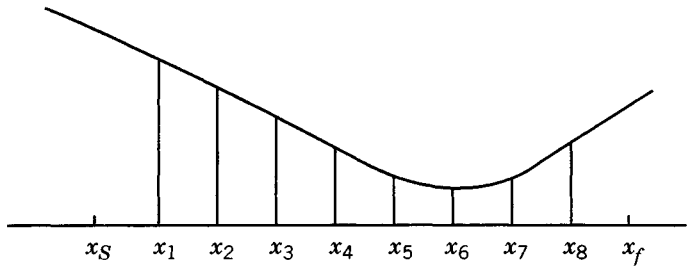


Figure 5.6 Exhaustive search.

The final interval of uncertainty obtainable for different number of trials in the exhaustive search method is given below.

Number of trials	2	3	4	5	6	· · ·	n
L_n/L_0	2/3	2/4	2/5	2/6	2/7	· · ·	$2/(n+1)$

Since the function is evaluated at all n points simultaneously, this method can be called a *simultaneous search method.* This method is relatively inefficient compared to the sequential search methods discussed next, where the information gained from the initial trials is used in placing the subsequent experiments.

Example 5.4 Find the minimum of $f = x(x - 1.5)$ in the interval (0.0,1.00) to within 10% of the exact value.

SOLUTION If the middle point of the final interval of uncertainty is taken as the approximate optimum point, the maximum deviation could be $1/(n + 1)$ times the initial interval of uncertainty. Thus, to find the optimum within 10% of the exact value, we should have

$$\frac{1}{n+1} \leq \frac{1}{10} \quad \text{or} \quad n \geq 9$$

By taking $n = 9$, the following function values can be calculated.

i	1	2	3	4	5	6	7	8	9
x_i	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$f_i = f(x_i)$	−0.14	−0.26	−0.36	−0.44	−0.50	−0.54	−0.56	−0.56	−0.54

Since $x_7 = x_8$, the assumption of unimodality gives the final interval of uncertainty as $L_9 = (0.7,0.8)$. By taking the middle point of L_9 (i.e., 0.75) as

an approximation to the optimum point, we find that it is, in fact, the true optimum point.

5.5 DICHOTOMOUS SEARCH

The exhaustive search method is a simultaneous search method in which all the experiments are conducted before any judgment is made regarding the location of the optimum point. The *dichotomous search method*, as well as the Fibonacci and the golden section methods discussed in subsequent sections, are sequential search methods in which the result of any experiment influences the location of the subsequent experiment.

In the dichotomous search, two experiments are placed as close as possible at the center of the interval of uncertainty. Based on the relative values of the objective function at the two points, almost half of the interval of uncertainty is eliminated. Let the positions of the two experiments be given by (Fig. 5.7)

$$x_1 = \frac{L_0}{2} - \frac{\delta}{2}$$

$$x_2 = \frac{L_0}{2} + \frac{\delta}{2}$$

where δ is a small positive number chosen so that the two experiments give significantly different results. Then the new interval of uncertainty is given by $(L_0/2 + \delta/2)$. The building block of dichotomous search consists of conducting a pair of experiments at the center of the current interval of uncertainty. The next pair of experiments is, therefore, conducted at the center of the remaining interval of uncertainty. This results in the reduction of the interval of uncertainty by nearly a factor of 2. The intervals of uncertainty at the end of different pairs of experiments are given in the following table.

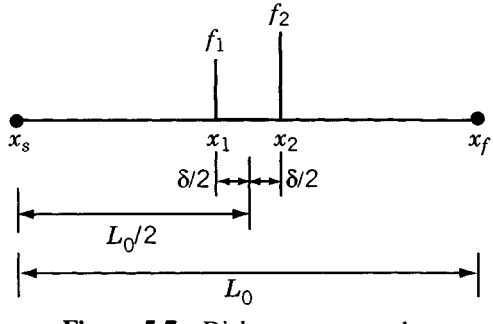


Figure 5.7 Dichotomous search.

Number of experiments	2	4	6
Final interval of uncertainty	$\frac{1}{2}(L_0 + \delta)$	$\frac{1}{2}\left(\frac{L_0 + \delta}{2}\right) + \frac{\delta}{2}$	$\frac{1}{2}\left(\frac{L_0 + \delta}{4} + \frac{\delta}{2}\right) + \frac{\delta}{2}$

In general, the final interval of uncertainty after conducting n experiments (n even) is given by

$$L_n = \frac{L_0}{2^{n/2}} + \delta\left(1 - \frac{1}{2^{n/2}}\right) \tag{5.3}$$

The following example is given to illustrate the method of search.

Example 5.5 Find the minimum of $f = x(x - 1.5)$ in the interval (0.0,1.00) to within 10% of the exact value.

SOLUTION The ratio of final to initial intervals of uncertainty is given by [from Eq. (5.3)]

$$\frac{L_n}{L_0} = \frac{1}{2^{n/2}} + \frac{\delta}{L_0}\left(1 - \frac{1}{2^{n/2}}\right)$$

where δ is a small quantity, say 0.001, and n is the number of experiments. If the middle point of the final interval is taken as the optimum point, the requirement can be stated as

$$\frac{1}{2}\frac{L_n}{L_0} \leq \frac{1}{10}$$

i.e.,

$$\frac{1}{2^{n/2}} + \frac{\delta}{L_0}\left(1 - \frac{1}{2^{n/2}}\right) \leq \frac{1}{5}$$

Since $\delta = 0.001$ and $L_0 = 1.0$, we have

$$\frac{1}{2^{n/2}} + \frac{1}{1000}\left(1 - \frac{1}{2^{n/2}}\right) \leq \frac{1}{5}$$

i.e.,

$$\frac{999}{1000}\frac{1}{2^{n/2}} \leq \frac{995}{5000} \quad \text{or} \quad 2^{n/2} \geq \frac{999}{199} \simeq 5.0$$

Since n has to be even, this inequality gives the minimum admissible value of n as 6.

The search is made as follows: The first two experiments are made at

$$x_1 = \frac{L_0}{2} - \frac{\delta}{2} = 0.5 - 0.0005 = 0.4995$$

$$x_2 = \frac{L_0}{2} + \frac{\delta}{2} = 0.5 + 0.0005 = 0.5005$$

with the function values given by

$$f_1 = f(x_1) = 0.4995(-1.0005) \simeq -0.49975$$

$$f_2 = f(x_2) = 0.5005(-0.9995) \simeq -0.50025$$

Since $f_2 < f_1$, the new interval of uncertainty will be (0.4995,1.0). The second pair of experiments is conducted at

$$x_3 = \left(0.4995 + \frac{1.0 - 0.4995}{2}\right) - 0.0005 = 0.74925$$

$$x_4 = \left(0.4995 + \frac{1.0 - 0.4995}{2}\right) + 0.0005 = 0.75025$$

which give the function values as

$$f_3 = f(x_3) = 0.74925(-0.75075) = -0.5624994375$$

$$f_4 = f(x_4) = 0.75025(-0.74975) = -0.5624999375$$

Since $f_3 > f_4$, we delete $(0.4995,x_3)$ and obtain the new interval of uncertainty as

$$(x_3,1.0) = (0.74925,1.0)$$

The final set of experiments will be conducted at

$$x_5 = \left(0.74925 + \frac{1.0 - 0.74925}{2}\right) - 0.0005 = 0.874125$$

$$x_6 = \left(0.74925 + \frac{1.0 - 0.74925}{2}\right) + 0.0005 = 0.875125$$

The corresponding function values are

$$f_5 = f(x_5) = 0.874125(-0.625875) = -0.5470929844$$

$$f_6 = f(x_6) = 0.875125(-0.624875) = -0.5468437342$$

Since $f_5 < f_6$, the new interval of uncertainty is given by $(x_3,x_6) = (0.74925,0.875125)$. The middle point of this interval can be taken as optimum, and hence

$$x_{\text{opt}} \simeq 0.8121875 \quad \text{and} \quad f_{\text{opt}} \simeq -0.5586327148$$

5.6 INTERVAL HALVING METHOD

In the *interval halving method*, exactly one-half of the current interval of uncertainty is deleted in every stage. It requires three experiments in the first stage and two experiments in each subsequent stage. The procedure can be described by the following steps:

1. Divide the initial interval of uncertainty $L_0 = [a,b]$ into four equal parts and label the middle point x_0 and the quarter-interval points x_1 and x_2.
2. Evaluate the function $f(x)$ at the three interior points to obtain $f_1 = f(x_1)$, $f_0 = f(x_0)$, and $f_2 = f(x_2)$.
3. (a) If $f_2 > f_0 > f_1$ as shown in Fig. 5.8*a*, delete the interval (x_0,b), label x_1 and x_0 as the new x_0 and b, respectively, and go to step 4.
   (b) If $f_2 < f_0 < f_1$ as shown in Fig. 5.8*b*, delete the interval (a,x_0), label x_2 and x_0 as the new x_0 and a, respectively, and go to step 4.
   (c) If $f_1 > f_0$ and $f_2 > f_0$ as shown in Fig. 5.8*c*, delete both the intervals (a,x_1) and (x_2,b), label x_1 and x_2 as the new a and b, respectively, and go to step 4.
4. Test whether the new interval of uncertainty, $L = b - a$, satisfies the convergence criterion $L \leq \epsilon$, where ϵ is a small quantity. If the convergence criterion is satisfied, stop the procedure. Otherwise, set the new $L_0 = L$ and go to step 1.

Remarks:

1. In this method, the function value at the middle point of the interval of uncertainty, f_0, will be available in all the stages except the first stage.
2. The interval of uncertainty remaining at the end of n experiments ($n \geq 3$ and odd) is given by

$$L_n = \left(\frac{1}{2}\right)^{(n-1)/2} L_0 \tag{5.4}$$

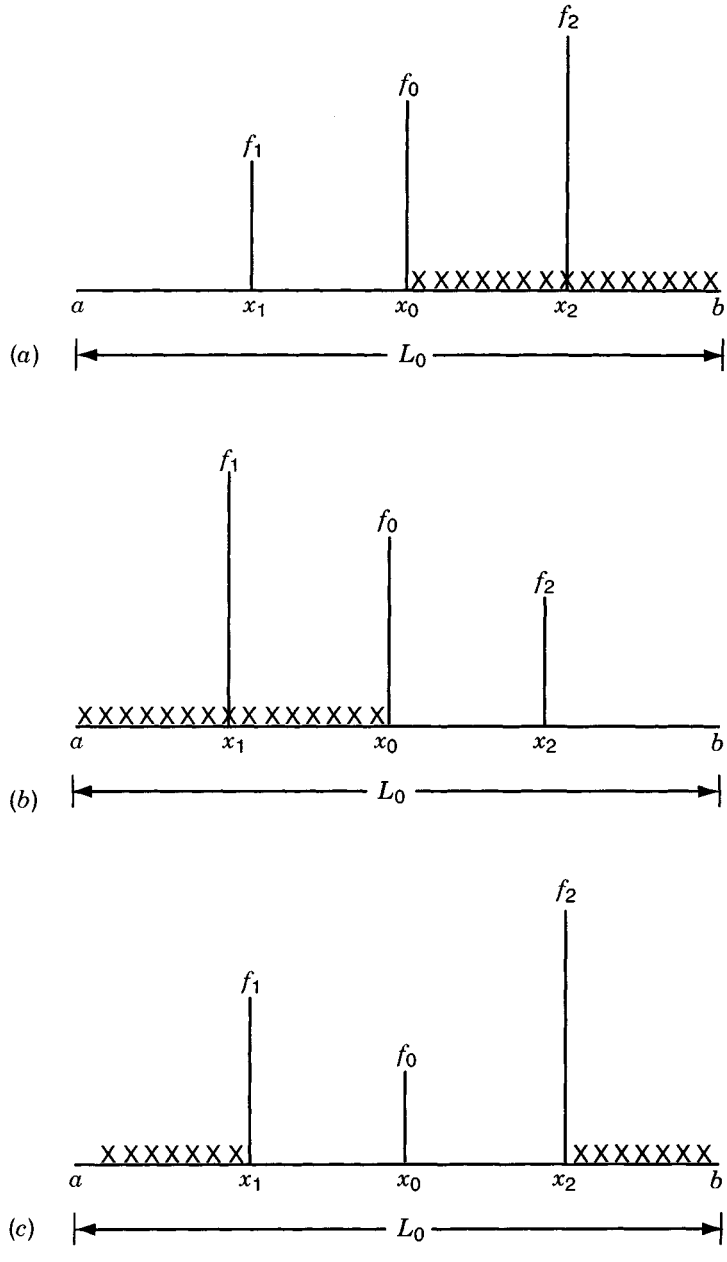


Figure 5.8 Possibilities in the interval halving method: (*a*) $f_2 > f_0 > f_1$; (*b*) $f_1 > f_0 > f_2$; (*c*) $f_1 > f_0$ and $f_2 > f_0$.

Example 5.6 Find the minimum of $f = x(x - 1.5)$ in the interval (0.0,1.0) to within 10% of the exact value.

SOLUTION If the middle point of the final interval of uncertainty is taken as the optimum point, the specified accuracy can be achieved if

$$\frac{1}{2}L_n \le \frac{L_0}{10} \quad \text{or} \quad \left(\frac{1}{2}\right)^{(n-1)/2} L_0 \le \frac{L_0}{5} \tag{E$_1$}$$

Since $L_0 = 1$, Eq. (E$_1$) gives

$$\frac{1}{2^{(n-1)/2}} \le \frac{1}{5} \quad \text{or} \quad 2^{(n-1)/2} \ge 5 \tag{E$_2$}$$

Since n has to be odd, inequality (E$_2$) gives the minimum permissible value of n as 7. With this value of $n = 7$, the search is conducted as follows. The first three experiments are placed at one-fourth points of the interval $L_0 = [a = 0, b = 1]$ as

$$x_1 = 0.25, \quad f_1 = 0.25(-1.25) = -0.3125$$
$$x_0 = 0.50, \quad f_0 = 0.50(-1.00) = -0.5000$$
$$x_2 = 0.75, \quad f_2 = 0.75(-0.75) = -0.5625$$

Since $f_1 > f_0 > f_2$, we delete the interval $(a,x_0) = (0.0,0.5)$, label x_2 and x_0 as the new x_0 and a so that $a = 0.5$, $x_0 = 0.75$, and $b = 1.0$. By dividing the new interval of uncertainty, $L_3 = (0.5,1.0)$ into four equal parts, we obtain

$$x_1 = 0.625, \quad f_1 = 0.625(-0.875) = -0.546875$$
$$x_0 = 0.750, \quad f_0 = 0.750(-0.750) = -0.562500$$
$$x_2 = 0.875, \quad f_2 = 0.875(-0.625) = -0.546875$$

Since $f_1 > f_0$ and $f_2 > f_0$, we delete both the intervals (a,x_1) and (x_2,b), and label x_1, x_0, and x_2 as the new a, x_0, and b, respectively. Thus the new interval of uncertainty will be $L_5 = (0.625,0.875)$. Next, this interval is divided into four equal parts to obtain

$$x_1 = 0.6875, \quad f_1 = 0.6875(-0.8125) = -0.558594$$
$$x_0 = 0.75, \quad f_0 = 0.75(-0.75) = -0.5625$$
$$x_2 = 0.8125, \quad f_2 = 0.8125(-0.6875) = -0.558594$$

Again we note that $f_1 > f_0$ and $f_2 > f_0$ and hence we delete both the intervals (a,x_1) and (x_2,b) to obtain the new interval of uncertainty as $L_7 = (0.6875,0.8125)$. By taking the middle point of this interval (L_7) as optimum, we obtain

$$x_{\text{opt}} \approx 0.75 \quad \text{and} \quad f_{\text{opt}} \approx -0.5625$$

(This solution happens to be the exact solution in this case.)

5.7 FIBONACCI METHOD

As stated earlier, the *Fibonacci method* can be used to find the minimum of a function of one variable even if the function is not continuous. This method, like many other elimination methods, has the following limitations:

1. The initial interval of uncertainty, in which the optimum lies, has to be known.
2. The function being optimized has to be unimodal in the initial interval of uncertainty.
3. The exact optimum cannot be located in this method. Only an interval known as the *final interval of uncertainty* will be known. The final interval of uncertainty can be made as small as desired by using more computations.
4. The number of function evaluations to be used in the search or the resolution required has to be specified beforehand.

This method makes use of the sequence of Fibonacci numbers, $\{F_n\}$, for placing the experiments. These numbers are defined as

$$F_0 = F_1 = 1$$

$$F_n = F_{n-1} + F_{n-2}, \qquad n = 2,3,4,\ldots$$

which yield the sequence 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, ...

Procedure. Let L_0 be the initial interval of uncertainty defined by $a \le x \le b$ and n be the total number of experiments to be conducted. Define

$$L_2^* = \frac{F_{n-2}}{F_n} L_0 \tag{5.5}$$

and place the first two experiments at points x_1 and x_2, which are located at a

distance of L_2^* from each end of L_0.[†] This gives[‡]

$$x_1 = a + L_2^* = a + \frac{F_{n-2}}{F_n} L_0$$
$$x_2 = b - L_2^* = b - \frac{F_{n-2}}{F_n} L_0 = a + \frac{F_{n-1}}{F_n} L_0 \tag{5.6}$$

Discard part of the interval by using the unimodality assumption. Then there remains a smaller interval of uncertainty L_2 given by[§]

$$L_2 = L_0 - L_2^* = L_0\left(1 - \frac{F_{n-2}}{F_n}\right) = \frac{F_{n-1}}{F_n} L_0 \tag{5.7}$$

and with one experiment left in it. This experiment will be at a distance of

$$L_2^* = \frac{F_{n-2}}{F_n} L_0 = \frac{F_{n-2}}{F_{n-1}} L_2 \tag{5.8}$$

from one end and

$$L_2 - L_2^* = \frac{F_{n-3}}{F_n} L_0 = \frac{F_{n-3}}{F_{n-1}} L_2 \tag{5.9}$$

from the other end. Now place the third experiment in the interval L_2 so that the current two experiments are located at a distance of

$$L_3^* = \frac{F_{n-3}}{F_n} L_0 = \frac{F_{n-3}}{F_{n-1}} L_2 \tag{5.10}$$

from each end of the interval L_2. Again the unimodality property will allow us to reduce the interval of uncertainty to L_3 given by

$$L_3 = L_2 - L_3^* = L_2 - \frac{F_{n-3}}{F_{n-1}} L_2 = \frac{F_{n-2}}{F_{n-1}} L_2 = \frac{F_{n-2}}{F_n} L_0 \tag{5.11}$$

[†]If an experiment is located at a distance of $(F_{n-2}/F_n)L_0$ from one end, it will be at a distance of $(F_{n-1}/F_n)L_0$ from the other end. Thus $L_2^* = (F_{n-1}/F_n)L_0$ will yield the same result as with $L_2^* = (F_{n-2}/F_n)L_0$.

[‡]It can be seen that

$$L_2^* = \frac{F_{n-2}}{F_n} L_0 \leq \frac{1}{2} L_0 \quad \text{for} \quad n \geq 2$$

[§]The symbol L_j is used to denote the interval of uncertainty remaining after conducting j experiments, while the symbol L_j^* is used to define the position of the jth experiment.

This process of discarding a certain interval and placing a new experiment in the remaining interval can be continued, so that the location of the jth experiment and the interval of uncertainty at the end of j experiments are, respectively, given by

$$L_j^* = \frac{F_{n-j}}{F_{n-(j-2)}} L_{j-1} \tag{5.12}$$

$$L_j = \frac{F_{n-(j-1)}}{F_n} L_0 \tag{5.13}$$

The ratio of the interval of uncertainty remaining after conducting j of the n predetermined experiments to the initial interval of uncertainty becomes

$$\frac{L_j}{L_0} = \frac{F_{n-(j-1)}}{F_n} \tag{5.14}$$

and for $j = n$, we obtain

$$\frac{L_n}{L_0} = \frac{F_1}{F_n} = \frac{1}{F_n} \tag{5.15}$$

The ratio L_n/L_0 will permit us to determine n, the required number of experiments, to achieve any desired accuracy in locating the optimum point. Table 5.2 gives the reduction ratio in the interval of uncertainty obtainable for different number of experiments.

Position of the Final Experiment. In this method the last experiment has to be placed with some care. Equation (5.12) gives

$$\frac{L_n^*}{L_{n-1}} = \frac{F_0}{F_2} = \frac{1}{2} \quad \text{for all } n \tag{5.16}$$

Thus, after conducting $n - 1$ experiments and discarding the appropriate interval in each step, the remaining interval will contain one experiment precisely at its middle point. However the final experiment, namely, the nth experiment, is also to be placed at the center of the present interval of uncertainty. That is, the position of the nth experiment will be same as that of $(n - 1)$th one, and this is true for whatever value we choose for n. Since no new information can be gained by placing the nth experiment exactly at the same location as that of the $(n - 1)$th experiment, we place the nth experiment very close to the remaining valid experiment, as in the case of the dichotomous search method. This enables us to obtain the final interval of uncertainty to within $\frac{1}{2}L_{n-1}$. A flowchart for implementing the Fibonacci method of minimization is given in Fig. 5.9.

TABLE 5.2 Reduction Ratios

Value of n	Fibonacci Number, F_n	Reduction Ratio, L_n/L_0
0	1	1.0
1	1	1.0
2	2	0.5
3	3	0.3333
4	5	0.2
5	8	0.1250
6	13	0.07692
7	21	0.04762
8	34	0.02941
9	55	0.01818
10	89	0.01124
11	144	0.006944
12	233	0.004292
13	377	0.002653
14	610	0.001639
15	987	0.001013
16	1,597	0.0006406
17	2,584	0.0003870
18	4,181	0.0002392
19	6,765	0.0001479
20	10,946	0.00009135

Example 5.7 Minimize $f(x) = 0.65 - [0.75/(1 + x^2)] - 0.65x \tan^{-1}(1/x)$ in the interval [0,3] by the Fibonacci method using $n = 6$. (Note that this objective is equivalent to the one stated in Example 5.2.)

SOLUTION Here $n = 6$ and $L_0 = 3.0$, which yield

$$L_2^* = \frac{F_{n-2}}{F_n} L_0 = \frac{5}{13} (3.0) = 1.153846$$

Thus the positions of the first two experiments are given by $x_1 = 1.153846$ and $x_2 = 3.0 - 1.153846 = 1.846154$ with $f_1 = f(x_1) = -0.207270$ and $f_2 = f(x_2) = -0.115843$. Since f_1 is less than f_2, we can delete the interval $[x_2,3.0]$ by using the unimodality assumption (Fig. 5.10*a*). The third experiment is placed at $x_3 = 0 + (x_2 - x_1) = 1.846154 - 1.153846 = 0.692308$, with the corresponding function value of $f_3 = -0.291364$.

Since $f_1 > f_3$, we delete the interval $[x_1,x_2]$ (Fig. 5.10*b*). The next experiment is located at $x_4 = 0 + (x_1 - x_3) = 1.153846 - 0.692308 = 0.461538$ with $f_4 = -0.309811$. Noting that $f_4 < f_3$, we delete the interval $[x_3,x_1]$ (Fig.

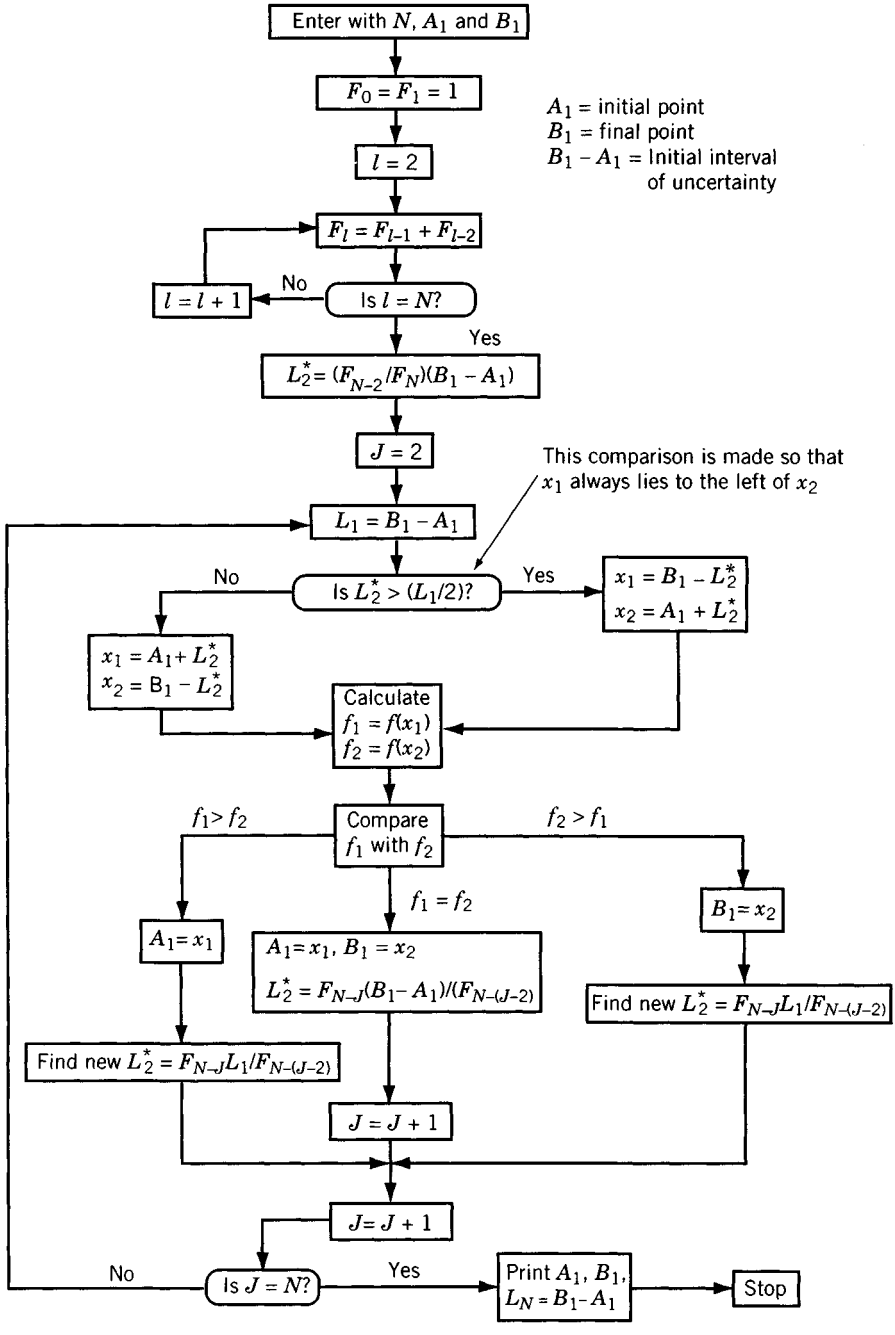


Figure 5.9 Flowchart for implementing Fibonacci search method.

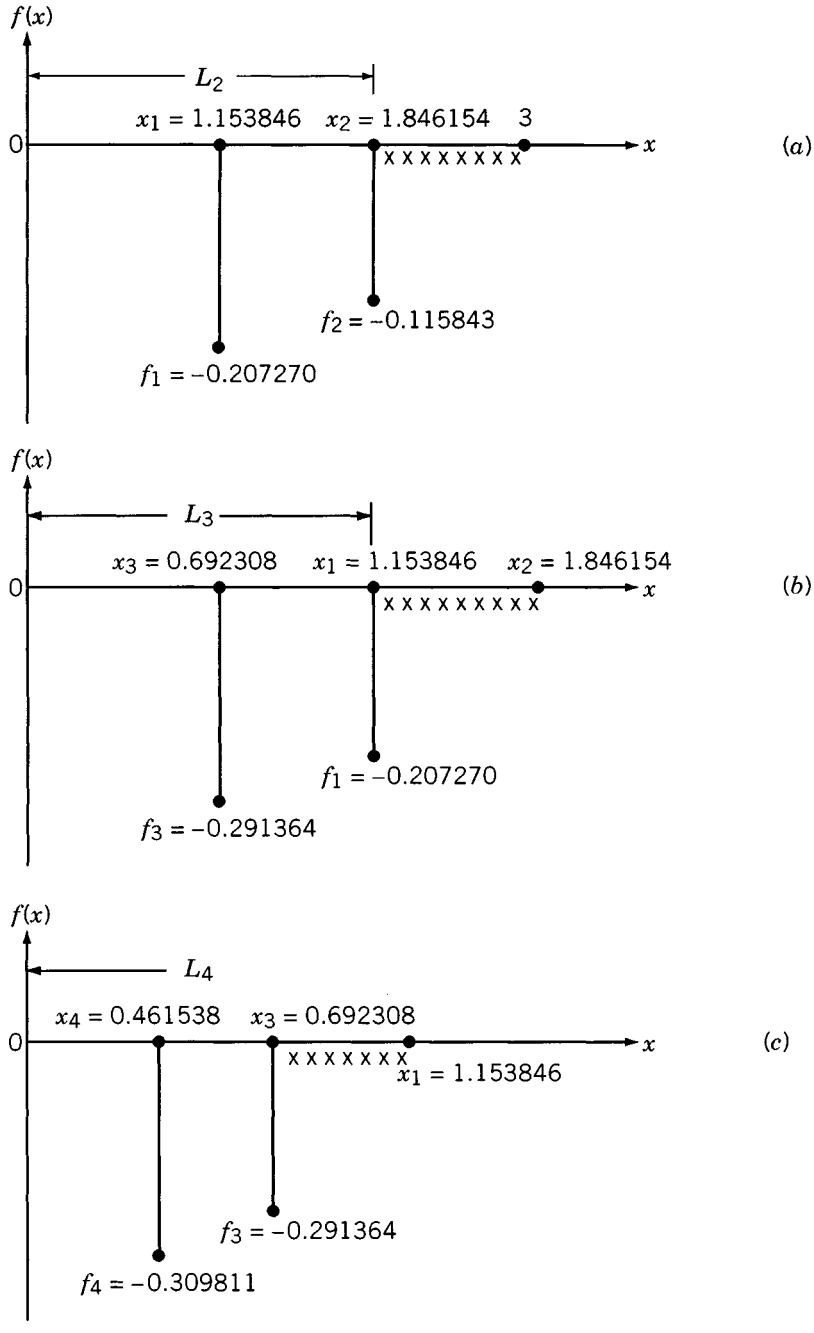
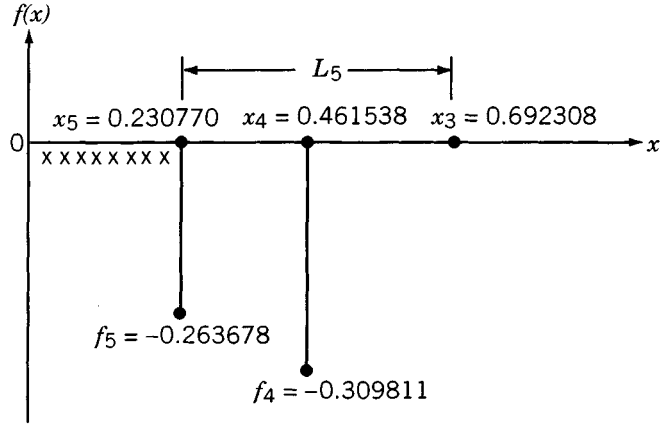
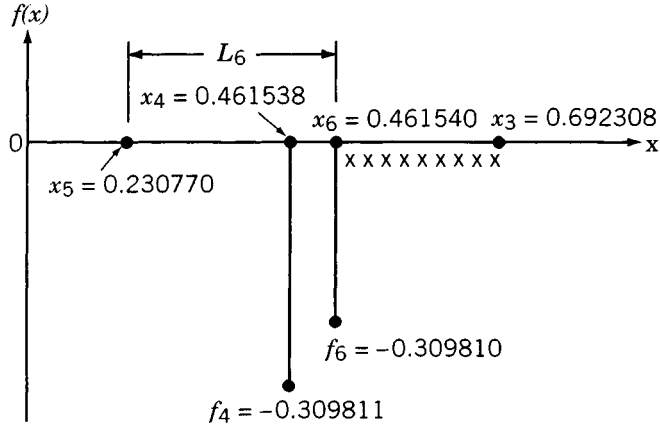


Figure 5.10 Graphical representation of the solution of Example 5.7.



(d)



(e)

Figure 5.10 (*Continued*)

5.10*c*). The location of the next experiment can be obtained as $x_5 = 0 + (x_3 - x_4) = 0.692308 - 0.461538 = 0.230770$ with the corresponding objective function value of $f_5 = -0.263678$. Since $f_5 > f_4$, we delete the interval $[0,x_5]$ (Fig. 5.10*d*). The final experiment is positioned at $x_6 = x_5 + (x_3 - x_4) = 0.230770 + (0.692308 - 0.461538) = 0.461540$ with $f_6 = -0.309810$. (Note that, theoretically, the value of x_6 should be same as that of x_4; however, it is slightly different from x_4, due to round-off error).

Since $f_6 > f_4$, we delete the interval $[x_6,x_3]$ and obtain the final interval of uncertainty as $L_6 = [x_5,x_6] = [0.230770,0.461540]$ (Fig. 5.10*e*). The ratio of the final to the initial interval of uncertainty is

$$\frac{L_6}{L_0} = \frac{0.461540 - 0.230770}{3.0} = 0.076923$$

This value can be compared with Eq. (5.15), which states that if n experiments ($n = 6$) are planned, a resolution no finer than $1/F_n = 1/F_6 = \frac{1}{13} = 0.076923$ can be expected from the method.

5.8 GOLDEN SECTION METHOD

The *golden section method* is same as the Fibonacci method except that in the Fibonacci method the total number of experiments to be conducted has to be specified before beginning the calculation, whereas this is not required in the golden section method. In the Fibonacci method, the location of the first two experiments is determined by the total number of experiments, n. In the golden section method we start with the assumption that we are going to conduct a large number of experiments. Of course, the total number of experiments can be decided during the computation.

The intervals of uncertainty remaining at the end of different number of experiments can be computed as follows:

$$L_2 = \lim_{N \to \infty} \frac{F_{N-1}}{F_N} L_0 \tag{5.17}$$

$$L_3 = \lim_{N \to \infty} \frac{F_{N-2}}{F_N} L_0 = \lim_{N \to \infty} \frac{F_{N-2}}{F_{N-1}} \frac{F_{N-1}}{F_N} L_0$$

$$\simeq \lim_{N \to \infty} \left(\frac{F_{N-1}}{F_N} \right)^2 L_0 \tag{5.18}$$

This result can be generalized to obtain

$$L_k = \lim_{N \to \infty} \left(\frac{F_{N-1}}{F_N} \right)^{k-1} L_0 \tag{5.19}$$

Using the relation

$$F_N = F_{N-1} + F_{N-2} \tag{5.20}$$

we obtain, after dividing both sides by F_{N-1},

$$\frac{F_N}{F_{N-1}} = 1 + \frac{F_{N-2}}{F_{N-1}} \tag{5.21}$$

By defining a ratio γ as

$$\gamma = \lim_{N \to \infty} \frac{F_N}{F_{N-1}} \tag{5.22}$$

Eq. (5.21) can be expressed as

$$\gamma \simeq \frac{1}{\gamma} + 1$$

that is,

$$\gamma^2 - \gamma - 1 = 0 \tag{5.23}$$

This gives the root $\gamma = 1.618$, and hence Eq. (5.19) yields

$$L_k = \left(\frac{1}{\gamma}\right)^{k-1} L_0 = (0.618)^{k-1} L_0 \tag{5.24}$$

In Eq. (5.18) the ratios F_{N-2}/F_{N-1} and F_{N-1}/F_N have been taken to be same for large values of N. The validity of this assumption can be seen from the following table:

Value of N	2	3	4	5	6	7	8	9	10	∞
Ratio $\frac{F_{N-1}}{F_N}$	0.5	0.667	0.6	0.625	0.6156	0.619	0.6177	0.6181	0.6184	0.618

The ratio γ has a historical background. Ancient Greek architects believed that a building having the sides d and b satisfying the relation

$$\frac{d+b}{d} = \frac{d}{b} = \gamma \tag{5.25}$$

will be having the most pleasing properties (Fig. 5.11). It is also found in Euclid's geometry that the division of a line segment into two unequal parts so that the ratio of the whole to the larger part is equal to the ratio of the larger to the smaller, being known as the *golden section* or *golden mean*—thus the term *golden section method*.

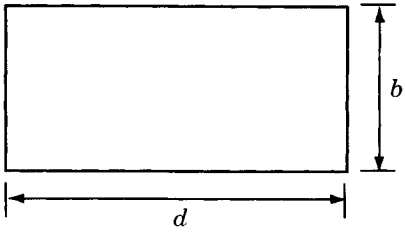


Figure 5.11 Rectangular building of sides b and d.

Procedure. The procedure is same as the Fibonacci method except that the location of the first two experiments is defined by

$$L_2^* = \frac{F_{N-2}}{F_N} L_0 = \frac{F_{N-2}}{F_{N-1}} \frac{F_{N-1}}{F_N} L_0 = \frac{L_0}{\gamma^2} = 0.382 L_0 \tag{5.26}$$

The desired accuracy can be specified to stop the procedure.

Example 5.8 Minimize the function $f(x) = 0.65 - [0.75/(1 + x^2)] - 0.65\, x \tan^{-1}(1/x)$ using the golden section method with $n = 6$.

SOLUTION The locations of the first two experiments are defined by $L_2^* = 0.382L_0 = (0.382)(3.0) = 1.1460$. Thus $x_1 = 1.1460$ and $x_2 = 3.0 - 1.1460 = 1.8540$ with $f_1 = f(x_1) = -0.208654$ and $f_2 = f(x_2) = -0.115124$. Since $f_1 < f_2$, we delete the interval $[x_2,3.0]$ based on the assumption of unimodality and obtain the new interval of uncertainty as $L_2 = [0,x_2] = [0.0,1.8540]$. The third experiment is placed at $x_3 = 0 + (x_2 - x_1) = 1.8540 - 1.1460 = 0.7080$. Since $f_3 = -0.288943$ is smaller than $f_1 = -0.208654$, we delete the interval $[x_1,x_2]$ and obtain the new interval of uncertainty as $[0.0,x_1] = [0.0,1.1460]$. The position of the next experiment is given by $x_4 = 0 + (x_1 - x_3) = 1.1460 - 0.7080 = 0.4380$ with $f_4 = -0.308951$.

Since $f_4 < f_3$, we delete $[x_3,x_1]$ and obtain the new interval of uncertainty as $[0,x_3] = [0.0,0.7080]$. The next experiment is placed at $x_5 = 0 + (x_3 - x_4) = 0.7080 - 0.4380 = 0.2700$. Since $f_5 = -0.278434$ is larger than $f_4 = -0.308951$, we delete the interval $[0,x_5]$ and obtain the new interval of uncertainty as $[x_5,x_3] = [0.2700,0.7080]$. The final experiment is placed at $x_6 = x_5 + (x_3 - x_4) = 0.2700 + (0.7080 - 0.4380) = 0.5400$ with $f_6 = -0.308234$. Since $f_6 > f_4$, we delete the interval $[x_6,x_3]$ and obtain the final interval of uncertainty as $[x_5,x_6] = [0.2700,0.5400]$. Note that this final interval of uncertainty is slightly larger than the one found in the Fibonacci method, [0.461540,0.230770]. The ratio of the final to the initial interval of uncertainty in the present case is

$$\frac{L_6}{L_0} = \frac{0.5400 - 0.2700}{3.0} = \frac{0.27}{3.0} = 0.09$$

5.9 COMPARISON OF ELIMINATION METHODS

The efficiency of an elimination method can be measured in terms of the ratio of the final and the initial intervals of uncertainty, L_n/L_0. The values of this ratio achieved in various methods for a specified number of experiments ($n = 5$ and $n = 10$) are compared in Table 5.3. It can be seen that the Fibonacci method is the most efficient method, followed by the golden section method, in reducing the interval of uncertainty.

TABLE 5.3 Final Intervals of Uncertainty

Method	Formula	$n = 5$	$n = 10$
Exhaustive search	$L_n = \frac{2}{n+1} L_0$	$0.33333L_0$	$0.18182L_0$
Dichotomous search ($\delta = 0.01$ and n = even)	$L_n = \frac{L_0}{2^{n/2}} + \delta\left(1 - \frac{1}{2^{n/2}}\right)$	$\frac{1}{4}L_0 + 0.0075$ with $n = 4$, $\frac{1}{8}L_0 + 0.00875$ with $n = 6$	$0.03125L_0 + 0.0096875$
Interval halving ($n \geq 3$ and odd)	$L_n = (\frac{1}{2})^{(n-1)/2} L_0$	$0.25L_0$	$0.0625L_0$ with $n = 9$, $0.03125L_0$ with $n = 11$
Fibonacci	$L_n = \frac{1}{F_n} L_0$	$0.125L_0$	$0.01124L_0$
Golden section	$L_n = (0.618)^{n-1} L_0$	$0.1459L_0$	$0.01315L_0$

TABLE 5.4 Number of Experiments for a Specified Accuracy

Method	Error: $\frac{1}{2}\frac{L_n}{L_0} \leq 0.1$	Error: $\frac{1}{2}\frac{L_n}{L_0} \leq 0.01$
Exhaustive search	$n \geq 9$	$n \geq 99$
Dichotomous search ($\delta = 0.01$, $L_0 = 1$)	$n \geq 6$	$n \geq 14$
Interval halving ($n \geq 3$ and odd)	$n \geq 7$	$n \geq 13$
Fibonacci	$n \geq 4$	$n \geq 9$
Golden section	$n \geq 5$	$n \geq 10$

A similar observation can be made by considering the number of experiments (or function evaluations) needed to achieve a specified accuracy in various methods. The results are compared in Table 5.4 for maximum permissible errors of 0.1 and 0.01. It can be seen that to achieve any specified accuracy, the Fibonacci method requires the least number of experiments, followed by the golden section method.

INTERPOLATION METHODS

The interpolation methods were originally developed as one-dimensional searches within multivariable optimization techniques, and are generally more efficient than Fibonacci-type approaches. The aim of all the one-dimensional minimization methods is to find λ^*, the smallest nonnegative value of λ, for

which the function

$$f(\lambda) = f(\mathbf{X} + \lambda\mathbf{S}) \tag{5.27}$$

attains a local minimum. Hence if the original function $f(\mathbf{X})$ is expressible as an explicit function of $x_i (i = 1,2,\ldots,n)$, we can readily write the expression for $f(\lambda) = f(\mathbf{X} + \lambda\mathbf{S})$ for any specified vector $\mathbf{S}$, set

$$\frac{df}{d\lambda}(\lambda) = 0 \tag{5.28}$$

and solve Eq. (5.28) to find λ^* in terms of $\mathbf{X}$ and $\mathbf{S}$. However, in many practical problems, the function $f(\lambda)$ cannot be expressed explicitly in terms of λ (as shown in Example 5.1). In such cases the interpolation methods can be used to find the value of λ^*.

Example 5.9 Derive the one-dimensional minimization problem for the following case:

$$\text{Minimize } f(\mathbf{X}) = (x_1^2 - x_2)^2 + (1 - x_1)^2 \tag{E_1}$$

from the starting point $\mathbf{X}_1 = \begin{Bmatrix} -2 \\ -2 \end{Bmatrix}$ along the search direction $\mathbf{S} = \begin{Bmatrix} 1.00 \\ 0.25 \end{Bmatrix}$.

SOLUTION The new design point $\mathbf{X}$ can be expressed as

$$\mathbf{X} = \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \mathbf{X}_1 + \lambda\mathbf{S} = \begin{Bmatrix} -2 + \lambda \\ -2 + 0.25\lambda \end{Bmatrix}$$

By substituting $x_1 = -2 + \lambda$ and $x_2 = -2 + 0.25\lambda$ in Eq. (E_1), we obtain f as a function of λ as

$$f(\lambda) = f\begin{pmatrix} -2 + \lambda \\ -2 + 0.25\lambda \end{pmatrix} = [(-2 + \lambda)^2 - (-2 + 0.25\lambda)]^2 + [1 - (-2 + \lambda)]^2 = \lambda^4 - 8.5\lambda^3 + 31.0625\lambda^2 - 57.0\lambda + 45.0$$

The value of λ at which $f(\lambda)$ attains a minimum gives λ^*.

In the following sections, we discuss three different interpolation methods with reference to one-dimensional minimization problems that arise during multivariable optimization problems.

5.10 QUADRATIC INTERPOLATION METHOD

The quadratic interpolation method uses the function values only; hence it is useful to find the minimizing step (λ^*) of functions $f(\mathbf{X})$ for which the partial derivatives with respect to the variables x_i are not available or difficult to compute [5.2, 5.5]. This method finds the minimizing step length λ^* in three stages. In the first stage the S-vector is normalized so that a step length of $\lambda = 1$ is acceptable. In the second stage the function $f(\lambda)$ is approximated by a quadratic function $h(\lambda)$ and the minimum, $\tilde{\lambda}^*$, of $h(\lambda)$ is found. If $\tilde{\lambda}^*$ is not sufficiently close to the true minimum λ^*, a third stage is used. In this stage a new quadratic function (refit) $h'(\lambda) = a' + b'\lambda + c'\lambda^2$ is used to approximate $f(\lambda)$, and a new value of $\tilde{\lambda}^*$ is found. This procedure is continued until a $\tilde{\lambda}^*$ that is sufficiently close to λ^* is found.

Stage 1. In this stage,[†] the **S** vector is normalized as follows: Find $\Delta = \max_i |s_i|$, where s_i is the ith component of **S** and divide each component of **S** by Δ. Another method of normalization is to find $\Delta = (s_1^2 + s_2^2 + \cdots + s_n^2)^{1/2}$ and divide each component of **S** by Δ.

Stage 2. Let

$$h(\lambda) = a + b\lambda + c\lambda^2 \tag{5.29}$$

be the quadratic function used for approximating the function $f(\lambda)$. It is worth noting at this point that a quadratic is the lowest-order polynomial for which a finite minimum can exist. The necessary condition for the minimum of $h(\lambda)$ is that

$$\frac{dh}{d\lambda} = b + 2c\lambda = 0$$

that is,

$$\tilde{\lambda}^* = -\frac{b}{2c} \tag{5.30}$$

The sufficiency condition for the minimum of $h(\lambda)$ is that

$$\left.\frac{d^2h}{d\lambda^2}\right|_{\tilde{\lambda}^*} > 0$$

[†]This stage is not required if the one-dimensional minimization problem has not arisen within a multivariable minimization problem.

that is,

$$c > 0 \tag{5.31}$$

To evaluate the constants a, b, and c in Eq. (5.29), we need to evaluate the function $f(\lambda)$ at three points. Let $\lambda = A$, $\lambda = B$, and $\lambda = C$ be the points at which the function $f(\lambda)$ is evaluated and let f_A, f_B, and f_C be the corresponding function values, that is,

$$\begin{aligned} f_A &= a + bA + cA^2 \\ f_B &= a + bB + cB^2 \\ f_C &= a + bC + cC^2 \end{aligned} \tag{5.32}$$

The solution of Eqs. (5.32) gives

$$a = \frac{f_A BC(C - B) + f_B CA(A - C) + f_C AB(B - A)}{(A - B)(B - C)(C - A)} \tag{5.33}$$

$$b = \frac{f_A(B^2 - C^2) + f_B(C^2 - A^2) + f_C(A^2 - B^2)}{(A - B)(B - C)(C - A)} \tag{5.34}$$

$$c = -\frac{f_A(B - C) + f_B(C - A) + f_C(A - B)}{(A - B)(B - C)(C - A)} \tag{5.35}$$

From Eqs. (5.30), (5.34), and (5.35), the minimum of $h(\lambda)$ can be obtained as

$$\bar{\lambda}^* = \frac{-b}{2c} = \frac{f_A(B^2 - C^2) + f_B(C^2 - A^2) + f_C(A^2 - B^2)}{2[f_A(B - C) + f_B(C - A) + f_C(A - B)]} \tag{5.36}$$

provided that c, as given by Eq. (5.35), is positive.

To start with, for simplicity, the points A, B, and C can be chosen as 0, t, and $2t$, respectively, where t is a preselected trial step length. By this procedure, we can save one function evaluation since $f_A = f(\lambda = 0)$ is generally known from the previous iteration (of a multivariable search). For this case, Eqs. (5.33) to (5.36) reduce to

$$a = f_A \tag{5.37}$$

$$b = \frac{4f_B - 3f_A - f_C}{2t} \tag{5.38}$$

$$c = \frac{f_C + f_A - 2f_B}{2t^2} \tag{5.39}$$

$$\bar{\lambda}^* = \frac{4f_B - 3f_A - f_C}{4f_B - 2f_C - 2f_A} t \tag{5.40}$$

provided that

$$c = \frac{f_C + f_A - 2f_B}{2t^2} > 0 \tag{5.41}$$

The inequality (5.41) can be satisfied if

$$\frac{f_A + f_C}{2} > f_B \tag{5.42}$$

(i.e., the function value f_B should be smaller than the average value of f_A and f_C). This can be satisfied if f_B lies below the line joining f_A and f_C as shown in Fig. 5.12.

The following procedure can be used not only to satisfy the inequality (5.42) but also to ensure that the minimum $\bar{\lambda}^*$ lies in the interval $0 < \bar{\lambda}^* < 2t$.

1. Assuming that $f_A = f(\lambda = 0)$ and the initial step size t_0 are known, evaluate the function f at $\lambda = t_0$ and obtain $f_1 = f(\lambda = t_0)$. The possible outcomes are shown in Fig. 5.13.
2. If $f_1 > f_A$ is realized (Fig. 5.13*c*), set $f_C = f_1$ and evaluate the function f at $\lambda = t_0/2$ and $\bar{\lambda}^*$ using Eq. (5.40) with $t = t_0/2$.
3. If $f_1 \leqslant f_A$ is realized (Fig. 5.13*a* or *b*), set $f_B = f_1$, and evaluate the function f at $\lambda = 2t_0$ to find $f_2 = f(\lambda = 2t_0)$. This may result in any one of the situations shown in Fig. 5.14.

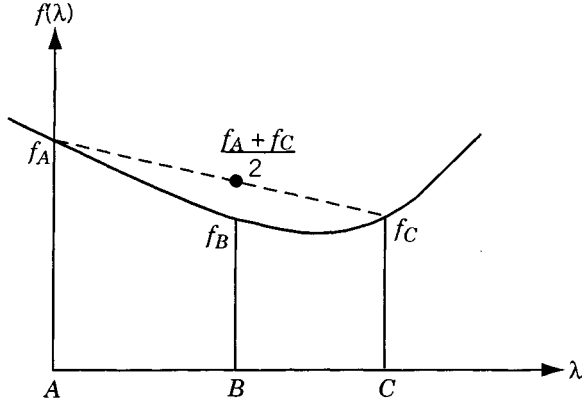


Figure 5.12 f_B smaller than $(f_A + f_C)/2$.

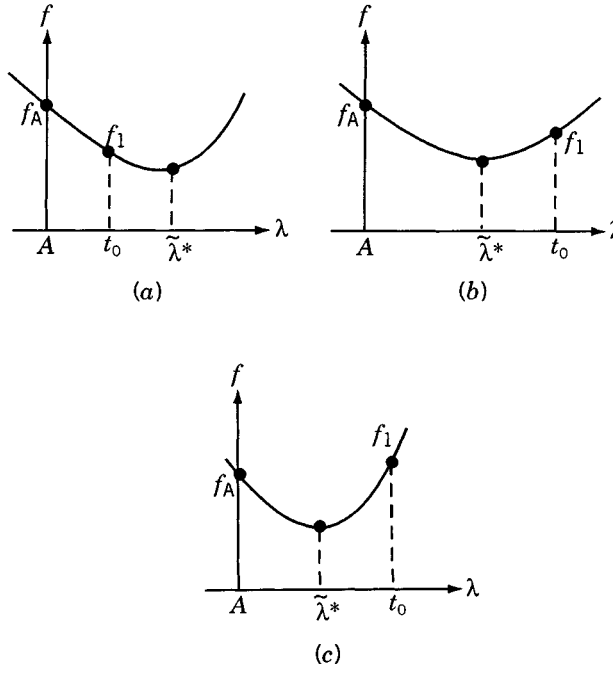


Figure 5.13 Possible outcomes when the function is evaluated at $\lambda = t_0$: (*a*) $f_1 < f_A$ and $t_0 < \bar{\lambda}^*$; (*b*) $f_1 < f_A$ and $t_0 > \bar{\lambda}^*$; (*c*) $f_1 > f_A$ and $t_0 > \bar{\lambda}^*$.

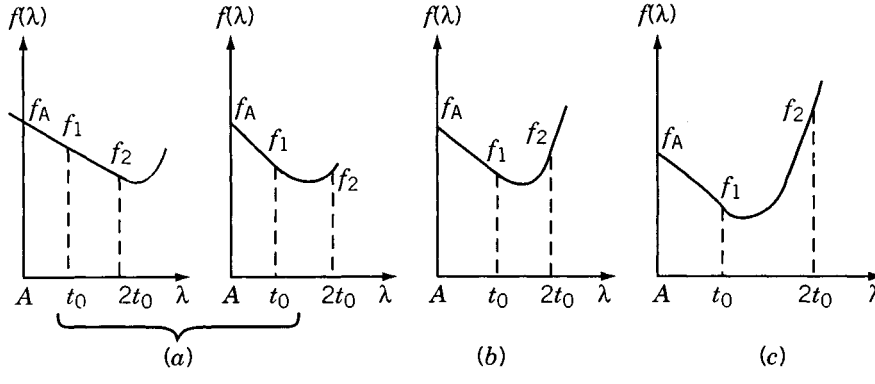


Figure 5.14 Possible outcomes when function is evaluated at $\lambda = t_0$ and $2t_0$: (*a*) $f_2 < f_1$ and $f_2 < f_A$; (*b*) $f_2 < f_A$ and $f_2 > f_1$; (*c*) $f_2 > f_A$ and $f_2 > f_1$.

4. If f_2 turns out to be greater than f_1 (Fig. 5.14*b* or *c*), set $f_C = f_2$ and compute $\tilde{\lambda}^*$ according to Eq. (5.40) with $t = t_0$.
5. If f_2 turns out to be smaller than f_1, set new $f_1 = f_2$ and $t_0 = 2t_0$, and repeat steps 2 to 4 until we are able to find $\tilde{\lambda}^*$.

Stage 3. The $\tilde{\lambda}^*$ found in stage 2 is the minimum of the approximating quadratic $h(\lambda)$ and we have to make sure that this $\tilde{\lambda}^*$ is sufficiently close to the true minimum λ^* of $f(\lambda)$ before taking $\lambda^* \simeq \tilde{\lambda}^*$. Several tests are possible to ascertain this. One possible test is to compare $f(\tilde{\lambda}^*)$ with $h(\tilde{\lambda}^*)$ and consider $\tilde{\lambda}^*$ a sufficiently good approximation if they differ not more than by a small amount. This criterion can be stated as

$$\left|\frac{h(\tilde{\lambda}^*) - f(\tilde{\lambda}^*)}{f(\tilde{\lambda}^*)}\right| \leq \varepsilon_1 \tag{5.43}$$

Another possible test is to examine whether $df/d\lambda$ is close to zero at $\tilde{\lambda}^*$. Since the derivatives of f are not used in this method, we can use a finite-difference formula for $df/d\lambda$ and use the criterion

$$\left|\frac{f(\tilde{\lambda}^* + \Delta\tilde{\lambda}^*) - f(\tilde{\lambda}^* - \Delta\tilde{\lambda}^*)}{2\Delta\tilde{\lambda}^*}\right| \leq \varepsilon_2 \tag{5.44}$$

to stop the procedure. In Eqs. (5.43) and (5.44), ε_1 and ε_2 are small numbers to be specified depending on the accuracy desired.

If the convergence criteria stated in Eqs. (5.43) and (5.44) are not satisfied, a new quadratic function

$$h'(\lambda) = a' + b'\lambda + c'\lambda^2$$

is used to approximate the function $f(\lambda)$. To evaluate the constants a', b' and c', the three best function values of the current $f_A = f(\lambda = 0)$, $f_B = f(\lambda = t_0)$, $f_C = f(\lambda = 2t_0)$, and $\tilde{f} = f(\lambda = \tilde{\lambda}^*)$ are to be used. This process of trying to fit another polynomial to obtain a better approximation to $\tilde{\lambda}^*$ is known as *refitting* the polynomial.

For refitting the quadratic, we consider all possible situations and select the best three points of the present A, B, C, and $\tilde{\lambda}^*$. There are four possibilities, as shown in Fig. 5.15. The best three points to be used in refitting in each case are given in Table 5.5. A new value of $\tilde{\lambda}^*$ is computed by using the general formula, Eq. (5.36). If this $\tilde{\lambda}^*$ also does not satisfy the convergence criteria stated in Eqs. (5.43) and (5.44), a new quadratic has to be refitted according to the scheme outlined in Table 5.5.

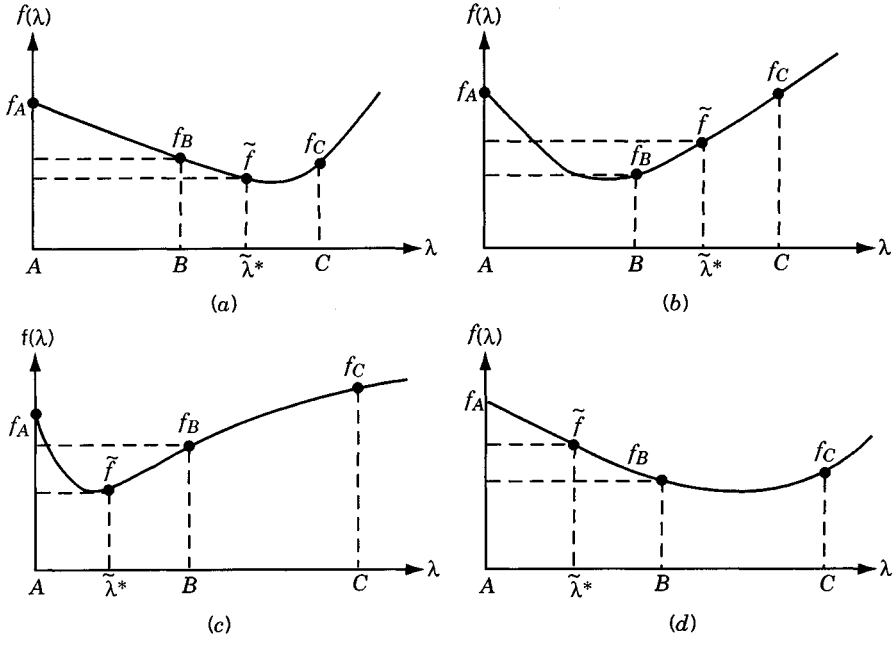


Figure 5.15 Various possibilities for refitting.

TABLE 5.5 Refitting Scheme

		New Points for Refitting	
Case	Characteristics	New	Old
1	$\tilde{\lambda}^* > B$	A	B
	$\tilde{f} < f_B$	B	$\tilde{\lambda}^*$
		C	C
		Neglect old A	
2	$\tilde{\lambda}^* > B$	A	A
	$\tilde{f} > f_B$	B	B
		C	$\tilde{\lambda}^*$
		Neglect old C	
3	$\tilde{\lambda}^* < B$	A	A
	$\tilde{f} < f_B$	B	$\tilde{\lambda}^*$
		C	B
		Neglect old C	
4	$\tilde{\lambda}^* < B$	A	$\tilde{\lambda}^*$
	$\tilde{f} > f_B$	B	B
		C	C
		Neglect old A	

Example 5.10 Find the minimum of $f = \lambda^5 - 5\lambda^3 - 20\lambda + 5$.

SOLUTION Since this is not a multivariable optimization problem, we can proceed directly to stage 2. Let the initial step size be taken as $t_0 = 0.5$ and $A = 0$.

Iteration 1

$$f_A = f(\lambda = 0) = 5$$

$$f_1 = f(\lambda = t_0) = 0.03125 - 5(0.125) - 20(0.5) + 5 = -5.59375$$

Since $f_1 < f_A$, we set $f_B = f_1 = -5.59375$, and find that

$$f_2 = f(\lambda = 2t_0 = 1.0) = -19.0$$

As $f_2 < f_1$, we set new $t_0 = 1$ and $f_1 = -19.0$. Again we find that $f_1 < f_A$ and hence set $f_B = f_1 = -19.0$, and find that $f_2 = f(\lambda = 2t_0 = 2) = -43$. Since $f_2 < f_1$, we again set $t_0 = 2$ and $f_1 = -43$. As this $f_1 < f_A$, set $f_B = f_1 = -43$ and evaluate $f_2 = f(\lambda = 2t_0 = 4) = 629$. This time $f_2 > f_1$ and hence we set $f_C = f_2 = 629$ and compute $\tilde{\lambda}^*$ from Eq. (5.40) as

$$\tilde{\lambda}^* = \frac{4(-43) - 3(5) - 629}{4(-43) - 2(629) - 2(5)}(2) = \frac{1632}{1440} = 1.135$$

Convergence test: Since $A = 0, f_A = 5, B = 2, f_B = -43, C = 4$, and $f_C = 629$, the values of a, b, and c can be found to be

$$a = 5, \quad b = -204, \quad c = 90$$

and

$$h(\tilde{\lambda}^*) = h(1.135) = 5 - 204(1.135) + 90(1.135)^2 = -110.9$$

Since

$$\tilde{f} = f(\tilde{\lambda}^*) = (1.135)^5 - 5(1.135)^3 - 20(1.135) + 5.0 = -23.127$$

we have

$$\left|\frac{h(\tilde{\lambda}^*) - f(\tilde{\lambda}^*)}{f(\tilde{\lambda}^*)}\right| = \left|\frac{-116.5 + 23.127}{-23.127}\right| = 3.8$$

As this quantity is very large, convergence is not achieved and hence we have to use *refitting*.

Iteration 2

Since $\tilde{\lambda}^* < B$ and $\tilde{f} > f_B$, we take the new values of A, B, and C as

$$A = 1.135, \quad f_A = -23.127$$
$$B = 2.0, \quad f_B = -43.0$$
$$C = 4.0, \quad f_C = 629.0$$

and compute new $\tilde{\lambda}^*$, using Eq. (5.36), as

$$\tilde{\lambda}^* = \frac{\begin{matrix}(-23.127)(4.0 - 16.0) + (-43.0)(16.0 - 1.29) \\ + (629.0)(1.29 - 4.0)\end{matrix}}{2[\begin{matrix}(-23.127)(2.0 - 4.0) + (-43.0)(4.0 - 1.135) \\ + (629.0)(1.135 - 2.0)]\end{matrix}} = 1.661$$

Convergence test: To test the convergence, we compute the coefficients of the quadratic as

$$a = 288.0, \quad b = -417.0, \quad c = 125.3$$

As

$$h(\tilde{\lambda}^*) = h(1.661) = 288.0 - 417.0(1.661) + 125.3(1.661)^2 = -59.7$$
$$\tilde{f} = f(\tilde{\lambda}^*) = 12.8 - 5(4.59) - 20(1.661) + 5.0 = -38.37$$

we obtain

$$\left|\frac{h(\tilde{\lambda}^*) - f(\tilde{\lambda}^*)}{f(\tilde{\lambda}^*)}\right| = \left|\frac{-59.70 + 38.37}{-38.37}\right| = 0.556$$

Since this quantity is not sufficiently small, we need to proceed to the next refit.

5.11 CUBIC INTERPOLATION METHOD

The cubic interpolation method finds the minimizing step length λ^* in four stages [5.5, 5.11]. It makes use of the derivative of the function f:

$$f'(\lambda) = \frac{df}{d\lambda} = \frac{d}{d\lambda} f(\mathbf{X} + \lambda\mathbf{S}) = \mathbf{S}^T \nabla f(\mathbf{X} + \lambda\mathbf{S})$$

The first stage normalizes the $\mathbf{S}$ vector so that a step size $\lambda = 1$ is acceptable. The second stage establishes bounds on λ^*, and the third stage finds the value

of $\tilde{\lambda}^*$ by approximating $f(\lambda)$ by a cubic polynomial $h(\lambda)$. If the $\tilde{\lambda}^*$ found in stage 3 does not satisfy the prescribed convergence criteria, the cubic polynomial is refitted in the fourth stage.

Stage 1. Calculate $\Delta = \max_i |s_i|$, where $|s_i|$ is the absolute value of the ith component of $\mathbf{S}$, and divide each component of $\mathbf{S}$ by Δ. An alternative method of normalization is to find

$$\Delta = (s_1^2 + s_2^2 + \cdots + s_n^2)^{1/2}$$

and divide each component of $\mathbf{S}$ by Δ.

Stage 2. To establish lower and upper bounds on the optimal step size λ^*, we need to find two points A and B at which the slope $df/d\lambda$ has different signs. We know that at $\lambda = 0$,

$$\left.\frac{df}{d\lambda}\right|_{\lambda=0} = \mathbf{S}^T \nabla f(\mathbf{X}) < 0$$

since $\mathbf{S}$ is presumed to be a direction of descent.[†]

Hence, to start with we can take $A = 0$ and try to find a point $\lambda = B$ at which the slope $df/d\lambda$ is positive. Point B can be taken as the first value out of $t_0, 2t_0, 4t_0, 8t_0, \ldots$ at which f' is nonnegative, where t_0 is a preassigned initial step size. It then follows that λ^* is bounded in the interval $A < \lambda^* \leq B$ (Fig. 5.16).

Stage 3. If the cubic equation

$$h(\lambda) = a + b\lambda + c\lambda^2 + d\lambda^3 \tag{5.45}$$

[†]In this case the angle between the direction of steepest descent and $\mathbf{S}$ will be less than 90°.

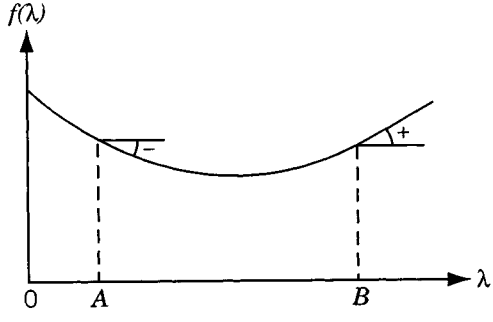


Figure 5.16 Minimum of $f(\lambda)$ lies between A and B.

is used to approximate the function $f(\lambda)$ between points A and B, we need to find the values $f_A = f(\lambda = A)$, $f'_A = df/d\lambda\ (\lambda = A)$, $f_B = f(\lambda = B)$, and $f'_B = df/d\lambda\ (\lambda = B)$ in order to evaluate the constants, a, b, c, and d in Eq. (5.45). By assuming that $A \neq 0$, we can derive a general formula for $\tilde{\lambda}^*$. From Eq. (5.45) we have

$$\begin{aligned} f_A &= a + bA + cA^2 + dA^3 \\ f_B &= a + bB + cB^2 + dB^3 \\ f'_A &= b + 2cA + 3dA^2 \\ f'_B &= b + 2cB + 3dB^2 \end{aligned} \tag{5.46}$$

Equations (5.46) can be solved to find the constants as

$$a = f_A - bA - cA^2 - dA^3 \tag{5.47}$$

with

$$b = \frac{1}{(A - B)^2}(B^2 f'_A + A^2 f'_B + 2ABZ) \tag{5.48}$$

$$c = -\frac{1}{(A - B)^2}[(A + B)Z + Bf'_A + Af'_B] \tag{5.49}$$

and

$$d = \frac{1}{3(A - B)^2}(2Z + f'_A + f'_B) \tag{5.50}$$

where

$$Z = \frac{3(f_A - f_B)}{B - A} + f'_A + f'_B \tag{5.51}$$

The necessary condition for the minimum of $h(\lambda)$ given by Eq. (5.45) is that

$$\frac{dh}{d\lambda} = b + 2c\lambda + 3d\lambda^2 = 0$$

that is,

$$\tilde{\lambda}^* = \frac{-c \pm (c^2 - 3bd)^{1/2}}{3d} \tag{5.52}$$

The application of the sufficiency condition for the minimum of $h(\lambda)$ leads to the relation

$$\left.\frac{d^2h}{d\lambda^2}\right|_{\tilde{\lambda}^*} = 2c + 6d\tilde{\lambda}^* > 0 \tag{5.53}$$

By substituting the expressions for b, c, and d given by Eqs. (5.48) to (5.50) into Eqs. (5.52) and (5.53), we obtain

$$\tilde{\lambda}^* = A + \frac{f'_A + Z \pm Q}{f'_A + f'_B + 2Z}(B - A) \tag{5.54}$$

where

$$Q = (Z^2 - f'_A f'_B)^{1/2} \tag{5.55}$$

$$2(B - A)(2Z + f'_A + f'_B)(f'_A + Z \pm Q)$$
$$-2(B - A)(f'^2_A + Zf'_B + 3Zf'_A + 2Z^2)$$
$$-2(B + A)f'_A f'_B > 0 \tag{5.56}$$

By specializing Eqs. (5.47) to (5.56) for the case where $A = 0$, we obtain

$$a = f_A$$

$$b = f'_A$$

$$c = -\frac{1}{B}(Z + f'_A)$$

$$d = \frac{1}{3B^2}(2Z + f'_A + f'_B)$$

$$\tilde{\lambda}^* = B\frac{f'_A + Z \pm Q}{f'_A + f'_B + 2Z} \tag{5.57}$$

$$Q = (Z^2 - f'_A f'_B)^{1/2} > 0 \tag{5.58}$$

where

$$Z = \frac{3(f_A - f_B)}{B} + f'_A + f'_B \tag{5.59}$$

The two values of $\tilde{\lambda}^*$ in Eqs. (5.54) and (5.57) correspond to the two possibilities for the vanishing of $h'(\lambda)$ [i.e., at a maximum of $h(\lambda)$ and at a minimum]. To avoid imaginary values of Q, we should ensure the satisfaction of the condition

$$Z^2 - f'_A f'_B \geq 0$$

in Eq. (5.55). This inequality is satisfied automatically since A and B are selected such that $f'_A < 0$ and $f'_B \geq 0$. Furthermore, the sufficiency condition (when $A = 0$) requires that $Q > 0$, which is already satisfied. Now we compute $\tilde{\lambda}^*$ using Eq. (5.57) and proceed to the next stage.

Stage 4. The value of $\tilde{\lambda}^*$ found in stage 3 is the true minimum of $h(\lambda)$ and may not be close to the minimum of $f(\lambda)$. Hence the following convergence criteria can be used before choosing $\lambda^* \approx \tilde{\lambda}^*$:

$$\left| \frac{h(\tilde{\lambda}^*) - f(\tilde{\lambda}^*)}{f(\tilde{\lambda}^*)} \right| \leq \varepsilon_1 \tag{5.60}$$

$$\left| \frac{df}{d\lambda} \right|_{\tilde{\lambda}^*} = \left| \mathbf{S}^T \nabla f \right|_{\tilde{\lambda}^*} \leq \varepsilon_2 \tag{5.61}$$

where ε_1 and ε_2 are small numbers whose values depend on the accuracy desired. The criterion of Eq. (5.61) can be stated in nondimensional form as

$$\left| \frac{\mathbf{S}^T \nabla f}{|\mathbf{S}| \, |\nabla f|} \right|_{\tilde{\lambda}^*} \leq \varepsilon_2 \tag{5.62}$$

If the criteria stated in Eqs. (5.60) and (5.62) are not satisfied, a new cubic equation

$$h'(\lambda) = a' + b'\lambda + c'\lambda^2 + d'\lambda^3$$

can be used to approximate $f(\lambda)$. The constants a', b', c', and d' can be evaluated by using the function and derivative values at the best two points out of the three points currently available: A, B, and $\tilde{\lambda}^*$. Now the general formula given by Eq. (5.54) is to be used for finding the optimal step size $\tilde{\lambda}^*$. If $f'(\tilde{\lambda}^*) < 0$, the new points A and B are taken as $\tilde{\lambda}^*$ and B, respectively; otherwise [if $f'(\tilde{\lambda}^*) > 0$], the new points A and B are taken as A and $\tilde{\lambda}^*$, and Eq. (5.54) is applied to find the new value of $\tilde{\lambda}^*$. Equations (5.60) and (5.62) are again used to test for the convergence of $\tilde{\lambda}^*$. If convergence is achieved, $\tilde{\lambda}^*$ is taken as λ^* and the procedure is stopped. Otherwise, the entire procedure is repeated until the desired convergence is achieved.

The flowchart for implementing the cubic interpolation method is given in Fig. 5.17.

Example 5.11 Find the minimum of $f = \lambda^5 - 5\lambda^3 - 20\lambda + 5$ by the cubic interpolation method.

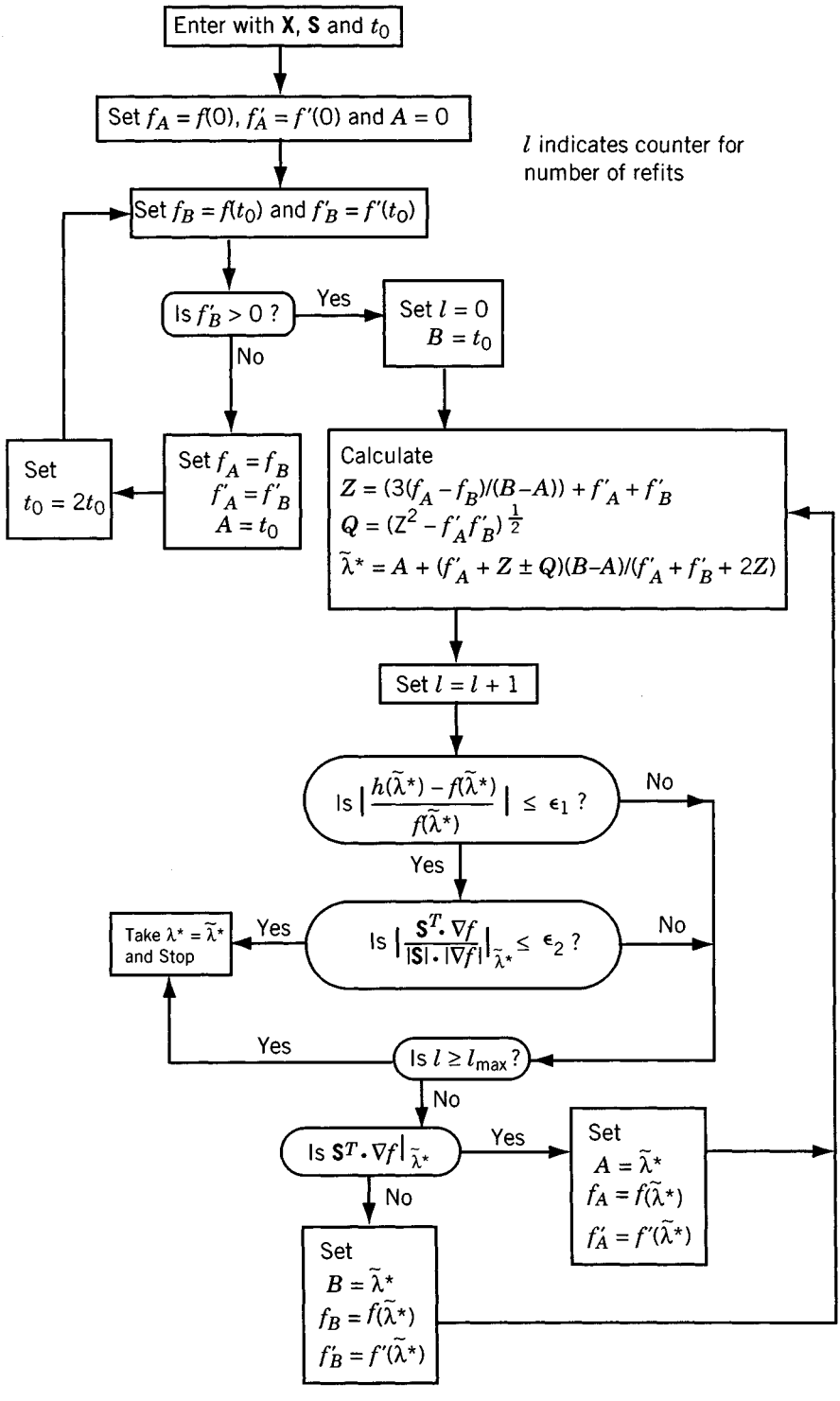


Figure 5.17 Flowchart for cubic interpolation method.

SOLUTION Since this problem has not arisen during a multivariable optimization process, we can skip stage 1. We take $A = 0$ and find that

$$\frac{df}{d\lambda}(\lambda = A = 0) = 5\lambda^4 - 15\lambda^2 - 20\Big|_{\lambda=0} = -20 < 0$$

To find B at which $df/d\lambda$ is nonnegative, we start with $t_0 = 0.4$ and evaluate the derivative at $t_0, 2t_0, 4t_0, \ldots$. This gives

$$f'(t_0 = 0.4) = 5(0.4)^4 - 15(0.4)^2 - 20.0 = -22.272$$

$$f'(2t_0 = 0.8) = 5(0.8)^4 - 15(0.8)^2 - 20.0 = -27.552$$

$$f'(4t_0 = 1.6) = 5(1.6)^4 - 15(1.6)^2 - 20.0 = -25.632$$

$$f'(8t_0 = 3.2) = (3.2)^4 - 15(3.2)^2 - 20.0 = 350.688$$

Thus we find that[†]

$$A = 0.0, \quad f_A = 5.0, \quad f'_A = -20.0$$

$$B = 3.2, \quad f_B = 113.0, \quad f'_B = 350.688$$

$$A < \lambda^* < B$$

Iteration 1

To find the value of $\tilde{\lambda}^*$ and to test the convergence criteria, we first compute Z and Q as:

$$Z = \frac{3(5.0 - 113.0)}{3.2} - 20.0 + 350.688 = 229.588$$

$$Q = [229.588^2 + (20.0)(350.688)]^{1/2} = 244.0$$

Hence

$$\tilde{\lambda}^* = 3.2\left(\frac{-20.0 + 229.588 \pm 244.0}{-20.0 + 350.688 + 459.176}\right) = 1.84 \quad \text{or} \quad -0.1396$$

By discarding the negative value, we have

$$\tilde{\lambda}^* = 1.84$$

[†]As f' has been found to be negative at $\lambda = 1.6$ also, we can take $A = 1.6$ for faster convergence.

Convergence criterion: If $\tilde{\lambda}^*$ is close to the true minimum, λ^*, then $f'(\tilde{\lambda}^*) = df(\tilde{\lambda}^*)/d\lambda$ should be approximately zero. Since $f' = 5\lambda^4 - 15\lambda^2 - 20$,

$$f'(\tilde{\lambda}^*) = 5(1.84)^4 - 15(1.84)^2 - 20 = -13.0$$

Since this is not small, we go to the next iteration or refitting. As $f'(\tilde{\lambda}^*) < 0$, we take $A = \tilde{\lambda}^*$ and

$$f_A = f(\tilde{\lambda}^*) = (1.84)^5 - 5(1.84)^3 - 20(1.84) + 5 = -41.70$$

Thus

$$A = 1.84, \quad f_A = -41.70, \quad f'_A = -13.0$$
$$B = 3.2, \quad f_B = 113.0, \quad f'_B = 350.688$$
$$A < \tilde{\lambda}^* < B$$

Iteration 2

$$Z = \frac{3(-41.7 - 113.0)}{3.20 - 1.84} - 13.0 + 350.688 = -3.312$$
$$Q = [(-3.312)^2 + (13.0)(350.688)]^{1/2} = 67.5$$

Hence

$$\tilde{\lambda}^* = 1.84 + \frac{-13.0 - 3.312 \pm 67.5}{-13.0 + 350.688 - 6.624}(3.2 - 1.84) = 2.05$$

Convergence criterion:

$$f'(\tilde{\lambda}^*) = 5.0(2.05)^4 - 15.0(2.05)^2 - 20.0 = 5.35$$

Since this value is large, we go the next iteration with $B = \tilde{\lambda}^* = 2.05$ [as $f'(\tilde{\lambda}^*) > 0$] and

$$f_B = (2.05)^5 - 5.0(2.05)^3 - 20.0(2.05) + 5.0 = -42.90$$

Thus

$$A = 1.84, \quad f_A = -41.70, \quad f'_A = -13.00$$
$$B = 2.05, \quad f_B = -42.90, \quad f'_B = 5.35$$
$$A < \lambda^* < B$$

Iteration 3

$$Z = \frac{3.0(-41.70 + 42.90)}{(2.05 - 1.84)} - 13.00 + 5.35 = 9.49$$

$$Q = [(9.49)^2 + (13.0)(5.35)]^{1/2} = 12.61$$

Therefore,

$$\tilde{\lambda}^* = 1.84 + \frac{-13.00 + 9.49 \pm 12.61}{-13.00 + 5.35 + 18.98}(2.05 - 1.84) = 2.0086$$

Convergence criterion:

$$f'(\tilde{\lambda}^*) = 5.0(2.0086)^4 - 15.0(2.0086)^2 - 20.0 = 0.855$$

Assuming that this value is close to zero, we can stop the iterative process and take

$$\lambda^* \simeq \tilde{\lambda}^* = 2.0086$$

5.12 DIRECT ROOT METHODS

The necessary condition for $f(\lambda)$ to have a minimum of λ^* is that $f'(\lambda^*) = 0$. The direct root methods seek to find the root (or solution) of the equation, $f'(\lambda) = 0$. Three root-finding methods—the Newton, the quasi-Newton, and the secant methods—are discussed in this section.

5.12.1 Newton Method

Consider the quadratic approximation of the function $f(\lambda)$ at $\lambda = \lambda_i$ using the Taylor's series expansion:

$$f(\lambda) = f(\lambda_i) + f'(\lambda_i)(\lambda - \lambda_i) + \tfrac{1}{2} f''(\lambda_i)(\lambda - \lambda_i)^2 \tag{5.63}$$

By setting the derivative of Eq. (5.63) equal to zero for the minimum of $f(\lambda)$, we obtain

$$f'(\lambda) = f'(\lambda_i) + f''(\lambda_i)(\lambda - \lambda_i) = 0 \tag{5.64}$$

If λ_i denotes an approximation to the minimum of $f(\lambda)$, Eq. (5.64) can be rearranged to obtain an improved approximation as

$$\lambda_{i+1} = \lambda_i - \frac{f'(\lambda_i)}{f''(\lambda_i)} \tag{5.65}$$

Thus the *Newton method*, Eq. (5.65), is equivalent to using a quadratic approximation for the function $f(\lambda)$ and applying the necessary conditions. The iterative process given by Eq. (5.65) can be assumed to have converged when the derivative, $f'(\lambda_{i+1})$, is close to zero:

$$|f'(\lambda_{i+1})| \leq \epsilon \tag{5.66}$$

where ϵ is a small quantity. The convergence process of the method is shown graphically in Fig. 5.18*a*.

Remarks:

1. The Newton method was originally developed by Newton for solving nonlinear equations and later refined by Raphson, and hence the method is also known as *Newton–Raphson method* in the literature of numerical analysis.
2. The method requires both the first- and second-order derivatives of $f(\lambda)$.
3. If $f''(\lambda_i) = 0$ [in Eq. (5.65)], the Newton iterative method has a powerful (fastest) convergence property, known as *quadratic convergence.*[†]
4. If the starting point for the iterative process is not close to the true solution λ^*, the Newton iterative process might diverge as illustrated in Fig. 5.18*b*.

Example 5.12 Find the minimum of the function

$$f(\lambda) = 0.65 - \frac{0.75}{1 + \lambda^2} - 0.65\lambda \tan^{-1} \frac{1}{\lambda}$$

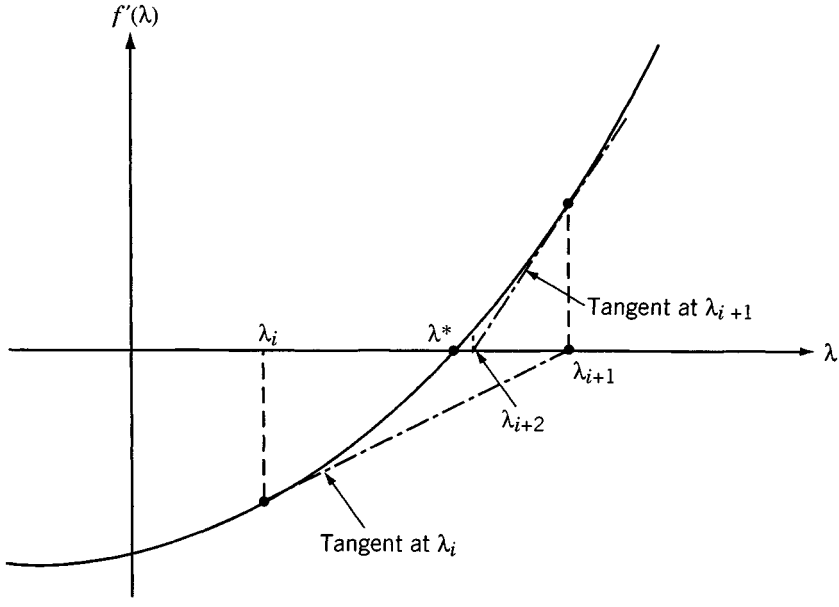
using the Newton–Raphson method with the starting point $\lambda_1 = 0.1$. Use $\epsilon = 0.01$ in Eq. (5.66) for checking the convergence.

SOLUTION The first and second derivatives of the function $f(\lambda)$ are given by

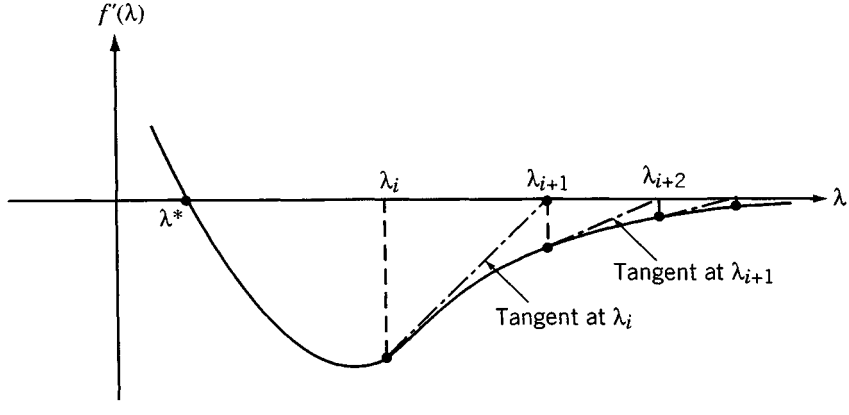
$$f'(\lambda) = \frac{1.5\lambda}{(1 + \lambda^2)^2} + \frac{0.65\lambda}{1 + \lambda^2} - 0.65 \tan^{-1} \frac{1}{\lambda}$$

$$f''(\lambda) = \frac{1.5(1 - 3\lambda^2)}{(1 + \lambda^2)^3} + \frac{0.65(1 - \lambda^2)}{(1 + \lambda^2)^2} + \frac{0.65}{1 + \lambda^2} = \frac{2.8 - 3.2\lambda^2}{(1 + \lambda^2)^3}$$

[†]The definition of quadratic convergence is given in Section 6.7.



(a)



(b)

Figure 5.18 Iterative process of Newton method: (*a*) convergence; (*b*) divergence.

Iteration 1

$$\lambda_1 = 0.1, \quad f(\lambda_1) = -0.188197, \quad f'(\lambda_1) = -0.744832, \quad f''(\lambda_1) = 2.68659$$

$$\lambda_2 = \lambda_1 - \frac{f'(\lambda_1)}{f''(\lambda_1)} = 0.377241$$

Convergence check: $|f'(\lambda_2)| = |-0.138230| > \epsilon$.

Iteration 2

$$f(\lambda_2) = -0.303279, \quad f'(\lambda_2) = -0.138230, \quad f''(\lambda_2) = 1.57296$$

$$\lambda_3 = \lambda_2 - \frac{f'(\lambda_2)}{f''(\lambda_2)} = 0.465119$$

Convergence check: $|f'(\lambda_3)| = |-0.0179078| > \epsilon$.

Iteration 3

$$f(\lambda_3) = -0.309881, \quad f'(\lambda_3) = -0.0179078, \quad f''(\lambda_3) = 1.17126$$

$$\lambda_4 = \lambda_3 - \frac{f'(\lambda_3)}{f''(\lambda_3)} = 0.480409$$

Convergence check: $|f'(\lambda_4)| = |-0.0005033| > \epsilon$.

Since the process has converged, the optimum solution is taken as $\lambda^* \approx \lambda_4 = 0.480409$.

5.12.2 Quasi-Newton Method

If the function being minimized $f(\lambda)$ is not available in closed form or is difficult to differentiate, the derivatives $f'(\lambda)$ and $f''(\lambda)$ in Eq. (5.65) can be approximated by the finite difference formulas as

$$f'(\lambda_i) = \frac{f(\lambda_i + \Delta\lambda) - f(\lambda_i - \Delta\lambda)}{2\Delta\lambda} \tag{5.67}$$

$$f''(\lambda_i) = \frac{f(\lambda_i + \Delta\lambda) - 2f(\lambda_i) + f(\lambda_i - \Delta\lambda)}{\Delta\lambda^2} \tag{5.68}$$

where $\Delta\lambda$ is a small step size. Substitution of Eqs. (5.67) and (5.68) into Eq. (5.65) leads to

$$\lambda_{i+1} = \lambda_i - \frac{\Delta\lambda[f(\lambda_i + \Delta\lambda) - f(\lambda_i - \Delta\lambda)]}{2[f(\lambda_i + \Delta\lambda) - 2f(\lambda_i) + f(\lambda_i - \Delta\lambda)]} \tag{5.69}$$

The iterative process indicated by Eq. (5.69) is known as the *quasi-Newton method.* To test the convergence of the iterative process, the following criterion can be used:

$$|f'(\lambda_{i+1})| = \left|\frac{f(\lambda_{i+1} + \Delta\lambda) - f(\lambda_{i+1} - \Delta\lambda)}{2\Delta\lambda}\right| \leq \epsilon \qquad (5.70)$$

where a central difference formula has been used for evaluating the derivative of f and ϵ is a small quantity.

Remarks:

1. The central difference formulas have been used in Eqs. (5.69) and (5.70). However, the forward or backward difference formulas can also be used for this purpose.
2. Equation (5.69) requires the evaluation of the function at the points $\lambda_i + \Delta\lambda$ and $\lambda_i - \Delta\lambda$ in addition to λ_i in each iteration.

Example 5.13 Find the minimum of the function

$$f(\lambda) = 0.65 - \frac{0.75}{1 + \lambda^2} - 0.65\lambda \tan^{-1}\frac{1}{\lambda}$$

using quasi-Newton method with the starting point $\lambda_1 = 0.1$ and the step size $\Delta\lambda = 0.01$ in central difference formulas. Use $\epsilon = 0.01$ in Eq. (5.70) for checking the convergence.

SOLUTION

Iteration 1

$$\lambda = 0.1, \quad \Delta\lambda = 0.01, \quad \epsilon = 0.01, \quad f_1 = f(\lambda_1) = -0.188197,$$

$$f_1^+ = f(\lambda_1 + \Delta\lambda) = -0.195512, \quad f_1^- = f(\lambda_1 - \Delta\lambda) = -0.180615$$

$$\lambda_2 = \lambda_1 - \frac{\Delta\lambda(f_1^+ - f_1^-)}{2(f_1^+ - 2f_1 + f_1^-)} = 0.377882$$

Convergence check: $|f'(\lambda_2)| = \left|\frac{f_2^+ - f_2^-}{2\Delta\lambda}\right| = 0.137300 > \epsilon.$

Iteration 2

$$f_2 = f(\lambda_2) = -0.303368, \quad f_2^+ = f(\lambda_2 + \Delta\lambda) = -0.304662,$$

$$f_2^- = f(\lambda_2 - \Delta\lambda) = -0.301916$$

$$\lambda_3 = \lambda_2 - \frac{\Delta\lambda(f_2^+ - f_2^-)}{2(f_2^+ - 2f_2 + f_2^-)} = 0.465390$$

Convergence check: $|f'(\lambda_3)| = \left|\frac{f_3^+ - f_3^-}{2\Delta\lambda}\right| = 0.017700 > \epsilon.$

Iteration 3

$$f_3 = f(\lambda_3) = -0.309885, \quad f_3^+ = f(\lambda_3 + \Delta\lambda) = -0.310004,$$

$$f_3^- = f(\lambda_3 - \Delta\lambda) = -0.309650$$

$$\lambda_4 = \lambda_3 - \frac{\Delta\lambda(f_3^+ - f_3^-)}{2(f_3^+ - 2f_3 + f_3^-)} = 0.480600$$

Convergence check: $|f'(\lambda_4) = \left|\frac{f_4^+ - f_4^-}{2\Delta\lambda}\right| = 0.000350 < \epsilon.$

Since the process has converged, we take the optimum solution as $\lambda^* \approx \lambda_4 = 0.480600$.

5.12.3 Secant Method

The secant method uses an equation similar to Eq. (5.64) as

$$f'(\lambda) = f'(\lambda_i) + s(\lambda - \lambda_i) = 0 \tag{5.71}$$

where s is the slope of the line connecting the two points $(A, f'(A))$ and $(B, f'(B))$, where A and B denote two different approximations to the correct solution, λ^*. The slope s can be expressed as (Fig. 5.19)

$$s = \frac{f'(B) - f'(A)}{B - A} \tag{5.72}$$

Equation (5.71) approximates the function $f'(\lambda)$ between A and B as a linear equation (secant), and hence the solution of Eq. (5.71) gives the new approximation to the root of $f'(\lambda)$ as

$$\lambda_{i+1} = \lambda_i - \frac{f'(\lambda_i)}{s} = A - \frac{f'(A)(B - A)}{f'(B) - f'(A)} \tag{5.73}$$

The iterative process given by Eq. (5.73) is known as the *secant method* (Fig. 5.19). Since the secant approaches the second derivative of $f(\lambda)$ at A as B approaches A, the secant method can also be considered as a quasi-Newton method. It can also be considered as a form of elimination technique since part

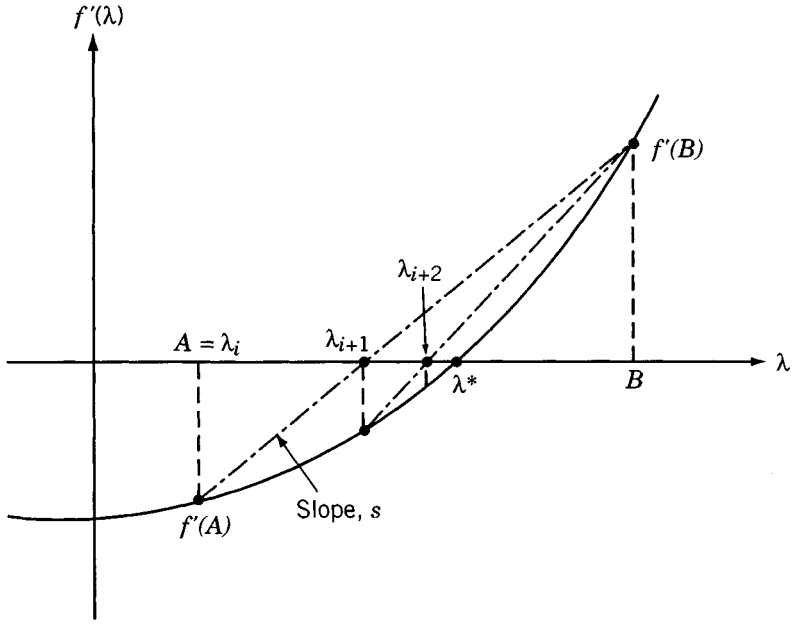


Figure 5.19 Iterative process of the secant method.

of the interval, (A,λ_{i+1}) in Fig. 5.19, is eliminated in every iteration. The iterative process can be implemented by using the following step-by-step procedure.

1. Set $\lambda_1 = A = 0$ and evaluate $f'(A)$. The value of $f'(A)$ will be negative. Assume an initial trial step length t_0. Set $i = 1$.
2. Evaluate $f'(t_0)$.
3. If $f'(t_0) < 0$, set $A = \lambda_i = t_0, f'(A) = f'(t_0)$, new $t_0 = 2t_0$, and go to step 2.
4. If $f'(t_0) \geq 0$, set $B = t_0, f'(B) = f'(t_0)$, and go to step 5.
5. Find the new approximate solution of the problem as

$$\lambda_{i+1} = A - \frac{f'(A)(B - A)}{f'(B) - f'(A)} \tag{5.74}$$

6. Test for convergence:

$$|f'(\lambda_{i+1})| \leq \epsilon \tag{5.75}$$

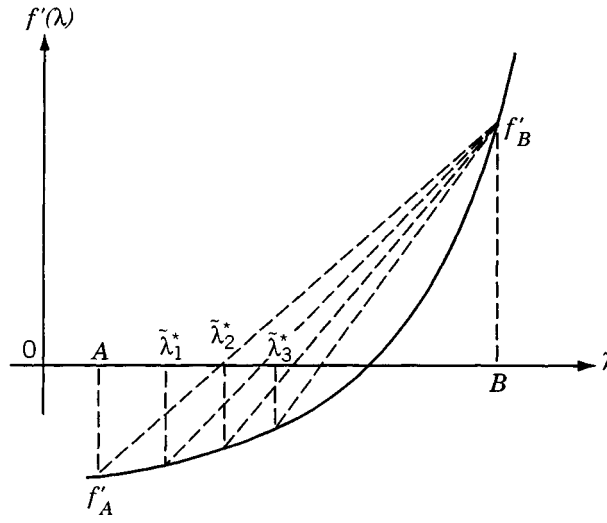


Figure 5.20 Situation when f'_A varies very slowly.

where ϵ is a small quantity. If Eq. (5.75) is satisfied, take $\lambda^* \approx \lambda_{i+1}$ and stop the procedure. Otherwise, go to step 7.

7. If $f'(\lambda_{i+1}) \geq 0$, set new $B = \lambda_{i+1}, f'(B) = f'(\lambda_{i+1}), i = i + 1$, and go to step 5.
8. If $f'(\lambda_{i+1}) < 0$, set new $A = \lambda_{i+1}, f'(A) = f'(\lambda_{i+1}), i = i + 1$, and go to step 5.

Remarks:

1. The secand method is identical to assuming a linear equation for $f'(\lambda)$. This implies that the original function, $f(\lambda)$, is approximated by a quadratic equation.
2. In some cases we may encounter a situation where the function $f'(\lambda)$ varies very slowly with λ, as shown in Fig. 5.20. This situation can be identified by noticing that the point B remains unaltered for several consecutive refits. Once such a situation is suspected, the convergence process can be improved by taking the next value of λ_{i+1} as $(A + B)/2$ instead of finding its value from Eq. (5.74).

Example 5.14 Find the minimum of the function

$$f(\lambda) = 0.65 - \frac{0.75}{1 + \lambda^2} - 0.65\lambda \tan^{-1} \frac{1}{\lambda}$$

using the secant method with an initial step size of $t_0 = 0.1$, $\lambda_1 = 0.0$, and $\epsilon = 0.01$.

SOLUTION $\lambda_1 = A = 0.0$, $t_0 = 0.1$, $f'(A) = -1.02102$, $B = A + t_0 = 0.1$, $f'(B) = -0.744832$. Since $f'(B) < 0$, we set new $A = 0.1$, $f'(A) = -0.744832$, $t_0 = 2(0.1) = 0.2$, $B = \lambda_1 + t_0 = 0.2$, and compute $f'(B) = -0.490343$. Since $f'(B) < 0$, we set new $A = 0.2$, $f'(A) = -0.490343$, $t_0 = 2(0.2) = 0.4$, $B = \lambda_1 + t_0 = 0.4$, and compute $f'(B) = -0.103652$. Since $f'(B) < 0$, we set new $A = 0.4$, $f'(A) = -0.103652$, $t_0 = 2(0.4) = 0.8$, $B = \lambda_1 + t_0 = 0.8$, and compute $f'(B) = +0.180800$. Since $f'(B) > 0$, we proceed to find λ_2.

Iteration 1
Since $A = \lambda_1 = 0.4$, $f'(A) = -0.103652$, $B = 0.8$, $f'(B) = +0.180800$, we compute

$$\lambda_2 = A - \frac{f'(A)(B - A)}{f'(B) - f'(A)} = 0.545757$$

Convergence check: $|f'(\lambda_2)| = |+0.0105789| > \epsilon$.

Iteration 2
Since $f'(\lambda_2) = +0.0105789 > 0$, we set new $A = 0.4$, $f'(A) = -0.103652$, $B = \lambda_2 = 0.545757$, $f'(B) = f'(\lambda_2) = +0.0105789$, and compute

$$\lambda_3 = A - \frac{f'(A)(B - A)}{f'(B) - f'(A)} = 0.490632$$

Convergence check: $|f'(\lambda_3)| = |+0.00151235| < \epsilon$.

Since the process has converged, the optimum solution is given by $\lambda^* \approx \lambda_3 = 0.490632$.

5.13 PRACTICAL CONSIDERATIONS

5.13.1 How to Make the Methods Efficient and More Reliable

In some cases, some of the interpolation methods discussed in Sections 5.10 to 5.12 may be very slow to converge, may diverge, or may predict the minimum of the function, $f(\lambda)$, outside the initial interval of uncertainty, especially when the interpolating polynomial is not representative of the variation of the function being minimized. In such cases we can use the Fibonacci or golden section method to find the minimum. In some problems it might prove to be more efficient to combine several techniques. For example, the unrestricted search with an accelerated step size can be used to bracket the minimum and then the Fibonacci or the golden section method can be used to find the optimum point. In some cases the Fibonacci or golden section method can be used in conjunction with an interpolation method.

5.13.2 Implementation in Multivariable Optimization Problems

As stated earlier, the one-dimensional minimization methods are useful in multivariable optimization problems to find an improved design vector $\mathbf{X}_{i+1}$ from the current design vector $\mathbf{X}_i$ using the formula

$$\mathbf{X}_{i+1} = \mathbf{X}_i + \lambda_i^* \mathbf{S}_i \tag{5.76}$$

where $\mathbf{S}_i$ is the known search direction and λ_i^* is the optimal step length found by solving the one-dimensional minimization problem as

$$\lambda_i^* = \min_{\lambda_i} [f(\mathbf{X}_i + \lambda_i \mathbf{S}_i)] \tag{5.77}$$

Here the objective function f is to be evaluated at any trial step length t_0 as

$$f(t_0) = f(\mathbf{X}_i + t_0 \mathbf{S}_i) \tag{5.78}$$

Similarly, the derivative of the function f with respect to λ corresponding to the trial step length t_0 is to be found as

$$\left.\frac{df}{d\lambda}\right|_{\lambda = t_0} = \mathbf{S}_i^T \, \Delta f|_{\lambda = t_0} \tag{5.79}$$

Separate function programs or subroutines can be written conveniently to implement Eqs. (5.78) to (5.79).

5.13.3 Comparison of Methods

It has been shown in Section 5.9 that the Fibonacci method is the most efficient elimination technique in finding the minimum of a function if the initial interval of uncertainty is known. In the absence of the initial interval of uncertainty, the quadratic interpolation method or the quasi-Newton method is expected to be more efficient when the derivatives of the function are not available. When the first derivatives of the function being minimized are available, the cubic interpolation method or the secant method are expected to be very efficient. On the other hand, if both the first and second derivatives of the function are available, the Newton method will be the most efficient one in finding the optimal step length, λ^*.

In general, the efficiency and reliability of the various methods are problem dependent and any efficient computer program must include many heuristic additions not indicated explicitly by the method. The heuristic considerations are needed to handle multimodal functions (functions with multiple extreme points), sharp variations in the slopes (first derivatives) and curvatures (second derivatives) of the function, and the effects of round-off errors resulting from

the precision used in the arithmetic operations. A comparative study of the efficiencies of the various search methods is given in Ref. [5.10].

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REVIEW QUESTIONS

5.1 What is an one-dimensional minimization problem?

5.2 What are the limitations of classical methods in solving a one-dimensional minimization problem?

5.3 What is the difference between elimination and interpolation methods?

5.4 Define Fibonacci numbers.

5.5 What is the difference between Fibonacci and golden section methods?

5.6 What is a unimodal function?

5.7 What is an interval of uncertainty?

5.8 Suggest a method of finding the minimum of a multimodal function.

5.9 What is an exhaustive search method?

5.10 What is a dichotomous search method?

5.11 Define the golden mean.

5.12 What is the difference between quadratic and cubic interpolation methods?

5.13 Why is refitting necessary in interpolation methods?

5.14 What is a regula falsi method?

5.15 What is the basis of the interval halving method?

5.16 What is the difference between Newton and quasi-Newton methods?

5.17 What is the secant method?

5.18 Answer true or false.

(a) A unimodal function cannot be discontinuous.

(b) All elimination methods assume the function to be unimodal.

(c) The golden section method is more accurate than the Fibonacci method.

(d) Nearly 50% of the interval of uncertainty is eliminated with each pair of experiments in the dichotomous search method.

(e) The number of experiments to be conducted is to be specified beforehand in both the Fibonacci and golden section methods.

PROBLEMS

5.1 Find the minimum of the function

$$f(x) = 0.65 - \frac{0.75}{1 + x^2} - 0.65x \tan^{-1} \frac{1}{x}$$

using the following methods.

(a) Unrestricted search with a fixed step size of 0.1 from the starting point 0.0

(b) Unrestricted search with an accelerated step size using an initial step size of 0.1 and starting point of 0.0

(c) Exhaustive search method in the interval (0,3) to achieve an accuracy of within 5% of the exact value

(d) Dichotomous search method in the interval (0,3) to achieve an accuracy of within 5% of the exact value using a value of $\delta = 0.0001$

(e) Interval halving method in the interval (0,3) to achieve an accuracy of within 5% of the exact value

5.2 Find the minimum of the function given in Problem 5.1 using the quadratic interpolation method with an initial step size of 0.1.

5.3 Find the minimum of the function given in Problem 5.1 using the cubic interpolation method with an initial step size of $t_0 = 0.1$.

5.4 Plot the graph of the function $f(x)$ given in Problem 5.1 in the range (0,3) and identify its minimum.

5.5 The shear stress induced along the z-axis when two cylinders are in contact with each other is given by

$$\frac{\tau_{zy}}{p_{\max}} = -\frac{1}{2}\left[-\frac{1}{\sqrt{1+\left(\frac{z}{b}\right)^2}} + \left\{2 - \frac{1}{\left(1+\left(\frac{z}{b}\right)^2\right)}\right\} \cdot \sqrt{1+\left(\frac{z}{b}\right)^2} - 2\left(\frac{z}{b}\right)\right] \tag{1}$$

where $2b$ is the width of the contact area and $p_{\max}$ is the maximum pressure developed at the center of the contact area (Fig. 5.21):

$$b = \left(\frac{2F}{\pi l}\,\frac{\dfrac{1-\nu_1^2}{E_1} + \dfrac{1-\nu_2^2}{E_2}}{\dfrac{1}{d_1} + \dfrac{1}{d_2}}\right)^{1/2} \tag{2}$$

$$p_{\max} = \frac{2F}{\pi b l} \tag{3}$$

F is the contact force; E_1 and E_2 are Young's moduli of the two cylinders; ν_1 and ν_2 are Poisson's ratios of the two cylinders; d_1 and d_2 the diameters of the two cylinders, and l the axial length of contact (length of the shorter cylinder). In many practical applications, such as roller bearings, when the contact load (F) is large, a crack originates at the point of maximum shear stress and propagates to the surface leading to a fatigue failure. To locate the origin of a crack, it is necessary to find the point at which the shear stress attains its maximum value. Show that the problem of finding the location of the maximum shear stress for

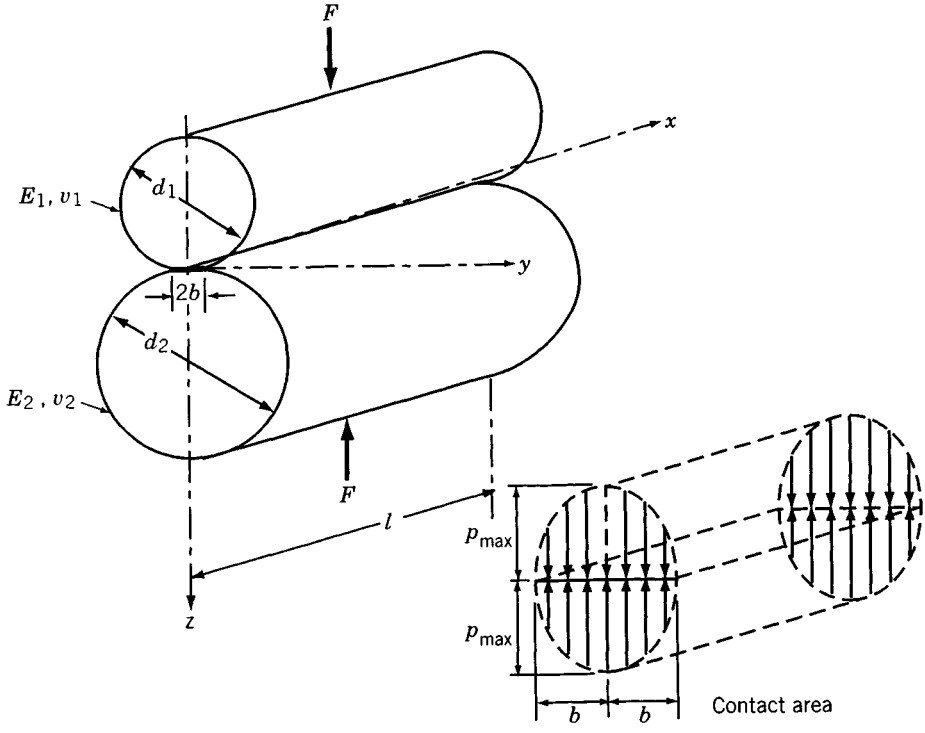

Figure 5.21 Contact stress between two cylinders.

$\nu_1 = \nu_2 = 0.3$ reduces to maximizing the function

$$f(\lambda) = \frac{0.5}{\sqrt{1 + \lambda^2}} - \sqrt{1 + \lambda^2}\left(1 - \frac{0.5}{1 + \lambda^2}\right) + \lambda \qquad (4)$$

where $f = \tau_{zy}/p_{max}$ and $\lambda = z/b$.

5.6 Plot the graph of the function $f(\lambda)$ given by Eq. (4) in Problem 5.5 in the range (0,3) and identify its maximum.

5.7 Find the maximum of the function given by Eq. (4) in Problem 5.5 using the following methods.

(a) Unrestricted search with a fixed step size of 0.1 from the starting point 0.0

(b) Unrestricted search with an accelerated step size using an initial step length of 0.1 and a starting point of 0.0

(c) Exhaustive search method in the interval (0,3) to achieve an accuracy of within 5% of the exact value

(d) Dichotomous search method in the interval (0,3) to achieve an accuracy of within 5% of the exact value using a value of $\delta = 0.0001$

(e) Interval halving method in the interval (0,3) to achieve an accuracy of within 5% of the exact value

5.8 Find the maximum of the function given by Eq. (4) in Problem 5.5 using the following methods.

(a) Fibonacci method with $n = 8$

(b) Golden section method with $n = 8$

5.9 Find the maximum of the function given by Eq. (4) in Problem 5.5 using the quadratic interpolation method with an initial step length of 0.1.

5.10 Find the maximum of the function given by Eq. (4) in Problem 5.5 using the cubic interpolation method with an initial step length of $t_0 = 0.1$.

5.11 Find the maximum of the function $f(\lambda)$ given by Eq. (4) in Problem 5.5 using the following methods.

(a) Newton method with the starting point 0.6

(b) Quasi-Newton method with the starting point 0.6 and a finite difference step size of 0.001

(c) Secant method with the starting point $\lambda_1 = 0.0$ and $t_0 = 0.1$

5.12 Prove that a convex function is unimodal.

5.13 Compare the ratios of intervals of uncertainty (L_n/L_0) obtainable in the following methods for $n = 2, 3, \ldots, 10$.

(a) Exhaustive search

(b) Dichotomous search with $\delta = 10^{-4}$

(c) Interval halving method

(d) Fibonacci method

(e) Golden section method

5.14 Find the number of experiments to be conducted in the following methods to obtain a value of $L_n/L_0 = 0.001$.

(a) Exhaustive search

(b) Dichotomous search with $\delta = 10^{-4}$

(c) Interval halving method

(d) Fibonacci method

(e) Golden section method

5.15 Find the value of x in the interval (0,1) which minimizes the function $f = x(x - 1.5)$ to within ± 0.05 by (a) the golden section method and (b) the Fibonacci method.

5.16 Find the minimum of the function $f = \lambda^5 - 5\lambda^3 - 20\lambda + 5$ by the following methods.

(a) Unrestricted search with a fixed step size of 0.1 starting from $\lambda = 0.0$

(b) Unrestricted search with accelerated step size from the initial point 0.0 with a starting step length of 0.1

(c) Exhaustive search in the interval (0,5)

(d) Dichotomous search in the interval (0,5) with $\delta = 0.0001$

(e) Interval halving method in the interval (0,5)

(f) Fibonacci search in the interval (0,5)

(g) Golden section method in the interval (0,5)

5.17 Find the minimum of the function $f = (\lambda/\log \lambda)$ by the following methods (take the initial trial step length as 0.1).

(a) Quadratic interpolation method

(b) Cubic interpolation method

5.18 Find the minimum of the function $f = \lambda/\log \lambda$ using the following methods.

(a) Newton method

(b) Quasi-Newton method

(c) Secant method

5.19 Consider the function

$$f = \frac{2x_1^2 + 2x_2^2 + 3x_3^2 - 2x_1x_2 - 2x_2x_3}{x_1^2 + x_2^2 + 2x_3^2}$$

Substitute $\mathbf{X} = \mathbf{X}_1 + \lambda\mathbf{S}$ into this function and derive an exact formula for the minimizing step length λ^*.

5.20 Minimize the function $f = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$ starting from the point $\mathbf{X}_1 = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix}$ along the direction $\mathbf{S} = \begin{Bmatrix} -1 \\ 0 \end{Bmatrix}$ using the quadratic interpolation method with an initial step length of 0.1.

5.21 Consider the problem:

$$\text{Minimize } f(\mathbf{X}) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

and the starting point, $\mathbf{X}_1 = \begin{Bmatrix} -1 \\ 1 \end{Bmatrix}$. Find the minimum of $f(\mathbf{X})$ along the direction, $\mathbf{S}_1 = \begin{Bmatrix} 4 \\ 0 \end{Bmatrix}$ using quadratic interpolation method. Use a maximum of two refits.

5.22 Solve Problem 5.21 using the cubic interpolation method. Use a maximum of two refits.

5.23 Solve Problem 5.21 using the direct root method. Use a maximum of two refits.

5.24 Solve Problem 5.21 using the Newton method. Use a maximum of two refits.

5.25 Solve Problem 5.21 using the Fibonacci method with $L_0 = (0,0.1)$.

5.26 Write a computer program, in the form of a subroutine, to implement the Fibonacci method.

5.27 Write a computer program, in the form of a subroutine, to implement the golden section method.

5.28 Write a computer program, in the form of a subroutine, to implement the quadratic interpolation method.

5.29 Write a computer program, in the form of a subroutine, to implement the cubic interpolation method.

5.30 Write a computer program, in the form of a subroutine, to implement the secant method.