APPROXIMATION THEORY AND APPROXIMATION PRACTICE

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Contents

1. Introduction

Welcome to a beautiful subject! — the constructive approximation of functions. And welcome to a rather unusual book.

Approximation theory is an established field, and our aim is to teach you some of its most important ideas and results. The style of this book, however, is quite different from what you will find elsewhere. Everything is illustrated computationally with the help of the Chebfun software package in Matlab, from Chebyshev interpolants to Lebesgue constants, from the Weierstrass Approximation Theorem to the Remez algorithm. Everything is practical and fast, so we will routinely compute polynomial interpolants or Gauss quadrature weights for tens of thousands of points. In fact, each chapter of this book is a single Matlab M-file, and the book has been produced by executing these files with Matlab's "publish" facility. The chapters come from M-files called `chap1.m`, `chap2.m`, ..., and you can download them and use them as templates to be modified for explorations of your own.

Beginners are welcome, and so are experts, who will find familiar topics approached from new angles and familiar conclusions turned on their heads. Indeed, the field of approximation theory came of age in an era of polynomials of degrees perhaps O(10). Now that O(1000) is easy and O(1,000,000) is not hard, different questions come to the fore. For example, we shall see that "best" approximants are hardly better than "near-best", though they are much harder to compute.

This is a book about approximation, not about Chebfun, and for the most part we shall use Chebfun tools with minimal explanation. For information about Chebfun, see `www.maths.ox.ac.uk/chebfun`. In the course of the book we shall use Chebfun overloads of the following Matlab functions, among others:

```
CONV, CUMSUM, DIFF, INTERP1, NORM, POLY, POLYFIT, ROOTS, SPLINE
```

as well as additional Chebfun commands such as

```
CF, CHEBELLIPSEPLOT, CHEBPADE, CHEBPOLY, CHEBPOLYPLOT,
CHEBPOLYVAL, CHEBPTS, LEBESGUE, LEGPOLY, LEGPTS, RATINTERP,
REMEZ.
```

There are quite a number of excellent books on approximation theory. Three classics are [Cheney 1966], [Davis 1963], and [Meinardus 1967], and a more recent computationally oriented classic is [Powell 1981]. The first approximation theory text was perhaps [Borel 1905].

A good deal of our emphasis will be on ideas related to Chebyshev points and polynomials, whose roots go back a century or more to mathematicians including Chebyshev (1821–1894), de la Vallée Poussin (1866–1962), Bernstein (1880–1968), and Dunham Jackson (1888–1946). In the computer era, some of the early

figures who developed "Chebyshev technology," in approximately chronological order, were Lanczos, Clenshaw, Specht, Good, Babenko, Fox, Elliott, Mason, Lebedev, and Orszag. Three books on Chebyshev polynomials are by Fox and Parker [1968], Rivlin [1990], and Mason and Handscomb [2003]. One reason we emphasize Chebyshev technology so much is that in practice, for working with functions on intervals, these methods are unbeatable. For example, we shall see in Chapter 16 that the difference in approximation power between Chebyshev and "optimal" interpolation points is utterly negligible. Another reason is that if you know the Chebyshev material well, this is the best possible foundation for work on other approximation topics.

Our style is conversational, but that doesn't mean the material is all elementary. The book aims to be more readable than most, and the numerical experiments help achieve this. At the same time, theorems are stated and proofs are given, often rather tersely, without all the details spelled out. It is assumed that the reader is comfortable with rigorous mathematical arguments and familiar with ideas like continuous functions on compact sets, Lipschitz continuity, contour integrals in the complex plane, and norms of operators. If you are a student, I hope you are an advanced undergraduate or graduate who has taken courses in numerical analysis and complex analysis. If you are a seasoned mathematician, I hope you are also a Matlab user!

Each chapter has a collection of exercises, which span a wide range from mathematical theory to Chebfun-based numerical experimentation. Do not skip the numerical exercises! If you are going to do that, you might as well put this book aside and read one of the classics from the 1960s.

The book was produced using `publish` in LaTeX mode: thus this chapter, for example, can be generated with the command `publish('chap1','latex')`. To achieve the desired layout we begin by setting a few default parameters:

```
set(0,'defaultfigureposition',[380 320 540 200],...
'defaultaxeslinewidth',0.9,'defaultaxesfontsize',8,...
'defaultlinelinewidth',1.1,'defaultpatchlinewidth',1.1,...
'defaultlinemarkersize',15), format compact, format long
FS='fontsize'; MS='markersize'; LW='linewidth'; CO='color';
chebfunpref('factory'); x = chebfun('x');
```

To make the chapters independently executable, it is necessary to include these statements at the beginning of each. This would lead to a clutter of text, so instead, at the beginning of each chapter we execute the command

```
ATAPformats
```

which calls an M-file containing the code above that is included in the standard distribution of Chebfun. For the actual production of the printed book, `publish` was executed not chapter-by-chapter but on a big file concatenating all the

chapters, and a few tweaks were made to the resulting LaTeX file, including the elimination of the `ATAPformats` calls so that they do not appear in this printed book.

The Lagrange interpolation formula was discovered by Waring, the Gibbs phenomenon was discovered by Wilbraham, and the Hermite integral formula is due to Cauchy. These are just some of the instances of Stigler's Law in approximation theory, and I have taken special pains in this book to try to cite the originator of each of the main ideas. Thus the entries in the references section stretch back several centuries, and each has an editorial comment attached. Often the original papers are surprisingly readable and insightful, at least if you are comfortable with French or German, and in any case, it seems particularly important to pay heed to original sources in a book like this that aims to reexamine material that has grown too standardized in the textbooks. Another reason for looking at original sources is that in the last few years it has become far easier to track them down, thanks to the digitization of journals, though there are always difficult special cases like [Wilbraham 1848], which I finally found in an elegant leather-bound volume in the Balliol College library. No doubt I have missed originators of certain ideas, and I would be glad to be corrected on such points by readers.

Perhaps I may add a further personal comment. As an undergraduate and graduate student in the late 1970s and early 1980s, one of my main interests was approximation theory. I regarded this subject as the foundation of my wider field of numerical analysis, but as the years passed, research in approximation theory came to seem dry and academic, and I moved into other areas. Now times have changed, computers have changed, and my perceptions have changed. I now again regard approximation theory as exceedingly close to computing, and in this book we shall discuss many practical numerical problems including interpolation, quadrature, rootfinding, analytic continuation, extrapolation of sequences and series, and the solution of differential equations.

Why is approximation theory useful? The answer goes much further than the rather tired old fact that your computer relies on approximations to evaluate functions like $\sin(x)$ and $\exp(x)$. For my personal answer to the question, take a look at the last three pages of Chapter 23, beginning with the quotes of Runge and Kirchberger from the beginning of the 20th century.

In summary, here are some distinctive features of this book:

- The emphasis is on topics close to numerical algorithms.
- Everything is illustrated numerically with Chebfun.
- Each chapter is a publishable M-file, available online.
- There is a bias toward theorems and methods for analytic functions, which appear so often in applications, rather than on functions at the edge of

discontinuity with their seductive theoretical challenges.

- Original sources are cited wherever possible, and each item in the bibliography is listed with an editorial comment.

At the more detailed level, virtually every chapter contains mathematical and scholarly novelties. Examples are the use of barycentric formulas in Chapter 5 and elsewhere, the tracing of barycentric formulas and the Hermite integral formula back to Jacobi in 1825 and Cauchy in 1826, Theorem 7.1 on the size of Chebyshev coefficients, the introduction to potential theory in Chapter 12, the discussion in Chapter 14 of prevailing misconceptions about interpolation, the presentation of colleague matrices for rootfinding in Chapter 18 with Jacobi matrices for quadrature as a special case in Chapter 19, Theorem 19.5 showing that Clenshaw–Curtis quadrature often converges about as fast as Gauss quadrature, the first textbook presentation of Carathódory–Fejér approximation in Chapter 20, the explanation in Chapter 22 of why polynomials are not optimal functions for linear approximation, the extensive discussion in Chapter 23 of the uses of rational approximations, and the SVD-based derivation of robust rational interpolation and Padé approximation in Chapters 26 and 27.

All in all, we shall see that there is scarcely an idea in classical approximation theory that cannot be illustrated compellingly in a few lines of Chebfun code, and as I first imagined around 1975, anyone who wants to be expert at numerical computation really does need to know this material.

Exercise 1.1. Chebfun download. Download Chebfun from `www.maths.ox.ac.uk/chebfun` and install it in your Matlab path as instructed at the web site. Execute the command `chebtest` to make sure things are working, and note the time taken. Execute `chebtest` again and see how much speedup there is now that various files have been brought into memory. Now read Chapter 1 of the Chebfun Guide.

Exercise 1.2. The publish command. Execute `help publish` and `doc publish` in Matlab to learn the basics of how the `publish` command works. Then download the files `chap1.m` and `chap2.m` from `www.maths.ox.ac.uk/chebfun/ATAP` and publish them with `publish('chap1','latex')` followed by appropriate LaTeX commands. (You will probably find that `chap1.tex` and `chap2.tex` appear in a subdirectory on your computer labeled `html`.) If you are a student taking a course for which you are expected to turn in writeups of the exercises, I recommend that you make it your habit to produce them with `publish`.

Exercise 1.3. Textbook X. Buy or borrow a copy of an approximation theory textbook, which we shall call X; good examples are the books of Achieser, Cheney, Davis, Lorentz, Natanson, Meinardus, Powell, Rice, Rivlin, and Timan listed in the References. As you work through *Approximation Theory and Approximation Practice*, keep X at your side and get in the habit of comparing treatments of each topic between *ATAP* and X. (a) What are the author, title, and publication date of X? (b) Where did/does the author work and what were/are his/her dates? (c) Look at the first three theorems in X and write down one of them that interests you. You do not have to write down the proof.

2. Chebyshev points and interpolants

Any interval $[a, b]$ can be scaled to $[-1, 1]$, so most of the time, we shall just talk about $[-1, 1]$.

Let n be a positive integer:

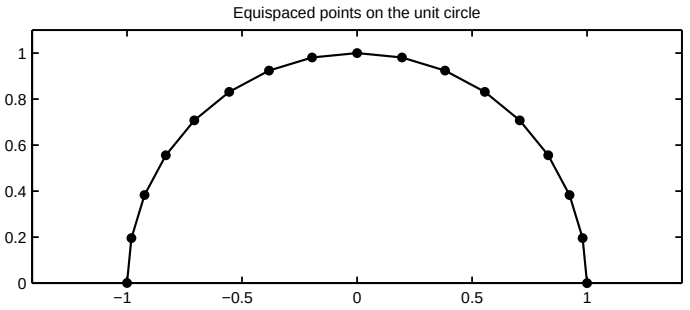
```
n = 16;
```

Consider $n+1$ equally spaced angles $\{\theta_j\}$ from 0 to π:

```
tt = linspace(0,pi,n+1);
```

We can think of these as the arguments of $n+1$ points $\{z_j\}$ on the upper half of the unit circle in the complex plane. These are the $(2n)$th roots of unity lying in the closed upper half-plane:

```
zz = exp(1i*tt);
hold off, plot(zz,'.-k'), axis equal, ylim([0 1.1])
title('Equispaced points on the unit circle')
```



The **Chebyshev points** associated with the parameter n are the real parts of these points,

$$x_j = \mathrm{Re}\, z_j = \frac{1}{2}(z_j + z_j^{-1}), \quad 0 \le j \le n : \tag{2.1}$$

```
xx = real(zz);
```

Some authors use the terms **Chebyshev–Lobatto points**, **Chebyshev extreme points**, or **Chebyshev points of the second kind**, but as these are the points most often used in practical computation, we shall just say Chebyshev points.

Another way to define the Chebyshev points is in terms of the original angles:

$$x_j = \cos(j\pi/n), \quad 0 \le j \le n, \tag{2.2}$$

```
xx = cos(tt);
```

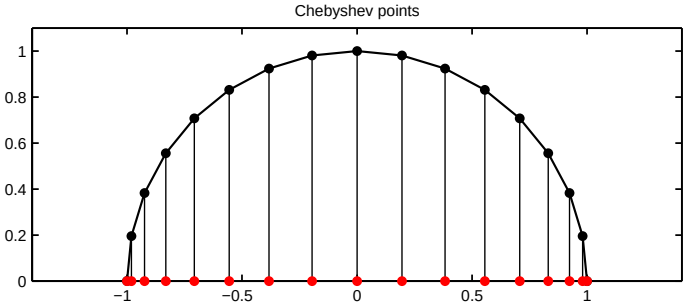
There is also an equivalent Chebfun command `chebpts`:

```
xx = chebpts(n+1);
```

Actually this result isn't exactly equivalent, as the ordering is left-to-right rather than right-to-left. Concerning rounding errors when these numbers are calculated numerically, see Exercise 2.3.

Let us add the Chebyshev points to the plot:

```
hold on
for j = 2:n
  plot([xx(n+2-j) zz(j)],'k',LW,0.7)
end
plot(xx,0*xx,'.r'), title('Chebyshev points')
```



They cluster near 1 and -1, with the average spacing as $n \to \infty$ being given by a density function with square root singularities at both ends (Exercise 2.2).

Let $\{f_j\}$, $0 \le j \le n$, be a set of numbers, which may or may not come from sampling a function $f(x)$ at the Chebyshev points. Then there exists a unique polynomial p of degree n that interpolates these data, i.e., $p(x_j) = f_j$ for each j. When we say "of degree n," we mean of degree less than or equal to n, and we let P_n denote the set of all such polynomials:

$$P_n = \{\text{polynomials of degree at most } n\}. \tag{2.3}$$

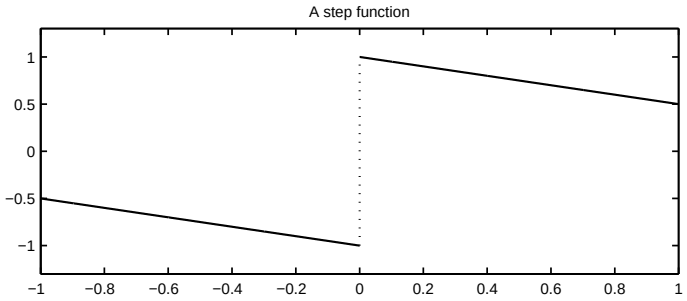
As we trust the reader already knows, the existence and uniqueness of polynomial interpolants applies for any distinct set of interpolation points. In the case of Chebyshev points, we call the polynomial the **Chebyshev interpolant**.

Polynomial interpolants through equally spaced points have terrible properties, as we shall see in Chapters 11–15. Polynomial interpolants through Chebyshev

points, however, are excellent. It is the clustering near the ends of the interval that makes the difference, and other sets of points with similar clustering, like Legendre points (Chapter 17), have similarly good behavior. The explanation of this fact has a lot to do with potential theory, a subject we shall introduce in Chapter 12. Specifically, what makes Chebyshev or Legendre points effective is that each one has approximately the same distance from the others, on average as measured in the sense of the geometric mean. On the interval $[-1, 1]$, this distance is about $1/2$ (Exercise 2.6).

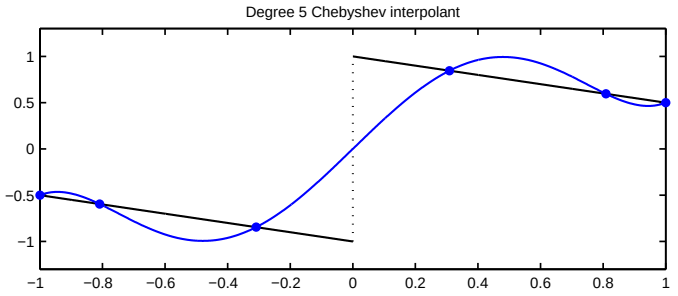
Chebfun is built on Chebyshev interpolants. For example, here is a certain step function:

```
x = chebfun('x');
f = sign(x) - x/2;
hold off, plot(f,'k'), ylim([-1.3 1.3])
title('A step function')
```



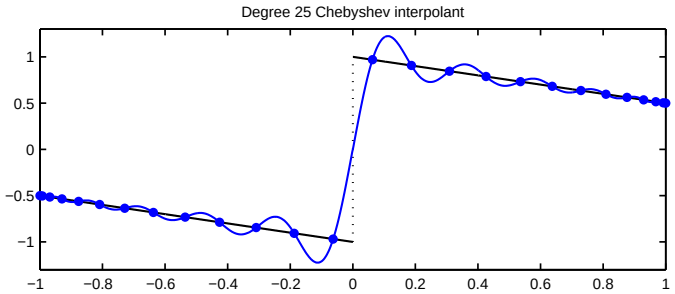
By calling `chebfun` with a second explicit argument of 6, we can construct the Chebyshev interpolant to f through 6 points, that is, of degree 5:

```
p = chebfun(f,6);
hold on, plot(p,'.-'), ylim([-1.3 1.3])
title('Degree 5 Chebyshev interpolant')
```



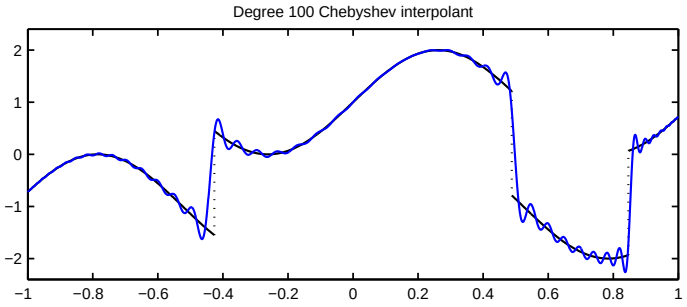
Similarly, here is the Chebyshev interpolant of degree 25:

```
hold off, plot(f,'k')
p = chebfun(f,26);
hold on, plot(p,'.-'), ylim([-1.3 1.3])
title('Degree 25 Chebyshev interpolant')
```



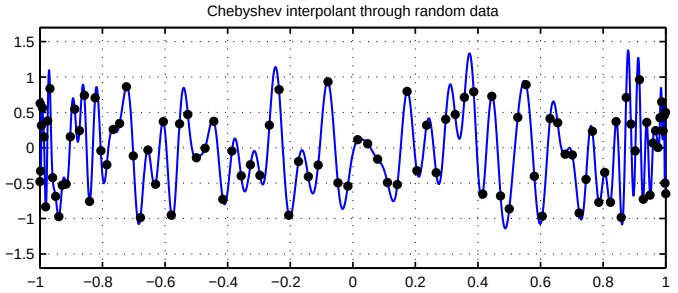
Here are a more complicated function and its Chebyshev interpolant of degree 100:

```
f = sin(6*x) + sign(sin(x+exp(2*x)));
hold off, plot(f,'k')
p = chebfun(f,101);
hold on, plot(p), ylim([-2.4 2.4])
title('Degree 100 Chebyshev interpolant')
```



Another way to use the `chebfun` command is by giving it an explicit vector of data rather than a function to sample, in which case it interprets the vector as data for a Chebyshev interpolant of the appropriate order. Here for example is the interpolant of degree 99 through 100 random data values in $[-1,1]$:

```
p = chebfun(2*rand(100,1)-1);
hold off, plot(p,'-')
hold on, plot(p,'.k')
ylim([-1.7 1.7]), grid on
title('Chebyshev interpolant through random data')
```



This experiment illustrates how robust Chebyshev interpolation is. If we had taken a million points instead of 100, the result would not have been much different mathematically, though it would have been a mess to plot. We shall return to this figure in Chapter 15.

For illustrations like these it is interesting to pick data with jumps or wiggles, and Chapter 9 discusses such interpolants systematically. In applications where polynomial interpolants are most useful, however, the data will typically be smooth.

SUMMARY OF CHAPTER 2. *Polynomial interpolants in equispaced points in* $[-1,1]$ *have very poor approximation properties, but polynomial interpolants in Chebyshev points, which cluster near* ± 1*, are excellent.*

Exercise 2.1. Chebyshev interpolants through random data. (a) Repeat the experiment of interpolation through random data for 10, 100, 1000, and 10000 points. In each case use `minandmax(p)` to determine the minimum and maximum values of the interpolant and measure the computer time required for this computation (e.g. using `tic` and `toc`). You may find it helpful to increase Chebfun's standard plotting resolution with a command like `plot(p,'numpts',10000)`. (b) In addition to the four plots over $[-1,1]$, use `plot(p,'.-','interval',[0.9999 1])` to produce another plot of the interpolant through 10000 values in the interval $[0.9999,1]$. How many of the 10000 grid points fall in this interval?

Exercise 2.2. Limiting density as $n \to \infty$. (a) Suppose $x_0,\dots,x_n$ are $n+1$ points equally spaced from -1 to 1. If $-1 \le a < b \le 1$, what fraction of the $n+1$ points fall in the interval $[a,b]$ in the limit $n \to \infty$? Give an exact formula. (b) Give the analogous formula for the case where $x_0,\dots,x_n$ are the Chebyshev points. (c) How does the result of (b) match the number found in $[0.9999,1]$ in the last exercise for the case $n = 9999$? (d) Derive the following formula for the density of the Chebyshev

points near $x \in (-1,1)$ in the limit $n \to \infty$: $\mu(x) = (\pi\sqrt{1-x^2})^{-1}$ (see equation (12.8)).

Exercise 2.3. Rounding errors in computing Chebyshev points. On a computer in floating point arithmetic, the formula (2.2) for the Chebyshev points is not so good because it lacks the expected symmetries. (a) Write a Matlab program that finds the smallest even value $n \geq 2$ for which, on your computer as computed by this formula, $x_{n/2} \neq 0$. (You will probably find that $n = 2$ is the first such value.) (b) Find the line in the code `chebfun/chebpts.m` in which Chebfun computes Chebyshev points. What alternative formula does it use? Explain why this formula achieves perfect symmetry for all n in floating point arithmetic. (c) Show that this formula is mathematically equivalent to (2.2).

Exercise 2.4. Chebyshev points of the first kind. The Chebyshev points of the first kind, also known as **Gauss–Chebyshev points**, are obtained by taking the real parts of points on the unit circle mid-way between those we have considered, i.e. $x_j = \cos((j+\frac{1}{2})\pi/(n+1))$ for integers $0 \leq j \leq n$. Call `help chebpts` and `help legpts` to find out how to generate these points in Chebfun and how to generate Legendre points for comparison (these are roots of Legendre polynomials — see Chapter 17). For $n+1 = 100$, what is the maximum difference between a Chebyshev point of the first kind and the corresponding Legendre point? Draw a plot to illustrate as informatively as you can how close these two sets of points are.

Exercise 2.5. Convergence of Chebyshev interpolants. (a) Use Chebfun to produce a plot on a log scale of $\|f - p_n\|$ as a function of n for $f(x) = e^x$ on $[-1,1]$, where p_n is the Chebyshev interpolant in P_n. Take $\|\cdot\|$ to be the supremum norm, which can be computed by `norm(f-p,inf)`. How large must n be for accuracy at the level of machine precision? What happens if n is increased beyond this point? (b) Same questions for $f(x) = 1/(1+25x^2)$. Convergence rates like these will be analyzed in Chapters 7 and 8.

Exercise 2.6. Geometric mean distance between points. Write a code `meandistance` which takes as input a vector of points $x_0, \ldots, x_n$ in $[-1,1]$ and produces a plot with x_j on the x axis and the geometric mean distance of x_j to the other points on the y axis. (That Matlab command `prod` may be useful.) (a) What are the results for Chebyshev points with $n = 5, 10, 20$? (b) Same for Legendre points (see Exercise 2.4). (c) Same for equally spaced points from $x_0 = -1$ to $x_n = 1$.

Exercise 2.7. Chebyshev points scaled to an interval $[a,b]$. (a) Use `chebpts(10)` to print the values of the Chebyshev points in $[-1,1]$ for $n = 9$. (b) Use `chebfun(@sin,10)` to compute the degree 9 interpolant $p(x)$ to $\sin(x)$ in these points. Make a plot showing $p(x)$ and $\sin(x)$ over the larger interval $[-6,6]$, and also a semilog plot of $|f(x) - p(x)|$ over that interval. Comment on the results. (c) Now use `chebpts(10,[0 6])` to print the values of the Chebyshev points for $n = 9$ scaled to the interval $[0,6]$. (d) Use `chebfun(@sin,[0 6],10)` to compute the degree 9 interpolant to $\sin(x)$ in these points, and make the same two plots as before over $[-6,6]$. Comment.

3. Chebyshev polynomials and series

One good way to specify a polynomial $p \in P_n$ on $[-1,1]$, as we saw in the last chapter, is by its values at $n+1$ Chebyshev points. Another is by its

coefficients in a **Chebyshev expansion**, that is, a linear combination of the Chebyshev polynomials $T_0, \ldots, T_n$. Depending on the application, one or the other of these two representations may be most useful, and one can go back and forth between them quickly with an algorithm based on the Fast Fourier Transform (FFT). This duality is analogous to the well-known relationship between "function space" and "Fourier space" in discrete Fourier analysis.

In (2.1) and (2.2) we defined Chebyshev points as the real parts of equally spaced points on the unit circle. Similarly, the kth **Chebyshev polynomial** can be defined as the real part of the function z^k on the unit circle:

$$x = \mathrm{Re}(z) = \tfrac{1}{2}(z + z^{-1}) = \cos\theta, \quad \theta = \cos^{-1} x, \tag{3.1}$$

$$T_k(x) = \mathrm{Re}(z^k) = \tfrac{1}{2}(z^k + z^{-k}) = \cos(k\theta). \tag{3.2}$$

Chebyshev polynomials were introduced by Chebyshev in the 1850s, though without the connection to the variables z and θ [Chebyshev 1854 & 1859]. The reason they are labelled by the letter T is probably that Chebyshev, de la Vallée Poussin, Bernstein, and other early experts published in French, and the French transliteration of the Russian name is Tchebychef. The Chebyshev polynomials are a family of orthogonal polynomials with respect to a certain weight function (Exercise 3.7), but we shall not make much use of orthogonality until Chapters 17–19.

It follows from (3.2) that T_k satisfies $-1 \leq T_k(x) \leq 1$ for $x \in [-1,1]$ and takes alternating values ± 1 at the $k+1$ Chebyshev points. What is not so obvious is that T_k is a polynomial. We can verify this property by induction. For example, we can calculate $T_2(x)$ like this:

$$T_2(x) = \tfrac{1}{2}(z^2 + z^{-2}) = \tfrac{1}{2}(z + z^{-1})^2 - 1 = 2x^2 - 1.$$

Similarly we calculate

$$T_3(x) = \tfrac{1}{2}(z^3 + z^{-3}) = \tfrac{1}{2}(z + z^{-1})(z^2 + z^{-2}) - \tfrac{1}{2}(z^1 + z^{-1}) = 2xT_2(x) - T_1(x),$$

so $T_3(x) = 4x^3 - 3x$. A further similar calculation gives the general formula

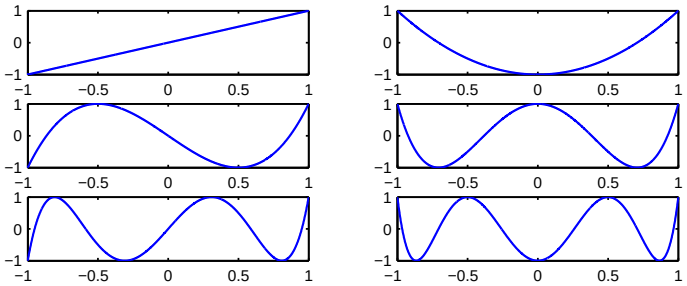
$$T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x), \tag{3.3}$$

implying that for each $k \geq 1$, T_k is a polynomial of degree exactly k with leading coefficient 2^{k-1}. In Chapter 18 the coefficients of this 3-term recurrence relation will be taken as the entries of a "colleague matrix" whose eigenvalues can be computed to find roots of polynomials or quadrature nodes.

The Chebfun command `chebpoly(n)` returns the chebfun corresponding to T_n.[1] Here for example are $T_1, \ldots, T_6$:

[1] The name of the software system is Chebfun, with a capital C. A representation of a particular function in Chebfun is called a chebfun, with a lower-case c.

```
for n = 1:6
    T{n} = chebpoly(n);
    subplot(3,2,n)
    plot(T{n}), axis([-1 1 -1 1])
end
```



These plots do not show the Chebyshev points, which are the extremes of each curve: thus the numbers of Chebyshev points in the six plots are 2, 3, 4, 5, 6, and 7.

Here are the coefficients of these polynomials with respect to the monomial basis $1, x, x^2, \ldots$. As usual, Matlab orders coefficients from highest degree down to degree zero.

```
for n = 1:6
    disp(poly(T{n}))
end
     1     0
     2     0    -1
     4     0    -3     0
     8     0    -8     0     1
    16     0   -20     0     5     0
    32     0   -48     0    18     0    -1
```

So, for example,

$$T_5(x) = 16x^5 - 20x^3 + 5x.$$

The monomial basis is familiar and comfortable, but you should never use it for numerical work with functions on an interval. Use the Chebyshev basis instead (Exercise 3.8). (If the domain is $[a, b]$ rather than $[-1, 1]$, the Chebyshev polynomials must be scaled accordingly, and Chebfun does this automatically when one works on other intervals.) For example, x^5 has the Chebyshev expansion

$$x^5 = \frac{5}{80}T_5(x) + \frac{5}{16}T_3(x) + \frac{5}{8}T_1(x).$$

We can calculate such expansion coefficients by using the command `chebpoly(p)`, where p is the chebfun whose coefficients we want to know:


```
format short
chebpoly(x.^5)

ans =
    0.0625         0    0.3125         0    0.6250         0
```

Any polynomial p can be written uniquely like this as a finite Chebyshev series: the functions $T_0(x), T_1(x), \ldots, T_n(x)$ form a *basis* for P_n. Since p is determined by its values at Chebyshev points, it follows that there is a one-to-one linear mapping between values at Chebyshev points and Chebyshev expansion coefficients. As mentioned at the beginning of this chapter, this mapping can be applied in $O(n \log n)$ operations with the aid of the Fast Fourier Transform (FFT) or the Fast Cosine Transform, an observation perhaps first made by Ahmed and Fisher and Orzsag around 1970 [Ahmed & Fisher 1970, Orszag 1971a and 1971b, Gentleman 1972b, Geddes 1978]. That is what Chebfun does when you type `chebpoly`. We shall not give details of the FFT in this book; see for example [Trefethen 2000, Chap. 8].

Just as a polynomial p has a finite Chebyshev series, a more general function f has an infinite Chebyshev series. Exactly what kind of "more general function" can we allow? For an example like $f(x) = e^x$ with a rapidly converging Taylor series, everything will surely be straightforward, but what if f is merely differentiable rather than analytic? Or what if it is continuous but not differentiable? Analysts have studied such cases carefully, identifying exactly what degrees of smoothness correspond to what kinds of convergence of Chebyshev series. We shall not concern ourselves with trying to state the sharpest possible result but will just make a particular assumption that covers almost every application. We shall assume that f is **Lipschitz continuous** on $[-1, 1]$. Recall that this means that there is a constant C such that $|f(x) - f(y)| \le C|x - y|$ for all $x, y \in [-1, 1]$. Recall also that a series is **absolutely convergent** if it remains convergent if each term is replaced by its absolute value, and that this implies that one can reorder the terms arbitrarily without changing the result. Such matters are discussed in books of advanced calculus such as [Kreyszig 2007].

Here is our basic theorem about Chebyshev series and their coefficients.

Theorem 3.1: Chebyshev series. *If f is Lipschitz continuous on $[-1, 1]$, it has a unique representation as an absolutely and uniformly convergent series*

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x), \tag{3.4}$$

and the coefficients are given for $k \ge 1$ by the formula

$$a_k = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x)T_k(x)}{\sqrt{1 - x^2}} dx, \tag{3.5}$$

and for $k = 0$ by the same formula with the factor $2/\pi$ changed to $1/\pi$.

Proof. Throughout this book, our approach to all kinds of results involving Chebyshev polynomials will always be the same: transplant them to the unit circle in the complex plane, where they become results involving powers of z. Integrals over $[-1,1]$ transplant to integrals over the unit circle, where one can generally get the results one wants from the Cauchy integral formula. This method of dealing with Chebyshev mathematics has the advantage that one never has to remember any trigonometric identities!

Here is how it goes for Chebyshev series and their coefficients. We are given a function $f(x)$ on $[-1,1]$. We transplant f by defining a function F on the unit circle whose value at a point z on the circle is the same as the value of f at the corresponding point $x \in [-1,1]$. In other words, $F(z) = F(z^{-1}) = f(x)$, where $x = \mathrm{Re}\, z = (z + z^{-1})/2$. Notice that each value $x \in (-1,1)$ corresponds to two different values z on the unit circle, one on the upper semicircle and the other on the lower semicircle.

To convert between integrals in x and z, we have to convert between dx and dz. We can do this by differentiating the formula for x to get

$$dx = \tfrac{1}{2}(1 - z^{-2})\, dz = \tfrac{1}{2} z^{-1}(z - z^{-1})\, dz.$$

Since

$$\tfrac{1}{2}(z - z^{-1}) = i\, \mathrm{Im}\, z = \pm i\sqrt{1 - x^2},$$

this implies

$$dx = \pm i\, z^{-1} \sqrt{1 - x^2}\, dz.$$

In these equations the plus sign applies for $\mathrm{Im}\, z \geq 0$ and the minus sign for $\mathrm{Im}\, z \leq 0$.

These formulas have implications for smoothness. Since $\sqrt{1 - x^2} \leq 1$ for all $x \in [-1,1]$, they imply that if $f(x)$ is Lipschitz continuous, then so is $F(z)$. By a standard result in complex variables, this implies that F has a unique representation as an absolutely and uniformly convergent Laurent series on the unit circle,

$$F(z) = \frac{1}{2} \sum_{k=0}^{\infty} a_k (z^k + z^{-k}) = \sum_{k=0}^{\infty} a_k T_k(x).$$

Recall that a **Laurent series** is an infinite series in both positive and negative powers of z, and that such series in general converge in the interior of an annulus. A good treatment of Laurent series can be found in [Markushevich 1985]; see also complex variables texts such as [Priestley 2003, Saff & Snider 2003]. Or one can derive results about F by converting them to results about Fourier series, for the Laurent series for F is equivalent to a Fourier series in the variable θ if $z = e^{i\theta}$.

The kth Laurent coefficient of an analytic function $G(z) = \sum_{k=-\infty}^{\infty} b_k z^k$ on the unit circle can be computed by the Cauchy integral formula,

$$b_k = \frac{1}{2\pi i} \int_{|z|=1} z^{-1-k} G(z)\, dz.$$

(We shall make more substantial use of the Cauchy integral formula in Chapters 11–12.) The notation $|z| = 1$ indicates that the contour consists of the unit circle traversed once in the positive (counterclockwise) direction. Here we have a function F with the special symmetry property $F(z) = F(z^{-1})$, and we have also introduced a factor $1/2$ in front of the series. Accordingly in the case of F we can compute the coefficients a_k from either of two contour integrals,

$$a_k = \frac{1}{\pi i} \int_{|z|=1} z^{-1+k} F(z)\, dz = \frac{1}{\pi i} \int_{|z|=1} z^{-1-k} F(z)\, dz, \tag{3.6}$$

with πi replaced by $2\pi i$ for $k = 0$.

In particular, we can get a formula for a_k that is symmetric in k and $-k$ by combining the two integrals like this:

$$a_k = \frac{1}{2\pi i} \int_{|z|=1} (z^{-1+k} + z^{-1-k}) F(z)\, dz = \frac{1}{\pi i} \int_{|z|=1} z^{-1}\, T_k(x) F(z)\, dz,$$

with πi replaced by $2\pi i$ for $k = 0$. Replacing $F(z)$ by $f(x)$ and $z^{-1}dz$ by $-i\, dx/(\pm\sqrt{1 - x^2})$ gives

$$a_k = -\frac{1}{\pi} \int_{|z|=1} \frac{f(x) T_k(x)}{\pm\sqrt{1 - x^2}}\, dx,$$

with π replaced by 2π for $k = 0$. We have now almost entirely converted to the x variable, except that the contour of integration is still the circle $|z| = 1$. When z traverses the circle all the way around in the positive direction, x decreases from 1 to -1 and then increases back to 1 again. At the turning point $z = x = -1$, the $\pm$ sign attached to the square root switches from $+$ to $-$. Thus instead of cancelling, the two traverses of $x \in [-1,1]$ contribute equal halves to a_k. Converting to a single integration from -1 to 1 in the x variable multiplies the integral by $-1/2$, hence multiplies the formula for a_k by -2, giving (3.5). ∎

Chebfun represents functions by their values at Chebyshev points. How does it figure out the right value of n? Given a set of $n + 1$ samples, it converts the data to a Chebyshev expansion of degree n and examines the resulting Chebyshev coefficients. If several of these in a row fall below a relative level of approximately 10^{-15}, then the grid is judged to be fine enough. For example, here are the Chebyshev coefficients of the chebfun corresponding to e^x:

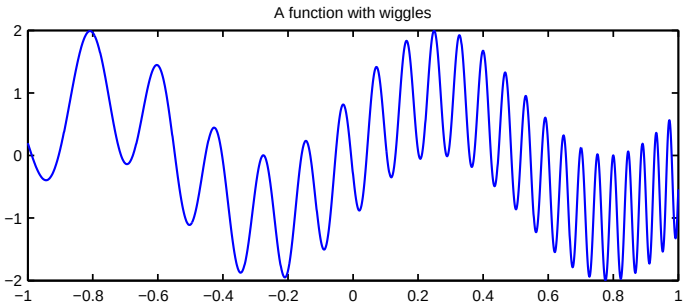
```
f = exp(x);
a = chebpoly(f);
format long
a(end:-1:1)'
```

```
ans =
   1.266065877752008
   1.130318207984970
   0.271495339534077
   0.044336849848664
   0.005474240442094
   0.000542926311914
   0.000044977322954
   0.000003198436462
   0.000000199212481
   0.000000011036772
   0.000000000550590
   0.000000000024980
   0.000000000001039
   0.000000000000040
   0.000000000000001
```

Notice that the last coefficient is about at the level of machine precision.

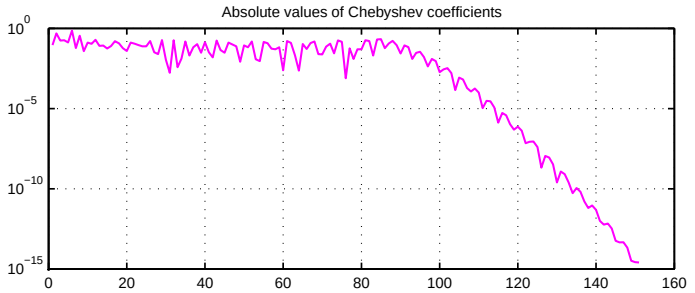
For complicated functions it is often more interesting to plot the coefficients than to list them. For example, here is a function with a number of wiggles:

```
f = sin(6*x) + sin(60*exp(x));
clf, plot(f), title('A function with wiggles')
```



If we plot the absolute values of the Chebyshev coefficients, here is what we find:

```
a = chebpoly(f);
semilogy(abs(a(end:-1:1)),'m')
grid on, title('Absolute values of Chebyshev coefficients')
```

One can explain this plot as follows. Up to degree about $k = 80$, a Chebyshev series cannot resolve f accurately, for the oscillations occur on too short wavelengths. After that, the series begins to converge rapidly. By the time we reach $k = 150$, the accuracy is about 15 digits, and the computed Chebyshev series is truncated there. We can find out exactly where the truncation took place with the command `length(f)`:

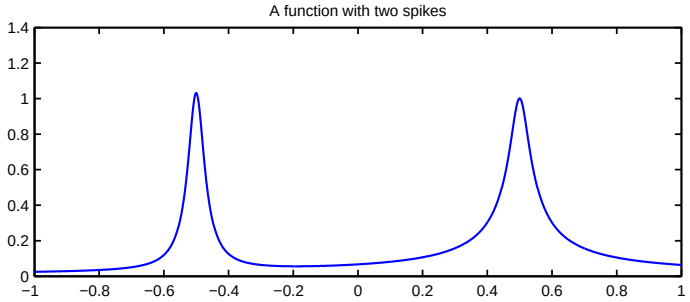
```
length(f)

ans = 151
```

This tells us that the chebfun is a polynomial interpolant through 151 points, that is, of degree 150.

Without giving all the engineering details, here is a fuller description of how Chebfun constructs its approximation. First it calculates the polynomial interpolant through the function sampled at 9 Chebyshev points, i.e., a polynomial of degree 8, and checks whether the Chebyshev coefficients appear to be small enough. For the example just given the answer is no. Then it tries 17 points, then 33, then 65, and so on. In this case Chebfun judges at 257 points that the Chebyshev coefficients have finally fallen to the level of rounding error. At this point it truncates the tail of terms deemed to be negligible, leaving a series of 151 terms. The corresponding degree 150 polynomial is then evaluated at 151 Chebyshev points via FFT, and these 151 numbers become the data defining this particular chebfun. Engineers would say that the signal has been *downsampled* from 257 points to 151.

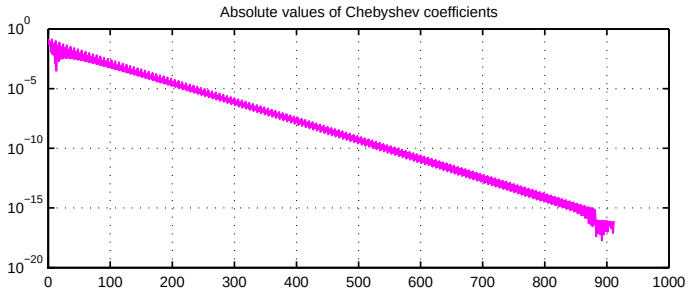
For another example we consider a function with two spikes:

```
f = 1./(1+1000*(x+.5).^2) + 1./sqrt(1+1000*(x-.5).^2);
clf, plot(f), title('A function with two spikes')
```



Here are the Chebyshev coefficients of the chebfun. This time, instead of `chebpoly` and `semilogy`, we execute the special command `chebpolyplot`, which does the same thing.

```
chebpolyplot(f,'m'), grid on
title('Absolute values of Chebyshev coefficients')
```



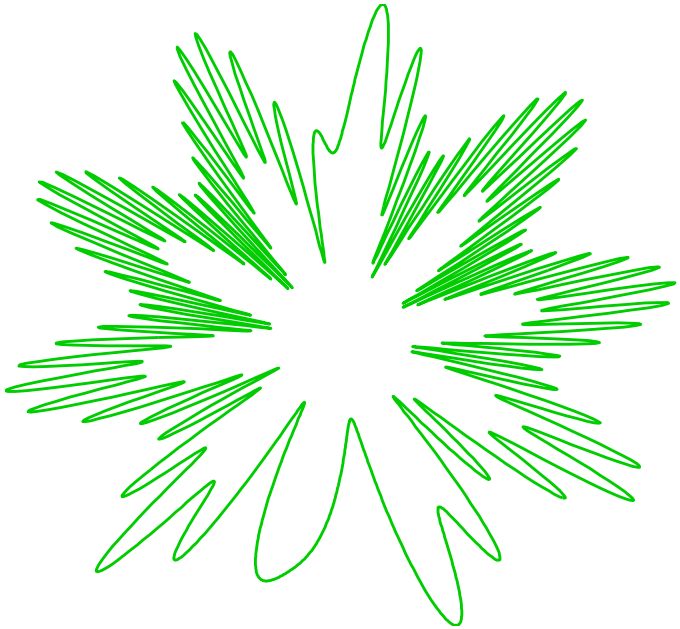
Note that although it is far less wiggly, this function needs six times as many points to resolve as the previous one.

Chebyshev interpolants are effective for complex functions (still defined on a real interval) as well as real ones. Here for example is a complex function that happens to be periodic, though the Chebyshev representation does not take advantage of this fact.

```
f = (3+sin(10*pi*x)+sin(61*exp(.8*sin(pi*x)+.7))).*exp(1i*pi*x);
```

A plot shows the image of $[-1,1]$ under f, which seems to the eye quite complicated:

```
plot(f,LW,0.6,CO,[0 .8 0]), axis equal, axis off
```

Yet the degree of the polynomial is not so high:

```
length(f)
```

```
ans = 617
```

People often ask, is there anything special about Chebyshev points and Chebyshev polynomials? Could we equally well interpolate in other points and expand in other sets of polynomials? From an approximation point of view, the answer is yes, and in particular, Legendre points and Legendre polynomials have much the same power for representing a general function f, as we shall see in Chapters 17–19. Legendre points and polynomials are neither better than Chebyshev for approximating functions, nor worse; they are essentially the same. One can improve both Legendre and Chebyshev — by a factor of up to $\pi/2$ — but to do so one must leave the class of polynomials. See Chapter 22.

Nevertheless, there is a big advantage of Chebyshev over Legendre points, and this is that one can use the FFT to go from point values to coefficients and back again. There are algorithms that make such computations practicable in the Legendre case too [Dutt, Gu & Rokhlin 1996, Potts, Steidl & Tasche 1998, Iserles 2010], but Chebyshev remains the lightning fast and easy case.

[To be added: (1) Original references for Chebyshev polynomials and Theorem 3.1. (2) In particular, pin down where the notation T_k comes from and confirm

the claim about transliteration. (3) Exercise on Chebyshev coeffs of $\exp(x)$. (4) Mention Dini–Lipschitz. This is also an exercise in Chap 14. (5) Exercise 3.6. (6) Exercise on Chebyshev polynomials in the complex plane.]

SUMMARY OF CHAPTER 3. *The Chebyshev polynomial $T_k(x)$ is an analogue for $[-1,1]$ of the monomial z^k on the unit circle. Each Lipschitz continuous function f on $[-1,1]$ has an absolutely and uniformly convergent Chebyshev series, that is, an expansion $f(x) = a_0T_0(x) + a_1T_1(x) + \cdots$.*

Exercise 3.1. Monomial and Chebyshev coefficients. Let $p \in P_n$ have coefficient vectors $a = (a_0, a_1, \ldots, a_n)^T$ for a Chebyshev series and $b = (b_0, b_1, \ldots, b_n)^T$ for a series in the monomials $1, x, \ldots, x^n$. Show that a and b are related by $Aa = b$, where A is an upper-triangular matrix, whose entries you should describe. Prove that any $p \in P_n$ has uniquely defined coefficient vectors a and b for both representations.

Exercise 3.2. An expansion coefficient. Determine numerically the coefficient of T_5 in the Chebyshev expansion of $\tan^{-1}(x)$ on $[-1,1]$.

Exercise 3.3. Chebyshev coefficients and "rat". (a) Use Chebfun to determine numerically the coefficients of the Chebyshev series for $1 + x^3 + x^4$. By inspection, identify these rational numbers. Use the Matlab command `[n,d] = rat(c)` to confirm this. (b) Use Chebfun and `rat` to make good guesses as to the Chebyshev coefficients of $x^7/7 + x^9/9$.

Exercise 3.4. Dependence on wave number. (a) Calculate the length L_k of the chebfun corresponding to $f(x) = \sin(kx)$ on $[-1,1]$ for $k = 1, 2, 4, 8, \ldots, 2^{10}$. (You can do this elegantly by defining a Matlab anonymous function `f = @(k)`.) Make a loglog plot of L_k as a function of k and comment on the result. (b) Do the same for $g(x) = 1/(1 + (kx)^2)$.

Exercise 3.5. Chebyshev series of a complicated function. (a) Make chebfuns of the three functions $f(x) = \tanh(x)$, $g(x) = 10^{-5}\tanh(10x)$, $h(x) = 10^{-10}\tanh(100x)$ on $[-1,1]$, and call `chebpolyplot` to show their Chebyshev coefficients. Comment on the results. (b) Now define $s = f + g + h$ and comment on the result of `chebpolyplot` applied to s. Chebfun does not automatically chop the tail of a Chebyshev series, but applying the `simplify` command will do this. What happens with `chebpolyplot(simplify(s))`? (c) Repeat (b) but with the function $t = f + 10^{-5}g + 10^{-10}h$. What does `chebpolyplot` reveal about the difference between `simplify(t)` and `simplify(s)`?

Exercise 3.6. Chebyshev series of $|x|$. Show that for $f(x) = |x|$, the Chebyshev coefficients are $a_k = 0$ for k odd, $a_0 = 2/\pi$, and for $k \geq 2$ even, $a_k = (-1)^{(k/2)}/(1-k^2)$. [This exercise is not yet finished and may be moved to a later chapter. See Bernstein 1914.]

Exercise 3.7. Orthogonality of Chebyshev polynomials. Equation (3.5) gives the Chebyshev coefficient a_k of f by integration of f against just the single Chebyshev polynomial T_k. This formula implies an orthogonality property for $\{T_j\}$ involving a weighted integral. State exactly what this orthogonality property is and show carefully how it follows from the equations of this chapter.

Exercise 3.8. Conditioning of the Chebyshev basis. Although the Chebyshev polynomials are not orthogonal with respect to the standard unweighted inner product, they are close enough to provide a well-behaved basis. Set `T = chebpoly(0:10)` and explore the Chebfun "quasimatrix" that results with commands like `size(T)`, `spy(T)`, `plot(T)`, `svd(T)`. Explain the meaning of `T` (you may find Chapter 6 of the Chebfun Guide helpful) and determine the condition number of this basis with `cond(T)`. (b) Now construct the corresponding quasimatrix of monomials by executing `x = chebfun('x'); M = T; for j = 0:10, M(:,j+1) = x.^j; end`. What is the condition number of `M`? (c) Produce a plot of these two condition numbers for matrices whose columns span P_n for $n = 0, 1, \ldots, 10$. (d) What happens to the condition numbers if M is constructed from monomials on $[0,1]$ rather than $[-1,1]$ via `x = chebfun('x',[0,1])`?

Exercise 3.9. Derivatives at endpoints. Prove from (3.3) that the derivatives of the Chebyshev polynomials satisfy $T_n'(1) = n^2$ for each $n \geq 0$. (**Markov's inequality** asserts that for any $p \in P_n$, $\|p'\| \leq n^2\|p\|$, where $\|\cdot\|$ is the supremum norm.)

Exercise 3.10. Odd and even functions. Show that if f is an odd function on $[-1,1]$, its Chebyshev coefficients of even order are zero; similarly if f is even its odd coefficients are zero.

Exercise 3.11. A function neither even nor odd. Apply `chebpolyplot` to the function $f(x) = \exp(x)/(1 + 10000x^2)$. Why does the plot have the appearance of a stripe? Can you explain quantitatively the height of the stripe?

Exercise 3.12. Extrema and roots of Chebyshev polynomials. Give formulas for the extrema and roots of T_n in $[-1,1]$.

Exercise 3.13. `chebpoly` on other intervals. [Not yet written.]

4. Interpolants, truncations, and aliasing

Suppose $f(x)$ is a Lipschitz continuous function on $[-1,1]$ with Chebyshev expansion coefficients $\{a_k\}$ as in Theorem 3.1:

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x). \tag{4.1}$$

One approximation to f in P_n is the polynomial obtained by **interpolation** in Chebyshev points:

$$p_n(x) = \sum_{k=0}^{n} c_k T_k(x). \tag{4.2}$$

Another is the polynomial obtained by **truncation** of the series at term n, whose coefficients through degree n are the same as those of f itself:

$$f_n(x) = \sum_{k=0}^{n} a_k T_k(x). \tag{4.3}$$

The relationship of the Chebyshev coefficients of f_n to those of f is obvious, and in a moment we shall see that the Chebyshev coefficients of p_n have simple

expressions too. In computational work generally, and in particular in Chebfun, the polynomials $\{p_n\}$ are usually almost as good approximations to f as the polynomials $\{f_n\}$, and easier to work with, since one does not need to evaluate the integral (3.5). The polynomials $\{f_n\}$, on the other hand, are also interesting and have received a great deal of attention over the years. In this book, most of our computations will make use of $\{p_n\}$, but many of our theorems will treat both cases. A typical example is Theorem 8.2, which asserts that if f is analytic on $[-1,1]$, then both $\|f-f_n\|$ and $\|f-p_n\|$ decrease geometrically to 0 as $n\to\infty$.

The key to understanding $\{c_k\}$ is the phenomenon of **aliasing,** a term which originated with radio engineers early in the 20th century. On the $(n+1)$-point Chebyshev grid, it is obvious that any function f is indistinguishable from a polynomial of degree n. But something more is true: any Chebyshev polynomial T_N, no matter how big N is, is indistinguishable on the grid from a *single* Chebyshev polynomial T_k for some k with $0\le k\le n$. We state this as a theorem.

Theorem 4.1: Aliasing of Chebyshev polynomials. *For any $n\ge 1$ and $0\le k\le n$, the following Chebyshev polynomials take the same values on the $(n+1)$-point Chebyshev grid:*

$$T_k,\ T_{2n-k},\ T_{2n+k},\ T_{4n-k},\ T_{4n+k},\ T_{6n-k},\ldots.$$

Equivalently, for any $k\ge 0$, T_k takes the same value on the grid as $T_{\tilde{k}}$ with

$$\tilde{k} = |(k+n-1)(\mathrm{mod}\, 2n) - (n-1)|. \tag{4.4}$$

Proof. Recall from (2.1) and (3.2) that Chebyshev polynomials on $[-1,1]$ are related to monomials on the unit circle by $T_k(x) = (z^k+z^{-k})/2$, and Chebyshev points are related to $(2n)$th roots of unity by $x_k = (z_k+z_k^{-1})/2$. It follows that the assertion of the theorem is equivalent to the statement that the following functions take the same values at the $(2n)$th roots of unity:

$$z^k+z^{-k},\ z^{2n-k}+z^{k-2n},\ z^{2n+k}+z^{-2n-k},\ldots.$$

Inspection of the exponents shows that in every case, modulo $2n$, we have one exponent equal to $+k$ and the other to $-k$. The conclusion now follows from the elementary phenomenon of aliasing of monomials on the unit circle: at the $(2n)$th roots of unity, $z^{2\nu n}=1$ for any integer ν. ∎

Here is a numerical illustration of Theorem 4.1. Taking $n=4$, let `X` be the Chebyshev grid with $n+1$ points, and let $T\{1\},\ldots,T\{10\}$ be the first ten Chebyshev polynomials:

```
n = 4; X = chebpts(n+1);
for k = 1:10
    T{k} = chebpoly(k);
end
```

Then T_3 and T_5 are the same on the grid:

```
disp([T{3}(X) T{5}(X)])
```

```
  -1.000000000000000  -1.000000000000000
   0.707106781186548   0.707106781186547
                   0                   0
  -0.707106781186548  -0.707106781186547
   1.000000000000000   1.000000000000000
```

So are T_1, T_7, and T_9:

```
disp([T{1}(X) T{7}(X) T{9}(X)])
```

```
  -1.000000000000000  -1.000000000000000  -1.000000000000000
  -0.707106781186547  -0.707106781186548  -0.707106781186547
                   0                   0                   0
   0.707106781186547   0.707106781186548   0.707106781186547
   1.000000000000000   1.000000000000000   1.000000000000000
```

As a corollary of Theorem 4.1, we can now derive the connection between $\{a_k\}$ and $\{c_k\}$. The following result can be found in [Clenshaw & Curtis 1960].

Theorem 4.2: Aliasing formula for Chebyshev coefficients. *Let f be Lipschitz continuous on $[-1,1]$ and let p_n be its Chebyshev interpolant in P_n, $n\ge 1$. Let $\{a_k\}$ and $\{c_k\}$ be the Chebyshev coefficients of f and p_n, respectively. Then*

$$c_0 = a_0 + a_{2n} + a_{4n} + \ldots, \tag{4.5}$$

$$c_n = a_n + a_{3n} + a_{5n} + \ldots, \tag{4.6}$$

and for $1\le k\le n-1$,

$$c_k = a_k + (a_{k+2n} + a_{k+4n} + \ldots) + (a_{-k+2n} + a_{-k+4n} + \ldots). \tag{4.7}$$

Proof. By Theorem 3.1, f has a unique Chebyshev series (3.4), and it converges absolutely. Thus we can rearrange the terms of the series without affecting convergence, and in particular, each of the three series expansions written above converges, so these formulas do indeed define certain numbers $c_0,\ldots,c_n$. Taking these numbers as coefficients multiplied by the corresponding Chebyshev polynomials $T_0,\ldots,T_n$ gives us a polynomial of degree n. By Theorem 4.1, this polynomial takes the same values as f at each point of the Chebyshev grid. Thus it is the unique interpolant $p_n\in P_n$. ∎

We can summarize Theorem 4.2 as follows. On the $(n+1)$-point grid, any function f is indistinguishable from a polynomial of degree n. In particular, the

Chebyshev series of the polynomial interpolant to f is obtained by reassigning all the Chebyshev coefficients in the infinite series for f to their aliases of degrees 0 through n.

As a corollary, the theorem gives us formulas for $f - f_n$ and $f - p_n$, which we shall exploit in Chapters 7 and 8:

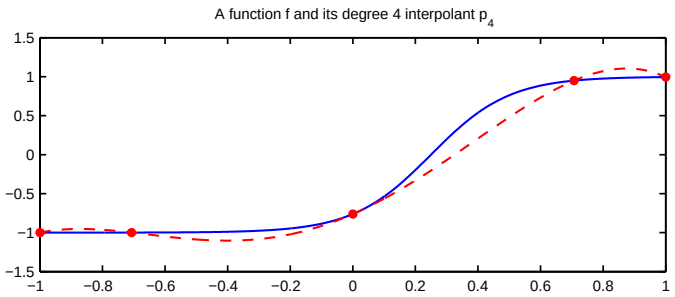
$$f(x) - f_n(x) = \sum_{k=n+1}^{\infty} a_k T_k(x), \tag{4.8}$$

$$f(x) - p_n(x) = \sum_{k=n+1}^{\infty} a_k (T_k(x) - T_{\tilde{k}}(x)), \tag{4.9}$$

where $\tilde{k}$ is given by (4.4).

To illustrate Theorem 4.2, here is the function $\tanh(4x-1)$ (solid) and its degree 4 Chebyshev interpolant (dashed):

```
f = tanh(4*x-1);
n = 4; pn = chebfun(f,n+1);
hold off, plot(f), hold on, plot(pn,'.--r')
title('A function f and its degree 4 interpolant p_4')
```



The first 5 Chebyshev coefficients of f,

```
a = chebpoly(f); a = a(end:-1:1)'; a(1:n+1)
```

```
ans =
  -0.166584582703135
   1.193005991160944
   0.278438064117869
  -0.239362401056012
  -0.176961398392888
```

are different from the Chebyshev coefficients of p_n,


```
c = chebpoly(pn); c = c(end:-1:1)'
```

```
c =
  -0.203351068209675
   1.187719968517890
   0.379583465333916
  -0.190237989543227
  -0.178659622412174
```

As asserted in (4.5) and (4.6), the coefficients c_0 and c_n are given by sums of coefficients a_k with a stride of $2n$:

```
c0 = sum(a(1:2*n:end))
```

```
c0 = -0.203351068209675
```

```
cn = sum(a(n+1:2*n:end))
```

```
cn = -0.178659622412174
```

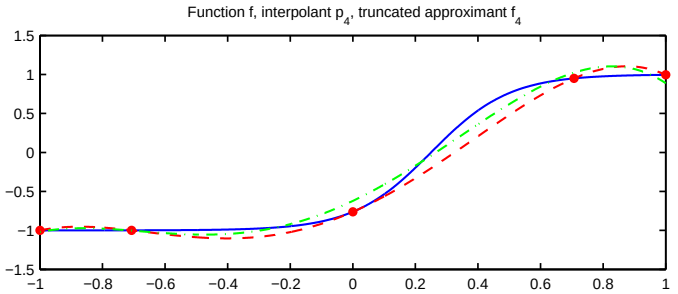
And as asserted in (4.7), the coefficients c_1 through c_{n-1} involve two sums of this kind:

```
for k = 1:n-1
  ck = sum(a(1+k:2*n:end)) + sum(a(1-k+2*n:2*n:end))
end
```

```
ck =
   1.187719968517889
ck =
   0.379583465333916
ck =
  -0.190237989543227
```

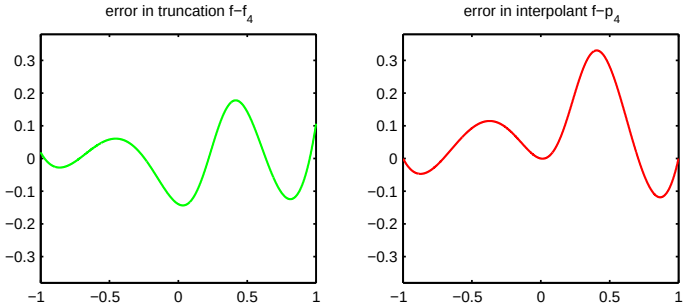
Following up on the last figure, how does the truncated series f_n compare with the interpolant p_n as an approximation to f? Chebfun includes a `'trunc'` option for computing f_n, which we now add to the plot as a dot-dash line:

```
fn = chebfun(f,'trunc',n+1);
plot(fn,'-.g')
title('Function f, interpolant p_4, truncated approximant f_4')
```



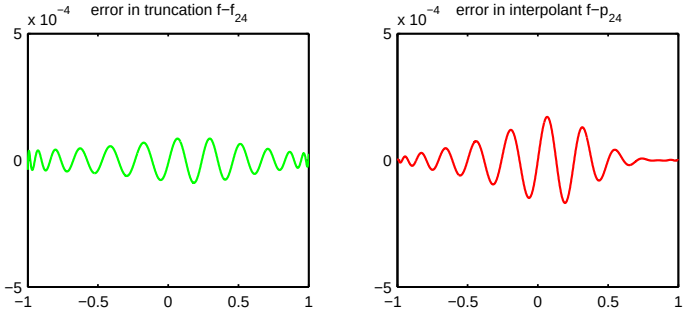
Here are the errors $f - f_n$ and $f - p_n$:

```
hold off
subplot(1,2,1), plot(f-fn,'g'), ylim(.38*[-1 1])
title('error in truncation f-f_4')
subplot(1,2,2), plot(f-pn,'r'), ylim(.38*[-1 1])
title('error in interpolant f-p_4')
```



Here is the analogous plot with $n = 4$ increased to 24:

```
n = 24; pn = chebfun(f,n+1);
fn = chebfun(f,'trunc',n+1);
subplot(1,2,1), plot(f-fn,'g'), ylim(.0005*[-1 1])
title('error in truncation f-f_{24}')
subplot(1,2,2), plot(f-pn,'r'), ylim(.0005*[-1 1])
title('error in interpolant f-p_{24}')
```



On the basis of plots like these, one might speculate that f_n may often be a better approximation than p_n, but that the difference is small. This is indeed the case, as we shall confirm in Theorems 7.2 and 8.2, both of which suggest a difference of a factor of 2, and Theorem 16.1, which suggests a factor of $\pi/2$.

Let us summarize where we stand. We have considered Chebyshev interpolants (Chapter 2) and Chebyshev expansions (Chapter 3) for a function $f(x)$ defined

on $[-1, 1]$. Mathematically speaking, each coefficient of a Chebyshev expansion is equal to the value of the integral (3.5). This formula, however, is not needed for effective polynomial approximation, since Chebyshev interpolants are approximately as accurate as truncations. Chebfun readily computes Chebyshev coefficients of polynomial interpolants, and this is done not by evaluating the integral but by taking the FFT of the sample values in Chebyshev points. If the degree of the interpolant is high enough that the polynomial matches f to machine precision, then the Chebyshev coefficients will match too.

[To be added: (1) Aliasing plots from NCN. (2) The projection/orthogonality interpretation.]

SUMMARY OF CHAPTER 4. *Two excellent methods of approximating a function f on $[-1, 1]$ by a polynomial are truncation of its Chebyshev series and interpolation in Chebyshev points. The Chebyshev interpolant is the polynomial obtained by reassigning contributions of degree $> n$ in the Chebyshev series to their aliases of degree $\le n$. The two approximations are typically within a factor of 2 of each other in accuracy.*

Exercise 4.1. Aliasing. (a) On the $(n+1)$-point Chebyshev grid with $n = 20$, which Chebyshev polynomials T_k take the same values as T_5? (b) Use Chebfun to draw plots illustrating some of these intersections.

Exercise 4.2. Aliasing in roots of unity. For each $n \ge 0$, let $p_n \in P_n$ be the degree n polynomial interpolant to the function $f(z) = z^{-1}$ at the $(n+1)$st roots of unity on the unit circle in the z-plane. Use the aliasing observation at the end of the proof of Theorem 4.1 to prove that p_n does not converge to f on the unit disk as $n \to \infty$, even though f is analytic there. (This example comes from [Méray 1884].)

Exercise 4.3. Fooling the Chebfun constructor. (a) Construct the anonymous function `f = @(M) chebfun(@(x) 1+exp(-(M*(x-0.4)).^4))` and plot `f(10)` and `f(100)`. This function has a narrow spike of width proportional to $1/M$. Confirm this by comparing `sum(f(10))` and `sum(f(100))`. (b) Plot `length(f(M))` as a function of M for $M = 1, 2, 3, \ldots$, going into the region where the length becomes 1. What do you think is happening? (c) Let `Mmax` be the largest integer for which the constructor behaves normally and execute `semilogy(f(Mmax)-1,'interval',[.3 .5])`. Superimpose on this plot information to show the locations of the points returned by `chebpts(9)`, which is the default initial grid on which Chebfun samples a function. Explain how this result fits with (b). (d) Now for `np` taking values 17, 33, 65, 129 execute `chebfunpref('minsamples',np)` and `length(f(np))`, and plot the Chebyshev points on your semilog plot of (c). The `minsamples` flag forces Chebfun to sample the function at the indicated number of points. How do these results match your observations of (b) and (c)? When you're done, be sure to return Chebfun to its default state with `chebfunpref('factory')`.

Exercise 4.4. Relative precision. Try Exercise 4.3 again but without the "1+" in the definition of `f`. The value of `Mmax` will be different, and the reason has to do with

Chebfun's aim of constructing each function to about 15 digits of relative precision, not absolute. Can you figure out what is happening and explain it quantitatively?

Exercise 4.5. Chebfun computation of truncations. In the text we computed Chebyshev truncations of $f(x) = \tanh(4x-1)$ using the `'trunc'` flag in the Chebfun constructor. Another method is to compute all the Chebyshev coefficients of f and then truncate the series. Compute f_4 by this method and verify that the results agree to machine precision.

Exercise 4.6. Least-squares projection. [not yet written]

5. Barycentric interpolation formula

How does one evaluate a Chebyshev interpolant? One good approach, involving $O(n \log n)$ work for a single point evaluation, is to compute Chebyshev coefficients and use the Chebyshev series. However, there is a direct method requiring just $O(n)$ work, not based on the series expansion, that is both elegant and numerically stable. It also has the advantage of generalizing to sets of points other than Chebyshev. It is called the **barycentric interpolation formula**, introduced by Salzer [1972], with an earlier closely related formula by Marcel Riesz [1916]. The more general barycentric formula for arbitrary interpolation points, of which Salzer's formula is an exceptionally simple special case, was developed earlier by Taylor [1945] and Dupuy [1948], with origins at least as early as Jacobi [1825]. For a survey of variations of barycentric formulas, though without references before 1945, see [Berrut & Trefethen 2004].

The study of polynomial interpolation goes back a long time; the word "interpolation" may be due to Wallis in 1655. In particular Newton addressed the topic and devised a method based on divided differences. Many textbooks claim that it is important to use this approach for reasons of numerical stability, but this is not true, and we shall not discuss the Newton approach here.

Instead, the barycentric formula is in the alternative **Lagrange form**, where the interpolant is written as a linear combination of **Lagrange** or **cardinal** or **fundamental polynomials**:

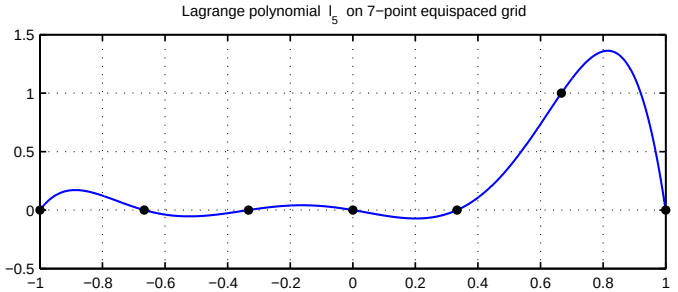
$$p(x) = \sum_{j=0}^{n} f_j \ell_j(x). \tag{5.1}$$

Here we have a set of distinct interpolation points $x_0, \dots, x_n$, which could be real or complex, and $\ell_j(x)$, the jth Lagrange polynomial, is the unique polynomial in P_n that takes the value 1 at x_j and 0 at the other points x_k:

$$\ell_j(x_k) = \begin{cases} 1 & k = j, \\ 0 & k \neq j. \end{cases} \tag{5.2}$$

For example, here is a plot of ℓ_5 on the equispaced 7-point grid (i.e., $n = 6$):


```
d = domain(-1,1);
s = linspace(-1,1,7);
y = [0 0 0 0 0 1 0];
p = interp1(s,y,d);
clf, plot(p), hold on, plot(s,p(s),'.k'), grid on
title('Lagrange polynomial  l_5  on 7-point equispaced grid')
```



It is easy to write down an explicit expression for ℓ_j:

$$\ell_j(x) = \frac{\prod_{k \neq j}(x - x_k)}{\prod_{k \neq j}(x_j - x_k)}. \tag{5.3}$$

Since the denominator is a constant, this function is a polynomial of degree n with zeros at the right places, and clearly it takes the value 1 when $x = x_j$. Equation (5.3) is very well known and can be found in many textbooks as a standard representation for Lagrange interpolants. Lagrange worked with (5.1) and (5.3) in 1795, and his name is firmly attached to these ideas, but the same formulas were published earlier by Waring [1779] and Euler [1783].

Computationally speaking, (5.1) is excellent but (5.3) is not so good. It requires $O(n)$ operations to evaluate $\ell_j(x)$ for each value of x, and then $O(n)$ such evaluations must be added up in (5.1), giving a total operation count of $O(n^2)$ for evaluating $p(x)$ at a single value of x.

By a little rearrangement we can improve the operation count. The key observation is that for the various values of j, the numerators in (5.3) are the same except that they are missing different factors $x - x_j$. To take advantage of this commonality, we define the **node polynomial** $\ell \in P_{n+1}$ for the given grid by

$$\ell(x) = \prod_{k=0}^{n} (x - x_k). \tag{5.4}$$

Then (5.3) becomes the elementary but extremely important identity

$$\ell_j(x) = \frac{\ell(x)}{\ell'(x_j)(x - x_j)}. \tag{5.5}$$

(We shall use this equation to derive the Hermite integral formula in Chapter 11.) Equivalently, let us define

$$\lambda_j = \frac{1}{\prod_{k\neq j}(x_j - x_k)}, \tag{5.6}$$

that is,

$$\lambda_j = \frac{1}{\ell'(x_j)}. \tag{5.7}$$

Then (5.3) becomes

$$\ell_j(x) = \ell(x)\frac{\lambda_j}{x - x_j}, \tag{5.8}$$

and the Lagrange formula (5.1) becomes

$$p(x) = \ell(x)\sum_{j=0}^{n}\frac{\lambda_j}{x - x_j}f_j. \tag{5.9}$$

These formulas were derived by Jacobi in his PhD thesis in Berlin [Jacobi 1825], and they appeared in 19th century textbooks.[2]

Equation (5.9) has been called the "modified Lagrange formula" (by N. J. Higham) and the "first form of the barycentric interpolation formula" (by H. Rutishauser). What is valuable here is that the dependence on x inside the sum is so simple. If the weights $\{\lambda_j\}$ are known, (5.9) produces each value $p(x)$ with just $O(n)$ operations. Computing the weights from (5.8) requires $O(n^2)$ operations, but this computation only needs to be done once and for all, independently of x; and for special grids $\{x_j\}$ such as Chebyshev, as we shall see in a moment, the weights are known analytically and don't need to be computed at all. (For Legendre and other grids associated with orthogonal polynomials, see Theorem 19.6.)

However, there is another barycentric formula that is more elegant. If we add up all the Lagrange polynomials ℓ_j, we get a polynomial in P_n that takes the value 1 at every point of the grid. Since polynomial interpolants are unique, this must be the constant polynomial 1:

$$\sum_{j=0}^{n}\ell_j(x) = 1.$$

Dividing (5.8) by this expression enables us to cancel the factor $\ell(x)$, giving

$$\ell_j(x) = \frac{\lambda_j}{x - x_j}\Bigg/\sum_{k=0}^{n}\frac{\lambda_k}{x - x_k}. \tag{5.10}$$

[2] I am grateful to Folkmar Bornemann for drawing this history to my attention.

By inserting these representations in (5.1), we get the "second form of the barycentric interpolation formula" for polynomial interpolation in an arbitrary set of $n+1$ points $\{x_j\}$.

Theorem 5.1: Barycentric interpolation formula. *The polynomial interpolant through data $\{f_j\}$ at $n+1$ points $\{x_j\}$ is*

$$p(x) = \sum_{j=0}^{n}\frac{\lambda_j f_j}{x - x_j}\Bigg/\sum_{j=0}^{n}\frac{\lambda_j}{x - x_j}, \tag{5.11}$$

with the special case $p(x) = f_j$ if $x = x_j$ for some j, where the weights $\{\lambda_j\}$ are defined by

$$\lambda_j = \frac{1}{\prod_{k\neq j}(x_j - x_k)}. \tag{5.12}$$

Proof. Given in the discussion above. ∎

If you look at (5.11), it is obvious that the function it defines interpolates the data. As x approaches one of the values x_j, one term in the numerator blows up and so does one term in the denominator. Their ratio is f_j, so this is clearly the value approached as x approaches x_j. On the other hand if x is equal to x_j, we can't use the formula: that would be a division of ∞ by ∞. That is why the theorem is stated with the qualification for the special case $x = x_j$.

What is not obvious is that the function defined by (5.11) is a polynomial, let alone a polynomial of degree n: it looks like a rational function. The fact that it is actually a polynomial depends on the special values (5.12) of the weights. For choices of weights that differ from (5.12), (5.11) will still interpolate the data, but in general it will be a rational function that is not a polynomial. These rational barycentric interpolants are extremely useful in certain applications, especially for work on irregular grids [Tee & Trefethen 2006], but they are not discussed in this book.

Chebfun's overload of Matlab's `interp1` command, which was illustrated at the beginning of this chapter, contains an implementation of (5.11)–(5.12). We shall make use of `interp1` again in Chapters 13 and 15. Now, however, let us turn to the special case that is so important in practice.

For Chebyshev points, the weights $\{\lambda_j\}$ are wonderfully simple: they are equal to $(-1)^j$ times the constant $2^{n-1}/n$, or half this value for $j = 0$ and n. This formula was worked out by Marcel Riesz in 1916 [Riesz 1916]. The constant cancels in the numerator and denominator when we divide by the constant 1 in (5.11), giving Salzer's amazingly simple result from 1972 [Salzer 1972]:

Theorem 5.2: Barycentric interpolation in Chebyshev points. *The*

polynomial interpolant through data $\{f_j\}$ *at* $n+1$ *Chebyshev points* $\{x_j\}$ *is*

$$p(x) = \sum_{j=0}^{n}{}' \frac{(-1)^j f_j}{x - x_j} \Bigg/ \sum_{j=0}^{n}{}' \frac{(-1)^j}{x - x_j}, \tag{5.13}$$

with the special case $p(x) = f_j$ *if* $x = x_j$*. The primes on the summation signs signify that the terms* $j = 0$ *and* $j = n$ *are multiplied by* $1/2$*.*

Equation (5.13) is scale-invariant: for interpolation in Chebyshev points scaled to any interval $[a, b]$, the formula is exactly the same.

Proof. Equation (5.13) is a special case of (5.11). To prove it, we will show that for Chebyshev points, the weights (5.12) reduce to $(-1)^j$ times the constant $2^{n-1}/n$, and half this value for $j = 0$ or n.

To do this, we begin by noting that for Chebyshev points, the node polynomial ℓ of (5.4) can be written

$$\ell(x) = 2^{-n}(T_{n+1}(x) - T_{n-1}(x)). \tag{5.14}$$

To verify this formula we note first that it is certainly a polynomial of degree $n+1$, and since T_{n+1} has leading coefficient 2^n, the polynomial is monic. Now by Theorem 4.1, T_{n-1} and T_{n+1} take the same values on the $(n+1)$-point Chebyshev grid. Thus $T_{n+1} - T_{n-1}$ has roots at all the nodes of that grid, confirming that (5.14) is exactly the polynomial (5.4).

Equations (5.8) and (5.14) imply that

$$\ell_j(x) = 2^{-n}\lambda_j \frac{T_{n+1}(x) - T_{n-1}(x)}{x - x_j},$$

and from (5.7) we have

$$\lambda_j = \frac{1}{\ell'(x_j)} = \frac{2^n}{T'_{n+1}(x_j) - T'_{n-1}(x_j)}.$$

Now it can be shown that

$$T'_{n+1}(x_j) - T'_{n-1}(x_j) = 2n(-1)^j, \quad 1 \le j \le n-1,$$

with twice this value for $j = 0$ and n (Exercise 5.3). So we have

$$\lambda_j = \frac{2^{n-1}}{n}(-1)^j, \quad 1 \le j \le n-1, \tag{5.15}$$

with half this value for $j = 0$ and n, as claimed. ∎

The formula (5.13) is extraordinarily effective, even if n is in the thousands or millions, even if p must be evaluated at thousands or millions of points. As a first example, let us construct a rather wiggly chebfun:

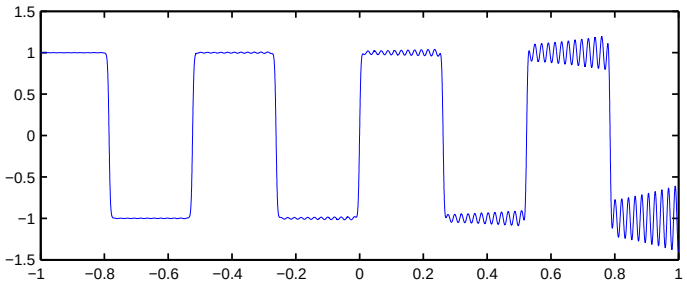

```
f = tanh(20*sin(12*x)) + .02*exp(3*x).*sin(300*x);
length(f)
```

```
ans = 5184
```

We now plot `f` using 10000 sample points and note the time required:

```
hold off
tic, plot(f,LW,.5,'numpts',10000), toc
```

```
Elapsed time is 0.605590 seconds.
```



In this short time Chebfun has evaluated a polynomial interpolant of degree about 5000 at 10000 sample points.

Raising the degree further, let p be the Chebyshev interpolant of degree 10^6 to the function $\sin(10^5 x)$ on $[-1, 1]$:

```
ff = @(x) sin(1e5*x);
p = chebfun(ff,1000001);
```

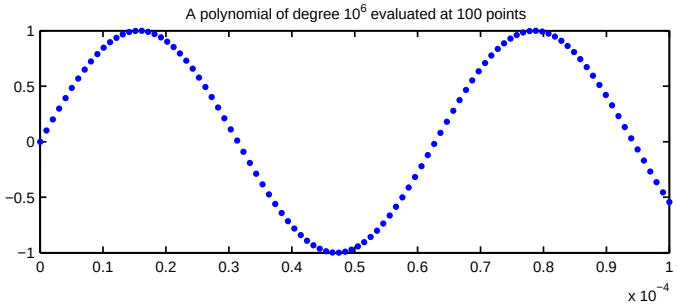
How long does it take to evaluate this interpolant at 100 points?

```
xx = linspace(0,0.0001);
tic, pp = p(xx); toc
```

```
Elapsed time is 1.316492 seconds.
```

Not bad for a million-degree polynomial! The result looks fine:

```
clf, plot(xx,pp,'.',MS,10)
axis([0 0.0001 -1 1])
title('A polynomial of degree 10^6 evaluated at 100 points')
```



and it matches the target function closely:

```
format long
for j = 1:5
    r = rand;
    disp([ff(r) p(r) ff(r)-p(r)])
end
```

```
  -0.953922024875663  -0.953922024881650   0.000000000005988
  -0.924684248370759  -0.924684248367095  -0.000000000003665
  -0.700448855358137  -0.700448855360117   0.000000000001980
  -0.814666653387460  -0.814666653397518   0.000000000010058
  -0.239538284491439  -0.239538284487261  -0.000000000004178
```

The apparent loss of 4 or 5 digits of accuracy is to be expected since the derivative of this function is of order 10^5: each evaluation is the correct result for a value of x within about 10^{-16} of the correct one (Exercise 5.5).

Experiments like these show that barycentric interpolation in Chebyshev points is a robust process in practice: it is numerically stable, untroubled by rounding errors on a computer. This may seem surprising if you look at (5.9) or (5.13) — won't cancellation errors on a computer cause trouble if x is close to one of the Chebyshev points x_j? In fact they do not, and these formulas have been proved stable in floating point arithmetic for all $x \in [-1,1]$ [Rack & Reimer 1982, Higham 2004]. This is in marked contrast to the more familiar algorithm of polynomial interpolation via solution of a Vandermonde linear system of equations, which is exponentially unstable (Exercise 5.2).

More precisely, Higham [2004] showed that for Chebyshev points, (5.13) has the property that numerical analysts call forward stability, whereas (5.9), with the Chebyshev weights $\{\lambda_j\}$, has the stronger property known as backward stability. This suggests that (5.9) has advantages, but it also has at least one disadvantage: it is not scale-invariant, and the weights scale inverse-exponentially as functions of the length of the interval of interpolation. We see this in (5.15), where the weights have size 2^n, and would in fact overflow on a computer in standard

IEEE double precision arithmetic for n bigger than about 1000. We shall have more to say about these matters in Chapters 11–15.

For interpolation in equispaced points or other sets that are far from the Chebyshev distribution, Higham showed that the forward stability of (5.13) is lost and it becomes more important to use the form (5.9). However, as we shall discuss in Chapters 13–14, in these cases the interpolation problem is so ill-conditioned that one should probably not be trying to solve it in the first place.

[To be added: (1) Concerning barycentric formulas Salzer recommends Winrich, *Computer J.* 12, 154–155. (2) Possible new exercises on weights for Cheb pts of the 1st kind. (3) More about interp1. (4) Does Exercise 5.2 mix discrete and continuous improperly? (5) Read Stiefel, Einfuehrung in die Numer Math]

SUMMARY OF CHAPTER 5. *Polynomial interpolants can be evaluated fast and stably by the barycentric formula, even for thousands or millions of interpolation points. The barycentric formula has the form of a rational function but reduces to a polynomial because of the use of specially determined weights.*

Exercise 5.1. Barycentric coefficients by hand. (a) Work out on paper the barycentric interpolation coefficients $\{\lambda_j\}$ for the case $n = 3$ and $x_0 = -1$, $x_1 = 0$, $x_2 = 1/2$, $x_3 = 1$. (b) Confirm that (5.9) gives the right value $p(-1/2)$ for the polynomial interpolant to data $1, 2, 3, 4$ in these points.

Exercise 5.2. Instability of Vandermonde interpolation. The best-known numerical algorithm for polynomial interpolation, unlike the barycentric formula, is unstable. This is the method implemented in Matlab's `polyfit` command, which forms a Vandermonde matrix of sampled powers of x and solves a corresponding linear system of equations. (In [Trefethen 2000], to my embarrassment, this unstable method is used throughout, forcing the values of n used for plots in that book to be kept small.) (a) Explore this instability by comparing a Chebfun evaluation of $p(0)$ with the result of `polyval(polyfit(xx,f(xx),n),0)` where `f = @(x) cos(k*x)` for $k = 10, 20, \ldots, 90, 100$, n is the degree of the corresponding chebfun, and `xx` is a fine grid. (b) Examining Matlab's `polyfit` code as appropriate, construct the Vandermonde matrices V for each of these 11 problems and compute their condition numbers. (You can also use Matlab's `vander` command.) By contrast, the underlying Chebyshev interpolation problem is well-conditioned.

Exercise 5.3. Calculating derivatives for the proof of Theorem 5.2. Derive the following identities used in the proof of Theorem 5.2. (a) For $1 \le j \le n-1$, $T'_{n+1}(x_j) - T'_{n-1}(x_j) = 2n(-1)^j$. (b) For $j = 0$ and $j = n$, $T'_{n+1}(x_j) - T'_{n-1}(x_j) = 4n(-1)^j$. One can derive this formula directly, or indirectly by a symmetry argument.

Exercise 5.4. Interpolating the sign function. Use `x = chebfun('x')`, `f = sign(x)` to construct the sign function on $[-1,1]$ and `p = chebfun('sign(x)',10000)` to construct its interpolant in 10000 Chebyshev points. Explore the difference in the

interesting region by defining `d = f-p`, `d = d{-0.002,0.002}`. What is the maximum value of `p`? In what subset of $[-1,1]$ is `p` smaller than 0.5 in absolute value?

Exercise 5.5. Accuracy of point evaluations. (a) Construct the chebfun g corresponding to $f(x) = \sin(\exp(10x))$ on $[-1,1]$. What is the degree of this polynomial? (b) Let `xx` be the vector of 1000 linearly spaced points from -1 to 1. How long does it take on your computer to evaluate f(`xx`)? g(`xx`)? (c) Draw a loglog plot of the vector of errors $|f(\texttt{xx}) - g(\texttt{xx})|$ against the vector of derivatives $|f'(\texttt{xx})|$. Comment on why the dots line up as they do.

Exercise 5.6. Equispaced points. [Not yet finished] Show that for equispaced points with spacing h the weights are $\lambda_j = (-1)^{n-j}\binom{n}{j}/h^n n!$, or after canceling common factors, $\lambda_j = (-1)^j\binom{n}{j}$.

Exercise 5.7. Adpative interpolation grids. [to be written – interpolate $|x|$ and keep adding worst point.]

Exercise 5.8. Peturbed Chebyshev grids. [perturb the grid and compare rational and polynomial interpolants]

Exercise 5.9. Barycentric formula for Chebyshev polynomials. Derive an elegant formula for $T_n(x)$ from (5.13) [Salzer 1972].

Exercise 5.10. Barycentric interpolation in roots of unity. Derive the barycentric weights $\{\lambda_j\}$ for polynomial interpolation in (a) $\{\pm 1\}$, (b) $\{1, i, -1, -i\}$, (c) The $(n+1)$st roots of unity for arbitrary $n \geq 0$.

Exercise 5.11. Barycentric weights for a general interval. (a) How does the formula for Chebyshev barycentric weights on $[-1,1]$ change for weights on an interval $[a,b]$? (b) The *capacity* of $[a,b]$ (see Chapter 12) is equal to $c = (b-a)/4$. How do the barycentric weights behave as $n \to \infty$ for an interval of capacity c? As a function of c, what is the maximal value of n for which they can be represented in IEEE double precision arithmetic without overflow or underflow? (You may assume the overflow and underflow limits are 10^{308} and 10^{-308}. The overflow/underflow problem goes away with the use of the divided form (5.13).)

6. Weierstrass Approximation Theorem

Every continuous function on a bounded interval can be approximated to arbitrary accuracy by polynomials. This is the famous Weierstrass Approximation Theorem, proved by Karl Weierstrass when he was 70 years old [Weierstrass 1885]. The theorem was independently discovered at about the same time, in essence, by Carl Runge: as pointed out in 1886 by Phragmén in remarks published as a footnote stretching over four pages in a paper by Mittag-Leffler [1900], it can be derived as a corollary of results Runge published in a pair of papers in 1885 and 1886 [Runge 1885 & 1885/1886] (Exercise 6.3).

Here and throughout this book, except where otherwise indicated, $\|\cdot\|$ denotes the supremum norm on $[-1,1]$.

Theorem 6.1: Weierstrass Approximation Theorem. *Let f be a continuous function on $[-1,1]$ and let $\varepsilon > 0$ be arbitrary. Then there exists a polynomial p such that*

$$\|f - p\| < \varepsilon.$$

Proof. We shall not spell out a proof in detail. However, here is an outline of the beautiful proof from Weierstrass's original paper. First, extend $f(x)$ to a continuous function $\tilde{f}$ with compact support on the whole real line. Now, take $\tilde{f}$ as initial data at $t = 0$ for the diffusion equation $\partial u/\partial t = \partial^2 u/\partial x^2$ on the real line. It is known that by convolving $\tilde{f}$ with the Gaussian kernel $\phi(x) = e^{-x^2/4t}/\sqrt{4\pi t}$, we get a solution to this partial differential equation that converges uniformly to f as $t \to 0$, and thus can be made arbitrarily close to f on $[-1,1]$ by taking t small enough. On the other hand, since $\tilde{f}$ has compact support, for each $t > 0$ this solution is an integral over a bounded interval of entire functions and is thus itself an entire function, that is, analytic throughout the complex plane. Therefore it has a convergent Taylor series on $[-1,1]$, which can be truncated to give polynomial approximations of arbitrary accuracy. ∎

For a fuller presentation of the argument just given as "one of the most amusing applications of the Gaussian kernel," where the result is stated for the more general case of a function of several variables approximated by multivariate polynomials, see Chapter 4 of [Folland 1995]. Many other proofs are also known, including these early ones:

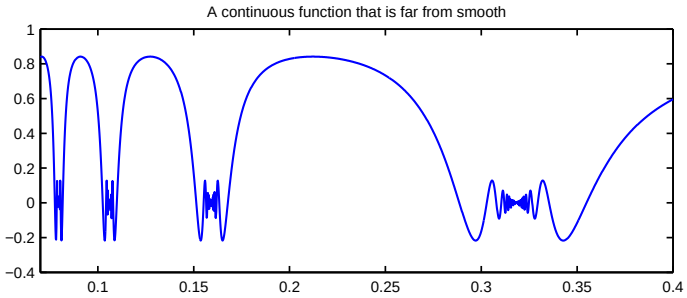
Runge (1885/86)
Picard (1891)
Lerch (1892 and 1903)
Volterra (1897)
Lebesgue (1898)
Mittag-Leffler (1900)
Fejér (1900)
Landau (1908)
de la Vallée Poussin (1908)
Jackson (1911)
Bernstein (1912)
Montel (1918)

For example, Bernstein's proof has a probabilistic flavor, and Lebesgue's proof, which appeared in his first paper published at age 23, is based on reducing approximation of general continuous functions to the approximation of $|x|$ [Lebesgue 1898]. This long list gives an idea of the great amount of mathematics stimulated by Weierstrass's theorem and the significant role it played in the development of analysis in the early 20th century. For a fascinating discussion of this piece of mathematical history, see [Pinkus 2000].

Weierstrass's theorem establishes that even extremely non-smooth functions can be approximated by polynomials, functions like $x\sin(x^{-1})$ or even $\sin(x^{-1})\sin(1/\sin(x^{-1}))$. The latter function has an infinite number of points near which it oscillates infinitely often, as we begin to see from the plot below

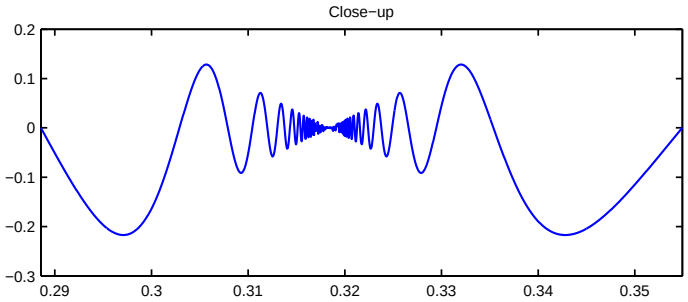
over the range $[0.07, 0.4]$. In this calculation Chebfun is called with a user-prescribed number of interpolation points, 30000, since the usual adaptive procedure has no chance of resolving the function to machine precision with a practicable number of points.

```
f = chebfun(@(x) sin(1./x).*sin(1./sin(1./x)),[.07 .4],30000);
plot(f), xlim([.07 .4])
title('A continuous function that is far from smooth')
```



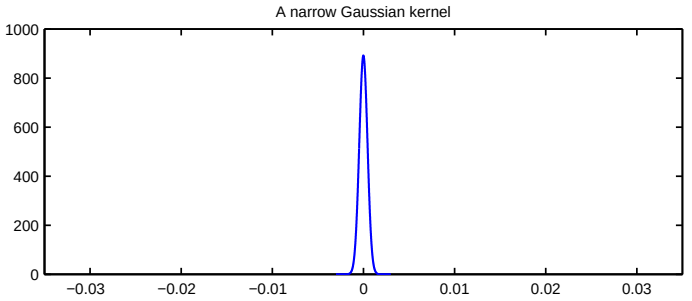
We can illustrate the idea of Weierstrass's proof by showing the convolution of this complicated function with a Gaussian. Here is the same function f recomputed over a subinterval extending from one of its zeros to another:

```
a = 0.2885554757; b = 0.3549060246;
f2 = chebfun(@(x) sin(1./x).*sin(1./sin(1./x)),[a,b],2000);
plot(f2), xlim([a b]), title('Close-up')
```



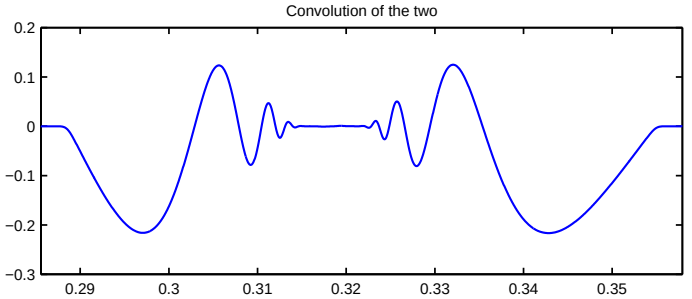
Here is a narrow Gaussian.

```
t = 1e-7;
phi = chebfun(@(x) exp(-x.^2/(4*t))/sqrt(4*pi*t),.003*[-1 1]);
plot(phi), xlim(.035*[-1 1])
title('A narrow Gaussian kernel')
```

Convolving the two gives a smoothed version of the close-up of f. Notice how the short wavelengths vanish while the long ones are nearly undisturbed.

```
f3 = conv(f2,phi);
plot(f3), xlim([a-.003,b+.003])
title('Convolution of the two')
```



This is an entire function, which means it can be approximated by polynomials merely by truncating the Taylor series.

For all its beauty, power, and importance, Weierstrass's theorem has in some respects served as an unfortunate distraction. Knowing that even troublesome functions can be approximated by polynomials, we naturally ask, how can we do it? A famous result of Faber and Bernstein asserts that there is no set of interpolation points, Chebyshev or otherwise, that achieves convergence as $n \to \infty$ for all continuous f [Bernstein 1919, Faber 1914]. So it becomes tempting to look at approximation methods that go beyond interpolation, and to warn people that interpolation is dangerous, and to try to characterize exactly what minimal properties of f suffice to ensure that interpolation will work after all. A great deal is known about these subjects. The trouble with this line of research is that for almost all the functions encountered in practice, Chebyshev interpolation works beautifully! Weierstrass's theorem has encouraged mathematicians over the years to give too much of their attention to pathological

functions at the edge of discontinuity, leading to the bizarre and unfortunate situation where many books on numerical analysis caution their readers that interpolation may fail without mentioning that for functions with a little bit of smoothness, it succeeds outstandingly. For a discussion of the history of such misrepresentations and misconceptions, see Chapter 14.

[To be added: (1) Can we speed up `conv`? (2) Runge & Mergelyan theorems.]

SUMMARY OF CHAPTER 6. *A continuous function on a bounded interval can be approximated arbitrarily closely by polynomials.*

Exercise 6.1. A pathological function of Weierstrass. Weierstrass was one of the first to give an example of a function continuous but nowhere differentiable on $[-1,1]$, and it is one of the early examples of a fractal [Weierstrass 1872]:

$$w(x) = \sum_{k=0}^{\infty} 2^{-k} \cos(3^k x).$$

(a) Construct a chebfun `w7` corresponding to this series truncated at $k = 7$. Plot `w7`, its derivative (use `diff`), and its indefinite integral (`cumsum`). What is the degree of the polynomial defining this chebfun? (b) Prove that w is continuous. (You can use the Weierstrass M-test.)

Exercise 6.2. Taylor series of an entire function. In illustrating the proof of the Weierstrass Approximation Theorem we plotted a Gaussian kernel. The key point of the proof is that this kernel is entire, so its Taylor series converges for all x. (a) For $x = 1$ at the given time $t = 10^{-7}$, how many terms of the Taylor series about $x = 0$ would you have to take before the terms fall below 1? Estimate the answer at least to within a factor of 2. You may find Stirling's formula helpful. (b) Also for $x = 1$ and $t = 10^{-7}$, approximately how big is the biggest term in the Taylor series?

Exercise 6.3. Runge's proof. [to be written]

Exercise 6.4. Resolving a difficult function. [Figure out how many points it would take in fact to resolve the wiggly function. To be written.]

7. Convergence for differentiable functions

The principle mentioned at the end of the last chapter might be regarded as the central fact of approximation theory: the smoother a function, the faster its approximants converge as $n \to \infty$. Connections of this kind were explored in the early years of the 20th century by three of the founders of approximation theory: Charles de la Vallée Poussin (1866–1962), a mathematician at Louvain in Belgium, Sergei Bernstein (1880–1968), a Ukrainian mathematician who had studied with Hilbert in Göttingen, and Dunham Jackson (1888–1946), an American student of Landau's also at Göttingen. (Henri Lebesgue in France

(1875–1941) also proved some of the early results. For remarks on the history see [Goncharov 2000, Steffens 2006].) Bernstein made the following comment concerning best approximation errors $E_n(f) = \|f - p_n^*\|_\infty$ (see Chapter 10) in his summary article for the International Congress of Mathematicians in 1912 [Bernstein 1912a].

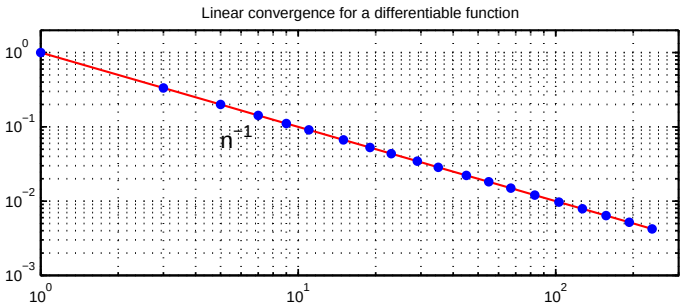
The general fact that emerges from this study is the existence of a most intimate connection between the differential properties of the function $f(x)$ and the asymptotic rate of decrease of the positive numbers $E_n[f(x)]$.[3]

In this and the next chapter our aim is to make the smoothness–approximability link precise in the context of Chebyshev truncations and interpolants. Everything here is analogous to results for Fourier analysis of periodic functions, and indeed, the whole theory of Chebyshev interpolation can be regarded as a transplant to nonperiodic functions on $[-1,1]$ of the theory of trigonometric interpolation of periodic functions on $[-\pi,\pi]$.

Suppose a function f is ν times differentiable on $[-1,1]$, possibly with jumps in the νth derivative, and suppose you look at the convergence of its Chebyshev interpolants as $n \to \infty$, measuring the error in the ∞-norm. You will typically see convergence at the rate $O(n^{-\nu})$. We can explore this effect readily in Chebfun. For example, the function $f(x) = |x|$ is once differentiable with a jump in the first derivative at $x = 0$, and the convergence curve nicely matches n^{-1} (shown as a straight line). Actually the match is more than just "nice" in this case — it is exact, with p_n taking its maximal error at the value $p(0) = 1/n$ for odd n. (For even n the error is somewhat smaller.)

```
f = abs(x);
nn = 2*round(2.^(0:.3:7))-1;
ee = 0*nn;
for j = 1:length(nn)
    n = nn(j); fn = chebfun(f,n+1); ee(j) = norm(f-fn,inf);
end
hold off, loglog(nn,1./nn,'r')
text(5,0.07,'n^{-1}',FS,12)
grid on, axis([1 300 1e-3 2])
hold on, loglog(nn,ee,'.')
title('Linear convergence for a differentiable function')
```

[3] "Le fait général qui se dégage de cette étude est l'existence d'une liaison des plus intimes entre les propriétés différentielles de la fonction $f(x)$ et la loi asymptotique de la décroissance des nombres positifs $E_n[f(x)]$."

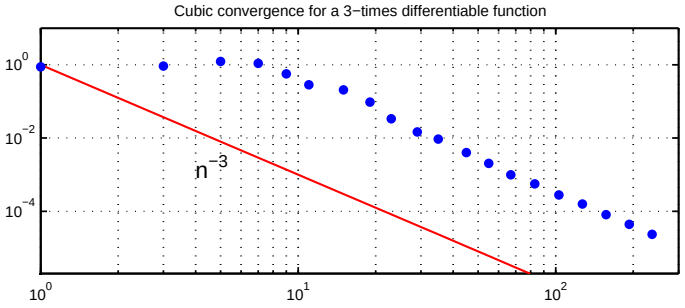


Similarly, we get cubic convergence for

$$f(x) = |\sin(5x)|^3, \tag{7.1}$$

which is three times differentiable with jumps in the third derivative at $x = 0$ and $\pm\pi/5$.

```
f = abs(sin(5*x)).^3;
for j = 1:length(nn)
    n = nn(j); fn = chebfun(f,n+1); ee(j) = norm(f-fn,inf);
end
hold off, loglog(nn,nn.^-3,'r')
text(4,.0015,'n^{-3}',FS,12)
grid on, axis([1 300 2e-6 10])
hold on, loglog(nn,ee,'.')
title('Cubic convergence for a 3-times differentiable function')
```



Encouraged by such experiments, you might look in a book to try to find theorems about $O(n^{-\nu})$. If you do, you'll run into two difficulties. First, it's hard to find theorems about Chebyshev interpolants, for most of the literature is about other approximations such as best approximations (see Chapters 10 and 16) or interpolants in Chebyshev polynomial roots rather than extrema. Second, you will probably fall one power of n short! In particular, the most commonly quoted

of the **Jackson theorems** asserts that if f is ν times *continuously* differentiable on $[-1, 1]$, then its best polynomial approximations converge at the rate $O(n^{-\nu})$ [Jackson 1911; Cheney 1966, sec. 4.6]. But the first and third derivatives of the functions we just looked at, respectively, are not continuous. Thus we must settle for the zeroth and second derivatives, respectively, if we insist on continuity, so this theorem would ensure only $O(n^0)$ and $O(n^{-2})$ convergence, not the $O(n^{-1})$ and $O(n^{-3})$ that are actually observed. And it would apply to best approximations, not Chebyshev interpolants.

We can get the result we want by recognizing that most functions encountered in applications have a property that is not assumed in most theorems: **bounded variation**. A function, whether continuous or not, has bounded variation if its total variation is finite. The **total variation** is the 1-norm of the derivative (as defined if necessary in the distributional sense; see [Ziemer 1989, chap. 5] or [Evans & Gariepy 1991, sec. 5.10]). We can compute this number conveniently with Chebfun by writing an anonymous function:

```
tv = @(f) norm(diff(f),1);
```

Here are the total variations of x and $\sin(10\pi x)$ over $[-1, 1]$:

```
disp([tv(x) tv(sin(10*pi*x))])
```

```
   2.000000000000000  40.000000000000007
```

Here is the total variation of the derivative of $|x|$:

```
tv(diff(abs(x)))
```

```
ans = 2
```

Here is the total variation of the third derivative of the function f of (7.1):

```
tv(diff(f,3))
```

```
ans = 1.652783663432566e+04
```

It is the finiteness of this number that allowed the Chebyshev interpolants to this function f to converge as fast as $O(n^{-3})$.

To get to a precise theorem we begin with a bound on Chebyshev coefficients, an improvement (in the definition of the quantity V) of a similar result in [Trefethen 2008]. The condition of *absolute continuity* is a standard one which we shall not make detailed use of, so we will not discuss. An absolutely continuous function is equal to the integral of its derivative, which exists almost everywhere and is Lebesgue integrable.

Theorem 7.1: Chebyshev coefficients of differentiable functions. *For an integer $\nu \geq 0$, let f have an absolutely continuous $(\nu-1)$st derivative $f^{(\nu-1)}$*

on $[-1,1]$ (if $\nu > 0$) and a νth derivative $f^{(\nu)}$ of bounded variation V. Then for $k \ge \nu+1$, the Chebyshev coefficients of f satisfy

$$|a_k| \le \frac{2V}{\pi k(k-1)\cdots(k-\nu)} \le \frac{2V}{\pi(k-\nu)^{\nu+1}}. \tag{7.2}$$

Proof. As in the proof of Theorem 3.1, setting $x = \frac{1}{2}(z+z^{-1})$ with z on the unit circle gives

$$a_k = \frac{1}{\pi i}\int_{|z|=1} f(\tfrac{1}{2}(z+z^{-1}))\, z^{k-1}\, dz,$$

and integrating by parts with respect to z converts this to

$$a_k = \frac{-1}{\pi i}\int_{|z|=1} f'(\tfrac{1}{2}(z+z^{-1}))\, \frac{z^k}{k}\, \frac{dx}{dz}\, dz\,; \tag{7.3}$$

the factor dx/dz appears since f' denotes the derivative with respect to x rather than z. Suppose now $\nu = 0$, so that all we are assuming about f is that it is of bounded variation $V = \|f'\|_1$. Then we note that this integral over the upper half of the unit circle is equivalent to an integral in x; the integral over the lower half gives another such integral. Combining the two gives

$$a_k = \frac{1}{\pi i}\int_{-1}^{1} f'(x)\, \frac{z^k - z^{-k}}{k}\, dx = \frac{2}{\pi}\int_{-1}^{1} f'(x)\, \mathrm{Im}\, \frac{z^k}{k}\, dx,$$

and since $|z^k/k| \le 1/k$ for $x \in [-1,1]$ and $V = \|f'\|_1$, this implies $|a_k| \le 2V/\pi k$, as claimed.

If $\nu > 0$, we replace dx/dz by $\frac{1}{2}(1-z^{-2})$ in (7.3), obtaining

$$a_k = -\frac{1}{\pi i}\int_{|z|=1} f'(\tfrac{1}{2}(z+z^{-1}))\, \left[\frac{z^k}{2k} - \frac{z^{k-2}}{2k}\right]\, dz.$$

Integrating by parts again with respect to z converts this to

$$a_k = \frac{1}{\pi i}\int_{|z|=1} f''(\tfrac{1}{2}(z+z^{-1}))\, \left[\frac{z^{k+1}}{2k(k+1)} - \frac{z^{k-1}}{2k(k-1)}\right]\, \frac{dx}{dz}\, dz.$$

Suppose now $\nu = 1$ so that we are assuming f' has bounded variation $V = \|f''\|_1$. Then again this integral is equivalent to an integral in x,

$$a_k = \frac{-2}{\pi}\int_{-1}^{1} f''(x)\, \mathrm{Im}\left[\frac{z^{k+1}}{2k(k+1)} - \frac{z^{k-1}}{2k(k-1)}\right]\, dx.$$

Since the term in square brackets is bounded by $1/k(k-1)$ for $x \in [-1,1]$ and $V = \|f''\|_1$, this implies $|a_k| \le 2V/\pi k(k-1)$, as claimed.

If $\nu > 1$, we continue in this fashion with a total of $\nu+1$ integrations by parts with respect to z, in each case first replacing dx/dz by $\frac{1}{2}(1-z^{-2})$. At the next step the term that appears in square brackets is

$$\left[\frac{z^{k+2}}{4k(k+1)(k+2)} - \frac{z^k}{4k^2(k+1)} - \frac{z^k}{4k^2(k-1)} + \frac{z^{k-2}}{4k(k-1)(k-2)}\right],$$

which is bounded by $1/k(k-1)(k-2)$ for $x \in [-1,1]$. And so on. ∎

From Theorems 3.1 and 7.1 we can derive consequences about the accuracy of Chebyshev truncations and interpolants. The estimate (7.5) can be found as Corollary 2 in [Mastroianni & Szabados 1995], though with a bound of the form $O(n^{-\nu}V)$ rather than an explicit constant, whose appearance here so far as we know is new. The analogous result for best approximations as opposed to Chebyshev interpolants or truncations was announced in [Bernstein 1911] and proved in [Bernstein 1912c].

Theorem 7.2: Convergence for differentiable functions. *If f satisfies the conditions of Theorem* 7.1*, with V again denoting the total variation of $f^{(\nu)}$ for some $\nu \ge 1$, then for any $n > \nu$, its Chebyshev truncations satisfy*

$$\|f - f_n\| \le \frac{2V}{\pi\nu(n-\nu)^\nu} \tag{7.4}$$

and its Chebyshev interpolants satisfy

$$\|f - p_n\| \le \frac{4V}{\pi\nu(n-\nu)^\nu}. \tag{7.5}$$

Proof. For (7.4), Theorem 7.1 applied to equation (4.8) gives us

$$\|f - f_n\| \le \sum_{k=n+1}^{\infty} |a_k| \le \frac{2V}{\pi}\sum_{k=n+1}^{\infty} (k-\nu)^{-\nu-1}$$

and this sum can in turn be bounded by

$$\int_n^\infty (s-\nu)^{-\nu-1} ds = \frac{1}{\nu(n-\nu)^\nu}.$$

For (7.5), we use (4.9) instead of (4.8) and get the same bound except with coefficients $2|a_k|$ rather than $|a_k|$. ∎

In a nutshell: a νth derivative of bounded variation implies convergence at the algebraic rate $O(n^{-\nu})$. Here is a way to remember this message. Suppose we try to approximate the step function $\mathrm{sign}(x)$ by polynomials. There is no hope of convergence, since polynomials are continuous and $\mathrm{sign}(x)$ is not, so all we can achieve is accuracy $O(1)$ as $n \to \infty$. That's the case $\nu = 0$. But now, each

time we make the function "one derivative smoother," ν increases by 1 and so does the order of convergence.

How sharp is Theorem 7.2 for our example functions? In the case of $f(x) = |x|$, with $\nu = 1$ and $V = 2$, it predicts $\|f - f_n\| \le 4/\pi(n-1)$ and $\|f - p_n\| \le 8/\pi(n-1) \approx 2.55/(n-1)$. As mentioned above, the actual value for Chebyshev interpolation is $\|f - p_n\| = 1/n$ for odd n. The minimal possible error in polynomial approximation, with p_n replaced by the best approximation p_n^* (Chapter 10), is $\|f - p_n^*\| \sim 0.280169\ldots n^{-1}$ as $n \to \infty$ [Varga & Carpenter 1985]. So we see that the range from best approximant, to Chebyshev interpolant, to bound on Chebyshev interpolant is less than a factor of 10. The approximation of $|x|$ was a central problem studied by Lebesgue, de la Vallée Poussin, Bernstein, and Jackson a century ago, and we shall consider it further in Chapter 24.

The results are similar for the other example, $f(x) = |\sin(5x)|^3$, whose third derivative, we saw, has variation $V \approx 16528$. Equation (7.5) implies that the Chebyshev interpolants satisfy $\|f - p_n\| < 7020/(n-1)^3$, whereas in fact, we have $\|f - p_n\| \approx 309/n^3$ for large odd n and $\|f - p_n^*\| \approx 80/n^3$.

We close with a comment about Theorem 7.2. We have assumed in this theorem that $f^{(\nu)}$ is of bounded variation. A similar but weaker condition would be that $f^{(\nu-1)}$ is Lipschitz continuous (Exercise 7.2). This weaker assumption is enough to ensure $\|f - p_n^*\| = O(n^{-\nu})$ for the best approximations $\{p_n^*\}$; this is one of the Jackson theorems. On the other hand it is not enough to ensure $O(n^{-\nu})$ convergence of Chebyshev truncations and interpolants. The reason we emphasize the stronger implication with the stronger conclusion is that in practice, one rarely deals with a function that is Lipschitz continuous while lacking a derivative of bounded variation, whereas one constantly deals with truncations and interpolants rather than best approximations.

Incidentally it was de la Vallée Poussin [1908] who first showed that the strong hypothesis is enough to reach the weak conclusion: if $f^{(\nu)}$ is of bounded variation, then $\|f - p_n^*\| = O(n^{-\nu})$ for the best approximation p_n^*. Three years later Jackson [1911] sharpened the result by weakening the hypothesis as just indicated.

[To be added: (1) Converse of Thm 7.2. (2) Jackson and other literature? (3) Check case $\nu = 0$ in Theorem 7.1 and make comment about Gibbs phenomenon. (4) Re Thm 7.2, check paper recommended by Tadmor: Canuto & Q, Approx results for orthog polys in Sobolev spaces, Math Comp 38 (1982), 67–82.]

SUMMARY OF CHAPTER 7. *The smoother a function f defined on $[-1,1]$ is, the faster its approximants converge. In particular, if the νth derivative of f is of bounded variation V, then the Chebyshev coefficients $\{a_k\}$ of f are bounded in absolute value by $2\pi^{-1}V(k-\nu)^{-\nu-1}$. It follows that the degree n Chebyshev truncation and interpolant of f have accuracy $O(Vn^{-\nu})$.*

Exercise 7.1. Total variation. (a) Determine numerically the total variation of $f(x) = \sin(100x)/(1+x^2)$ on $[-1,1]$. (b) It is no coincidence that the answer is close to 100, and indeed the total variation of $\sin(Mx)/(1+x^2)$ on $[-1,1]$ is asymptotic to M as $M \to \infty$. Explain why.

Exercise 7.2. Lipschitz continuous vs. derivative of bounded variation. (a) Prove that if the derivative f' of a function f has bounded variation, then f is Lipschitz continuous. (b) Give an example to show that the converse does not hold.

Exercise 7.3. Convergence for Weierstrass's function. Exercise 6.1 considered a "pathological function of Weierstrass" $w(x)$ which is continuous but nowhere differentiable on $[-1,1]$. (a) Make an anonymous function in Matlab that evaluates $w(\mathtt{xx})$ for a vector `xx` to machine precision by taking the sum to 53 terms. (b) Use Chebfun to produce a plot of $\|w - p_n\|$ accurate enough and for high enough values of n to confirm that convergence appears to take place as $n \to \infty$. Thus w is not one of the functions for which interpolants fail to converge, a fact we shall prove in Chapter 15 while also showing how such troublesome functions can be constructed.

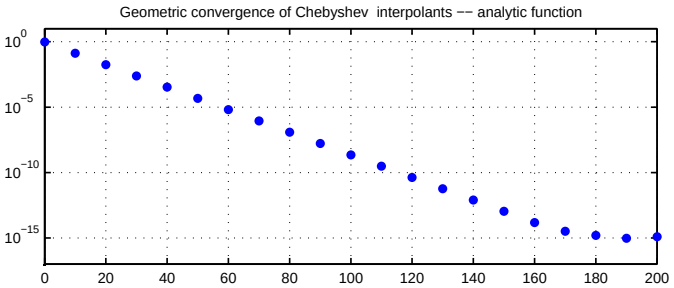
Exercise 7.4. Sharpness of Theorem 7.2. Consider the functions (a) $f(x) = |x|$, (b) $f(x) = |x|^5$, (c) $f(x) = \sin(100x)$. In each case plot as functions of n the error $\|f - p_n\|$ in Chebyshev interpolation on $[-1,1]$ and the bound on this quantity from (7.5). How close are the bounds? In cases (a) and (b) take ν as large as possible, and in case (c) take $\nu = 2$, 4, and 8.

8. Convergence for analytic functions

Suppose f is not just k times differentiable but infinitely differentiable and in fact analytic on $[-1,1]$. (Recall that this means that for any $s \in [-1,1]$, f has a Taylor series about s that converges to f in a neighborhood of s.) Then without any further assumptions we may conclude that the Chebyshev truncations and interpolants converge **geometrically**, that is, at the rate $O(C^{-n})$ for some constant $C > 1$. This means the errors will look like straight lines (or better) on a semilog scale rather than a loglog scale. This kind of connection was first announced by Bernstein in 1911, who showed that the best approximations to a function f on $[-1,1]$ converge geometrically as $n \to \infty$ if and only if f is analytic [Bernstein 1911 & 1912c].

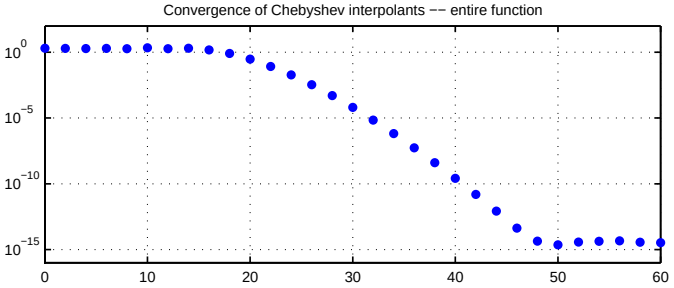
For example, for Chebyshev interpolants of the function $(1+25x^2)^{-1}$, known as the **Runge function** (Chapter 13), we get steady geometric convergence down to the level of rounding errors:

```
f = 1./(1+25*x.^2);
nn = 0:10:200; ee = 0*nn;
for j = 1:length(nn)
    n = nn(j); fn = chebfun(f,n+1); ee(j) = norm(f-fn,inf);
end
hold off, semilogy(nn,ee,'.'), grid on, axis([0 200 1e-17 10])
title(['Geometric convergence of Chebyshev ' ...
      ' interpolants -- analytic function'])
```



If f is analytic not just on $[-1,1]$ but in the whole complex plane — such a function is said to be **entire** — then the convergence is even faster than geometric. Here, for the function $\cos(20x)$, the dots are not approaching a fixed straight line but a curve that gets steeper as n increases, until rounding errors cut off the progress.

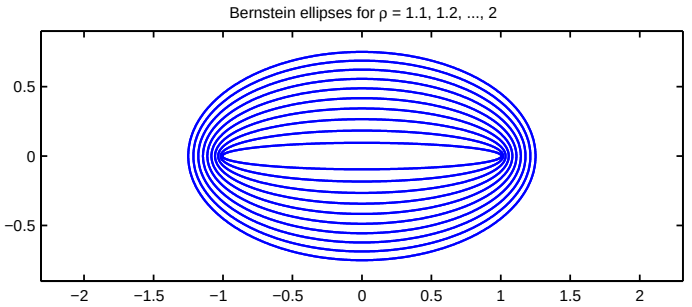
```
f = cos(20*x);
nn = 0:2:60; ee = 0*nn;
for j = 1:length(nn)
    n = nn(j); fn = chebfun(f,n+1); ee(j) = norm(f-fn,inf);
end
semilogy(nn,ee,'.'), grid on, axis([0 60 1e-16 100])
title('Convergence of Chebyshev interpolants -- entire function')
```



There are elegant theorems that explain these effects. If f is analytic on $[-1,1]$, then it can be analytically continued to a neighborhood of $[-1,1]$ in the complex

plane. (The idea of analytic continuation is explained in complex variables textbooks; see also Chapter 28.) The bigger the neighborhood, the faster the convergence. In particular, for polynomial approximations, the neighborhoods that matter are the regions in the complex plane bounded by ellipses with foci at -1 and 1. We call these **Bernstein ellipses**, for they were introduced into approximation theory by Bernstein [1912b, 1912c, 1913a & 1914a]. It is easy to plot these ellipses: pick a number $\rho > 1$ and plot the image in the complex x-plane of the circle of radius ρ in the z-plane under the Joukowsky map $x = (z+z^{-1})/2$. We let E_ρ denote the open region bounded by this ellipse. Here, for example, are the Bernstein ellipses corresponding to the parameters $\rho = 1.1, 1.2, \dots, 2$:

```
z = exp(2i*pi*x);
for rho = 1.1:0.1:2
    e = (rho*z+(rho*z).^(-1))/2;
    plot(e), hold on
end
ylim([-.9 .9]), axis equal
title('Bernstein ellipses for \rho = 1.1, 1.2, ..., 2')
```



It is not hard to verify that the length of the semimajor axis of E_ρ plus the length of the semiminor axis is equal to ρ (Exercise 8.1).

Here is the basic bound on Chebyshev coefficients of analytic functions from which many other things follow. It first appeared in Section 61 of [Bernstein 1912c].

Theorem 8.1: Chebyshev coefficients of analytic functions. *Let a function f analytic in $[-1,1]$ be analytically continuable to the open ρ-ellipse E_ρ, where it satisfies $|f(z)| \le M$ for some M. Then its Chebyshev coefficients satisfy*

$$|a_k| \le 2M\rho^{-k}, \tag{8.1}$$

with $|a_0| \le M$ in the case $k = 0$.

Proof. As in the proofs of Theorems 3.1, 4.1, and 7.1, we make use of the transplantation from $f(x)$ and $T_k(x)$ on $[-1,1]$ in the x-plane to $F(z)$ and $(z^k+z^{-k})/2$ on the unit circle in the z-plane, with $x=(z+z^{-1})/2$ and $F(z)=F(z^{-1})=f(x)$. The ellipse E_ρ in the x-plane corresponds under this formula in a 1-to-2 fashion to the annulus $\rho^{-1}<|z|<\rho$ in the z-plane. By this we mean that for each x in $E_\rho\backslash[-1,1]$ there are two corresponding values of z which are inverses of one another, and both the circles $|z|=\rho$ and $|z|=\rho^{-1}$ map onto the ellipse itself. (We can no longer use the formula $x=\mathrm{Re}\,z$, which is valid only for $|z|=1$.) The first thing to note is that if f is analytic in the ellipse, then F is analytic in the annulus since it is the composition of the two analytic functions $z\mapsto(z+z^{-1})/2$ and $x\mapsto f(x)$. Now we make use of the contour integral formula (3.6),

$$a_k=\frac{1}{\pi i}\int_{|z|=1} z^{-1-k}F(z)\,dz,$$

with πi replaced by $2\pi i$ for $k=0$. Suppose for a moment that F is analytic not just in the annulus but in its closure $\rho^{-1}\le|z|\le\rho$. Then we can expand the contour to $|z|=\rho$ without changing the value of the integral, giving

$$a_k=\frac{1}{\pi i}\int_{|z|=\rho} z^{-1-k}F(z)\,dz,$$

again with πi replaced by $2\pi i$ for $k=0$. Since the circumference is $2\pi\rho$ and $|F(z)|\le M$, the required bound now follows from an elementary estimate. If F is analytic only in the open annulus, we can move the contour to $|z|=s$ for any $s<\rho$, leading to the same bound for any $s<\rho$ and hence also for $s=\rho$. ∎

Here are two of the consequences of Theorem 8.1. Equation (8.2) first appeared in [Bernstein 1912c, Sec. 61]. I do not know where (8.3) may have appeared, though similar slightly weaker bounds can be found in (4.13) and (4.16) of [Tadmor 1986].

Theorem 8.2: Convergence for analytic functions. *If f has the properties of Theorem* 8.1*, then for each $n\ge0$ its Chebyshev truncations satisfy*

$$\|f-f_n\|\le\frac{2M\rho^{-n}}{\rho-1} \tag{8.2}$$

and its Chebyshev interpolants satisfy

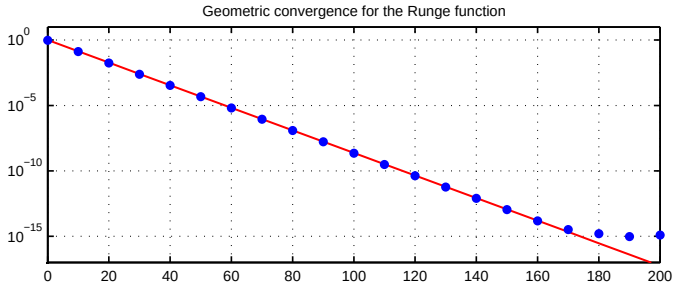
$$\|f-p_n\|\le\frac{4M\rho^{-n}}{\rho-1}. \tag{8.3}$$

Proof. Equation (8.2) follows from Theorem 8.1 and (4.8), and (8.3) follows from Theorem 8.1 and (4.9). ∎

We can apply Theorem 8.2 directly if f is analytic and bounded in E_ρ. If it is analytic but unbounded in E_ρ, then it will be analytic and bounded in E_s for any $s<\rho$, so we still get convergence at the rate $O(s^{-n})$ for any $s<\rho$.

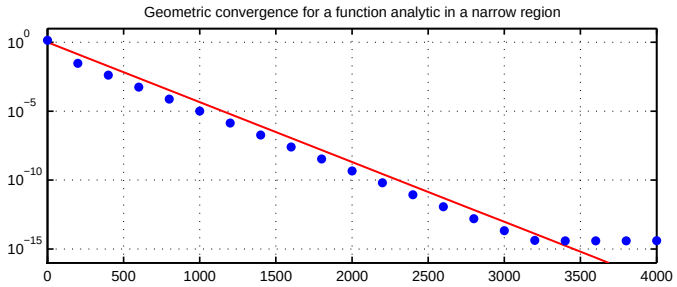
For example, the Runge function $(1+25x^2)^{-1}$ considered above has poles at $\pm i/5$. The corresponding value of ρ is $(1+\sqrt{26})/5\approx1.220$, and the errors in Chebyshev interpolation match this rate beautifully:

```
f = 1./(1+25*x.^2);
nn = 0:10:200; ee = 0*nn;
for j = 1:length(nn)
    n = nn(j); fn = chebfun(f,n+1);
    ee(j) = norm(f-fn,inf);
end
rho = (1+sqrt(26))/5;
hold off, semilogy(nn,rho.^(-nn),'-r')
hold on, semilogy(nn,ee,'.')
grid on, axis([0 200 1e-17 10])
title('Geometric convergence for the Runge function')
```



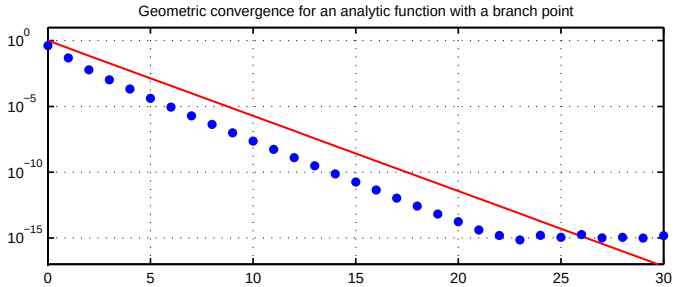
Here is a more extreme but entirely analogous example: $\tanh(50\pi x)$, with poles at $\pm0.01i$. These poles are so close to $[-1,1]$ that the convergence is much slower, but it is still robust. The only difference in this code segment is that `norm(f-fn,inf)`, a relatively slow Chebfun operation that depends on finding zeros of the derivative of `f-fn`, has been replaced by the default 2-norm `norm(f-fn)`, which is quick. This makes little difference to the figure, as the exponential decay rates are the same. (In the ∞-norm, the dots in the figure would appear just above the red line instead of just below it.)

```
f = tanh(50*pi*x);
nn = 0:200:4000; ee = 0*nn;
for j = 1:length(nn)
    n = nn(j); fn = chebfun(f,n+1); ee(j) = norm(f-fn);
end
rho = (1+sqrt(10001))/100;
hold off, semilogy(nn,rho.^(-nn),'-r')
hold on, semilogy(nn,ee,'.')
grid on, axis([0 4000 1e-16 10])
title(['Geometric convergence for a function ' ...
       'analytic in a narrow region'])
```



For another example, the function $\sqrt{2-x}$ has a branch point at $x = 2$, corresponding to $\rho = 2 + \sqrt{3}$. Again we see a good match, with the curve gradually bending over to the expected slope as $n \to \infty$.

```
f = sqrt(2-x);
nn = 0:30; ee = 0*nn;
for j = 1:length(nn)
    n = nn(j); fn = chebfun(f,n+1); ee(j) = norm(f-fn,inf);
end
rho = 2+sqrt(3);
hold off, semilogy(nn,rho.^(-nn),'-r')
hold on, semilogy(nn,ee,'.')
grid on, axis([0 30 1e-17 10])
title(['Geometric convergence for an analytic ' ...
       'function with a branch point'])
```



We conclude this chapter by stating a converse of Theorem 8.2, also due to Bernstein [1912c, Section 9]. The converse is not quite exact: Theorem 8.2 assumes analyticity and boundedness in E_ρ, whereas the conclusion of Theorem 8.3 is analyticity in E_ρ but not necessarily boundedness.

Theorem 8.3: Converse of Theorem 8.2. *Suppose f is a function on $[-1,1]$*

for which there exist polynomial approximations $\{q_n\}$ satisfying

$$\|f - q_n\| \le C\rho^{-n}, \quad n \ge 0$$

for some constants $\rho > 1$ and $C > 0$. Then f can be analytically continued to an analytic function in the open ρ-ellipse E_ρ.

Proof. The assumption implies that the polynomials $\{q_n\}$ satisfy $\|q_n - q_{n-1}\| \le 2C\rho^{1-n}$ on $[-1,1]$. Since $q_n - q_{n-1} \in P_n$, it can be shown that this implies $\|q_n - q_{n-1}\|_{E_s} \le 2Cs^n\rho^{1-n}$ for any $s > 1$, where $\|\cdot\|_{E_s}$ is the supremum norm on the s-ellipse E_s. (This estimate is one of **Bernstein's inequalities**, from Section 9 of [Bernstein 1912c]; see Exercise 8.6.) For $s < \rho$, this gives us a representation for f in E_s as a series of analytic functions,

$$f = q_0 + (q_1 - q_0) + (q_2 - q_1) + \cdots,$$

which according to the Weierstrass M test is uniformly convergent. According to another well-known theorem of Weierstrass, this implies that the limit is a bounded analytic function [Ahlfors 1953, Markushevich 1985]. Since this is true for any $s < \rho$, the analyticity applies throughout E_ρ. ∎

Note that Theorem 8.2 and 8.3 together establish a simple fact: a function defined on $[-1,1]$ can be approximated by polynomials with geometric accuracy if and only if it is analytic.

[To be added: (1) What did Bernstein 1912 (Sur l'ordre...) show about geom conv for Cheb pts of the 1st kind? (2) Can we prove Bernstein's inequality from the barycentric formula, following Riesz 1916? (3) Make it clearer how you work out ρ, given a function. In particular there should be more exercises giving practice finding singularities in the complex plane. (4) Exercise exploring convergence in the complex plane, in a Bernstein ellipse. (5) Fix reference Bernstein 1913a. (6) Exercise about sqrt(kappa) convergence of CG.]

SUMMARY OF CHAPTER 8. *If f is analytic, its Chebyshev coefficients $\{a_k\}$ decrease geometrically. In particular, if f is analytic and bounded by M in the Bernstein ρ-ellipse about $[-1,1]$, then $|a_k|$ is bounded by $2M\rho^{-k}$. It follows that the degree n Chebyshev truncation and interpolant of f have accuracy $O(M\rho^{-n})$.*

Exercise 8.1. Bernstein ellipses. Verify that for the Bernstein ellipse E_ρ for any $\rho > 1$, the length of the semimajor axis plus the length of the semiminor axis is equal to ρ.

Exercise 8.2. A Chebyshev series. With `x = chebfun('x')`, execute the command `chebpolyplot(sin(100*(x-.1))+.01*tanh(20*x))`. Explain the various features of the resulting plot as quantitatively as you can.

Exercise 8.3. Interpolation of an entire function. The function $f(x) = \exp(-x^2)$ is analytic throughout the complex x-plane, so Theorem 8.2 can be applied for any value of the parameter $\rho > 1$. Produce a semilog plot of $\|f - p_n\|$ as a function of n together with lines corresponding to the upper bound of the theorem for $\rho = 1.1, 1.2, 1.4, 2, 3, 5, 8$. Be sure to use the right value of M in each case. How well do your bounds fit the data?

Exercise 8.4. Convergence rates for different functions. Based on the theorems of this chapter, what can you say about the convergence as $n \to \infty$ of the Chebyshev interpolants to (a) $\log((x+3)/4)/(x-1)$, (b) $\int_{-1}^{x} \cos(t^2)\,dt$, (c) $\tan(\tan(x))$, (d) $(1+x)\log(1+x)$? In each case compare theoretical bounds with numerically computed results. Which is the case that converges much faster than the theorems predict? Can you speculate as to why?

Exercise 8.5. Total variation. Let f be a smooth function defined on $[0,1]$ and $t(x)$ its total variation over the interval $[0,x]$. What is the total variation of t over $[0,1]$?

Exercise 8.6. Proof of Bernstein inequality. Prove Bernstein's inequality used in the proof of Theorem 8.3: if p is a polynomial of degree d, then $\|p\|_{E_\rho} \le \rho^d \|p\|$, where $\|\cdot\|_{E_\rho}$ is the ∞-norm over the ρ-ellipse and $\|\cdot\|$ is the ∞-norm over $[-1,1]$. Hint: Show that if the branch cut is taken to be the unit interval $[-1,1]$, the function $q(z) = p(z)/(z+(z^2-1)^{1/2})^d$ is analytic throughout the region consisting of the complex plane plus the point $z=\infty$ minus $[-1,1]$. Apply the maximum modulus principle.

Exercise 8.7. Absolute value function. The function $|x-i|$ is analytic for $x \in [-1,1]$. Write it in another equivalent form that makes it clear exactly what form of singularities it has in the complex plane.

Exercise 8.8. Chebyshev polynomials on the Bernstein ellipse. Show that for any $\rho > 1$ and any z on the boundary of the ellipse E_ρ, $\lim_{n\to\infty} |T_n(z)|^{1/n} = \rho$.

Exercise 8.9. You can't judge smoothness by eye. Define $f(x) = 2 + \sin(50x)$ and $g(x) = f(x)^{1.0001}$ and construct chebfuns for these functions on $[-1,1]$. What are their lengths? Explain this effect as quantitatively as you can using the theorems of this chapter.

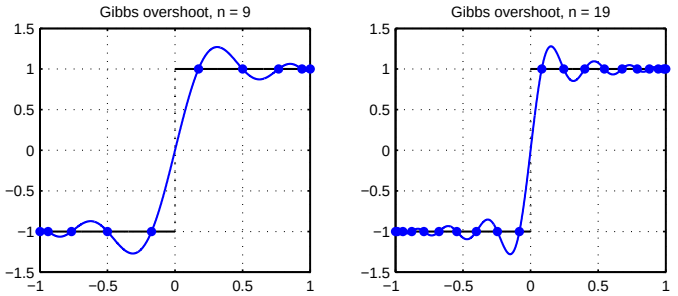
9. Gibbs phenomenon

Polynomial interpolants and truncations oscillate and overshoot near discontinuities. We have observed this **Gibbs phenomenon** already in Chapter 2, and now we shall look at it more carefully. We shall see that the Gibbs effect for interpolants can be regarded as a consequence of the oscillating inverse-linear tails of Lagrange polynomials, i.e., interpolants of Kronecker delta functions. Chapter 15 will show that these same tails, combined together in a different manner, are also the origin of Lebesgue constants of size $O(\log n)$, with implications throughout approximation theory.

To start, let us consider the function `sign(x)`, which we interpolate in $n+1 = 10$ and 20 Chebyshev points. We take n to be odd to avoid having a gridpoint at

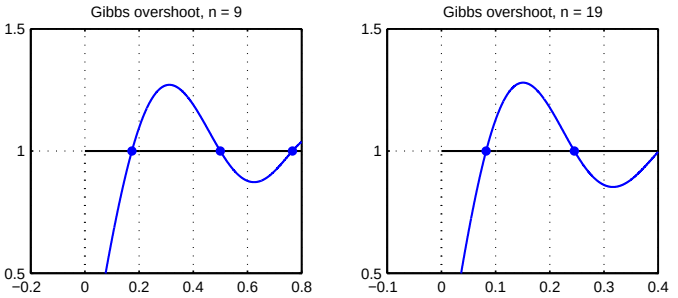
the middle of the step.

```
f = sign(x);
subplot(1,2,1), hold off, plot(f,'k'), hold on, grid on
f9 = chebfun(f,10); plot(f9,'.-')
title('Gibbs overshoot, n = 9')
subplot(1,2,2), hold off, plot(f,'k'), hold on, grid on
f19 = chebfun(f,20); plot(f19,'.-')
title('Gibbs overshoot, n = 19')
```



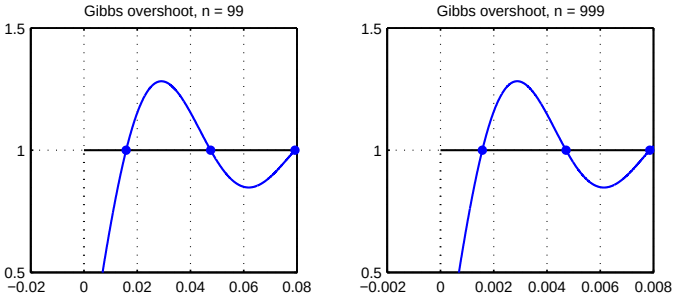
Both of these figures show a substantial overshoot near the jump. As n increases from 9 to 19, the overshoot gets narrower, but not shorter, and it will not go away as $n \to \infty$. Let us zoom in, using the $\{\cdot,\cdot\}$ feature to construct chebfuns on subintervals:

```
subplot(1,2,1), hold off, plot(f,'k'), hold on, grid on
plot(f9,'.'), plot(f9{0,0.8}), axis([-.2 .8 .5 1.5])
title('Gibbs overshoot, n = 9')
subplot(1,2,2), hold off, plot(f,'k'), hold on, grid on
plot(f19,'.'), plot(f19{0,0.4}), axis([-.1 .4 .5 1.5])
title('Gibbs overshoot, n = 19')
```



We now zoom in further with analogous plots for $n = 99$ and 999.

```
subplot(1,2,1), hold off, plot(f,'k'), hold on
f99 = chebfun(f,100); plot(f99,'.')
title('Gibbs overshoot, n = 99')
plot(f99{0,0.08}), grid on, axis([-.02 .08 .5 1.5])
subplot(1,2,2), hold off, plot(f,'k'), hold on
f999 = chebfun(f,1000); plot(f999,'.')
title('Gibbs overshoot, n = 999')
set(gca,'xtick',-.002:.002:.01)
set(gca,'xticklabel',{'-0.002','0','0.002','0.004','0.006','0.008'})
plot(f999{0,0.008}), grid on, axis([-.002 .008 .5 1.5])
```



Notice that in these figures, the vertical scale is always fixed while the horizontal scale is adjusted proportionally, confirming that the Gibbs overshoot gets narrower but approaches a constant height in the limit $n \to \infty$.

What is this height? We can measure it numerically with the `max` command:

```
disp('     n       Gibbs amplitude')
for n = 2.^(1:8)-1
   gibbs = max(chebfun(f,n+1));
   fprintf('%7d  %17.8f\n', n, gibbs)
end
```

```
     n       Gibbs amplitude
     1        1.00000000
     3        1.18807518
     7        1.26355125
    15        1.27816423
    31        1.28131717
    63        1.28204939
   127        1.28222585
   255        1.28226917
```

Clearly as $n \to \infty$, the maximum of the Chebyshev interpolant to the sign function converges to a number bigger than 1. The total variation of the interpolant, meanwhile, diverges slowly to ∞, at a rate proportional to $\log n$:


```
disp('     n          variation')
for n = 2.^(1:8)-1
   tv = norm(diff(chebfun(f,n+1)),1);
   fprintf('%7d  %14.2f\n', n, tv)
end
```

```
     n          variation
     1           2.00
     3           2.75
     7           3.64
    15           4.56
    31           5.47
    63           6.37
   127           7.26
   255           8.15
```

The following theorem summarizes the Gibbs phenomenon for Chebyshev interpolants. Well, perhaps it is not right to call it a "theorem", since it is not clear that a proof has ever been written down. The formulas necessary to represent the interpolant (in the equivalent trigonometric case — see Exercise 9.4) can be found in various forms in [Runck 1962] and [Helmberg & Wagner 1997], which relates the interpolating polynomial to the beta function and reports the numbers 1.282 and 1.066 to three digits of accuracy. The more precise results presented here have been privately communicated to us by Wagner based on calculations to more than 500 digits.

Theorem 9.1. Gibbs phenomenon for Chebyshev interpolants. *Let p_n be the degree n Chebyshev interpolant of the function $f(x) = \mathrm{sign}(x)$ on $[-1,1]$. Then as $n \to \infty$,*

$$\lim_{n\to\infty,\, n \text{ odd}} \|p_n\| = c_1 = 1.2822834557754285 4813\ldots, \tag{9.1}$$

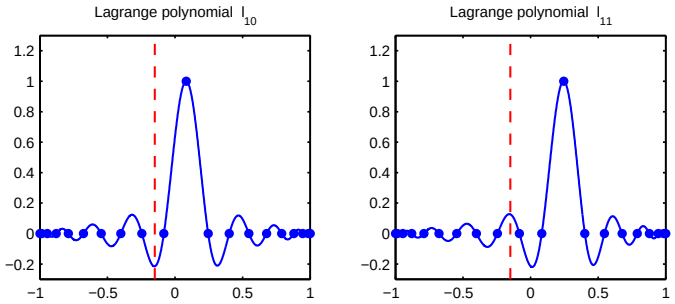
$$\lim_{n\to\infty,\, n \text{ even}} \|p_n\| = c_2 = 1.0657838882664480 9905\ldots. \tag{9.2}$$

(The case of n even differs in having a gridpoint at the middle of the jump.)

Although we are not going to prove Theorem 9.1, we do want to indicate where the fixed-overshoot effect comes from. Everything falls into place when we consider the Lagrange polynomials introduced in Chapter 5. Recall from (5.2) that the jth Lagrange polynomial $\ell_j(x)$ for the $(n+1)$-point Chebyshev grid is the unique polynomial in P_n that takes the values 1 at x_j and 0 at the other grid points x_k. On the 20-point grid, i.e. $n = 19$, here are the Lagrange polynomials ℓ_{10} and ℓ_{11}, with a dashed line marked at $x = -0.15$, which will be our point of special interest.

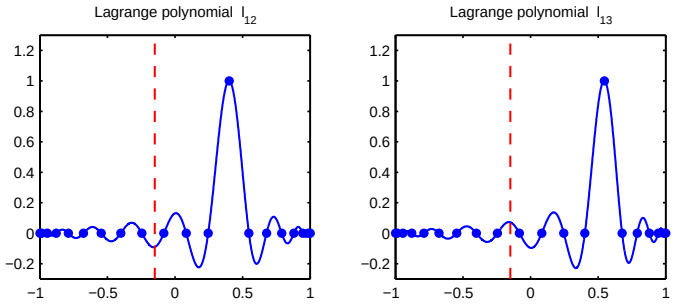
```
clf, yl = [-0.3 1.3];
xc = -0.15*[1 1];
```

```
p10 = chebfun([zeros(1,10) 1 zeros(1,9)]);
p11 = chebfun([zeros(1,11) 1 zeros(1,8)]);
subplot(1,2,1), plot(p10,'.-')
hold on, plot(xc,yl,'--r'), ylim(yl)
title('Lagrange polynomial  l_{10}')
subplot(1,2,2), plot(p11,'.-')
hold on, plot(xc,yl,'--r'), ylim(yl)
title('Lagrange polynomial  l_{11}')
```



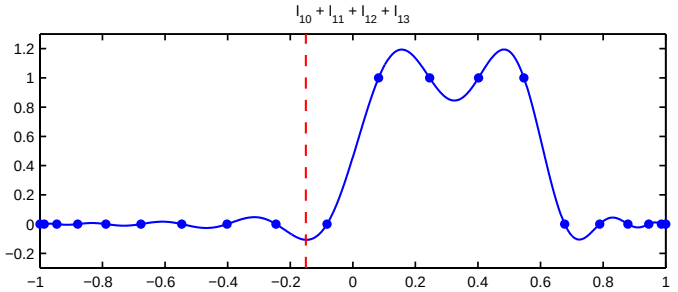
Here are ℓ_{12} and ℓ_{13}:

```
p12 = chebfun([zeros(1,12) 1 zeros(1,7)]);
p13 = chebfun([zeros(1,13) 1 zeros(1,6)]);
subplot(1,2,1), hold off, plot(p12,'.-')
hold on, plot(xc,yl,'--r'), ylim(yl)
title('Lagrange polynomial  l_{12}')
subplot(1,2,2), hold off, plot(p13,'.-')
hold on, plot(xc,yl,'--r'), ylim(yl)
title('Lagrange polynomial  l_{13}')
```



Following (5.1), we note that the by taking the sum of a sequence of such Lagrange functions, we get the interpolant to the function that jumps from 0 for $x < 0$ to 1 for $x > 0$. Here is the sum of the four just plotted, which is beginning to look like a square wave:


```
clf, plot(p10+p11+p12+p13,'.-')
hold on, plot(xc,yl,'--r'), ylim(yl)
title('l_{10} + l_{11} + l_{12} + l_{13}')
```



If we went all the way to the last grid point we would get the interpolant

$$p(x) = \sum_{j=(n+1)/2}^{n} \ell_j(x).$$

Note that for any fixed $x < x_{(n-1)/2}$, this is an *alternating series* of small terms whose amplitudes decrease inverse-linearly to zero. The finite but nonzero sum of such a series in the limit $n \to \infty$ is what gives rise to the fixed overshoot Gibbs effect in polynomial interpolation.

In particular, suppose we focus on the dashed line at $x = -0.15$ in the figures. Notice the alternating signs of the values of $\ell_{10}, \ell_{11}, \ell_{12}, \ell_{13}$ at this point. In the figure for $\ell_{10} + \ell_{11} + \ell_{12} + \ell_{13}$ we accordingly see the Gibbs overshoot beginning to converge to its asymptotic amplitude ≈ 0.141. This number is half of the value $0.282\ldots$ of Theorem 9.1, since the jump for this function is of amplitude 1 instead of 2.

In Chapter 15 we shall consider the same alternating series but with signs multiplied by $(-1)^j$. This eliminates the alternation, so that we have approximately a harmonic series of inverse-linear terms. The partial sums of such a series grow at a logarithmic rate, as we saw above with the calculation of the variation.

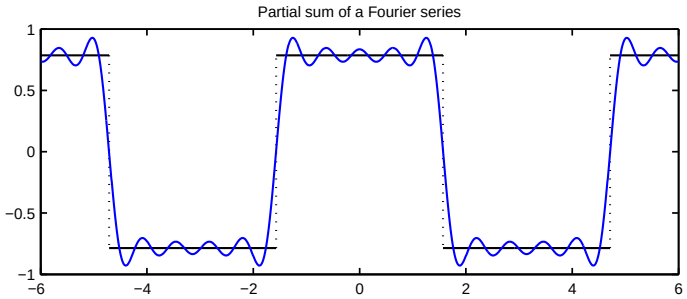
Our discussion so far has concerned interpolants, but there is a parallel theory of the Gibbs phenomenon for truncations — in the notation of this book, polynomials f_n rather than p_n. (The required Chebyshev coefficients are defined by the same integral (3.5) of Theorem 3.1, even though we are now dealing with functions f that are not Lipschitz continuous as in the assumption stated for that theorem.) As always, though the interpolants are closer to practical computation, the truncations may appear to be more fundamental mathematically. Historically speaking, it was the case of Fourier (trigonometric) truncation that was analyzed first. The original discoverer was not Gibbs but Henry Wilbraham,

a 22-year-old fellow of Trinity College, Cambridge, in 1848, who unfortunately made the mistake of publishing his fine paper in the short-lived *Cambridge and Dublin Journal of Mathematics* [Wilbraham 1848]. Fourier series for certain functions with jumps were already long known in Wilbraham's day — in fact they go back to Euler, half a century before Fourier. The particular series studied by Wilbraham, originally due to Euler in 1772, is

$$\cos(t) - \frac{1}{3}\cos(3t) + \frac{1}{5}\cos(5t) - \cdots, \tag{9.3}$$

which, as we can readily verify numerically, approximates a square wave of height $\pm\pi/4$:

```
t = chebfun('t',[-6,6]);
f = (pi/4)*sign(cos(t));
clf, plot(f,'k')
f9 = cos(t) - cos(3*t)/3 + cos(5*t)/5 - cos(7*t)/7 + cos(9*t)/9;
hold on, plot(f9), xlim([-6 6])
title('Partial sum of a Fourier series')
```



Wilbraham worked out the magnitude of the overshoot, and thus the following analogue of Theorem 9.1 is due to him.

Theorem 9.2. Gibbs phenomenon for Chebyshev truncations. *Let f_n be the degree n Chebyshev truncation of the sign function $f(x) = \mathrm{sign}(x)$ on $[-1,1]$. Then as $n \to \infty$,*

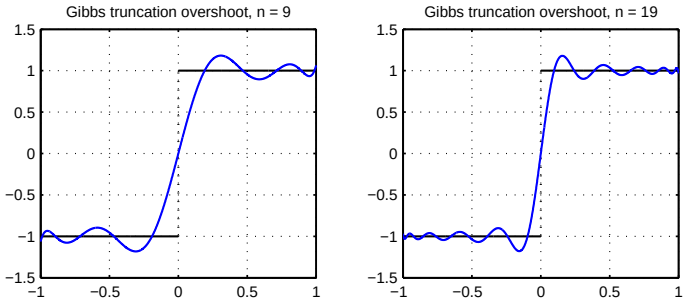
$$\lim_{n\to\infty} \|f_n\| = \frac{2}{\pi}\int_0^\pi \frac{\sin x}{x}\,dx = 1.178979744472167\ldots. \tag{9.4}$$

(The function $\mathrm{Si}(x) = \int_0^x t^{-1}\sin t\,dt$ is known as the *sine integral*; see Exercise 9.6.) To see this number experimentally we can use the `'trunc'` option in the Chebfun constructor. The overshoots look similar to what we saw before, but with smaller amplitude.

```
f = sign(x);
```



```
subplot(1,2,1), hold off, plot(f,'k'), hold on, grid on
f9 = chebfun(f,'trunc',10); plot(f9,'-')
title('Gibbs truncation overshoot, n = 9')
subplot(1,2,2), hold off, plot(f,'k'), hold on, grid on
f19 = chebfun(f,'trunc',20); plot(f19,'-')
title('Gibbs truncation overshoot, n = 19');
```



The numbers behave as predicted:

```
disp('     n       Gibbs amplitude')
for np = 2.^(4:7)
  g = chebfun(f,'trunc',np);
  fprintf('%7d  %17.8f\n', np, max(g{0,5/np}))
end
limit = (2/pi)*sum(chebfun('sin(x)./x',[0 pi]))
```

```
     n       Gibbs amplitude
    16         1.18028413
    32         1.17930541
    64         1.17906113
   128         1.17900009
limit =
   1.178979744472167
```

In all the experiments of this chapter we have worked with polynomials rather than trigonometric series, but the effects are the same (Exercise 9.4).

It is worth commenting on a particular property of series such as (9.3) that we have taken for granted throughout this discussion: even though each partial sum is continuous, a series may converge pointwise to a discontinuous limit, everywhere except at the points of discontinuity themselves. This kind of behavior seems familiar enough nowadays, but in the century beginning with Fourier's work in 1807, it often seemed paradoxical and confusing to mathematicians. The same pointwise convergence to discontinuous functions can also occur with interpolants, as in Theorem 9.1.

In this chapter we have focussed on the height of the overshoot of a Gibbs oscillation, because this is the effect so readily seen in plots. Perhaps the most important property of Gibbs oscillations for practical applications, however, is not their height but their slow decay as one moves away from the point of discontinuity. If f has a jump, the oscillations at a distance k gridpoints away must be expected to be of size $O(k^{-1})$; if f' has a jump we expect oscillations of size $O(k^{-2})$, and so on. This algebraic rate of decay of information in polynomial interpolants can be contrasted with the exponential decay that one gets with spline approximations, which is the the key advantage of splines for certain applications. Chebfun responds to this problem by representing functions with discontinuities by piecewise polynomials rather than global ones, with breakpoints at the discontinuities. For example, the location of the discontinuity in the function $\exp(|x-0.1|^3)$ will be determined automatically in response to the command

```
f = chebfun(@(x) abs(x-0.1).^3,'splitting','on');
```

The result is a chebfun consisting of two pieces each of degree 3, and the break in the middle appears at the right place:

```
f.ends(2)
```

```
ans = 0.099999999999999
```

Let us return to 22-year-old Mr. Wilbraham. Unfortunately, his published paper had little impact, and the effect was rediscovered and discussed in the pages of *Nature* during 1898–1899 by James Michelson, A. E. H. Love, and J. Willard Gibbs. These authors got more attention for a number of reasons. First, they were leading scientists. Second, their problem arose in a practical application (a mechanical graphing machine called a "harmonic analyser" used by Michelson and Stratton). Third, they published their observations in a major journal. Fourth, they failed to get it right at first, so several publications appeared in succession! Other mathematicians got involved too, notably Poincaré. Finally, they were lucky enough to have "Gibbs's phenomenon" named and highlighted a few years later in a major research article on Fourier analysis by the mathematician Maxime Bôcher [1906].

For a fascinating discussion of the history of the Gibbs phenomenon (for truncation, not interpolation), which they more properly call the **Gibbs–Wilbraham phenomenon**, see [Hewitt & Hewitt 1979]. Hewitt and Hewitt end their article with a charming coda.

Gibbs's phenomenon, while not a fundamental part of mathematics, displays in parvo *a number of central features of the development of mathematics. We find forgotten pioneers. We encounter shocking disputes over priority. We study brilliant achievements, some... never properly appreciated. We discover a remarkable succession of blunders, which could hardly have arisen save through copying from predecessors without checking.*

In short, Gibbs's phenomenon and its history offer ample evidence that mathematics, for all of its majesty and austere exactitude, is carried on by humans.

[To be added: (1) Check books on Gibbs phenomenon by Atreas and Karanikas, Abdul Jerri. (2) Exercise with moving midpoint following Helmber and Wagner.]

SUMMARY OF CHAPTER 9. *Chebyshev truncations and interpolants, as well as other polynomial and trigonometric approximations, tend to oscillate near discontinuities. The oscillations decay algebraically with distance from the discontinuity, not exponentially.*

Exercise 9.1. Calculations for larger n. We measured the height of the Gibbs overshoot for a step function for $n = 1, 3, 7, \ldots, 255$. Larger values of n get a bit slow, but knowing that the maximum occurs around $x = 3/n$, compute these numbers up to $n = 4095$ using a command of the form `max(g{0,5/n})`. How great a speedup does this trick produce?

Exercise 9.2. A function with many jumps. Use Chebfun to produce an attractive plot of the degree 200 Chebyshev interpolant to the function `round(exp(sin(2*pi*x)))` on $[-1, 1]$.

Exercise 9.3. Lagrange polynomials. Take $n \geq 2$ to be even and let p be the degree n Chebyshev interpolant to the Kronecker delta function at $x = x_{n/2} = 0$. (a) Use the barycentric formula of Theorem 5.2 to obtain a simple formula for p. (b) Derive a formula for the values of p at the "Chebyshev midpoints" defined by the usual formula $x_j = \cos(j\pi/n)$ of Chapter 2 except with half-integer values of j. (c) For $n = 100$, use Chebfun to produce an elegant plot showing the inverse-linear amplitudes of these values. (You can get the Chebyshev midpoints from `x=chebpts(2*n)`, `x=x(2:2:end)`.)

Exercise 9.4. Fourier and Chebyshev Gibbs phenomena. We have repeatedly made the connection between Chebyshev polynomials $T_n(x)$ on the unit interval, Laurent polynomials $(z^n + z^{-n})/2$ on the unit circle, and trigonometric polynomials $\cos(n\theta)$ on $[-\pi, \pi]$. Use these connections to show that the Gibbs overshoot in Chebyshev interpolation of $\mathrm{sign}(x)$ on $[-1, 1]$, with n even, is identical to the overshoot for a certain problem of trigonometric interpolation in θ.

Exercise 9.5. Local minima of a truncated sine series. (a) Plot ϕ_n with $n = 10, 100, 1000$ for a sum going back to Euler in 1755,

$$\phi_n(x) = \sum_{k=1}^{n} \frac{\sin(kx)}{x}.$$

What function does the sum evidently converge to? Is the Gibbs overshoot of the same relative magnitude as for (9.3)? (b) For each case, determine the first four local minimum values of $\phi_n(x)$ in $(0, \pi)$. (c) Write an elegant Chebfun program that determines the smallest value of n for which these minima are not monotoncally decreasing. (This effect was investigated by Gronwall [1912].)

Exercise 9.6. Sine integral. (a) Construct and plot a chebfun for the sine integral $\mathrm{Si}(x) = \int_0^x t^{-1} \sin t$ for $x \in [0, 10]$. What is its length? (b) Same for $x \in [0, 100]$. (c) Same for $x \in [0, 1000]$.

Exercise 9.7. Decay at points away from the discontinuity. [To be written.]

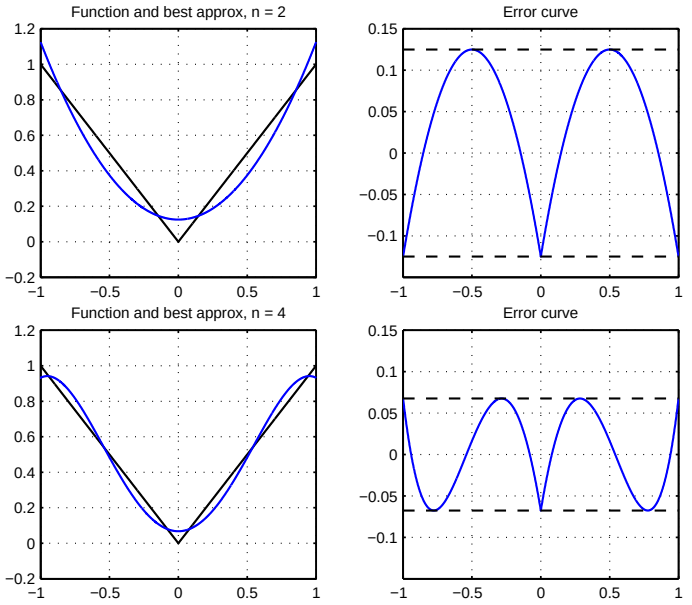
10. Best approximation

An old idea, going back to Chebyshev himself and earlier to Poncelet, is to look for a polynomial p^* of specified degree n that is the **best approximation** to a given continuous function f in the sense of minimizing the ∞-norm of the difference on an interval [Chebyshev 1854 & 1859]. (A best approximation is also called a **Chebyshev approximation**, but we shall avoid this usage to minimize confusion. A third term is **minimax approximation**.) It is known that p^* exists and is unique, as we shall prove below. There is a Chebfun command `remez` for computing these approximants, due to Ricardo Pachón: if f is a chebfun, then `remez(f,n)` is the chebfun corresponding to its best approximation of degree n. For details see [Pachón & Trefethen 2009].

We shall argue in Chapter 16 that best approximations are not always in fact very useful; Chebyshev interpolants are often as good or even better. Nevertheless, they represent an elegant and fundamental idea and a line of investigation going back more than 150 years. So for the moment, let us enjoy them.

For example, here are the best approximants of degree 2 and 4 to $|x|$, together with their **error curves** $(f - p^*)([-1, 1])$:

```
f = abs(x);
for n = 2:2:4
  subplot(1,2,1), hold off, plot(f,'k'), grid on
  [p,err] = remez(f,n); hold on
  plot(p,'b'), axis([-1 1 -.2 1.2])
  title(['Function and best approx, n = ' int2str(n)])
  subplot(1,2,2), hold off, plot(f-p), grid on
  hold on, axis([-1 1 -.15 .15]), title('Error curve')
  plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
  snapnow
end
```

Notice the **equioscillation** property: the error curve takes on its extreme value with alternating signs at a succession of values of x. Chebyshev knew this in the 1850s, though he seems not to have written down a proof that would satisfy modern standards of rigor. More systematic treatments came at the beginning of the 20th century with work by Blichfeldt [1901], Kirchberger [1902,1903], and Borel [1905]. It seems to have been Kirchberger, in a PhD thesis written under Hilbert, who first stated and proved the characterization theorem that is now so well known [Kirchberger 1902]. Note that in the characterization part of this theorem, f is assumed to be real, whereas most of the discussion in this book allows f to be real or complex. Existence and uniqueness in the complex case were established by Tonelli [1908]. Complex generalizations of the characterization originate with [Kolmogorov 1948, Remez 1951]. Many further generalizations can also be found in the approximation theory literature, for example with the set of polynomials on an interval replaced by a more general set of functions satisfying a property known as the *Haar condition.*

Theorem 10.1: Equioscillation characterization of best approximants. *A continuous function f on $[-1, 1]$ has a unique best approximation $p^* \in P_n$. If f is real, then p^* is real too, and in this case a polynomial $p \in P_n$ is equal to p^* if and only if $f - p$ equioscillates in at least $n + 2$ extreme points.*

Proof. To prove existence of a best approximation, we note that $\|f - p\|$ is a continuous function of $p \in P_n$. Since one candidate approximation is the zero function, we know that if p^* exists, it lies in $\{p \in P_n : \|f - p\| \le \|f\|\}$. This

is a closed and bounded subset of a finite-dimensional space, hence compact (the Bolzano–Weierstrass property), and thus the minimum is attained. This argument originates with F. Riesz [1918].

Next we show that equioscillation implies optimality. Suppose f and p are real and $(f-p)(x)$ takes equal extreme values with alternating signs at $n+2$ points $x_0 < x_1 < \cdots < x_{n+1}$, and suppose $\|f-q\| < \|f-p\|$ for some real polynomial $q \in P_n$. Then $p-q$ must take nonzero values with alternating signs at the equioscillation points, implying that it takes the value zero in at least $n+1$ points in-between. This implies that $p-q$ is identically zero, a contradiction.

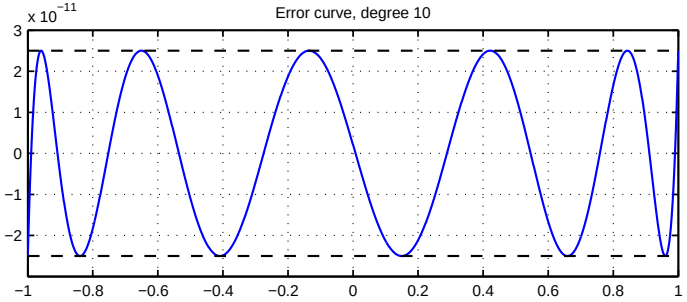
The third step is to show that optimality implies equioscillation (this part of the argument was given in Blichfeldt [1901]). Suppose $f-p$ equioscillates at fewer than $n+2$ points, and set $E = \|f-p\|$. Without loss of generality suppose the leftmost extremum is one where $f-p$ takes the value $-E$. Then there are numbers $-1 < x_1 < \cdots < x_k < 1$ with $k \le n$ such that $(f-p)(x) < E$ for $x \in [-1,x_1] \cup [x_2,x_3] \cup [x_4,x_5] \cup \cdots$ and $(f-p)(x) > -E$ for $x \in [x_1,x_2] \cup [x_3,x_4] \cup \cdots$. If we define $\delta p(x) = (x_1 - x)(x_2 - x) \cdots (x_k - x)$, then $(p - \varepsilon \delta p)(x)$ will be a better approximation than p to f for all sufficiently small $\varepsilon > 0$.

Finally, to prove uniqueness of best approximations (this part of the theorem was proved by Chebyshev [1859] — we treat the real case only), we refine the argument that equioscillation implies optimality. Suppose p is a best approximation with equioscillation extreme points $x_0 < x_1 < \cdots < x_{n+1}$, and suppose $\|f-q\| \le \|f-p\|$ for some real polynomial $q \in P_n$. Then (without loss of generality) $(p-q)(x)$ must be ≤ 0 at $x_0, x_2, x_4, \ldots$ and ≥ 0 at $x_1, x_3, x_5, \ldots$. This implies that $p-q$ has roots in each of the $n+1$ closed intervals $[x_0,x_1], [x_1,x_2], \ldots, [x_n,x_{n+1}]$. We wish to conclude that $p-q$ has at least $n+1$ roots in total, counted with multiplicity, implying that $p = q$. To make the argument we prove by induction that $p-q$ has at least k roots in $[x_0,x_k]$ for each k. The case $k=1$ is easy. For the general case, suppose $p-q$ has at least j roots in $[x_0,x_j]$ for each $j \le k-1$ but only $k-1$ roots in $[x_0,x_k]$. Then there must be a simple root at x_{k-1}. By the induction hypothesis, $p-q$ must have exactly $k-2$ roots in $[x_0,x_{k-2}]$ with a simple root at x_{k-2}, $k-3$ roots in $[x_0,x_{k-3}]$ with a simple root at x_{k-3}, and so on down to 1 root in $[x_0,x_1]$, a simple root at x_1. It follows that $p-q$ must be nonzero at x_0 and at x_k, and since the sign of $p-q$ changes at each of the simple roots $x_1, \ldots x_{k-1}$, the signs at x_0 and x_k must be the same if k is odd and opposite if k is even. On the other hand from the original alternation condition we know that $p-q$ must take the same signs at x_0 and x_k if k is even and opposite signs if k is odd. ∎

Note that the error curve for a best approximation may have more than $n+2$ points of equioscillation, and indeed this will always happen if f and n are both even or both odd (Exercise 10.4). For example, for the function $f(x) = |x|$ considered above, the degree 2 approximation equioscillates at 5 points, not 4, and the degree 4 approximation equioscillates at 7 points, not 6.

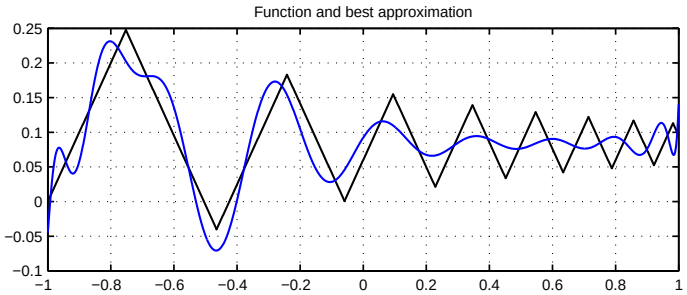
Here is another example, the degree 10 best approximation to $\exp(x)$. There are 12 points of equioscillation.

```
f = exp(x);
[p,err] = remez(f,10);
clf, plot(f-p), grid on, hold on
title('Error curve, degree 10')
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
```



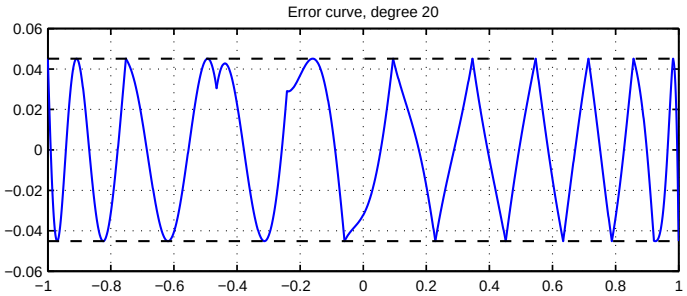
And here is another. The Chebfun `cumsum` command returns the indefinite integral, producing in this case a zigzag function.

```
f = cumsum(sign(sin(20*exp(x))));
clf, plot(f,'k'), hold on
[p,err] = remez(f,20);
plot(p), grid on, title('Function and best approximation')
```



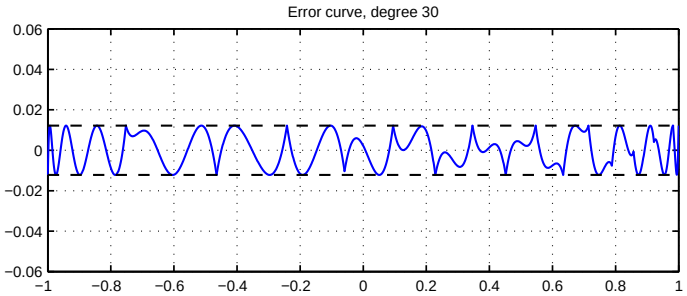
The corresponding error curve reveals $20+2 = 22$ points of equioscillation:

```
hold off, plot(f-p), grid on, hold on, axis([-1 1 -.06 .06])
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
title('Error curve, degree 20')
```



Here's the analogous curve for degree 30, plotted on the same scale.

```
[p,err] = remez(f,30);
hold off, plot(f-p), grid on, hold on, axis([-1 1 -.06 .06])
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
title('Error curve, degree 30')
```



The algorithm underlying `remez` goes back to the Soviet mathematician Evgeny Remez in 1934 [Remez 1934a, 1934b, 1957]. We shall not give details here, but in fact, Chebfun is an excellent platform for such computations since the algorithm depends on repeatedly finding the local extrema of trial error curves, an operation carried out easily in Chebfun via the `roots` command (see Chapter 18). Also crucial to the success of `remez` is the use of the barycentric representation (5.11) for all polynomials, based not at Chebyshev points but at the points of the so-called "reference set" that gets adjusted in the course of the iteration. See [Pachón & Trefethen 2009].

The history of the Remez algorithm is interesting, or perhaps we should say the sociology. It stands out as one of the preeminent examples of a nontrivial algorithm for a challenging computational problem that was developed before the invention of computers. Perhaps in part because of this early appearance, it became remarkably well known, a fixture in numerical analysis courses worldwide. One might imagine, based on its fame, that the Remez algorithm must

be very important in practice, used all the time, but in fact it seems there is not much software and just a moderate amount of use of these ideas. The best known area of application is the field of digital signal processing, where special variants of the Remez ideas were developed by Parks and McClellan beginning in the 1970s with tremendous success for designing low-pass, high-pass, and other digital filters [Parks & McClellan 1972]. Parks and McClellan too found that the use of a barycentric representation was crucial.

Chapter 16 will show that Chebyshev interpolants are usually as good as best approximations in practice, and this fact surely has something to do with why the Remez algorithm is used rather little. Chapter 20 will show that if you really want a best approximation, it may be more practical to compute it by CF approximation than by the Remez algorithm, at least if f is smooth.

[To be added: (1) See de Vore and Lorentz for possible further history of equioscillation theorem. (2) Give details of Remez algorithm? (See Powell.) (3) Follow up on Chebyshev's history with communications from Bogatyrev.]

SUMMARY OF CHAPTER 10. *Any $f \in C[-1,1]$ has a unique best approximation $p^* \in P_n$ with respect to the ∞-norm. If f is real, p^* is characterized by having an error curve that equioscillates in at least $n+2$ points.*

Exercise 10.1. A function with spikes. Compute numerically the degree 10 polynomial best approximation to $\mathrm{sech}^2(5(x+0.6))+\mathrm{sech}^4(50(x+0.2))+\mathrm{sech}^6(500(x-0.2))$ on $[-1,1]$ and plot f together with p^* as well as the error curve. What is the error? How does this compare with the error in 11-point Chebyshev interpolation? (Hint: for these Chebfun computations to be practical, be sure to use `'splitting','on'`.)

Exercise 10.2. Best approximation of $|x|$. (a) Use Chebfun to determine the errors $E_n = \|f - p_n\|$ in degree n best approximation of $f(x) = |x|$ on $[-1,1]$ for $n = 2, 4, 8, \ldots, 256$, and make a table of the values $\beta_n = nE_n$ as a function of n. (b) Use Richardson extrapolation to improve your data. How many digits can you appear to find for the limiting number $\beta = \lim_{n\to\infty} \beta_n$? (We shall discuss this problem in detail in Chapter 24.)

Exercise 10.3. de la Vallée Poussin lower bound. Suppose an approximation $p \in P_n$ to $f \in C[-1,1]$ approximately equioscillates in the sense that there are points $-1 \le s_0 < s_1 < \cdots < s_{n+1} \le 1$ at which $f-p$ alternates in sign with $|f(s_j)-p(s_j)| \ge \varepsilon$ for some $\varepsilon > 0$. Show that $\|f - p^*\| \ge \varepsilon$.

Exercise 10.4. Best approximation of even functions. Let $f \in C[-1,1]$ be an even function, i.e., $f(-x) = f(x)$ for all x. (a) Prove as a corollary of Theorem 10.1 that for any $n \ge 0$, the best approximation p_n^* is even. (b) Prove that for any $n \ge 0$, $p_{2n}^* = p_{2n+1}^*$. (c) Conversely, suppose $f \in C[-1,1]$ is not even. Prove that for all sufficiently large n, its best approximations p_n^* are not even.

Exercise 10.5. An invalid theorem. The first two figures of this chapter appear to confirm the following principle: *if f is an even function on $[-1,1]$ and p^* is its*

best approximation of some degree n, then one of the extreme points of $|(f-p^*)(x)|$ occurs at $x=0$. Find the flaw in the following "proof". By Exercise 10.4(b), p^* is the best approximation to f for all n in some range of the form even $\le n \le$ odd, such as $4 \le n \le 5$ or $10 \le n \le 13$. By Theorem 10.1, the number of equioscillation points of $f-p^*$ must accordingly be of the form odd $+\,2$, that is, odd. By symmetry, 0 must be one of these points.

Exercise 10.6. Nonlinearity of best approximation operator. We have mentioned that for given n, the operator that maps a function $f \in C[-1,1]$ to its best approximation p_n^* is nonlinear. Prove this (on paper, not numerically) by finding two functions f_1 and f_2 and an integer $n \to 0$ such that the best approximation of the sum in P_n is not the sum of the best approximations.

Exercise 10.7. Weierstrass function again. Exercise 6.1 considered a function of Weierstrass, continuous but nowhere differentiable. A variant of the same function based on Chebyshev polynomials would be

$$f(x) = \sum_{k=0}^{\infty} 2^{-k} T_{3^k}(x).$$

Show that the truncation

$$f_{3^K}(x) = \sum_{k=0}^{K} 2^{-k} T_{3^k}(x)$$

is the best approximation to f in the spaces P_n for certain n. What is the complete set of n for which this is true? What is the error?

Exercise 10.8. Continuity of best approximation operator. For any $n \ge 0$, the mapping from functions $f \in C[-1,1]$ to their best approximants $p^* \in P_n$ is continuous with respect to the usual ∞-norm in $C[-1,1]$. Prove this by an argument combining the uniqueness of best approximations with compactness. (In fact the mapping is not just continuous but Lipschitz continuous, a property known as *strong uniqueness,* but this is harder to prove.)

Exercise 10.9. Approximation of e^x. (a) Prove using the de la Vallée Poussin bound of Exercise 10.3 that asymptotically as $n \to \infty$, the best approximation errors for $f(x) = e^x$ on $[-1,1]$ satisfy $E_n \sim n!/2^n n!(n+1)!$. (b) Make a table comparing this estimate with the actual numbers E_n for $0 \le n \le 10$.

11. Hermite integral formula

If there is a single most valuable mathematical tool in the analysis of polynomial approximations, it is contour integrals in the complex plane.[4] From a contour integral one can see why some approximations are extraordinarily accurate, like interpolation in Chebyshev points, and others are impossibly bad, like interpolation in equispaced points. This chapter presents the basics of the contour integrals, and the next applies them to take some first steps toward the subject of potential theory, which relates the accuracy of approximations to

[4]This and the next chapter are probably the hardest in the book, with a good deal of mathematics presented in a few pages and heavy use of complex variables. Later chapters get easier again.

equipotential or minimal-energy problems for electrostatic charge distributions in the plane.

The starting ingredients have already appeared in Chapter 5. Following the formulation there, let $x_0, \dots, x_n$ be a set of $n+1$ distinct interpolation or "grid" points, which may be real or complex, and define the node polynomial $\ell \in P_{n+1}$ as in (5.4) by

$$\ell(x) = \prod_{k=0}^{n} (x - x_k). \tag{11.1}$$

Repeating (5.5), the function

$$\ell_j(x) = \frac{\ell(x)}{\ell'(x_j)\,(x - x_j)} \tag{11.2}$$

is the Lagrange polynomial associated with x_j, that is, the unique polynomial in P_n that takes the value 1 at x_j and 0 at the other points x_k. Following (5.1), a linear combination of these functions gives the interpolant in P_n to an arbitrary function f defined on the grid:

$$p(x) = \sum_{j=0}^{n} f(x_j) \ell_j(x). \tag{11.3}$$

We now make a crucial observation. Let Γ_j be a contour in the complex x-plane that encloses x_j but none of the other grid points, nor the point x. (By "encloses" we always mean that it winds around the specified set once in the counterclockwise direction, in the usual sense of complex variables.) Then the expression on the right in (11.2) can be written

$$\frac{\ell(x)}{\ell'(x_j)\,(x - x_j)} = \frac{1}{2\pi i} \int_{\Gamma_j} \frac{\ell(x)}{\ell(t)\,(x - t)}\, dt. \tag{11.4}$$

To verify this formula we ignore the $\ell(x)$ term on both sides, which has nothing to do with the integral, and use the fact that $1/(\ell'(x_j)(x-x_j))$ is the *residue* of the function $1/(\ell(t)(x-t))$ at the pole $t = x_j$.

From (11.2) and (11.4) we thus have an expression for $\ell_j(x)$ as a contour integral:

$$\ell_j(x) \;= \frac{1}{2\pi i} \int_{\Gamma_j} \frac{\ell(x)}{\ell(t)\,(x - t)}\, dt, \tag{11.5}$$

where Γ_j encloses x_j. Now let Γ' be a contour that encloses all of the grid points $\{x_j\}$, but still not the point x, and let f be a function analytic on and interior to Γ'. Then we can combine together these integrals to get an expression for the interpolant p to f in $\{x_j\}$:

$$p(x) = \frac{1}{2\pi i} \int_{\Gamma'} \frac{\ell(x) f(t)}{\ell(t)\,(x - t)}\, dt. \tag{11.6}$$

Note how neatly this formula replaces the sum of (11.3) by a contour integral with contributions from the same points x_j.

Now suppose we enlarge the contour of integration to a new contour Γ that encloses x as well as $\{x_j\}$, and we assume f is analytic on and inside Γ. The residue of the integrand of (11.6) at $t = x$ is $-f(x)$, so this brings in a new contribution $-f(x)$ to the integral, yielding an equation for the error in polynomial interpolation:

$$p(x) - f(x) = \frac{1}{2\pi i} \int_\Gamma \frac{\ell(x) f(t)}{\ell(t)\,(x-t)}\,dt. \tag{11.7}$$

And thus we have derived one of the most powerful formulas in all of approximation theory, the **Hermite interpolation formula**. This name comes from Hermite [1878], but the same result had been stated 52 years earlier by Cauchy [1826]. (Hermite, however, generalized the formulation significantly to nondistinct or "confluent" interpolation points and corresponding interpolation of derivatives as well as function values; see Exercise 11.2.)

Theorem 11.1. Hermite interpolation formula. *Let f be analytic in a region Ω containing distinct points $x_0, \ldots, x_n$, and let Γ be a contour in Ω enclosing these points in the positive direction. The polynomial interpolant $p \in P_n$ to f at $\{x_j\}$ is*

$$p(x) = \frac{1}{2\pi i} \int_\Gamma \frac{f(t)\,(\ell(t) - \ell(x))}{\ell(t)\,(t-x)}\,dt, \tag{11.8}$$

and if x is enclosed by Γ, the error in the interpolant is given by

$$f(x) - p(x) = \frac{1}{2\pi i} \int_\Gamma \frac{\ell(x)}{\ell(t)} \frac{f(t)}{(t-x)}\,dt. \tag{11.9}$$

Proof. Equation (11.9) is the same as (11.7). For (11.8), we note that if Γ encloses x, then $f(x)$ can be written

$$f(x) = \frac{1}{2\pi i} \int_\Gamma \frac{\ell(t)\, f(t)}{\ell(t)\,(t-x)}\,dt,$$

and combining this with (11.7) gives the result. But the integrand of (11.8) has no pole at $t = x$, so the same result also applies if Γ does not enclose x. ∎

It is perhaps interesting to sketch Cauchy's slightly different derivation from 1826, outlined in [Smithies 1997, p. 117], which may have been influenced by Jacobi's thesis a year earlier [Jacobi 1825]. Cauchy started from the observation that $p(x)/\ell(x)$ is a rational function with denominator degree greater than the numerator degree. This implies that it must be equal to the sum of the $n+1$ inverse-linear functions $r_j/(x - x_j)$, where r_j is the residue of $p(t)/\ell(t)$ at $t = x_j$ (a partial fraction decomposition, to be discussed further in Chapter 23). Since

p interpolates f at $\{x_j\}$, r_j is also the residue of $f(t)/\ell(t)$ at $t = x_j$. By residue calculus we therefore have

$$\frac{p(x)}{\ell(x)} = \frac{1}{2\pi i} \int_{\Gamma'} \frac{f(t)}{\ell(t)\,(x-t)}\,dt$$

if Γ' is again a contour that encloses the points $\{x_k\}$ but not x itself, or equivalently, (11.6).

Now let us see how Theorem 11.1 can be used to estimate the accuracy of polynomial interpolants.

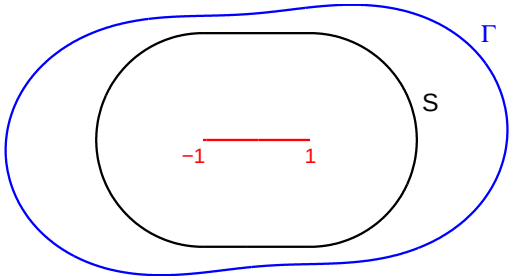
Suppose f and x are fixed and we want to estimate $f(x) - p(x)$ for various degrees n and corresponding sets of $n+1$ points $\{x_j\}$. On a fixed contour Γ, the quantities $f(t)$ and $t - x$ in (11.9) are independent of n. The ratio

$$\frac{\ell(x)}{\ell(t)} = \frac{\prod_{j=0}^n (x - x_j)}{\prod_{j=0}^n (t - x_j)}, \tag{11.10}$$

however, is another matter. If Γ is far enough from $\{x_j\}$, then for each $t \in \Gamma$, this ratio will shrink exponentially as $n \to \infty$, and if this happens, we may conclude from (11.9) that $p(x)$ converges exponentially to $f(x)$ as $n \to \infty$. The crucial condition for this argument to work is that it must be possible for f to be analytically continued as far out as Γ.

Here is a warm-up example mentioned in [Gaier 1987, p. 63]. Suppose the interpolation points $\{x_j\}$ lie in $[-1, 1]$ for each n and $x \in [-1, 1]$ also. Let S be the "sports ground" in the complex x-plane consisting of all numbers x lying at a distance ≤ 2 from $[-1, 1]$, and suppose f is analytic in a larger region Ω that includes a contour Γ enclosing S. We can sketch the situation like this:

```
hold off, plot(real(x),imag(x),'r')
semi = 2*exp(0.5i*pi*x);
S = [x-2i; 1+semi; 2i-x; -1-semi];
hold on, plot(S,'k'), axis equal off
z = exp(1i*pi*x);
Gamma = (2.8+.2i)*(sinh(z)+.5*real(z));
plot(Gamma,'b')
text(4.2,2,'\Gamma',CO,'b',FS,12)
text(3.1,.7,'S',FS,12)
text(.9,-.3,'1',CO,'r')
text(-1.4,-.3,'-1',CO,'r')
```



Under these assumptions, there is a constant $\gamma > 1$ such that for every $t \in \Gamma$ and every x_j, $|t - x_j| \geq \gamma |x - x_j|$. This implies

$$|\ell(x)/\ell(t)| \leq \gamma^{-n-1}$$

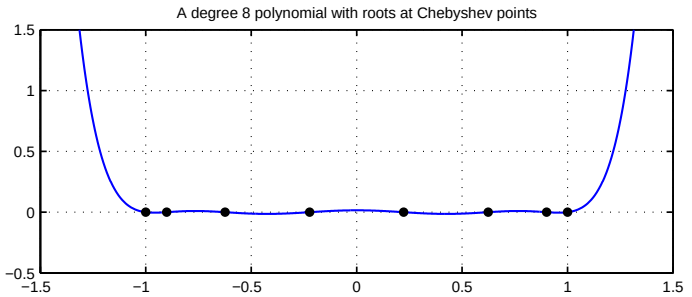
and thus by (11.9),

$$\|f - p\| = O(\gamma^{-n}).$$

Note that this conclusion applies regardless of the distribution of the interpolation points in $[-1, 1]$. They could be equally spaced or random, for example. (At least that is true in theory. In practice, such choices would be undone by rounding errors on a computer, as we shall see in the next chapter.)

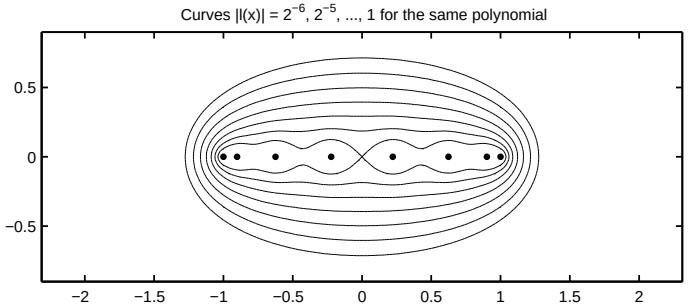
So convergence of polynomial interpolants to analytic functions on $[-1, 1]$ is all about how small $\ell(x)$ is on $[-1, 1]$, compared with how big it is on a contour Γ inside which f is analytic. From this point of view we can begin to see why Chebyshev points are so good: because a polynomial with roots at the Chebyshev points has approximately uniform magnitude on $[-1, 1]$. Suppose for example we consider the polynomial $\ell \in P_8$ with roots at 8 Chebyshev points. On $[-1, 1]$ it has size $O(2^{-8})$, roughly speaking, but it grows rapidly for x outside this interval. Here is a plot for $x \in [-1.5, 1.5]$:

```
np = 8; xj = chebpts(np);
d = domain([-1.5,1.5]);
ell = poly(xj,d);
hold off, plot(ell), grid on
hold on, plot(xj,ell(xj),'.k'), ylim([-.5 1.5])
title('A degree 8 polynomial with roots at Chebyshev points')
```

With Matlab's `contour` command we can examine the size of $\ell(x)$ for complex values of x. The following code plots contours at $|\ell(x)| = 2^{-6}, 2^{-5}, \ldots, 1$.

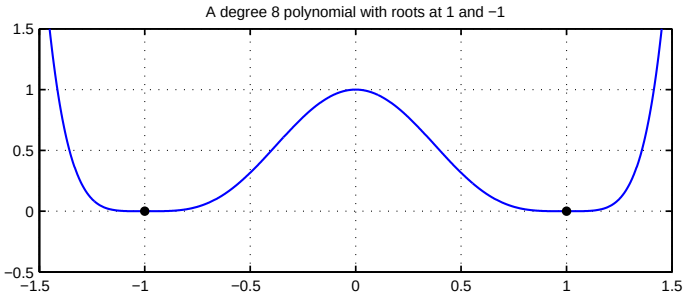
```
hold off, plot(xj,ell(xj),'.k',MS,10)
hold on, ylim([-0.9,0.9]), axis equal
xgrid = -1.5:.02:1.5; ygrid = -0.9:.02:0.9;
[xx,yy] = meshgrid(xgrid,ygrid); zz = xx+1i*yy;
ellzz = ell(zz); levels = 2.^(-6:0);
contour(xx,yy,abs(ellzz),levels,'k')
title(['Curves |l(x)| = 2^{-6}, 2^{-5}, ..., 1 '...
    'for the same polynomial'])
```



We can see a great deal in this figure. On $[-1, 1]$, it confirms that $\ell(x)$ is small, with maximum value $|\ell(x)| = 2^{-6}$ at $x = 0$. Away from $[-1, 1]$, $|\ell(x)|$ grows rapidly and takes constant values on curves that look close to ellipses. For t on the outermost of the curves plotted, the ratio $|\ell(x)/\ell(t)|$ will be bounded by 2^{-6} for any $x \in [-1, 1]$.

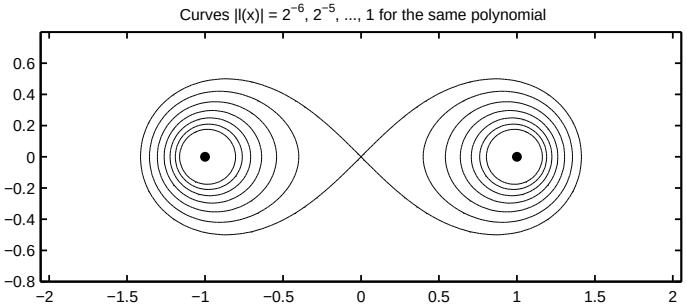
Let us compare this to the very different behavior if we take points that are not close to the Chebyshev distribution. To make a specific and quite arbitrary choice, let us again take 8 points, four of them at -1 and four at 1. Here is the plot on the real axis.

```
xj = [-1 -1 -1 -1 1 1 1 1];
ell = poly(xj,d);
hold off, plot(ell), grid on
hold on, plot(xj,ell(xj),'.k'), ylim([-.5 1.5])
title('A degree 8 polynomial with roots at 1 and -1')
```



And here are the contours in the complex plane.

```
hold off, plot(xj,ell(xj),'.k'), hold on
ylim([-0.8,0.8]), axis equal, ellzz = ell(zz);
contour(xgrid,ygrid,abs(ellzz),levels,'k')
title(['Curves |l(x)| = 2^{-6}, 2^{-5}, ..., 1 '...
    'for the same polynomial'])
```

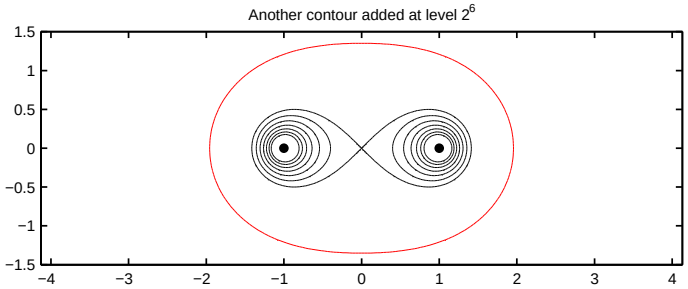


These figures show that the size of $\ell(x)$ on $[-1,1]$ is not at all uniform: it is far smaller than 2^{-6} for $x \approx \pm 1$, but as big as 1 at $x = 0$. Now, for $x \in [-1,1]$ and t on the outermost curve shown, the maximum of the ratio $|\ell(x)/\ell(t)|$ is no better than 1 since that curve touches $[-1,1]$. If we wanted to achieve $|\ell(x)/\ell(t)| \le 2^{-6}$ as in the last example, Γ would have to be a much bigger curve — closer to the "sports ground":

```
xgrid = -2:.04:2; ygrid = -1.5:.04:1.5;
[xx,yy] = meshgrid(xgrid,ygrid); zz = xx+1i*yy;
```



```
ellzz = ell(zz); levels = 2.^(-6:0); levels = [2^6,2^6];
hold on, contour(xgrid,ygrid,abs(ellzz),levels,'r')
ylim([-1.5 1.5]), axis equal
title('Another contour added at level 2^6')
```



The function f would have to be analytic within this much larger region for the bound (11.9) to apply with a ratio $|\ell(x)/\ell(t)|$ as favorable as 2^{-6}.

[To be added: (1) Hermite formula and points per wavelength for equispaced interpolation, following T & Weideman eigenvalues paper. Or put that in Chap. 13. (2) Find a way to shrink and center the contours figure.]

SUMMARY OF CHAPTER 11. *Polynomial interpolants and their errors can be represented by a contour integral in the complex plane, the Hermite integral formula. This provides the standard method for showing geometric convergence for certain approximations of analytic functions.*

Exercise 11.1. Chebfun computation of Cauchy integrals. (a) Figure out (on paper) the polynomial $p \in P_2$ that takes the values $p(-1) = 1$, $p(1/2) = 2$, and $p(1) = 2$. What is $p(2)$? (b) Read about the numerical computation of Cauchy integrals in Chapter 5 of the online *Chebfun Guide*. Write a program to confirm Theorem 11.1 by computing $p(2)$ numerically by a Cauchy integral for the function $f(x) = (x+1)(x-0.5)(x-1)e^x + 11/6 + x/2 - x^2/3$. Take both $|x| = 3/2$ and $|x| = 3$ as contours to confirm that it does not matter whether or not Γ encloses x. (c) Write an anonymous function `p = @(x) ...` to apply the above calculation not just for $x = 2$ but for arbitrary x, and construct a chebfun on $[-1,1]$ from this anonymous function. Do its coefficients as reported by `poly` match your expectations?

Exercise 11.2. Confluent interpolation points. Modify the above problem to require $p(-1) = 1$, $p(1) = 2$, and $p'(1) = 0$. This is a **Hermite interpolation problem,** in which some interpolation points are specified multiply with corresponding values specified for derivatives. What is the analytic solution to this interpolation problem? Do the computations involving contour integrals and anonymous functions deliver the right result?

Exercise 11.3. Interpolation in a disk. Suppose a function f is interpolated by polynomials in arbitrary points of the disk $|x| \le r'$ and we measure the accuracy $f(x) - p(x)$ for x in the disk $|x| \le r$. Show that geometric convergence is assured (in exact arithmetic, ignoring rounding errors) if f is analytic in the disk $|x| \le r + 2r'$. Give the constant ρ for convergence at the rate $O(\rho^{-n})$. (This result originates with [Méray 1884].)

Exercise 11.4. A contour integral. [Practice problem as found in complex variables books – to be written.]

12. Potential theory and approximation

The explorations of the last chapter are glimmerings of potential theory, a centuries-old subject that has been closely connected to approximation theory since the work of Walsh in the early 20th century [Walsh 1969]. Let us now outline how this subject works. A general treatment of potential theory in the complex plane is [Ransford 1995], and surveys of applications to approximation theory can be found in [Finkelshtein 2006, Levin & Saff 2006].

We begin by looking more carefully at (11.10), the formula giving the ratio of the size of the node polynomial ℓ at an approximation point x to its size at a point t on a contour Γ. Suppose we define $\gamma(x,t)$ to be the inverse of the $(n+1)$st root of this ratio,

$$\gamma(x,t)^{-1} = \frac{\left(\prod_{j=0}^n |x - x_j|\right)^{1/(n+1)}}{\left(\prod_{j=0}^n |t - x_j|\right)^{1/(n+1)}}. \tag{12.1}$$

Then the magnitude of the quotient in (11.10) is

$$\left|\frac{\ell(x)}{\ell(t)}\right| = \gamma(x,t)^{-(n+1)}. \tag{12.2}$$

Equation (12.1) has an interesting interpretation. The numerator is the geometric mean distance of x to the grid points, and the denominator is the geometric mean distance of t to the grid points. With a slight abuse of notation, suppose now that $\gamma = \min_{x,t} \gamma(x,t)$, where x ranges over $[-1,1]$ and t ranges over a contour Γ. Thus (11.9), (12.1) and (12.2) tell us that $p(x)$ is guaranteed to converge to $f(x)$ at the rate $O(\gamma^{-n})$ if f is analytic in the region bounded by Γ and each $x \in [-1,1]$ is at least γ times closer to the grid points, on average in the geometric mean sense, than to every point $t \in \Gamma$.

Now we linearize the products by taking logarithms. From (12.1) we find

$$-\log\gamma = \frac{1}{n+1}\sum_{j=0}^n \log|x - x_j| - \frac{1}{n+1}\sum_{j=0}^n \log|t - x_j|. \tag{12.3}$$

We define a **discrete potential function** by

$$u_n(x) = \frac{1}{n+1}\sum_{j=0}^n \log|x - x_j|. \tag{12.4}$$

Note that u_n is a harmonic function throughout the complex x-plane away from the points x_j, that is, a solution of the Laplace equation. We may think of each point x_j as a point charge like an electron and u_n as the harmonic potential generated by all these charges, whose gradient would define an "electric" field. A difference from the electrical case is that whereas electrons are points in 3-space that repel one another with an inverse-square force whose potential function is inverse-linear, here in the plane the repulsion is inverse-linear and the potential is logarithmic. (Some authors put a minus sign in front of (12.4), so that the potential approaches ∞ rather than $-\infty$ as $x \to x_j$, making u_n an energy rather than the negative of an energy.)

With the new definition of γ, (12.2) becomes

$$\left|\frac{\ell(x)}{\ell(t)}\right| = \exp(-(n+1)[u_n(t) - u_n(x)]). \tag{12.5}$$

If the minimum of u_n on Γ is stritly larger than its maximum on $[-1,1]$,

$$\min_{t\in\Gamma} u_n(t) \ge \max_{x\in[-1,1]} u_n(x) + \alpha$$

for some $\alpha > 0$ and all sufficiently large n, then together with (11.9) this implies

$$\|f - p\| = O(e^{-\alpha n}).$$

Notice the flavor of this result: the accuracy of interpolants depends exponentially on the difference of a potential function — the difference being taken between the interpolation point and a contour inside which f is analytic.

We now take the step from discrete to continuous potentials. Another way to write (12.4) is

$$u(x) = \int_{-1}^1 \log|x - t|\, d\mu(t), \tag{12.6}$$

where μ is a measure consisting of a sum of Dirac delta functions,

$$\mu(t) = \frac{1}{n+1}\sum_{j=0}^n \delta(t - x_j).$$

This is the **potential** or **logarithmic potential** associated with the measure μ. The same formula (12.6) also applies if μ is a continuous measure, which will typically be obtained from discrete measures in the limit $n \to \infty$. (The precise

notion of convergence appropriate for this limit is known as weak* convergence.) Equally spaced grids in $[-1,1]$ converge to the limiting measure

$$\mu(x) = \frac{1}{2}. \tag{12.7}$$

Chebyshev grids in $[-1,1]$ converge to the measure identified in Exercise 2.2,

$$\mu(x) = \frac{1}{\pi\sqrt{1-x^2}}. \tag{12.8}$$

So do pretty much all grids associated with zeros and/or extrema of orthogonal polynomials on $[-1,1]$, such as Legendre, Jacobi, or Gegenbauer polynomials.

And now we can identify the crucial property of this **Chebyshev measure** (12.8): the potential (12.6) it generates is *constant* on $[-1,1]$. The measure is known as an **equilibrium measure** for $[-1,1]$, and physically, it corresponds to one unit of charge adjusting itself into an equilibrium, minimal-energy distribution. Given a unit charge distribution μ with support on $[-1,1]$, the associated energy is the integral

$$I(\mu) = -\int_{-1}^{1} u(x)\,d\mu(x) = -\int_{-1}^{1}\int_{-1}^{1} \log|x-t|\,d\mu(t)\,d\mu(x). \tag{12.9}$$

It is clear physically, and can be proved mathematically, that for $I(\mu)$ to be minimized $u(x)$ must be constant, so the gradient of the potential is zero and there are no net forces on the points in $(-1,1)$.

We thus find ourselves with the following problem related to Green's functions: find a function $u(x)$ in the complex x-plane that is harmonic outside $[-1,1]$, approaches a constant value as $x \to [-1,1]$, and is equal to $\log|x| + O(x^{-1})$ as $x \to \infty$. We can solve this problem by introducing a conformal map to transplant the exterior of the interval to the exterior of a disk, where the solution is trivial. Such a mapping is the function

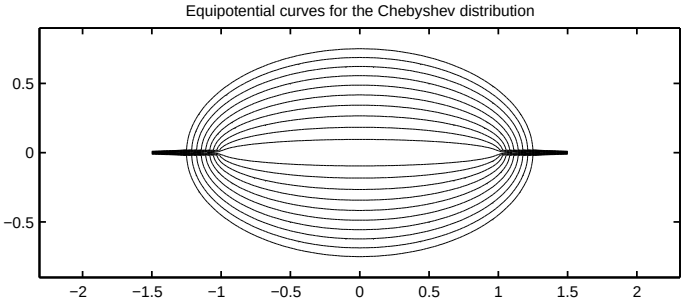
$$z = \phi(x) = \frac{1}{2}(x + i\sqrt{1-x^2}), \tag{12.10}$$

which maps the exterior of $[-1,1]$ in the x-plane onto the exterior of the disk $|z| \le 1/2$ in the z-plane. There, the solution of the potential problem is $\log|z|$. Mapping back to x, we find that the **Chebyshev potential** is given by $u(x) = \log|\phi(x)|$, that is,

$$u(x) = \log|x + i\sqrt{1-x^2}\,| - \log 2, \tag{12.11}$$

with constant value $u(x) = -\log 2$ on $[-1,1]$. For values $u_0 > -\log 2$, the equipotential curve $u(x) = u_0$ is the ρ-ellipse E_ρ with $\rho = 2\exp(u_0)$. Here is a contour plot of (12.11), confirming that the contours looks the same as the ellipses plotted in Chapter 8. The factor `sign(imag(x))` is included to make `u` return the right branch of the square root when $\mathrm{Im}\,x < 0$.


```
u = @(x) log(abs(x+1i*sign(imag(x)).*sqrt(1-x.^2))) - log(2);
xgrid = -1.5:.02:1.5; ygrid = -0.9:.02:0.9;
[xx,yy] = meshgrid(xgrid,ygrid); zz = xx+1i*yy;
uzz = u(zz);
levels = -log(2) + log(1.1:0.1:2);
hold off, contour(xgrid,ygrid,uzz,levels,'k')
ylim([-0.9,0.9]), axis equal
title('Equipotential curves for the Chebyshev distribution')
```



The **capacity** (or **logarithmic capacity** or **transfinite diameter**) of $[-1,1]$ is the radius of that equivalent disk,

$$c = \frac{1}{2}.$$

The associated minimal energy is the **Robin constant** of $[-1,1]$:

$$\min_{\mu} I(\mu) = -\log(c) = \log 2.$$

The fact that the capacity of $[-1,1]$ is $1/2$ has the following interpretation. For Chebyshev or other asymptotically optimal grids, in the limit $n \to \infty$, each grid point lies at a distance $1/2$ from the others in the geometric mean sense.

All these ideas of equilibrium measure, minimal energy, Robin constant and capacity generalize to other compact sets E in the complex plane. If E is connected, then μ and u can be obtained from a conformal map of its exterior onto the exterior of a disk, whereas if it is disconnected, a more general Green's function problem must be solved. In any case, the equilibrium measure, which is supported on the outer boundary of E, describes a good asymptotic distribution of interpolation points as $n \to \infty$, and the limiting geometric mean distance from one point to the others is the capacity, which is related to the Robin constant by $c(E) = \exp(-\min_\mu I(\mu))$.

Having discussed the continuous limit, let us return to the finite problem of finding good sets of $n+1$ points $\{x_j\}$ for interpolation by a polynomial $p \in P_n$

on a compact set E in the complex plane. Three particular families of points have received special attention. We say that $\{x_j\}$ is a set of **Fekete points** for the given n and E if the quantity

$$\left(\prod_{j \neq k} |x_j - x_k| \right)^{2/n(n+1)}, \tag{12.12}$$

which is the geometric mean of the distances between the points, is as large as possible, that is, the points are exactly in a minimal-energy configuration. As $n \to \infty$, these maximal quantities decrease monotonically to $c(E)$, the fact which gives rise to the expression "transfinite diameter". As a rule Fekete points have some of the cleanest mathematical properties for a given set E but are the hardest to compute numerically. Next, if E is connected and $\phi(x)$ is a map of its exterior to the exterior of a disk in the z-plane centered at the origin, a set of **Fejér points** is a set $\phi^{-1}(\{z_j\})$, where $\{z_j\}$ consists of $n+1$ points equally spaced around the boundary circle. Fejér points are more readily computable since it is often possible to get one's hands on a suitable mapping ϕ. Finally, **Leja points** are approximations to Fekete points obtained by a "greedy algorithm". Here, one starts with an arbitrary first point $x_0 \in E$ and then computes successive points $x_1, x_2, \ldots$ by an incremental version of the Fekete condition: with $x_0, \ldots, x_{n-1}$ known, x_n is chosen to maximize the same quantity (12.12), or equivalently, to maximize

$$\prod_{j=0}^{n-1} |x_j - x_n|. \tag{12.13}$$

All three of these families of points can be shown, under reasonable assumptions, to converge to the equilibrium measure as $n \to \infty$, and all work well in practice for interpolation.

In Chapter 8 we proved a very precise theorem (Theorem 8.2): if f is analytic and bounded by M in the ρ-ellipse E_ρ, then $\|f - p_n\| \le 4M\rho^{-n}/(\rho - 1)$, where $p_n \in P_n$ is the interpolant in $n+1$ Chebyshev points. The proof made use of the Chebyshev expansion of f and the aliasing properties of Chebyshev polynomials at Chebyshev points. By the methods of potential theory and the Hermite integral formula discussed in this chapter one can derive the following less sharp but much more general theorem to similar effect.

Theorem 12.1: Interpolation in asymptotically optimal points. *Let f be analytic in $[-1,1]$ but not entire, let ρ be the parameter of the largest ρ-ellipse E_ρ to which f can be analytically continued, and let $\{p_n\}$ be the interpolants to f in any sequence of sets $\{x_n\}$ of $n+1$ points in $[-1,1]$ asymptotically distributed according to the Chebyshev distribution* (12.8)*. Then the errors satisfy*

$$\lim_{n \to \infty} \|f - p_n\|^{1/n} = \rho^{-1}. \tag{12.14}$$

Proof. [Reference to be given.] ∎

So Chebyshev points, Legendre points, Jacobi points and the like all give the same exponential convergence factors for analytic functions — the convergence rates differ only at the margins, in possible algebraic factors like n or $\log n$.

[To be added: (1) Explain where the $O(x^{-1})$ condition for the Green's function comes from. (2) Clarify the branch in (12.10). (3) Who first made the connections between potentials and approximation – was it Walsh? (4) In the mention of general complex sets above (12.12), cite some references such as Smirnov & Lebedev, Walsh, Gaier, Levin & Saff, Finkelshtein. (5) Call Theorem 12.1 the Bernstein-Walsh theorem? Or is that name just for its generalization to a set E? (6) Reference to proof for Theorem 12.1. (7) Exercise 12.3. (8) Mention that barycentric weights grow at the rate *capacity*$^{-n}$. (9) Make the whole discussion more leisurely–indeed, rework this chapter.]

SUMMARY OF CHAPTER 12. *Polynomial interpolants to analytic functions converge geometrically if the grids are asymptotically ditributed like Chebyshev grids.*

Exercise 12.1. Fekete points in an interval. It can be shown that the equilibrium configuration for $n+1$ points in $[-1,1]$ consists of the roots of $(x^2-1)J_{n-1}^{(1,1)}(x)$, where $J_{n-1}^{(1,1)}$ is the degree $n-1$ Jacobi polynomial with parameters $(1,1)$ [Stieltjes 1885]. (An equivalent statement is that the points lie at the local extrema in $[-1,1]$ of the Legendre polynomial of degree $n+1$ — see Chapter 16.) Thus $(x^2-1)J_{n-1}^{(1,1)}(x)$ is the degree $n-1$ Fekete polynomial in $[-1,1]$. Verify numerically using the Chebfun `jacpts` command that in the case $n = 10$, the net forces on the 9 interior points are zero.

Exercise 12.2. Capacity of an ellipse. Let E be an ellipse in the complex plane of semiaxis lengths a and b. Show that $c(E) = (a+b)/2$.

Exercise 12.3. Leja points in an interval. [to be written — are they known explicitly for $[-1,1]$?]

13. Equispaced points, Runge phenomenon

So far in this book, we have considered three good methods for approximating functions by polynomials: Chebyshev interpolation, Chebyshev truncation, and best approximation. Now we shall look at a catastrophically bad method! — interpolation in equally spaced points. This procedure is so bad that for generations, it has unjustly tainted people's views of the whole subject of polynomial interpolation. The mathematical tools we will need to understand what is going on are the Hermite integral formula and potential theory, as discussed in the last two chapters.

As mentioned in Chapter 5, polynomial interpolation was an established tool by the 19th century. The question of whether or not polynomial interpolants would converge to an underlying function as $n \to \infty$ was not given much attention. Presumably many mathematicians would have supposed that if the function was analytic, the answer would be yes. In 1884 and 1896, Méray published a pair of papers in which he identified the fact that certain interpolation schemes do not converge [Méray 1884 & 1896]. In the first paper he writes,

It is rather astonishing that practical applications have not yet turned up any cases in which the interpolation is illusory.[5]

Méray's derivations had the key idea of making use of the Hermite integral formula. However, the examples he devised were rather contrived, and his idiosyncratically written papers had little impact. It was Runge in 1901 who made the possibility of divergence famous by showing that divergence of interpolants occurs in general even for equispaced points in an real interval and evaluation points in the interior of that interval [Runge 1901].

Runge illustrated his discovery with an example that has become known as the **Runge function:** $1/(1+x^2)$ on $[-5,5]$, or equivalently on $[-1,1]$,

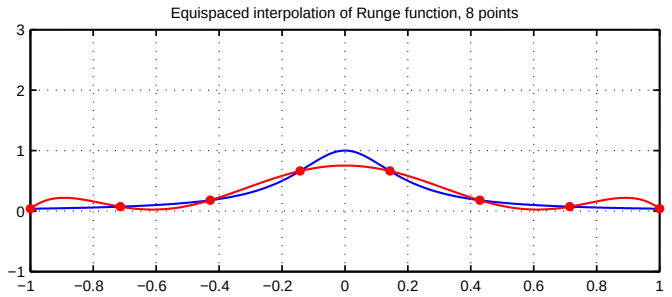
```
f = 1./(1+25*x.^2);
```

We already know from Chapter 8 that there is nothing wrong with this function for polynomial interpolation in Chebyshev points: f is analytic, and the polynomial interpolants converge geometrically. Now, however, let us follow Runge and look at interpolants in equally spaced points, which we can compute using the Chebfun overload of Matlab's `interp1` command.

Here is what we get with 8 points:

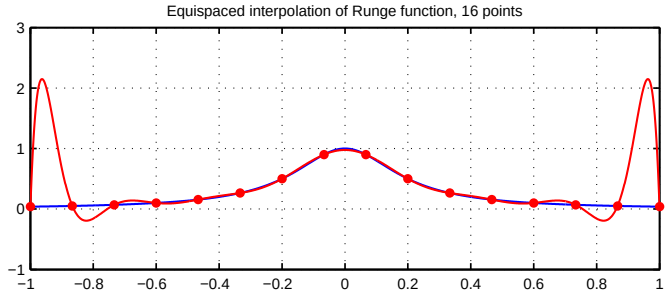
```
s = linspace(-1,1,8);
p = interp1(s,f);
hold off, plot(f), hold on, plot(p,'r'), grid on
plot(s,p(s),'.r'), axis([-1 1 -1 3])
title('Equispaced interpolation of Runge function, 8 points')
```

[5] "Il est assez étonnant que les hasards de la pratique n'aient encore fait connaître aucun cas dans lequel l'interpolation soit illusoire." By illusory, Méray means nonconvergent.



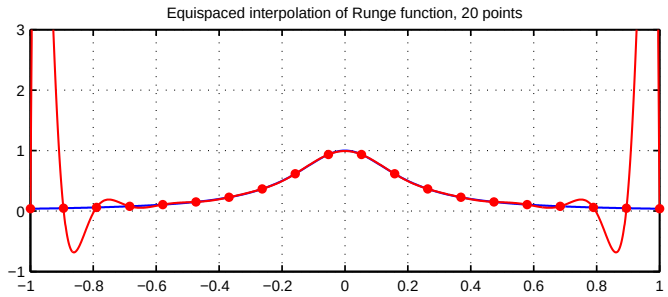
Here is the result for 16 points:

```
s = linspace(-1,1,16);
p = interp1(s,f);
hold off, plot(f), hold on, plot(p,'r'), grid on
plot(s,p(s),'.r'), axis([-1 1 -1 3])
title('Equispaced interpolation of Runge function, 16 points')
```



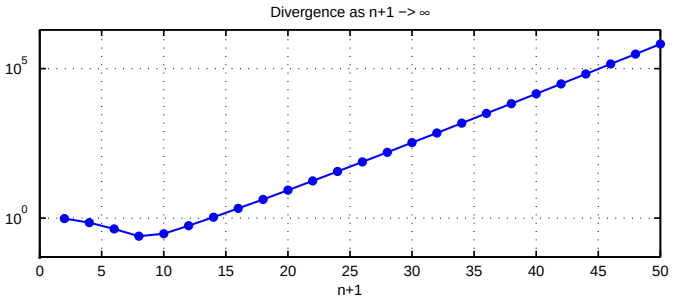
Is this going to converge as $n \to \infty$? Things look pretty good in the middle, but not so good at the edges. Here is the result for 20 points:

```
s = linspace(-1,1,20);
p = interp1(s,f);
hold off, plot(f), hold on, plot(p,'r'), grid on
plot(s,p(s),'.r'), axis([-1 1 -1 3])
title('Equispaced interpolation of Runge function, 20 points')
```



What is happening is exponential convergence in the middle of the interval but exponential divergence near the ends. The next figure shows the maximum error over $[-1,1]$ as a function of the number of equally spaced points. We get a hint of convergence at first, but after $n = 10$, things just get worse. Note the log scale.

```
ee = []; nn = 2:2:50;
for np = nn
  s = linspace(-1,1,np);
  p = interp1(s,f);
  ee = [ee norm(f-p,inf)];
end
hold off, semilogy(nn,ee,'.-'), grid on, axis([0 50 5e-2 2e6])
title('Divergence as n+1 -> \infty')
xlabel('n+1')
```

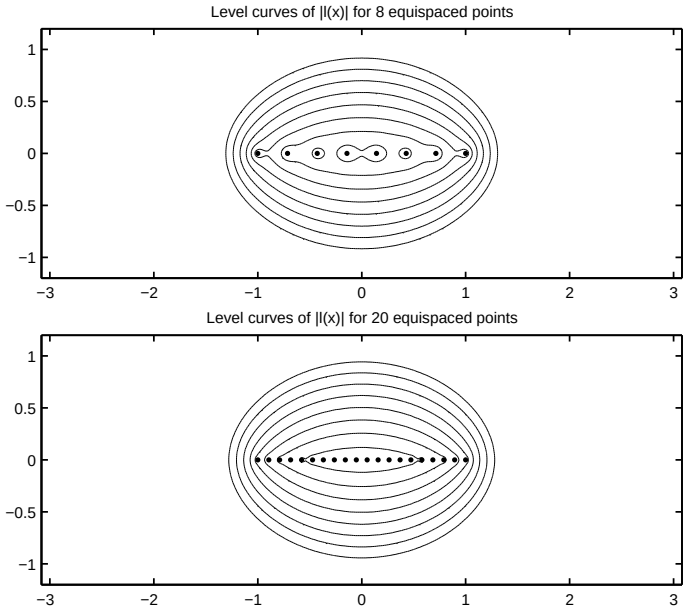


By now the reader may have suspected that what is going wrong here can be understood by looking at potentials, as in the last two chapters. Here is an adaptation of a code segment from Chapter 11 to plot equipotential curves for $n+1 = 8$ and 20.

```
d = domain([-1.5,1.5]);
xgrid = -1.5:.02:1.5; ygrid = -1:.02:1;
```



```
[xx,yy] = meshgrid(xgrid,ygrid); zz = xx+1i*yy;
for np = [8 20]
  xj = linspace(-1,1,np);
  ell = poly(xj,d);
  hold off, plot(xj,ell(xj),'.k',MS,8)
  hold on, ylim([-1.2 1.2]), axis equal
  ellzz = ell(zz);
  levels = ((1.25:.25:3)/exp(1)).^np;
  contour(xx,yy,abs(ellzz),levels,'k')
  title(['Level curves of |l(x)| for '...
    int2str(np) ' equispaced points'])
  snapnow
end
```



What we see here is that $[-1,1]$ is very far from being a level curve for equispaced interpolation points. From the last two chapters, we expect serious consequences of this irregularity. In the second plot just shown, for example, it is the fourth curve (from inside out) that approximately touches the endpoints ± 1. For Theorem 11.1 to be of any use in such a landscape, f will have to be analytic in a region larger than the "football" enclosed by that curve. Analyticity on $[-1,1]$ is not enough for convergence; we will need analyticity in a much bigger region of the complex plane. This is what Runge discovered in 1901.

Following the method of the last chapter, we now consider the limit $n \to \infty$,

where the distribution of interpolation points approaches the constant measure (12.7),

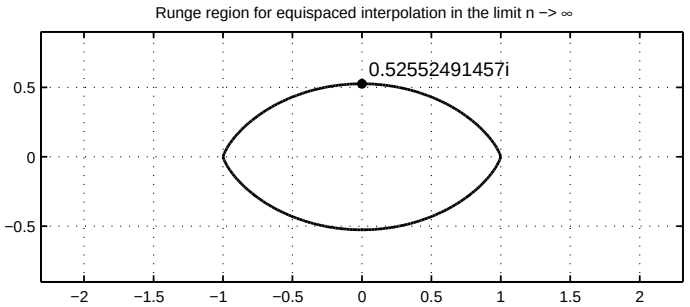
$$\mu(x) = \frac{1}{2}. \tag{13.1}$$

The potential (12.6) associated with this measure is

$$u(z) = -1 + \frac{1}{2}\mathrm{Re}\left[(z+1)\log(z+1) - (z-1)\log(z-1)\right]. \tag{13.2}$$

Here is a code that plots just one level curve of this potential, the one passing through ± 1, where the value of the potential is $-1 + \log 2$.

```
x1 = -1.65:.02:1.65; y1 = -0.7:.02:0.7;
[xx,yy] = meshgrid(x1,y1); zz = xx+1i*yy;
u = @(z) -1 + 0.5*real((z+1).*log(z+1)-(z-1).*log(z-1));
hold off
contour(x1,y1,u(zz),(-1+log(2))*[1 1],'k',LW,1.4)
set(gca,'xtick',-2:.5:2,'ytick',-.5:.5:.5), grid on
ylim([-.9 .9]), axis equal
hold on, plot(.5255i,'.k')
text(0.05,.63,'0.52552491457i')
title(['Runge region for equispaced interpolation ' ...
       'in the limit n -> \infty'])
```



For the interpolants to a function f in equispaced nodes to converge as $n \to \infty$ for all $x \in [-1,1]$, f must be analytic, not just on $[-1,1]$, but throughout this **Runge region,** which crosses the real axis at ± 1 and the imaginary axis at $\pm 0.52552491457\ldots i$. Runge reports this number correctly to 4 digits, and writes

The curve has somewhat the shape of an ellipse. At the ends of the long axis, however, our curve is more pointed than an ellipse.[6]

[6] "Die Kurve... hat etwa die Gestalt einer Ellipse.... An den Enden der grossen Achse ist unsere Kurve aber spitzer als eine Ellipse."

Here are the values of (13.2) at the endpoints and the middle:

$$u(\pm 1) = -1 + \log 2, \quad u(0) = -1,$$

and thus

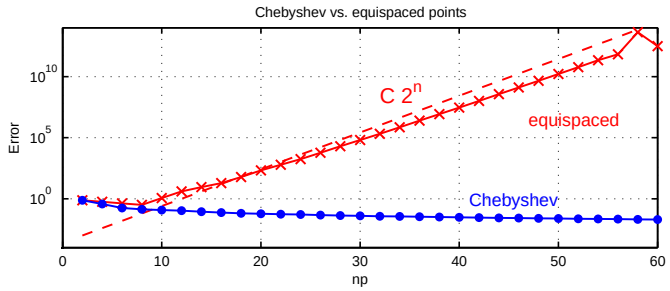
$$\exp(u(\pm 1)) = \frac{2}{e}, \quad \exp(u(0)) = \frac{1}{e}.$$

These numbers indicate that in the limit $n \to \infty$, the endpoints of an equispaced grid in $[-1,1]$ lie at an average distance $2/e$ from the other grid points, in the geometric mean sense, whereas the midpoint lies at an average distance of just $1/e$. As emphasized in the last chapter, for example in equation (11.15), the effect of such a discrepancy grows exponentially with n.

Here are some examples. Equispaced interpolation will converge throughout $[-1,1]$ for $f(x) = \exp(-x^2)$, which is analytic everywhere, and for $f(x) = (1+x^2)^{-1}$, which has poles at $\pm i$. On the other hand it will not converge for $f(x) = (1+16x^2)^{-1}$, which has poles at $\pm i/4$. It will converge slowly for $f(x) = (1+(x/0.53)^2)^{-1}$, and diverge slowly for $f(x) = (1+(x/0.52)^2)^{-1}$ (Exercise 13.3).

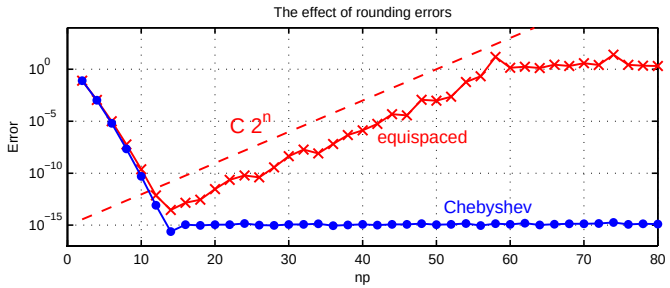
The worst-case rate of divergence is 2^n, and this rate will always appear if f is not analytic on $[-1,1]$. To be precise, for such a function the errors will be of size $O(2^n)$ as $n \to \infty$ but not of size $O(C^n)$ for any $C < 2$. Here, for example, we take f to be a hat function, with just one derivative of bounded variation. The dots show errors in Chebyshev interpolation, converging at the rate $O(n^{-1})$ in keeping with Theorem 7.2, and the crosses show errors in equispaced interpolation, with a dashed line parallel to 2^n for comparison.

```
f = max(0,1-2*abs(x));
eequi = []; echeb = []; nn = 2:2:60;
for n = nn
  s = linspace(-1,1,n+1);
  pequi = interp1(s,f); eequi = [eequi norm(f-pequi,inf)];
  pcheb = chebfun(f,n+1); echeb = [echeb norm(f-pcheb,inf)];
end
hold off, semilogy(nn,2.^(nn-12),'--r')
hold on, axis([0 60 1e-4 1e14]), grid on
semilogy(nn,eequi,'x-r',MS,8), semilogy(nn,echeb,'.-b')
text(47,3e6,'equispaced',CO,'r')
text(41,0.8,'Chebyshev',CO,'b')
text(32,4e8,'C 2^n',FS,12,CO,'r')
xlabel np, ylabel Error
title('Chebyshev vs. equispaced points')
```



All of the above remarks about equispaced interpolation concern the ideal mathematics of the problem. On a computer in floating point arithmetic, however, a further complication arises: even if convergence ought to take place in theory, rounding errors will be amplified by $O(2^n)$, causing divergence in practice. Here, for example, are the errors in equispaced and Chebyshev interpolation of $\exp(x)$:

```
f = exp(x);
eequi = []; echeb = []; nn = 2:2:80;
for n = nn
  s = linspace(-1,1,n+1);
  pequi = interp1(s,f); eequi = [eequi norm(f-pequi,inf)];
  pcheb = chebfun(f,n+1); echeb = [echeb norm(f-pcheb,inf)];
end
hold off, semilogy(nn,2.^(nn-50),'--r')
hold on, axis([0 80 1e-17 1e4]), grid on
semilogy(nn,eequi,'x-r',MS,8), semilogy(nn,echeb,'.-b')
text(22,6e-6,'C 2^n',FS,12,CO,'r')
text(42,3e-7,'equispaced',CO,'r')
text(51,6e-14,'Chebyshev',CO,'b')
xlabel np, ylabel Error
title('The effect of rounding errors')
```



In exact arithmetic we would see convergence for both sets of points, but on a computer the divergence for equispaced points sets in early. The rate is cleanly $O(2^n)$ until we reach $O(1)$. Notice that the line of crosses, if extended backward to $n = 0$, meets the y axis at approximately 10^{-18}, i.e., a digit or two below machine precision.

The 2^n divergence of equispaced polynomial interpolants is a fascinating subject, and we must remind ourselves that one should only go into so much detail in analyzing a method that should never be used! But perhaps we should qualify that "never" in one respect. As Runge himself emphasized, though interpolants in equispaced points do not converge on the whole interval of interpolation, they may still do very well near the middle. In the numerical solution of differential equations, for example, higher order centered difference formulas are successfully used based on 5 or 7 equally spaced grid points. A less happy example would be Newton–Cotes quadrature formulas, based on polynomial interpolation in equally spaced points, where the $O(2^n)$ effect is unavoidable and causes serious problems for larger n and divergence as $n \to \infty$, as first proved by Pólya [1933]. We shall discuss quadrature in Chapter 19.

We close this chapter with an observation that highlights the fundamental nature of the Runge phenomenon and its associated mathematics. Suppose you want to persuade somebody that it's important to know something about the complex plane, even for dealing with real functions. I still remember the argument my calculus teacher explained to me: to understand why the Taylor series for $1/(1+x^2)$ only converges for $-1 < x < 1$, you need to know that Taylor series converge within disks in the complex plane and this function has poles at $\pm i$.

Runge's observation is precisely a generalization of this fact to interpolation points equispaced in an interval rather than all at $x = 0$. The convergence or divergence of polynomial interpolants to a function f again depends on whether f is analytic in a certain region; the change is only that the region is not a disk but more elongated. Even the phenomenon of divergence in floating-point arithmetic for functions whose interpolants "ought" to converge is a generalization of familiar facts about Taylor series. Just try to evaluate $\exp(x)$ on a computer for $x = -20$ using the Taylor series!

[To be added: (1) Discuss phenomenon of convergence on a subinterval, which also goes back to Runge. (2) Where does (13.2) come from? (It's an exercise in SMIM.) (3) Exercise 13.5. (4) Compute $0.5255i$ with ROOTS.]

SUMMARY OF CHAPTER 13. *Polynomial interpolation in equispaced points is exponentially ill-conditioned: the interpolant p_n may have oscillations near the edge of the interval nearly 2^n times larger than the function f being interpolated, even if f is analytic. In particular, even if f is analytic and the interpolant is computed exactly without rounding errors, p_n need not converge to f as $n \to \infty$.*

Exercise 13.1. Three examples. Draw plots comparing accuracy of equispaced and Chebyshev interpolants as functions of n for $\exp(x^2)$, $\exp(-x^2)$, $\exp(-1/x^2)$.

Exercise 13.2. Computing geometric means in Chebfun. (a) What output is produced by the program below? (b) Why?

```
x = chebfun('x',[0 1]);
f = chebfun(@(y) prod(abs(x-1i*y)),[0.1 1],'vectorize');
roots(f-2/exp(1))
```

Exercise 13.3. Borderline convergence. The claim was made in the text that equispaced polynomial interpolants on $[-1,1]$ will converge for $f(x) = (1 + (x/0.53)^2)^{-1}$ and diverge for $f(x) = (1 + (x/0.52)^2)^{-1}$. Can you observe this difference numerically? Run appropriate experiments and discuss the results.

Exercise 13.4. Approaching the sinc function. The sinc function is defined for all x by $S(x) = \sin(\pi x)/(\pi x)$ (and $S(0) = 1$). For any $n \geq 1$, an approximation to S is given by

$$S_n = \prod_{k=1}^{n} (1 - x^2/k^2).$$

Construct S_{20} in Chebfun on the interval $[-20, 20]$ and compare it with S. On what interval around $x = 0$ do you find $|S_{20}(x) - S(x)| < 0.1$? (It can be shown that for every x, $\lim_{n\to\infty} S_n(x) = S(x)$.)

Exercise 13.5. Barycentric weights and ill-conditioning. [Exercise 5.6 showed weights $(-1)^j \binom{n}{j}$ for equispaced points. Relate this to Runge phenomenon. Not yet written.]

14. Discussion of high-order polynomial interpolation

As mentioned at various points in this book, high-order polynomial interpolation has a bad reputation. For equispaced points this is entirely appropriate, as shown in the last chapter, but for Chebyshev points it is entirely inappropriate. Here are some illustrative quotes from numerical analysis textbooks, which we present anonymously.

We cannot rely on a polynomial to be a good approximation if exact matching at the sample points is the criterion used to select the polynomial. The explanation of this phenomenon is, of course, that the derivatives grow too rapidly. (1962)

However, for certain functions the approximate representation of $f(x)$ by a single polynomial throughout the interval is not satisfactory. (1972)

But there are many functions which are not at all suited for approximation by a single polynomial in the entire interval which is of interest. (1974)

Polynomial interpolation has drawbacks in addition to those of global convergence. The determination and evaluation of interpolating polynomials of high degree can be too time-consuming for certain applications. Polynomials of high degree can also lead to difficult problems associated with roundoff error. (1977)

We end this section with two brief warnings, one against trusting the interpolating polynomial outside [the interval] and one against expecting too much of polynomial interpolation inside [the interval]. (1980)

Although Lagrangian interpolation is sometimes useful in theoretical investigations, it is rarely used in practical computations. (1985)

Polynomial interpolants rarely converge to a general continuous function. Polynomial interpolation is a bad idea. (1989)

While theoretically important, Lagrange's formula is, in general, not as suitable for actual calculations as some other methods to be described below, particularly for large numbers n of support points. (1993)

Unfortunately, there are functions for which interpolation at the Chebyshev points fails to converge. Moreoever, better approximations of functions like $1/(1 + x^2)$ can be obtained by other interpolants — e.g., cubic splines. (1996)

Increasing the number of interpolation points, i.e., increasing the degree of the polynomials, does not always lead to an improvement in the approximation. The spline interpolation *that we will study in this section remedies this deficiency.* (1998)

The surprising state of affairs is that for most continuous functions, the quantity $\|f - p_n\|_\infty$ will not coverge to 0. (2002)

By their very nature, polynomials of a very high degree do not constitute reasonable models for real-life phenomena, from the approximation and from the handling point-of-view. (2004)

Because its derivative has $n-1$ zeros, a polynomial of degree n has $n-1$ extreme or inflection points. Thus, simply put, a high-degree polynomial necessarily has many "wiggles," which may bear no relation to the data to be fit. (2004)

The oscillatory nature of high degree polynomials, and the property that a fluc-

tuation over a small portion of the interval can induce large fluctuations over the entire range, restricts their use. (2005)

A great deal of confusion underlies remarks like these. Some of them are literally correct, but they are all misleading. In fact, polynomial interpolants in Chebyshev points are problem-free when evaluated by the the barycentric interpolation formula. They have the same behavior as discrete Fourier series for periodic functions, whose practicability nobody worries about. The mention of splines is a red herring: the true advantage of splines, as mentioned in Chapter 9, is not that they converge where polynomials fail to do so, but that they are more easily adapted to irregular point distributions and more localized, giving errors that decay exponentially away from singularities rather than just algebraically.

It is interesting to speculate as to how the distrust of high-degree polynomials became so firmly established. I think the crucial circumstance is that not one but several combined problems affect certain computations with polynomials, a situation complex enough to have obscured the truth from easy elucidation. If working with polynomials had been the central task of scientific computing, the truth would have been worked out nonetheless, but over the years there were always bigger problems pressing upon the attention of numerical analysts, like matrix computations and differential equations. Polynomial computations were always a sideline.

At the most fundamental level there are the two issues of conditioning and stability: both crucial, and not the same (see [Trefethen & Bau 1997] for a general discussion of conditioning and stability).

(1) *Conditioning of the problem.* The interpolation points must be properly spaced (e.g. Chebyshev or Legendre) for the interpolation problem to be well-conditioned. This means that the interpolant should depend not too sensitively on the data. The Runge phenomenon for equally spaced points is the well-known consequence of extreme ill-conditioning, with sensitivities of order 2^n. The next chapter makes such statements precise through the use of Lebesgue constants.

(2) *Stability of the algorithm.* The interpolation algorithm must be stable (e.g. barycentric interpolation formula) for a computation to be accurate, even when the problem is well-conditioned. This means that in the presence of rounding errors, the computed solution should be close to an exact solution for some interpolation data close to the exact data. In particular, the best-known algorithm of all, namely solving a Vandermonde linear system of equations to find the coefficients of the interpolant expressed as a linear combination of monomials, is exponentially unstable (Exercise 5.2).

These facts would be enough to explain a good deal of confusion, but another consideration has muddied the water further, namely crosstalk with the notoriously troublesome problem of finding roots of a polynomial from its coefficients (to be discussed in Chapter 18). The difficulties of polynomial rootfinding were widely publicized by Wilkinson beginning in the 1950s, who later wrote an article called the "The perfidious polynomial" that won the Chauvenet Prize of the Mathematical Association of America [Wilkinson 1984]. Undoubtedly this negative publicity further discouraged people from the use of polynomials, even though interpolation and rootfinding are different problems. They are related, with related widespread misconceptions about accuracy: just as interpolation on an interval is trouble-free for a stable algorithm based on Chebyshev points, rootfinding on an interval is trouble-free for a stable algorithm based on expansions in Chebyshev polynomials (Chapter 18). But very few numerical analysis textbooks tell readers these facts.

[To be added: (1) Concerning Newton-Cotes quadrature, see [Trefethen 2008], refs 18,46,47.]

SUMMARY OF CHAPTER 14. *Generations of textbooks have warned readers that polynomial interpolation is dangerous. In fact, if the interpolation points are clustered and a stable algorithm is used, it is bulletproof.*

Exercise 14.1. Convergence as $n \to \infty$. The 1998 quote asserts that increasing n "does not always lead to an improvement". Based on the theorems of this book, for interpolation in Chebyshev points, for which functions f do we know that increasing n must lead to an improvement?

Exercise 14.2. Too many wiggles. Using Chebfun's `roots(f,'all')` option, plot all the roots in the complex plane of the chebfun corresponding to $f(x) = \exp(x)\tanh(2x-1)$ on $[-1,1]$. What is the error in the argument in the second 2004 quote used to show that "a high-degree polynomial necessarily has many wiggles"?

Exercise 14.3. Your own textbook. Find a textbook of numerical analysis and examine its treatment of polynomial interpolation. (a) What does it say about behavior for large n? If it asserts that this behavior is problematic, is this conclusion based on the assumption of equally spaced points, and does the text make this clear? (b) Does it mention interpolation in Chebyshev points? Does it state that such interpolants converge exponentially for analytic functions? (c) Does it mention the barycentric formula? (d) Does it claim that one should use a Newton rather than a Lagrange interpolation formula for numerical work? (This is a myth.)

Exercise 14.4. Spline interpolants. (a) Look up Matlab's `spline` command and use it to interpolate $f(x) = 1/(1+25x^2)$ in $n+1$ equally spaced points on $[-1,1]$. Compare the ∞-norm error as $n \to \infty$ with that of polynomial interpolation in Chebyshev points. You may find it convenient to construct a chebfun from the spline with a command like `f = chebfun(@(x) spline(nodes,f(nodes),x),nodes)`. (b) Same problem for $f(x) = |x + 1/\pi|$. (c) Same problem for $f(x) = |x + 1/\pi|$, but measuring the error by the ∞-norm over the interval $[0,1]$.

15. Lebesgue constants

There is a well developed theory that quantifies the convergence or divergence of polynomial interpolants. A key notion is that of the **Lebesgue constant**, Λ, for interpolation in a given set of points. The Lebesgue constant is the ∞-norm of the linear mapping from data to interpolant:

$$\Lambda = \sup_f \frac{\|p\|}{\|\{f_j\}\|}, \tag{15.1}$$

where $\|\cdot\|$ denotes the ∞-norm on $[-1,1]$ (in the numerator) or $\mathbf{C}^{n+1}$ (in the denominator). In words, if you have data values on an $(n+1)$-point grid, and the data are no greater than 1 in absolute value, what is the largest possible value of the interpolant p somewhere in $[-1,1]$?

In the plots of Chapter 13 for interpolation of Runge's function, for example, we saw that the interpolants grew much bigger than the data. Thus the Lebesgue constants must be large for equispaced interpolation. For example, for $n = 50$, the data are bounded by 1 for all n, yet the interpolant is bigger than 10^5. Thus the Lebesgue constant for interpolation in 50 equispaced points must be greater than 10^5. (In fact it is about 4.2×10^{12}.)

From the basic Lagrange formula (5.1) for polynomial interpolation,

$$p(x) = \sum_{j=0}^{n} f_j \, \ell_j(x), \tag{15.2}$$

we can get a formula for Λ in terms of the Lagrange polynomials $\{\ell_j\}$. At any point $x \in [-1,1]$, the maximum possible value of $|p(x)|$ for data bounded by 1 in absolute value will be

$$\lambda(x) = \sum_{j=0}^{n} |\ell_j(x)|. \tag{15.3}$$

This sum of absolute values is known as the **Lebesgue function** for the given grid, and the Lebesgue constant is its maximum value,

$$\Lambda = \sup_{x \in [-1,1]} \lambda(x). \tag{15.4}$$

The reason Lebesgue constants are interesting is that interpolants are guaranteed to be good if and only if the Lebesgue constants are small. We can make this statement precise as follows. Let Λ be the Lebesgue constant for interpolation in a certain set of points. Without loss of generality, suppose the samples have absolute value 1. If p is the interpolant in these points to a function f, we know that $\|p\|$ might be as great as Λ; yet $\|f\|$ might be as small as 1. Thus $\|f - p\|$ might be as great as $\Lambda - 1$, showing that a large Lebesgue constant rigorously implies the possibility of a large interpolation error.

Conversely, let p^* be the best approximation to f in the ∞-norm. If p is the polynomial interpolant to f in the given points, then $p - p^*$ is the polynomial interpolant to $f - p^*$. By the definition of the Lebesgue constant, $\|p - p^*\|$ is no greater than $\Lambda\|f - p^*\|$. Since $f - p = (f - p^*) - (p - p^*)$, this implies that $\|f - p\|$ is no greater than $(\Lambda + 1)\|f - p^*\|$. Thus a small Lebesgue constant implies that interpolation will be close to best.

Actually, the discussion of the last two paragraphs is not limited to interpolation. What is really in play here is any approximation process that is *linear* and a *projection*, of which Chebyshev projection (truncation of the Chebyshev series) would be an example as well as interpolation. Suppose we let L denote the operator that maps a function $f \in C[-1,1]$ to its approximation by a polynomial $p \in P_n$. For L to be linear means that $L(f_1 + f_2) = Lf_1 + Lf_2$ for any $f_1, f_2 \in C[-1,1]$ and $L(\alpha f) = \alpha Lf$ for any scalar α, and for L to be a projection means that if $p \in P_n$, then $Lp = p$. By the argument above we have established the following result applicable to any such approximation operator.

Theorem 15.1: Near-best approximation and Lebesgue constants. *Let Λ be the Lebesgue constant for a linear projection L of $C[-1,1]$ onto P_n. Let f be a function in $C([-1,1])$, $p = Lf$ the corresponding polynomial approximant to f, and p^* the best approximation. Then*

$$\|f - p\| \le (\Lambda + 1)\|f - p^*\|. \tag{15.5}$$

Proof. Given in the paragraphs above. ∎

So it all comes down to the question, how big is Λ? According to the theorem of Faber mentioned in Chapter 6 [Faber 1914], no set of interpolation points can lead to convergence for all f, so it follows from Theorems 6.1 and 15.1 that

$$\lim_{n \to \infty} \Lambda_n = \infty \tag{15.6}$$

for interpolation in any sets of points. However, for well chosen sets of points, the growth of Λ_n as $n \to \infty$ may be exceedingly slow. Chebyshev points turn out to be nearly optimal, whereas equispaced points are very bad.

The following theorem summarizes a great deal of knowledge accumulated over the past century about interpolation processes. At the end of the chapter an analogous theorem is stated for Cheybshev projection. As always in this book, by "Chebyshev points" we mean Chebyshev points of the second kind, defined by (2.2).

Theorem 15.2: Lebesgue constants for polynomial interpolation. *The Lebesgue constants Λ_n for degree $n \ge 0$ polynomial interpolation in any set of $n+1$ distinct points in $[-1,1]$ satisfy*

$$\Lambda_n \ge \frac{2}{\pi} \log(n+1) + 0.52125\ldots; \tag{15.7}$$

the number $0.52125\ldots$ *is* $(2/\pi)(\gamma + \log(4/\pi))$*, where* $\gamma \approx 0.577$ *is Euler's constant. For Chebyshev points, they satisfy*

$$\Lambda_n \le 1 + \frac{2}{\pi}\log(n+1) \quad \textit{and} \quad \Lambda_n \sim \frac{2}{\pi}\log n, \quad n \to \infty. \tag{15.8a,b}$$

For equispaced points they satisfy

$$\Lambda_n > \frac{2^{n-2}}{n^2} \quad \textit{and} \quad \Lambda_n \sim \frac{2^{n+1}}{e\, n \log n}, \quad n \to \infty, \tag{15.9a,b}$$

with the inequality (15.9a) *applying for* $n \ge 1$.

Proof. The fact that Lebesgue constants for polynomial interpolation always grow at least logarithmically goes back to Bernstein [1912c], Jackson [1913], and Faber [1914]. Bernstein knew that $(2/\pi)\log n$ was the appropriate asymptotic behavior for interpolation in an interval, and the proof of (15.7) in this sharp form is due to Erdős [1961], who got a constant C, and Brutman [1978], who improved the constant to $0.52125\ldots$. Equation (15.8a) is a consequence of Theorem 4 of [Ehlich & Zeller 1966]; see also [Brutman 1997] and [McCabe & Phillips 1973]. Equation (15.8b) follows from this together with Erdős's result. (Bernstein [1918] did the essential work, deriving this asymptotic result for Chebyshev points of the first kind, i.e., zeros rather than extrema of Chebyshev polynomials — see Exercise 15.2.) Equation (15.9b) is due to Turetskii [1940] and independently Schönhage [1961], and for (15.9a) and a discussion of related work, see [Trefethen & Weideman 1991]. ∎

Equation (15.8a) shows that Lebesgue constants for Chebyshev points grow more slowly than any polynomial: for many practical purposes they might as well be 1. It is interesting to relate this bound to the interpolant through 100 random data points plotted at the end of Chapter 2. The Lebesgue constant is the maximum amplitude this curve could possibly have attained, if the data had been as bad as possible. For 100 points this number is about 3.94. In the plot we see that random data have in fact come nowhere near even this modest limit.

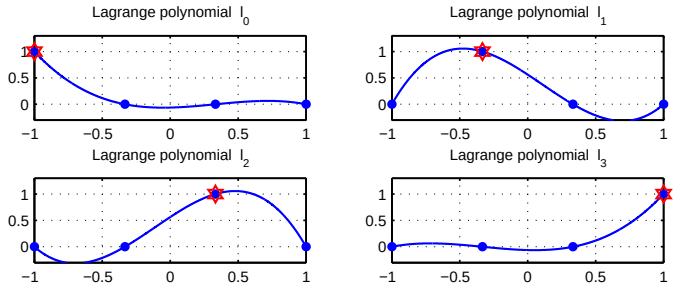
On the other hand, (15.9a) shows that Lebesgue constants for equispaced points grow faster than any polynomial: for many practical purposes, unless n is very small, they might as well be ∞.

Taking advantage again of the `interp1` command, as in Chapter 13, we can use Chebfun as a laboratory in which to see how such widely different Lebesgue constants emerge. Consider for example the case of four equally spaced points. Here are plots of the four Lagrange polynomials $\{\ell_j\}$. In Chapter 9 we have already seen plots of Lagrange polynomials, but on a grid of 20 Chebyshev points instead of 4 equispaced points.

```
npts = 4; clear p
```

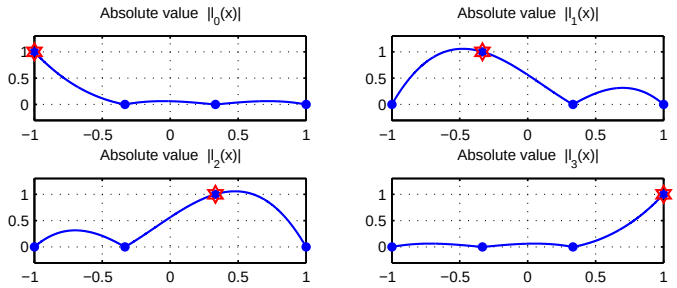


```
d = domain(-1,1); s = linspace(-1,1,4);
for k = 1:npts
  subplot(2,2,k)
  y = [zeros(1,k-1) 1 zeros(1,npts-k)];
  p{k} = interp1(s,y,d);
  hold off, plot(p{k}), grid on
  hold on, plot(s,p{k}(s),'.')
  plot(s(k),p{k}(s(k)),'hr',MS,9), ylim([-.3 1.3])
  title(['Lagrange polynomial  l_' int2str(k-1)])
end
```



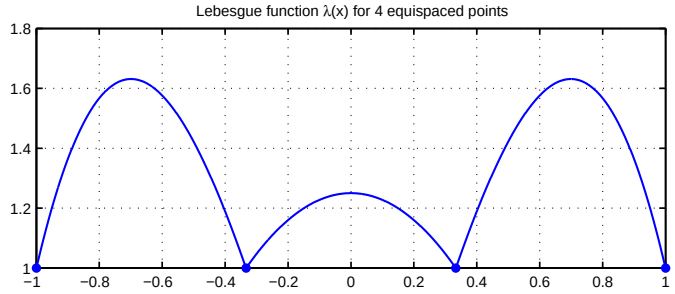
By taking the absolute values of these curves, we see the largest possible effect at each point in $[-1,1]$ of data that is nonzero at just one point of the grid:

```
for k = 1:npts
  subplot(2,2,k)
  absp = abs(p{k});
  hold off, plot(absp), grid on
  hold on, plot(s,absp(s),'.')
  plot(s(k),absp(s(k)),'hr',MS,9), ylim([-.3 1.3])
  title(['Absolute value  |l_' int2str(k-1) '(x)|'])
end
```



Now let us add up these absolute values as in (15.3):

```
L = 0*x;
for k = 1:npts, L = L + abs(p{k}); end
clf, plot(L), grid on
hold on, plot(s,L(s),'.')
title('Lebesgue function \lambda(x) for 4 equispaced points')
```



This is the Lebesgue function $\lambda(x)$, a piecewise polynomial, telling us the largest possible effect at each point $x \in [-1,1]$ of interpolating data of norm 1. The Lebesgue constant (15.4) is the height of the curve:

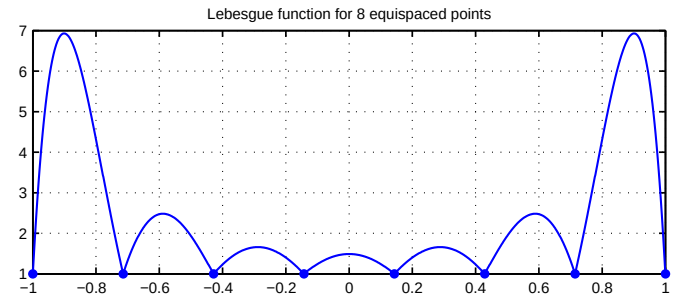
```
Lconst = norm(L,inf)
```

```
Lconst = 1.631130309440899
```

A code `lebesgue` for automating the above computation (actually based on a more efficient method) is included in Chebfun, and it optionally returns the Lebesgue constant as well as the Lebesgue function. Here are the results for 8 equispaced points:

```
s = linspace(-1,1,8); [L,Lconst] = lebesgue(s);
hold off, plot(L), grid on, hold on, plot(s,L(s),'.')
title('Lebesgue function for 8 equispaced points')
Lconst
```

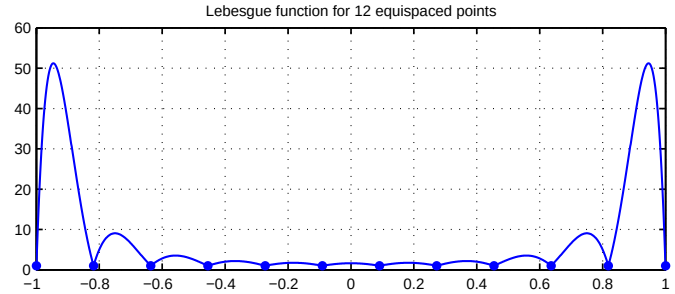
```
Lconst = 6.929739656126465
```



And here they are for 12 points. Note that the Lebesgue constant has jumped from 7 to 51.

```
s = linspace(-1,1,12); [L,Lconst] = lebesgue(s);
hold off, plot(L), grid on, hold on, plot(s,L(s),'.')
title('Lebesgue function for 12 equispaced points')
Lconst
```

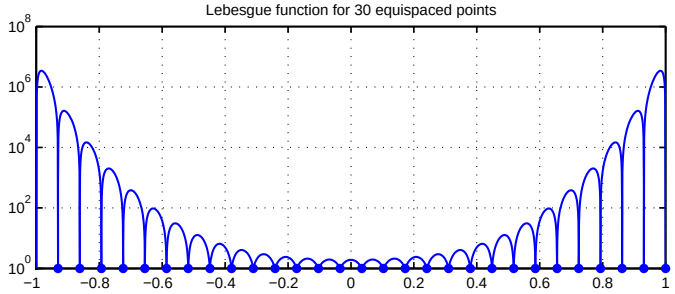
```
Lconst = 51.214223185730020
```



The function takes large values near ± 1, as we expect from Chapter 13 since the Runge phenomenon is associated with interpolants becoming very large near the endpoints. In fact the Lebesgue function for interpolation in equispaced points is more naturally displayed on a log scale. Here it is for $n = 30$:

```
s = linspace(-1,1,30); [L,Lconst] = lebesgue(s);
hold off, semilogy(L), grid on, hold on, semilogy(s,L(s),'.')
title('Lebesgue function for 30 equispaced points')
Lconst
```

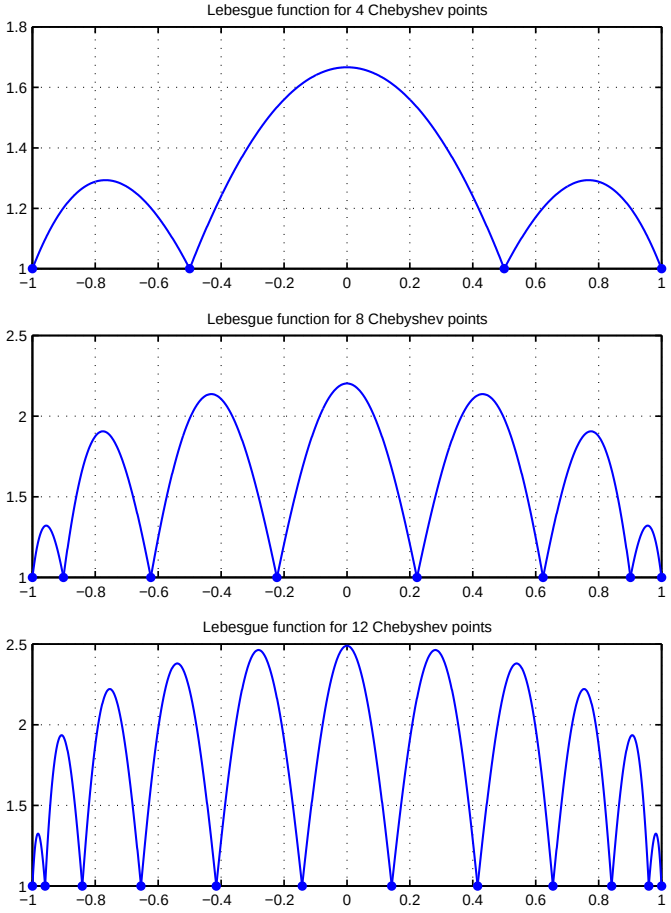
```
Lconst = 3.447738672687561e+06
```



For comparison, here are the corresponding results for 4, 8, and 12 Chebyshev points, now back again on a linear scale.

```
for npts = 4:4:12
  s = chebpts(npts); [L,Lconst] = lebesgue(s);
  hold off, plot(L), grid on, hold on, plot(s,L(s),'.')
  title(['Lebesgue function for ' int2str(npts) ' Chebyshev points'])
  snapnow, Lconst
end
```

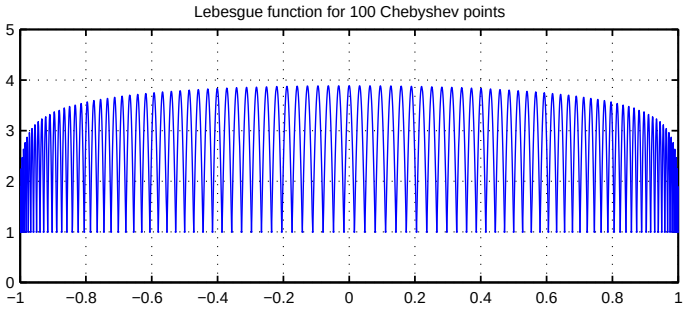
```
Lconst = 1.666666666666667
Lconst = 2.202214555205528
Lconst = 2.489430376881968
```



Here are 100 Chebyshev points, with a comparison of the actual Lebesgue constant with the bound from Theorem 15.2:


```
npts = 100;
s = chebpts(npts); [L,Lconst] = lebesgue(s);
clf, plot(L,LW,0.7), grid on, ylim([0 5])
Lconst
Lbound = 1 + (2/pi)*log(npts)
title('Lebesgue function for 100 Chebyshev points')
```

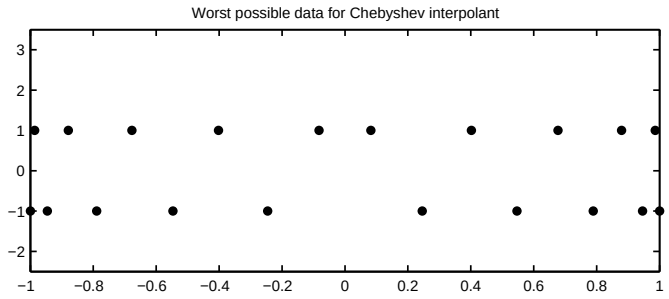
```
Lconst =
   3.887871431579913
Lbound =
   3.931742395517711
```



The low height of this curve shows how stable a process Chebyshev interpolation is.

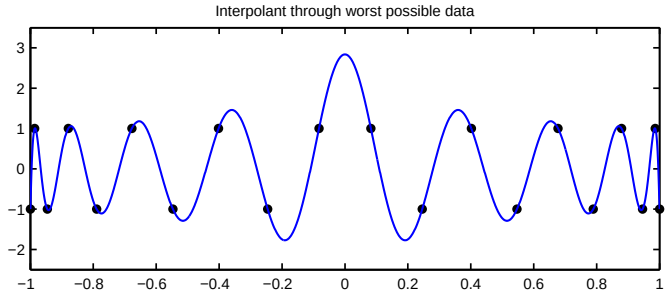
In Chapter 9 it was mentioned that combinations of Lagrange polynomials can explain both the Gibbs phenomenon and the size of Lebesgue functions. Let us now explain this remark. To analyze the Gibbs oscillations near a step, we added up a succession of Lagrange polynomials with constant amplitude 1. Since a single Lagrange polynomial has an oscillatory inverse-linear tail, the sum corresponds to an alternating series that converges as $n \to \infty$ to a constant. Lebesgue functions, on the other hand, are defined by taking a *maximum* at each point on the grid. The maximum is achieved by adding up Lagrange polynomials with equal but alternating coefficients, so as to make the combined signs all equal. For example, on the 20-point Chebyshev grid, the maximum possible value of an interpolant is achieved at $x = 0$ by taking data with this pattern:

```
s = chebpts(20);
d = (-1).^[1:10 10:19];
plot(s,d,'.k'), ylim([-2.5 3.5])
title('Worst possible data for Chebyshev interpolant')
```



Here is the Chebyshev interpolant:

```
p = chebfun(d);
hold on, plot(p)
title('Interpolant through worst possible data')
```



We readily confirm that the maximum of this interpolant is indeed the Lebesgue constant for this grid:

```
max(p)
[L,Lconst] = lebesgue(s);
Lconst
```

```
ans = 2.837131699740443
Lconst = 2.837131699740441
```

We can now summarize why Lebesgue constants for Chebyshev points, and indeed for any sets of interpolation points, must grow at least logarithmically with n. The fastest a Lagrange polynomial can decay is inverse-linearly, and the Lebesque function adds up those alternating tails with alternating coefficients, giving a harmonic series.

Our discussion in this chapter has focussed on Chebyshev interpolation rather than projection. However, as usual, there are parallel results for projection,

which historically were worked out earlier (for the Fourier case, not Chebyshev). We record here a theorem analogous to Theorem 15.2.

Theorem 15.3: Lebesgue constants for Chebyshev projection. *The Lebesgue constants Λ_n for degree $n \ge 1$ Chebyshev projection in $[-1,1]$ are given by*

$$\Lambda_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left| \frac{\sin((n+1/2)t)}{\sin(t/2)} \right| \, dt. \tag{15.10}$$

They satisfy

$$\Lambda_n \le 3 + \frac{4}{\pi^2} \log(n+1) \quad \text{and} \quad \Lambda_n \sim \frac{4}{\pi^2} \log n, \quad n \to \infty. \tag{15.11a,b}$$

Proof. See [Rivlin 1969]. Equation (15.11b) is due to Fejér in 1910 [Fejér 1910]. ∎

Related to Theorem 15.3 is another result concerning the norm of projection operators, proved by Landau [1913]. If f is analytic in the unit disk and continuous on the boundary, and $p \in P_n$ is the **Taylor projection** of f obtained by truncating its Taylor series, how much bigger can p be than f on the unit disk? Landau shown that these norms grow at the rate $(1/\pi)\log n$ as $n \to \infty$, a discovery which is perhaps the starting point of all results about logarithmic growth of norms of approximation operators.

For details about Lebesgue constants, the outstanding source is the survey article by Brutman [1997].

[To be added: (1) Original references on everything. Look up Tietze 1917 (cf. also Brutman survey), Fejér 1916, Faber 1914, Luttman & Rivlin 1965, Bernstein 1918, Cheney & Price 1970, Brutman, Powell, Smith. Get Bernstein reference right for 1914. (2) Pin down (15.7) with a suitable reference. (3) Make the discussion of worst possible data more leisurely. (4) Landau 1913 (Ex. 15.8) may have only done Taylor projection. (5) Mention Landau's constant? (6) Mention that Taylor projections are minimal? (Mason and Geddes 1975). (7) Is the logic around (15.6) backwards?]

SUMMARY OF CHAPTER 15. *The Lebesgue constant for interpolation or any other linear projection is the ∞-norm of the approximation operator. For interpolation in $n+1$ Chebyshev points the Lebesgue constant is bounded by $1 + 2\pi^{-1}\log(n+1)$, whereas for $n+1$ equispaced points it is asymptotic to $2^{n+1}/en\log(n)$.*

Exercise 15.1. Plots of Lebesgue functions. Plot the Lebesgue functions for the following distributions of interpolation points. (a) -0.9, -0.8, 0, 0.1, 0.2, 0.8. (b) Same as in (a) but with additional points at a distance 0.01 to the right of the others.

Exercise 15.2. Chebyshev points of the first kind. The Lebesgue constants for degree n Chebyshev interpolation are bounded by those for degree n interpolation in Chebyshev points of the first kind, mentioned in the last exercise, with equality when n is odd (Ehlich and Zeller [1966], McCabe and Phillips [1973]). Verify this numerically for $0 \le n \le 20$.

Exercise 15.3. Reproducing a table by Brutman. Page 698 of [Brutman 1978] gives a table of various quantities associated with the Lebesgue function for interpolation in Chebyshev points of the first kind. Track down this paper and write the shortest, most elegant Chebfun program you can to duplicate this table. Are all of Brutman's digits correct?

Exercise 15.4. Omitting the endpoints. Suppose one performs polynomial interpolation in the usual Chebyshev points (2.2), but omitting the endpoints $x = \pm 1$. Perform numerical experiments to determine what happens to the Lebesgue constants in this case. Does the growth appear to still be of order $\log n$, or n^α for some α, or what?

Exercise 15.5. Optimal interpolation points. Starting from the $n+1$ Chebyshev points, one could attempt to use one of Matlab's optimization codes to adjust the points to minimize the Lebesque constant. Do this and give the Lebesgue constant and plot the Lebesgue function for (a) $n = 4$, (b) $n = 5$, (c) $n = 6$, (d) $n = 7$, and (e) $n = 8$. How much improvement do you find in the Lebesgue constants as compared with Chebyshev points?

Exercise 15.6. Improving Turetskii's estimate. For interpolation in equispaced points, Schönhage [1961] derived a more accurate estimate than (15.9b): $\Lambda_n \sim 2^{n+1}/en(\log n + \gamma)$, where $\gamma = 0.577\ldots$ is again Euler's constant. Perform a numerical study of Λ_n as a function of n and see what difference this correction makes. For example it might be helpful to have a table showing the percentage errors in both estimates as functions of n.

Exercise 15.7. Interpolating data with a gap. (a) Consider polynomial interpolation in $n+1$ points of a function f defined on $[-1, 1]$, with half the points equally spaced from -1 to $-1/4$ and the other half equally spaced from $1/4$ to 1. Determine the Lebesgue constants for this interpolation process numerically for the cases $n + 1 = 20$ and 40. (b) Suppose f is analytic and bounded by 1 in the ρ-ellipse E_ρ with $\rho = 2$. Carefully quoting theorems from this book as appropriate, give upper bounds for the error $|f(0) - p(0)|$ for these two cases.

Exercise 15.8. Smallest local minimum of the Lebesgue function. Interpolation in equispaced points is much better near the middle of an interval than at the ends. In particular, the smallest local maximum of the Lebesgue function λ is $\sim \log n/\pi$ as $n \to \infty$ (Landau 1913). Make a plot of these minima as a function of n to verify this behavior numerically.

Exercise 15.9. Convergence for Weierstrass's function. Exercise 7.3 promised that in Chapter 15, we would show that Chebyshev interpolants to Weierstrass's nowhere-differentiable function of Exercise 6.1 converge as $n \to \infty$. Write down such a proof based on combining various theorems of this book.

Exercise 15.10. Random interpolation points. (a) Compute Lebesgue functions and constants numerically for degree n interpolation in uniformly distributed random points in $[-1, 1]$. How does Λ appear to grow with n? (b) Same question for points randomly distributed according to the Chebyshev density (11.18).

Exercise 15.11. Leja points. [to be written]

Exercise 15.12. Dini–Lipschitz continuity. [To be written. Show convergence in this case from Lebesgue constants together with the Weierstrass theorem (see Natanson book, 389–392). Early case may be Lebesgue, Sur les integrale singulieres, 1909.]

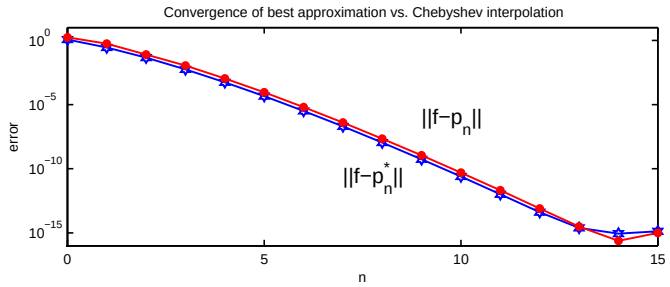
Exercise 15.13. A wiggly function. (a) Let f be the function $T_m(x) + T_{m+1}(x) + \cdots + T_n(x)$ with $m = 20$ and $n = 40$, and let p^* be the best approximation of f of degree $m - 1$. Plot f and $f - p^*$. What are their ∞-norms and 2-norms? (b) Same with $m = 200$ and $n = 300$.

16. Best and near-best

Traditionally, approximation theory has given a great deal of attention to best approximations and rather less to alternatives such as Chebyshev interpolants. One might think that this is because best approximations are much better than the alternatives. However, this is not true.

In a moment we shall continue with Lebesgue constants to shed some light on this matter, but first, let us do some experiments. We start with the extreme case of a very smooth function, $\exp(x)$, and compare convergence of its Chebyshev interpolants p and best approximants p^*. (The difference between n and $n + 1$ in this code is intentional, since `chebfun` takes as argument the number of interpolation points whereas `remez` takes the degree of the polynomial.)

```
f = exp(x); nn = 0:15;
errbest = []; errcheb = []; i = 0;
for n = nn
    i = i+1;
    [p,err] = remez(f,n);
    errbest(i) = err;
    errcheb(i) = norm(f-chebfun(f,n+1),inf);
end
hold off, semilogy(nn,errbest,'h-b',MS,6)
hold on, semilogy(nn,errcheb,'.-r')
text(7,3e-12,'||f-p_n^*||',FS,12)
text(9,2e-7,'||f-p_n||',FS,12)
ylim([1e-16 10])
xlabel n, ylabel error
title(['Convergence of best approximation '...
       'vs. Chebyshev interpolation'])
```



Clearly the stars for p^* aren't much better than the dots for p. The ratio of the two converges toward 2 until the rounding errors set in for larger degrees:

```
format short
ratio = errcheb./errbest;
disp('       n       ratio')
disp([nn' ratio'])
```

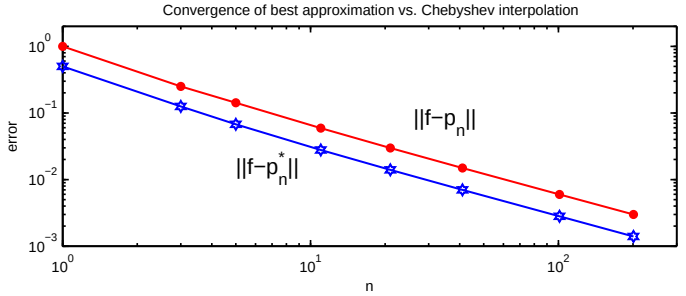
```
       n       ratio
         0    1.4621
    1.0000    2.0000
    2.0000    1.7444
    3.0000    1.9681
    4.0000    1.9499
    5.0000    1.9819
    6.0000    1.9818
    7.0000    1.9886
    8.0000    1.9910
    9.0000    1.9922
   10.0000    1.9947
   11.0000    1.9913
   12.0000    1.9629
   13.0000    1.2731
   14.0000    0.2723
   15.0000    0.7545
```

At the other extreme of smoothness, consider $|x|$:

```
f = abs(x); nn = [0 2 4 10 20 40 100 200];
errbest = []; errcheb = []; i = 0;
for n = nn
    i = i+1;
    [p,err] = remez(f,n);
    errbest(i) = err;
    errcheb(i) = norm(f-chebfun(f,n+1),inf);
end
```



```
hold off, loglog(nn+1,errbest,'h-b',MS,6)
hold on, loglog(nn+1,errcheb,'.-r')
axis([1 300 .001 2])
text(5,.01,'||f-p_n^*||',FS,12)
text(26,.06,'||f-p_n||',FS,12)
xlabel n, ylabel error
title(['Convergence of best approximation '...
       'vs. Chebyshev interpolation'])
```



Again the stars are only a little bit better than the dots, by a constant factor of about 2.13060:

```
ratio = errcheb./errbest;
disp('       n       ratio')
disp([nn' ratio'])
```

```
       n       ratio
         0    2.0000
    2.0000    2.0000
    4.0000    2.1023
   10.0000    2.1268
   20.0000    2.1297
   40.0000    2.1304
  100.0000    2.1306
  200.0000    2.1306
```

(For odd values of n the ratio is somewhat larger, approaching a constant of about 3.57.)

So for these examples at least, you don't buy much with best approximations. And the cost in computing time is tremendous. Here is the time for computing a Chebyshev interpolant p of degree 200 and evaluating it at 100 points:

```
xx = rand(100,1);
tic, p = chebfun(f,201); p(xx); toc
```

```
Elapsed time is 0.012117 seconds.
```

Here is the time for finding the best approximation p^* and evaluating it at the same points:

```
tic, p = remez(f,200); p(xx); toc
```

```
Elapsed time is 0.863739 seconds.
```

The reason computing p^* is more expensive is that the mapping from f to p^* is nonlinear, hence requiring iteration in a numerical implementation, whereas the mapping from f to p is linear (Exercise 10.5). It is perfectly feasible to compute p for degrees in the millions, whereas for p^* we would rarely attempt degrees higher than hundreds.

Why has p^* received so much more attention than p over the years? One reason is that in the days before fast computers, the degrees were low, so small differences in accuracy were more important. Another is that the theory of best approximations is so beautiful! Indeed, their very nonlinearity makes best approximations seemingly a richer field for research than the simpler Chebyshev interpolants. Everybody remembers Theorem 10.1, the equioscillation theorem, from the moment they first hear it. Perhaps there is a lesson here.

Yet in actual computation, true best approximations are not so often used, as we have mentioned earlier (Chapter 10). This is a clue that the world of practice has its own wisdom, independent of the theorists.

Now let us see what theoretical results might tell us about the difference between p and p^*. The first such results pertain to Theorems 7.2 and 8.2 given earlier. Those theorems concerned convergence rates of p_n to f, depending on the smoothness of f. What about analogous theorems for p_n^*? Apart from constant factors, they turn out to be the same! For example, exactly the same bound (8.3) was published by de la Vallée Poussin [1919, pp. 123–124], except with the Chebyshev interpolant p_n replaced by the best approximation p_n^*. So within the two classes of functions considered in Chapters 7 and 8 — f having a kth derivative of bounded variation, or f being analytic — there is no clear reason to expect p_n^* to be much better than p_n.

An observation for arbitrary functions f is the following consequence of Theorems 15.1–15.3:

Theorem 16.1: Chebyshev truncations and interpolants are near-best. *Let f be continuous on $[-1,1]$ with degree n Chebyshev truncation f_n, Chebyshev interpolant p_n and best approximant p_n^*, $n \geq 1$. Then*

$$\|f - f_n\| \leq \left(4 + \frac{4}{\pi^2}\log(n+1)\right)\|f - p^*\| \tag{16.1}$$

and

$$\|f - p_n\| \leq \left(2 + \frac{2}{\pi}\log(n+1)\right)\|f - p^*\|. \tag{16.2}$$

Proof. Follows from Theorems 15.1, 15.2, and 15.3. ∎

So the loss of accuracy in going from p_n^* to p_n, say, can never be larger than a factor of $2 + (2/\pi)\log(n+1)$. It is interesting to examine the size of this quantity for various values of n. For $n = 10^5$, for example:

```
2 + (2/pi)*log(100001)
```

```
ans = 9.3294
```

Since this number is less than 10, we see that in dealing with polynomials of degree up to $n = 100000$, the non-optimality of Chebyshev interpolation can never cost us more than one digit of accuracy. Here is the computation for $n = 10^{66}$:

```
2 + (2/pi)*log(1e66)
```

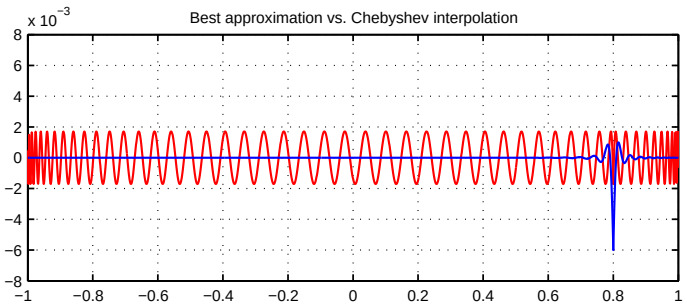
```
ans = 98.7475
```

So we never lose more than 2 digits for degrees all the way up to 10^{66} — which might as well be ∞ for practical purposes. One can give a talk on these matters with the title "10^{66} and All That".

In fact, one might question whether best approximations are really better than near-best ones at all! Of course they are better in a literal sense, as measured in the ∞-norm. However, consider the following error curves, which are quite typical for a function that is smoother in some regions than others.

```
f = abs(x-0.8);
tic, pbest = remez(f,100); toc
hold off, plot(f-pbest,'r')
tic, pcheb = chebfun(f,101); toc
hold on, plot(f-pcheb)
axis([-1 1 -.008 .008]), grid on
title('Best approximation vs. Chebyshev interpolation')
```

```
Elapsed time is 0.288806 seconds.
Elapsed time is 0.002654 seconds.
```



We see that `pbest` is worse than `pcheb` for almost all values of x, because the damage done by the singularity at $x = 0.8$ is global. By contrast, the effect of the singularity on `pcheb` decays with distance. Of course, `pbest` is better in the ∞-norm:

```
errcheb = norm(f-pcheb,inf)
errbest = norm(f-pbest,inf)
```

```
errcheb =
    0.0060
errbest =
    0.0017
```

In the 2-norm, however, it is a good deal worse:

```
errcheb2 = norm(f-pcheb,2)
errbest2 = norm(f-pbest,2)
```

```
errcheb2 =
   4.3337e-04
errbest2 =
    0.0017
```

One may seriously question how many applications there might be in which `pbest` was truly better than `pcheb` as an approximation to this function f. To echo a title of Corless and Watt [2004], minimax approximations are optimal, but Chebyshev interpolants are better!

Li [2004] takes another angle on the near-optimality of Chebyshev interpolants, pointing out that for applications to elementary functions, bounds on certain derivatives usually apply that ensure that the error in interpolation in Chebyshev points of the first kind typically exceeds that of the best approximation by less than a factor of 2, or as he calls it, "a fractional bit."

Finally, we mention another kind of optimality that has received attention in the approximation literature since Bernstein [Erdős 1961, de Boor & Pinkus 1978,

Kilgore 1978]: **optimal interpolation points** (Exercise 15.5). Chebyshev points are very good, but they do not quite minimize the Lebesgue constant. Optimal points minimize the Lebesgue constant (by definition), and they even out the peaks of the Lebesgue function exactly (it has been proved) — but the improvement is negligible. The first statement of Theorem 15.2 establishes that like Chebyshev points, they lead to Lebesgue constants that are asymptotic to $(2/\pi)\log n$ as $n \to \infty$, which means they don't even improve upon Chebyshev points by a constant factor.

To be added: (1) References on limiting ratios 2, 2.13060, and 3.57? (2) Proper discussion with references of the theorems analogous to Thms 7.2 and 8.2 alluded to above Theorem 16.1. (3) Original refs on optimal interpolation points. (4) For Cheb interp as near-best, see Fraser JACM 12 (1965), 310-313; Gavrilyuk & Maz USSR Comp Math & Math Phys 6 (1966), 209–222; pp 72-74 of Meinardus 1967 book. (5) Check whether REMEZ is giving warning messages.]

SUMMARY OF CHAPTER 16. *The ∞-norm error in degree n Chebyshev interpolation is never greater than $2 + 2\pi^{-1}\log(n+1)$ times the ∞-norm error in degree n best approximation, and in practice, the ratio of errors rarely exceeds even a factor of 2. In the 2-norm, the interpolant is often better than the "best" approximation.*

Exercise 16.1. Speed of interpolation vs. Remez. (a) Repeat the experiment of this chapter involving $|x - 0.8|$ but for all the values $n = 100, 200, 300, \ldots, 1000$. In each case measure the computing times for Chebyshev interpolation and best approximation, the L^2 errors of both approximants, and the L^∞ errors. Plot these results and comment on what you find. (b) In particular, produce a plot of error curves like that in the text. You may find it helpful to use a flag like `'numpts',10000` in your Chebfun plotting command.

Exercise 16.2. Approximation of a wiggly function. Define $f(x) = T_{200}(x) + T_{201}(x) + \cdots + T_{220}(x)$. Construct the Chebyshev interpolant p and best approximation p^* of degree 199. Plot the errors and measure the ∞- and 2-norms.

Exercise 16.3. Rounding errors on a grid of 10^{66} points.

17. Legendre and other orthogonal polynomials

This book gives special attention to Chebyshev polynomials, since they are so useful in applications. However, Chebyshev polynomials are just one example of a family of orthogonal polynomials defined on the interval $[-1, 1]$, and in this chapter we note some of the other possibilities, especially Legendre polynomials, which are the starting point for Gauss quadrature (Chapter 19). The study of orthogonal polynomials was initiated by Jacobi [1826] and already well

developed by the end of the 19th century thanks to work by mathematicians including Christoffel [1858], Darboux [1878], and Stieltjes [1884].

Let $w \in C(-1,1)$ be a **weight function** with $w(x) > 0$ for all $x \in (-1,1)$ and $\int_{-1}^{1} w(x)\, dx = 1$; we allow $w(x)$ to approach 0 or ∞ as $x \to \pm 1$. The function w defines an **inner product** for functions defined on $[-1,1]$:

$$(f,g) = \int_{-1}^{1} w(x)\overline{f(x)}g(x)dx. \tag{17.1}$$

(More precisely one can regard the inner product as applying in the Hilbert space $L^2[-1,1]$.) The family of **orthogonal polynomials** associated with w is the family

$$p_0, p_1, p_2, \dots$$

where $p_0 = 1$, p_n has degree exactly n for each n, and the polynomials satisfy the **orthogonality condition**

$$(p_j, p_k) = \delta_{jk} = \begin{cases} 1 & k = j, \\ 0 & k \neq j. \end{cases} \tag{17.2}$$

As we have seen in Chapter 3, Chebyshev polynomials come from the choice

$$w(x) = \frac{2}{\pi\sqrt{1-x^2}}. \tag{17.3}$$

The first three Chebyshev polynomials are

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_2(x) = 2x^2 - 1,$$

as we can confirm with the `chebpoly` command:

```
for j = 0:5
  disp(fliplr(poly(chebpoly(j))))
end
```

```
     1
     0     1
    -1     0     2
     0    -3     0     4
     1     0    -8     0     8
     0     5     0   -20     0    16
```

Legendre polynomials come from the simplest weight function of all, a constant function:

$$w(x) = 1.$$

If we normalize according to (17.1), the first three Legendre polynomials are

$$p_0(x) = \sqrt{1/2}, \quad p_1(x) = \sqrt{3/2}x, \quad p_2(x) = \sqrt{45/8}x^2 - \sqrt{5/8},$$

as can confirm with the `legpoly` command:


```
format short
for j = 0:5
  disp(fliplr(poly(legpoly(j,'norm'))))
end
```

```
    0.7071
         0    1.2247
   -0.7906         0    2.3717
         0   -2.8062         0    4.6771
    0.7955         0   -7.9550         0    9.2808
         0    4.3973         0  -20.5206         0   18.4685
```

However, it is more common to normalize Legendre polynomials by the condition $p_j(1) = 1$, in which case the first three are

$$p_0(x) = 1, \quad p_1(x) = x, \quad p_2(x) = \frac{3}{2}x^2 - \frac{1}{2}:$$

```
for j = 0:5
  disp(fliplr(poly(legpoly(j))))
end
```

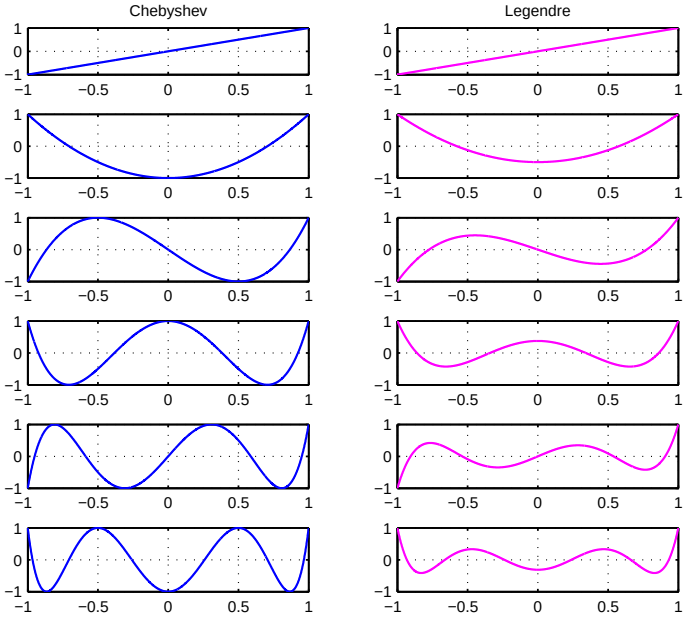
```
    1
    0     1
 -0.5000         0    1.5000
         0   -1.5000         0    2.5000
    0.3750         0   -3.7500         0    4.3750
         0    1.8750         0   -8.7500         0    7.8750
```

Given w, the family $\{p_j\}$ always exists and is unique.

The rest of this chapter is devoted to comparing Legendre and Chebyshev polynomials. The comparison, and the consideration of orthogonal polynomials in general, will continue into the next two chapters on roots (Chapter 18) and quadrature (Chapter 19). For example, Theorem 19.6 presents a fast method for calculating the barycentric weights for **Legendre points**, the zeros of Legendre polynomials. On the whole, different families of orthogonal polynomials have similar approximation properties, but Chebyshev points have the particular advantage that one can convert back and forth between interpolant and expansion by the FFT.

We begin with a visual comparison of the Chebyshev and Legendre polynomials of degrees 1–6. To avoid confusion with our notation P_n for the set of polynomials of degree at most n, we denote Legendre polynomials in this book by L rather than the standard letter P.

```
ax = [-1 1 -1 1]; T = []; L = [];
for n = 1:6
    T{n} = chebpoly(n);
    subplot(3,2,1), plot(T{n}), axis(ax), grid on
    if n==1, title Chebyshev, end
    L{n} = legpoly(n);
    subplot(3,2,2), plot(L{n},'m'), axis(ax), grid on
    if n==1, title Legendre, end
    snapnow
end
```



For Legendre polynomials normalized by $L_j(1) = 1$, the orthgonality condition turns out to be

$$\int_{-1}^{1} L_j(x)\, L_k(x)\, dx = \begin{cases} 0 & j \neq k, \\ \dfrac{2}{2k+1} & j = k. \end{cases} \tag{17.4}$$

We can verify this formula numerically by constructing what Chebfun calls a **quasimatrix** X, that is, a "matrix" whose columns are chebfuns, and then taking inner products via the quasimatrix product $X^T X$. One way to construct X is like this:

```
X = [L{1} L{2} L{3} L{4} L{5} L{6}];
```


Another equivalent method is built in to `legpoly`:

```
X = legpoly(1:6);
```

Here is the quasimatrix product.

```
X'*X
```

```
ans =
    0.6667         0   -0.0000         0    0.0000         0
         0    0.4000         0    0.0000         0   -0.0000
   -0.0000         0    0.2857         0    0.0000    0.0000
         0    0.0000         0    0.2222    0.0000    0.0000
    0.0000         0    0.0000    0.0000    0.1818   -0.0000
         0   -0.0000    0.0000    0.0000   -0.0000    0.1538
```

This matrix of inner products looks diagonal, as it should, and we can confirm the diagonal structure by checking the norm of the off-diagonal terms:

```
norm(ans-diag(diag(ans)))
```

```
ans = 1.6454e-16
```

The entries on the diagonal are the expected numbers $2/3, 2/5, 2/7, \ldots$.

Legendre polynomials satisfy the 3-term recurrence relation

$$(k+1)L_{k+1}(x) = (2k+1)xL_k(x) - kL_{k-1}(x). \tag{17.5}$$

This may be compared with the recurrence relation (3.3) for Chebyshev polynomials.

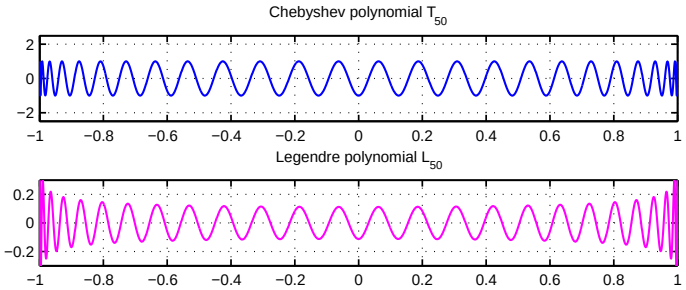
Chebyshev polynomials are not orthogonal in the standard inner product:

```
X = chebpoly(1:6);
X'*X
```

```
ans =
    0.6667         0   -0.4000         0   -0.0952         0
         0    0.9333         0   -0.3619         0   -0.0825
   -0.4000         0    0.9714         0   -0.3492         0
         0   -0.3619         0    0.9841   -0.0000   -0.3434
   -0.0952         0   -0.3492   -0.0000    0.9899   -0.0000
         0   -0.0825         0   -0.3434   -0.0000    0.9930
```

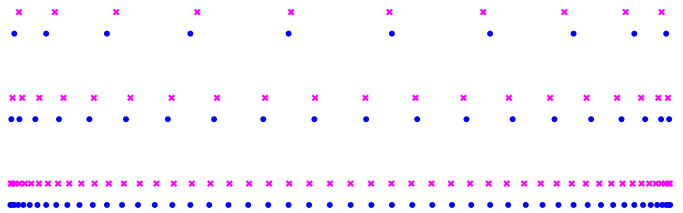
Nevertheless, Legendre and Chebyshev polynomials have much in common, as is further suggested by plots of T_{50} and L_{50}:

```
T50 = chebpoly(50); L50 = legpoly(50);
subplot(2,1,1), plot(T50), axis([-1 1 -2.5 2.5])
grid on, title('Chebyshev polynomial T_{50}')
subplot(2,1,2), plot(L50,'m'), axis([-1 1 -.3 .3])
grid on, title ('Legendre polynomial L_{50}')
```



The zeros of the two families of polynomials are similar, as can be confirmed by comparing Chebyshev (dots) and Legendre (crosses) zeros for degrees 10, 20, and 50. (Instead of using the `roots` command here, one could achieve the same effect with `chebpts(n,1)` and `legpts(n)` — see the next chapter.)

```
T10 = chebpoly(10); L10 = legpoly(10);
Tr = roots(T10); Lr = roots(L10);
clf, plot(Tr,.8,'.b',MS,9), hold on
plot(Lr,0.9,'xm',MS,4)
T20 = chebpoly(20); L20 = legpoly(20);
Tr = roots(T20); Lr = roots(L20);
plot(Tr,0.4,'.b',MS,9), plot(Lr,0.5,'xm',MS,4)
Tr = roots(T50); Lr = roots(L50);
plot(Tr,0,'.b',MS,9), plot(Lr,0.1,'xm',MS,4)
axis([-1 1 -.1 1.1]), axis off
```



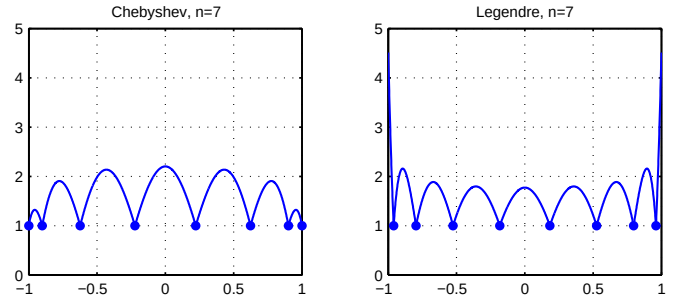
Asymptotically as $n \to \infty$, both sets of zeros cluster near ± 1 with the same density distribution $n\mu(x)$, with μ given by (11.18).

Another comparison between Chebyshev and Legendre points concerns their Lebesgue functions and Lebesgue constants. Here we repeat a computation

of Lebesgue functions from Chapter 15 for 8 Chebyshev points and compare it with the analogous computation for 8 Legendre points. Chebyshev and Legendre points as we have defined them so far differ not just in which polynomials they are connected with, but in that Chebyshev points come from extrema whereas Legendre points come from zeros.

```
hold off
s = chebpts(8); [L,Lconst] = lebesgue(s);
subplot(1,2,1), plot(L), grid on, hold on, plot(s,L(s),'.'), Lconst
ylim([0,5]), title('Chebyshev, n=7')
s = legpts(8); [L,Lconst] = lebesgue(s);
subplot(1,2,2), plot(L), grid on, hold on, plot(s,L(s),'.'), Lconst
ylim([0,5]), title('Legendre, n=7')
```

```
Lconst =
    2.2022
Lconst =
    4.5135
```

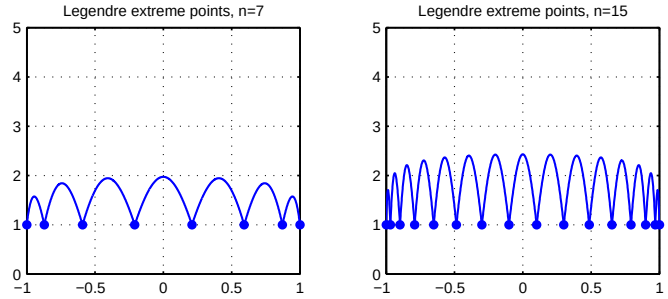


The Lebesgue functions and constants for Legendre points are a little bigger than for Chebyshev points, having size $O(n^{1/2})$ rather than $O(\log n)$ because of behavior near the endpoints [Szegő 1939, p. 338]. This small difference is of little significance for most applications: the Lebesgue constants are still quite small and either set of points will usually deliver excellent interpolants.

Moreover, an alternative is to consider **Legendre extreme points** — the $n+1$ points in $[-1,1]$ at which $|L_n(x)|$ attains a local maximum. (The Legendre extreme points in $(-1,1)$ are also the roots of the Jacobi polynomial $J^{(1,1)}(x)$.) The Lebesgue function in this case looks very satisfactory:

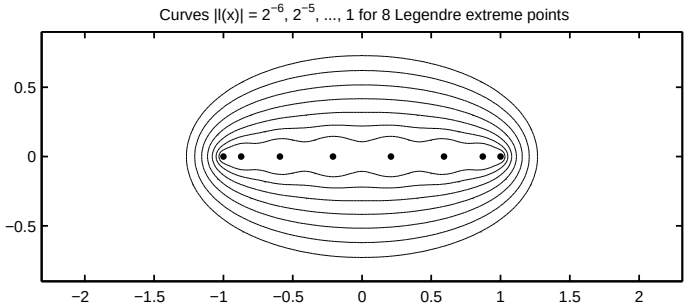
```
clf
s = [-1; roots(diff(legpoly(7))); 1]; [L,Lconst] = lebesgue(s);
subplot(1,2,1), plot(L), grid on, hold on, plot(s,L(s),'.'), Lconst
ylim([0,5]), title('Legendre extreme points, n=7')
s15 = [-1; roots(diff(legpoly(15))); 1]; [L,Lconst] = lebesgue(s15);
subplot(1,2,2), plot(L), grid on, hold on, plot(s15,L(s15),'.'), Lconst
ylim([0,5]), title('Legendre extreme points, n=15')
```

```
Lconst =
    1.9724
Lconst =
    2.4303
```



The Legendre extreme points have a memorable property: as shown by Stieltjes [1885], they are the Fekete or minimal-energy points in $[-1,1]$, solving the equipotential problem on that interval for a finite number of equal charges (Exercise 12.1). Here, for example, is a repetition of a figure from Chapter 11 but now for 8 Legendre extreme points instead of 8 Chebyshev points. Again the behavior is excellent.

```
ell = poly(s,domain(-1,1));
clf, plot(s,ell(s),'.k',MS,10)
hold on, ylim([-0.9,0.9]), axis equal
xgrid = -1.5:.02:1.5; ygrid = -0.9:.02:0.9;
[xx,yy] = meshgrid(xgrid,ygrid); zz = xx+1i*yy;
ellzz = ell(zz); levels = 2.^(-6:0);
contour(xx,yy,abs(ellzz),levels,'k')
title(['Curves |l(x)| = 2^{-6}, 2^{-5}, ..., 1 '...
    'for 8 Legendre extreme points'])
```



[To be added: (1) Computation of Legendre series: see Piessens 1974, Alpert & Rokhlin 1991, Iserles 2010. (2) Davis p. 313: bounds on Legendre coefficients.

(3) Talk about more general orthogonal polynomials and their 3-term recurrence relations. (4) Discuss Szego's explanation on p. 297 of the similarity between L50 and T50 — the envelope is known. (Make this an exercise?) (5) Clarify μ vs. μ_n vs. $n\mu$ vs. $n\mu_n$ in discussion of the measure. (6) Check normalization of weight function w. For example, $w = 1$ doesn't integrate to 1; the Chebyshev weight seems wrong for T_0.]

SUMMARY OF CHAPTER 17. *Chebyshev polynomials are just one example of a family of polynomials orthogonal with respect to a weight function on* $[-1,1]$. *If the weight function is a constant, one gets the Legendre polynomials.*

Exercise 17.1. Chebyshev and Legendre Lebesgue constants. Extend the experiments of the text to a table and a plot of Lebesgue constants of Chebyshev, Legendre, and Legendre extreme points for interpolation in $n+1$ points with $n = 1, 2, 4, \ldots, 256$. (To compute Legendre extreme points you can use the trick mentioned in Exercise 12.4.) What asymptotic behavior do you observe as $n \to \infty$? [The wording of this exercise needs to be made more precise.]

Exercise 17.2. Chebyshev and Legendre interpolation points. [Not yet written. Interpolate a particular function in Chebyshev and in Legendre points for various n and show it doesn't make much difference.]

Exercise 17.3. Orthogonal polynomials via QR decomposition. (a) Construct a Chebfun quasimatrix `A` with columns corresponding to $1, x, \ldots, x^5$ on $[-1,1]$. Execute `[Q,R] = qr(A)` to find an equivalent set of orthonormal functions, the columns of `Q`, and plot these with `plot(Q)`. How do the columns of `Q` compare with the Legendre polynomials normalized by (17.2)? (b) Write a **for** loop to normalize the columns of `Q` in a fashion corresponding to $L_j(1) = 1$ and to adjust R correspondingly so that the product `Q*R` continues to be equal to `A`, up to rounding errors, and plot the new quasimatrix with `plot(Q)`. How do the columns of the new `Q` compare with the Legendre polynomials normalized by $L_j(1) = 1$?

Exercise 17.4. Orthogonal polynomials via Gram–Schmidt. [Not yet written. Construct orthog. polys. via Gram–Schmidt and/or Householder. Unweighted, Chebyshev weight, e^{-10x^2} weight.]

Exercise 17.5. Three-term recurrence relation. [Derivation of (17.5).]

Exercise 17.6. Jacobi polynomials. [To be written.]

Exercise 17.7. Gegenbauer polynomials. [To be written.]

18. Polynomial roots and colleague matrices

It is well known that if p is a polynomial expressed as a linear combination of monomials x^k, then the roots of p are equal to the eigenvalues of a certain **companion matrix** formed from its coefficients (Exercise 18.8). Indeed, from

its beginning in the late 1970s Matlab has included a command `roots` that finds roots of polynomials by using this identity. This method of zerofinding is effective and numerically stable, but only in a very narrow sense. It is a numerically stable algorithm for precisely the problem just posed: given the monomial coefficients, find the roots [Goedecker 1994, Toh & Trefethen 1994]. The trouble is, this problem is an awful one! As Wilkinson made famous beginning in the 1960s, it is exponentially ill-conditioned in general [Wilkinson 1984]. The roots tend to be so sensitive to perturbations that even though the algorithm is stable in the sense that it produces roots that are exactly correct for a polynomial whose coefficients match the specified ones to a relative error on the order of machine precision, this slight perturbation is enough to cause terrible inaccuracy.

There is an exception to this dire state of affairs. Finding roots from polynomial coefficients is a well-conditioned problem in the special case of polynomials with roots on or near the unit circle [Sitton, Burrus, Fox & Treitel 2003]. The trouble is, most applications are not of this kind. Much more often, the roots of interest lie in or near a real interval, and in such cases one should avoid monomials, companion matrices, and Matlab's `roots` command completely.

Fortunately, there is a well-conditioned alternative for such problems, and that is the subject of this chapter. By now we are experts in approximating functions on $[-1,1]$ by Chebyshev interpolants and Chebyshev series. Within this class of tools, there is a natural way of computing the roots of a polynomial by solving an eigenvalue problem. Here is the crucial result, due independently to Wilhelm Specht [1960, p. 222] and Jack Good [1961].

Theorem 18.1: Polynomial roots and colleague matrix eigenvalues. *The roots of the polynomial*

$$p(x) = \sum_{k=0}^{n} a_k T_k(x), \quad a_n \neq 0$$

are the eigenvalues of the matrix

$$C = \begin{pmatrix} 0 & 1 & & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & & \\ & \frac{1}{2} & 0 & \frac{1}{2} & & \\ & & \ddots & \ddots & \ddots & \\ & & & & & \frac{1}{2} \\ & & & & \frac{1}{2} & 0 \end{pmatrix} - \frac{1}{2a_n} \begin{pmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ a_0 & a_1 & a_2 & \dots & a_{n-1} \end{pmatrix}.$$

(Entries not displayed are zero.) If there are multiple roots, these correspond to multiple eigenvalues with corresponding multiplicities.

Proof. Let x be any number, and consider the nonzero n-vector

$$v = (T_0(x), T_1(x), \dots, T_{n-1}(x))^T.$$

If we multiply C by v, then in every row but the first and last the result is

$$T_k(x) \mapsto \tfrac{1}{2}T_{k-1}(x) + \tfrac{1}{2}T_{k+1}(x) = xT_k(x),$$

thanks to the three-term recurrence relation (3.3) for Chebyshev polynomials, $T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x)$. In the first row we likewise have

$$T_0(x) \mapsto T_1(x) = xT_0(x)$$

since $T_0(x) = 1$ and $T_1(x) = x$. It remains to examine the bottom row. Here it is convenient to imagine that in the difference of matrices defining C above, the "missing" entry $1/2$ is added in the $(n, n+1)$ position of the first matrix and subtracted again from the $(n, n+1)$ position of the second matrix. Then by considering the recurrence relation again we find

$$T_{n-1}(x) \mapsto xT_{n-1}(x) - \frac{1}{2a_n}(a_0T_0(x) + a_1T_1(x) + \cdots + a_nT_n(x)).$$

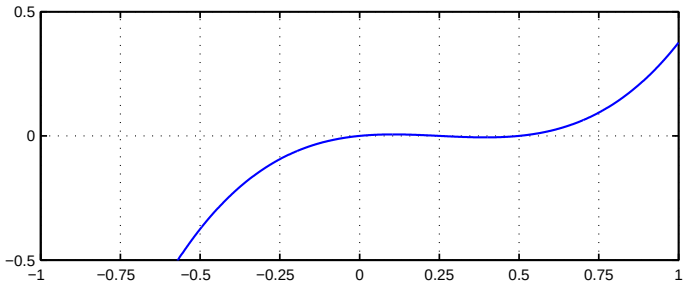
This equation holds for any x, but if x is a root of p, then the term in parentheses on the right vanishes. In other words, if x is a root of p, then Cv is equal to xv in every entry, making v is an eigenvector of C with eigenvalue x. If p has n distinct roots, this implies that they are precisely the eigenvalues of C, and this completes the proof in the case where p has distinct roots.

If p has multiple roots, we must show that each one corresponds to an eigenvalue of C with the same multiplicity. For this we consider perturbations of the coefficients $a_0, \dots, a_{n-1}$ of p with the property that the roots become distinct. Each root must then correspond to an eigenvalue of the correspondingly perturbed matrix C, and since both roots of polynomials and eigenvalues of matrices are continuous functions of the parameters, the multiplicities must be preserved in the limit as the amplitude of the perturbations goes to zero. ∎

The matrix C is called a **colleague matrix**. Theorem 18.1 has been rediscovered several times in the past half-century, for example by Day & Romero [2005]. Since Specht [1957] there have also been generalizations to other families of orthogonal polynomials besides Chebyshev polynomials, and the associated generalized colleague matrices are called **comrade matrices** [Barnett 1975a & 1975b]. The generalization is immediate: one need only change the entries of rows 1 to n to correspond to the appropriate recurrence relation.

For an example to illustrate Theorem 18.1, the polynomial

```
p = x.*(x-1/4).*(x-1/2);
clf, plot(p)
axis([-1 1 -.5 .5]), grid on
set(gca,'xtick',-1:.25:1)
```



obviously has roots 0, 1/4, and 1/2. The Chebyshev coefficients of p are $-3/8, 7/8, -3/8, 1/4$:

```
format short
a = fliplr(chebpoly(p))
```

```
a =
   -0.3750    0.8750   -0.3750    0.2500
```

As expected, the colleague matrix

```
C = [0 1 0; 1/2 0 1/2; 0 1/2 0] - ...
    (1/(2*a(4)))*[0 0 0; 0 0 0; a(1:3)]
```

```
C =
         0    1.0000         0
    0.5000         0    0.5000
    0.7500   -1.2500    0.7500
```

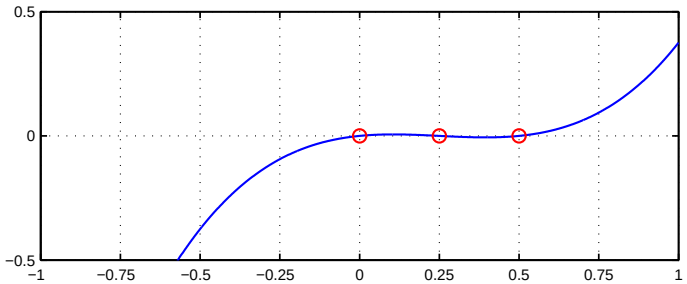
has eigenvalues that match the roots of p:

```
format long
eig(C)
```

```
ans =
                   0
   0.500000000000002
   0.249999999999999
```

In Chebfun, every function is represented by a polynomial (or a piecewise polynomial). Thus Theorem 18.1 provides Chebfun with its method of numerical rootfinding, implemented in the Chebfun `roots` command. For this polynomial `p`, we can call `roots` to add the roots to the plot, like this:

```
r = roots(p);
hold on, plot(r,p(r),'or',MS,7)
```

In this example, `p` was a polynomial from the start. The real power of Theorem 18.1, however, comes when it is applied to the problem of finding the roots on $[-1,1]$ of a general function f. To do this, we first approximate f by a polynomial, then find the roots of the polynomial. This powerful idea is proposed in Good's original 1961 paper [Good 1961]. In a more numerical era, it has been advocated in a number of papers by John Boyd, including [Boyd 2002], and it is applied virtually every time Chebfun is used.

For example, here is the chebfun corresponding to $\cos(50\pi x)$ on $[-1,1]$:

```
f = cos(50*pi*x); length(f)
```

```
ans = 253
```

It doesn't take long to compute its roots,

```
tic, r = roots(f); toc
```

```
Elapsed time is 0.039600 seconds.
```

Inspecting a few of the computed results shows they are accurate to close to machine precision:

```
r([1 2 51 99 100])
```

```
ans =
  -0.990000000000000
  -0.970000000000000
   0.010000000000000
   0.970000000000000
   0.990000000000000
```

Changing the function to $\cos(500\pi x)$ makes the chebfun ten times longer,

```
f = cos(500*pi*x); length(f)
```

```
ans = 2045
```

One might think this would increase the rootfinding time enormously, since the number of operations for an eigenvalue computation grows with the cube of the matrix dimension. (The colleague matrix has special structure that can be used to bring the operation count down to $O(n^2)$, but this is not done in a straightforward Matlab call to `eigs`.) However, an experiment shows that the timing is still quite good,

```
tic, r = roots(f); toc
```

```
Elapsed time is 0.600108 seconds.
```

and the accuracy is still outstanding

```
r([1 2 501 999 1000])
```

```
ans =
  -0.999000000000000
  -0.997000000000000
   0.001000000000000
   0.997000000000000
   0.999000000000000
```

The explanation of this great speed in finding the roots of a polynomial of degree in the thousands is that the complexity of the algorithm has been improved to $O(n^2)$ by recursion. If a chebfun has length greater than 100, the interval is divided recursively into subintervals, with a chebfun constructed on each subinterval of appropriately lower degree. Thus no eigenvalue problem is ever solved of dimension larger than about 100. This idea of rootfinding based on recursive subdivision of intervals and Chebyshev eigenvalue problems was developed by John Boyd in the 1980s and 1990s and published by him in 2002 [Boyd 2002]. Details of the original Chebfun implementation of `roots` were presented in [Battles 2006], and the algorithm was later speeded up substantially by Pedro Gonnet.

These techniques are remarkably powerful for practical computations. For example, how many zeros does the Bessel function J_0 have in the interval $[0, 5000]$? Chebfun finds the answer in less than a second:

```
tic, f = chebfun(@(x) besselj(0,x),[0,5000]);
r = roots(f); toc
length(r)
```

```
Elapsed time is 1.305023 seconds.
ans = 1591
```

What is the the 1000th zero?

```
r(1000)
```



```
ans = 3.140807295225079e+03
```

We readily verify that zero is an accurate one:

```
besselj(0,ans)
```

```
ans = 5.761964670423015e-17
```

This example is almost the first occasion in this book in which we have used chebfuns on an interval other than $[-1, 1]$. The mathematics is the same; $[0, 5000]$ is reduced to $[-1, 1]$ by a linear transformation.

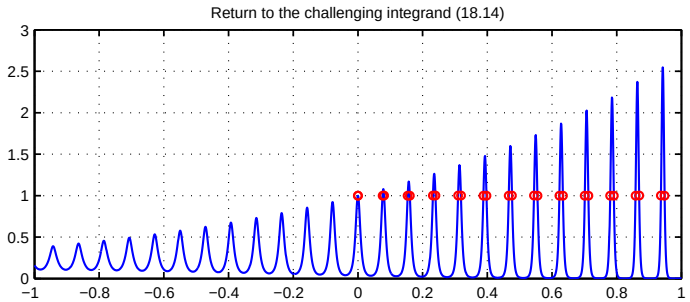
Here is another illustration of recursive colleague matrix rootfinding for a high-order polynomial. The function

$$f(x) = e^x[\mathrm{sech}(4\sin(40x))]^{\exp(x)} \tag{18.1}$$

exhibits a sequence of narrower and narrower spikes. Where in $[-1, 1]$ does it take the value 1? We can find the answer by using `roots` to find the zeros of the equation $f(x) - 1 = 0$:

```
ff = @(x) exp(x).*sech(4*sin(40*x)).^exp(x);
tic, f = ff(x); r = roots(f-1); toc
clf, plot(f), grid on
title('Return to the challenging integrand (18.14)')
hold on, plot(r,f(r),'or',MS,4)
```

```
Elapsed time is 1.561658 seconds.
```



Notice that we have found the roots here of a polynomial of quite high degree:

```
length(f)
```

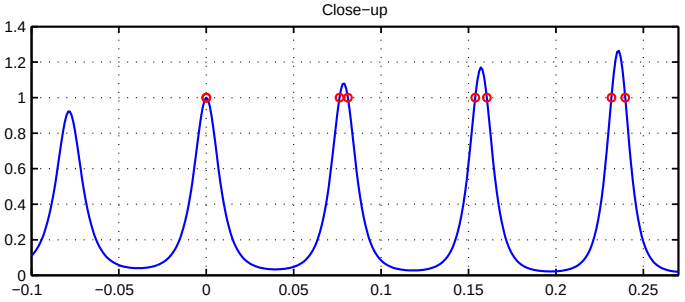
```
ans = 3521
```

A numerical check confirms that the roots are accurate,

```
max(abs(ff(r)-1))
```
```
ans = 8.315570454442422e-14
```

and zooming in gives perhaps a more convincing plot:

```
xlim([-.1 .27])
title('Close-up')
```



Computations like this are examples of *global rootfinding*, a special case of *global optimization*. They are made possible by the combination of fast methods of polynomial approximation with the extraordinarily fast and accurate methods for matrix eigenvalue problems that have been developed in the years since Francis invented the QR algorithm in the very same year as Good proposed his colleague matrices [Francis 1961].

Global rootfinding is a step in many other practical computations. It is used by Chebfun, for example, in computing minima, maxima, 1-norms, and absolute values.

It may be worth mentioning that as an alternative to eigenvalue problems based on Chebyshev expansion coefficients, it is possible to relate roots of polynomials to eigenvalue problems constructed from function values themselves at Chebyshev or other points. Mathematical processes along these lines are described in [Fortune 1981] and [Amiraslani, et al. 2004], but there has not been much numerical application, and whether such methods may one day compete with the robustness and speed of colleague matrix methods is not known.

We close this chapter by clarifying a point that may have puzzled the reader. In plots like the last two, we see only real roots of a function. Yet if the function is a chebfun based on a polynomial representation, won't there be complex roots too? This is indeed the case, but the Chebfun `roots` command by default returns only those roots in the interval where the function is defined. This default behavior can be overridden by the use of the flags `'all'` or `'complex'` (see Exercise 14.2). For example, suppose we make a chebfun corresponding to the function $f(x) = (x - i)\exp(x)$, which has just one complex root:


```
f = (x-1i).*exp(x);
length(f)
```
```
ans = 16
```

Typing `roots` alone gives an empty result,

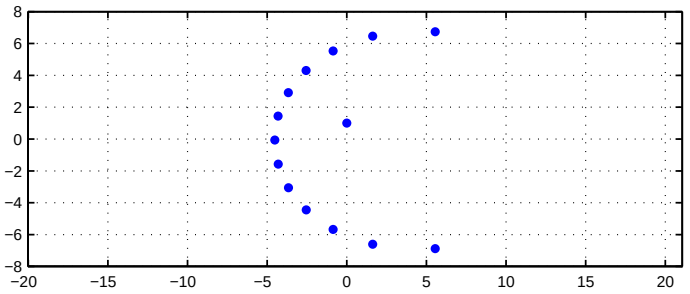
```
roots(f)
```
```
ans = Empty matrix: 0-by-1
```

With `roots(f,'all')` we get 15 complex roots, one of which is close to the exact value i:

```
roots(f,'all')
```
```
ans =
  5.547449161867402 - 6.881939962715025i
  5.549228934990555 + 6.742658291769258i
  1.621208524576572 - 6.600976209539127i
  1.622778153691944 + 6.459369547219920i
 -0.862071641931589 - 5.672970550178491i
 -0.863167878985637 + 5.529849812380652i
 -2.549964559078775 - 4.444767251346623i
 -3.664930599540194 - 3.055332374662211i
 -2.554485468502298 + 4.303049289549812i
 -4.305640171640882 - 1.579505420838914i
 -3.670759826319950 + 2.917470067938329i
 -4.516455458908681 - 0.066308326942409i
 -4.309583570325588 + 1.445394701241379i
 -0.000000000160410 + 0.999999999890419i
```

The other roots are meaningless from the point of view of the underlying function f; they are an epiphenomenon that arises in the process of approximating f on $[-1, 1]$. A plot reveals that they have a regular distribution, which is related to potential theory and has been the subject of considerable interest by some mathematicians [Saff & Varga 1978b]:

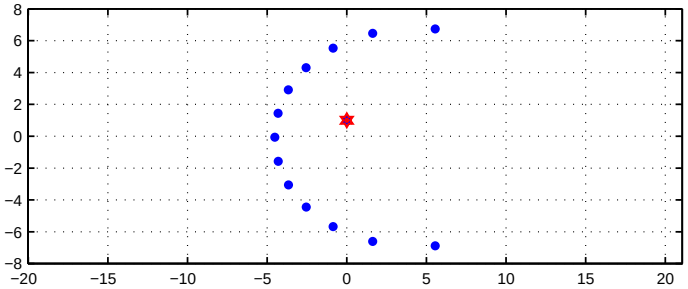
```
hold off, plot(ans,'.',MS,14)
ylim([-8 8]), grid on, axis equal
```



With the `roots(f,'complex')` option, Chebfun does its best to return just those roots in the complex plane that are near the interval of approximation and are considered reliable — that is, well within the Bernstein ellipse where the Chebyshev series appears to be valid. For this example, it correctly singles out $x = i$ as the genuine root.

```
roots(f,'complex')
hold on, plot(ans,'.r',MS,8), plot(ans,'hr',MS,7)
```

```
ans =
 -0.000000000160410 + 0.999999998890419i
```



[To be added: (1) Discussion of stability. (2) Look up Barnett's book. (3) Add references to Boyd after "more numerical era".]

SUMMARY OF CHAPTER 18. *The roots of a polynomial are equal to the eigenvalues of a colleague matrix formed from its coefficients in a Chebyshev series and the recurrence relation for Chebyshev polynomials. This identity, combined with recursive subdivision, leads to a stable and efficient numerical method for computing roots of a polynomial in an interval. For orthogonal polynomials other than Chebyshev, the colleague matrix generalizes to a comrade matrix.*

Exercise 18.1. Four forms of colleague matrix. A matrix C has the same eigenvalues and eigenvalue multiplicities as C^T and also as SCS^{-1}, where S is any nonsingular matrix. Use these properties to derive three alternative forms of the colleague matrix in which the Chebyshev coefficients appear in (a) the first row, (b) the first column, (c) the last column.

Exercise 18.2. Some forms stabler than others. Mathematically, all the matrices described in the last exercise have the same eigenvalues. Numerically, however, some may suffer more than others from rounding errors, and in fact Chebfun works with the first-column option for just this reason. (a) Determine the 11×11 colleague matrix corresponding to roots $-1, -0.8, -0.6, \ldots, 1$. Get the entries of the matrix exactly,

either analytically or by intelligent guesswork based on Matlab's `rat` command. (b) How does the accuracy of the eigenvalues of the four matrix variants compare? Which one is best? Is the difference significant? (c) What happens if you solve the four eigenvalue problems again using Matlab's `nobalance` option in the `eig` command?

Exercise 18.3. Legendre polynomials. The Legendre polynomials satisfy $L_0(x) = 1$, $L_1(x) = x$, and for $k \geq 1$, the recurrence relation (17.5). (a) Derive the "comrade matrix" analogue of Theorem 18.1 for the roots of a polynomial expanded as a linear combination of Legendre polynomials. (b) Verify numerically that the roots of the particular polynomial $L_0 + L_1 + \cdots + L_5$ match the prediction of your theorem. (Try `sum(legpoly(0:5),2)` to construct this polynomial slickly in Chebfun and don't forget `roots(...,'all')`.)

Exercise 18.4. Complex roots. Pick six quite varied functions defined on $[-1, 1]$, construct corresponding chebfuns, and plot all of their roots in the complex plane. Comment on the patterns you observe. [This needs to be made more precise.]

Exercise 18.5. Polishroots. Explore rootfinding in Chebfun in the two modes `chebfunpref('polishroots',1)` and `chebfunpref('polishroots',0)`. When this preference is set to 1, one step of Newton's method is used to improve each real root obtained from the colleague matrix eigenvalue problem. What is the effect on the accuracy of the algorithm? The speed? [to be written more properly]

Exercise 18.6. Random polynomials. [To be written. Use Matlab roots for a polynomial with random coeffs, and show the roots are near the unit circle. Similarly in the Chebyshev basis. Then point to Shiffman & Zelditch 2003.]

Exercise 18.7. Wilkinson polynomial. [To be written.]

Exercise 18.8. Companion matrix. [To be written.]

19. Clenshaw–Curtis and Gauss quadrature

One thing that is famous about Legendre points and polynomials is their connection with **Gauss quadrature**, invented by Gauss [1814]. Chebyshev points, similarly, are the basis of **Clenshaw–Curtis quadrature** [Clenshaw & Curtis 1960]. Quadrature is the standard term for the numerical calculation of integrals. It is one of the areas where approximation theory has an immediate link to applications, as we shall see in Theorems 19.3–19.5.

In the basic quadrature problem, we are given a function $f \in C[-1, 1]$ and wish to calculate

$$I = \int_{-1}^{1} f(x)\,dx. \tag{19.1}$$

There is a standard idea for doing this which is the basis of the Gauss and Clenshaw–Curtis formulas and many others besides. Given $n \geq 0$, we sample f at a certain set of $n + 1$ distinct **nodes** $x_0, \ldots, x_n$ in $[-1, 1]$. Clenshaw–Curtis quadrature uses Chebyshev points, and Gauss quadrature uses Legendre points. We then approximate I by I_n, the exact integral of the degree n polynomial

interpolant p_n of f at these nodes:

$$I_n = \int_{-1}^{1} p_n(x)\,dx. \tag{19.2}$$

One might wonder, why use a polynomial rather than some other interpolant? This is a very good question, and in Chapter 22 we shall see that other interpolants may in fact be up to $\pi/2$ times more efficient. Nevertheless polynomial interpolants have been the standard idea in numerical quadrature since the 18th century.

To integrate p_n, we do not construct it explicitly. Instead, I_n is computed from the formula

$$I_n = \sum_{k=0}^{n} w_k f(x_k), \tag{19.3}$$

where the numbers $w_0, \ldots, w_n$ are a set of $n+1$ **weights** that have been predetermined so that the value of I_n will come out right. From (5.1) it is clear that the weights must be the integrals of the Lagrange polynomials,

$$w_k = \int_{-1}^{1} \ell_k(x)\,dx. \tag{19.4}$$

Another way to write (19.3) is to say that I_n is given by an inner product,

$$I_n = w^T v, \tag{19.5}$$

where w and v are column vectors of the weights w_k and function values $f(x_k)$. Any linear process of computing an approximate integral from $n+1$ sample points must be representable in this inner product form, and the integration of polynomial interpolants is a linear process. The proper term is that the mapping from $\{f(x_k)\}$ to I_n is a *linear functional* (Exercise 19.1).

The following exactness properties of the Clenshaw–Curtis and Gauss formulas are very well known. (We say that a formula is "exact" when applied to f if the result it gives is the exactly correct integral of f.) The proof we give, the standard one based on orthogonal polynomials, comes from [Jacobi 1826]. Gauss's original work twelve years earlier was based on continued fractions rather than orthogonal polynomials.

Theorem 19.1: Polynomial degree of quadrature formulas. *For any $n \geq 0$, the $(n+1)$-point Clenshaw–Curtis formula is exact if $f \in P_n$, and the $(n+1)$-point Gauss formula is exact if $f \in P_{2n+1}$.*

Proof. Since both formulas are constructed by integration of a polynomial interpolant of degree n, it is immediate that they are exact for $f \in P_n$. The nontrivial property to be established is that Gauss quadrature achieves more than this, being exact for polynomials all the way up to degree $2n+1$.

Suppose then that $f \in P_{2n+1}$. Such a function can be written in the form $f(x) = L_{n+1}(x)\,q_n(x) + r_n(x)$, where L_{n+1} is the $(n+1)$st Legendre polynomial and $q_n, r_n \in P_n$. This implies

$$I = \int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} L_{n+1}(x)\,q_n(x)\,dx + \int_{-1}^{1} r_n(x)\,dx.$$

The first of the integrals on the right is zero because of the orthogonality property of Legendre polynomials, leaving us with

$$I = \int_{-1}^{1} r_n(x)\,dx.$$

Now consider I_n, the $(n+1)$-point Gauss quadrature approximation to I. The nodes of this formula are the zeros of $L_{n+1}(x)$. Accordingly, at each node x_k we have $f(x_k) = r_n(x_k)$. Thus the value I_n the Gauss formula gives for f will be the same as the value it gives for r_n. But $r_n \in P_n$, so this value is exactly the integral of r_n, that is, $I_n = I$. ∎

Theorem 19.1 is famous, but we shall see that it is misleading. It suggests that Clenshaw–Curtis quadrature will typically need twice as many points as Gauss to deliver a certain accuracy, but this is not true.

First let us give some more details of these quadrature formulas. For Clenshaw–Curtis quadrature, one way to compute I_n is by constructing the weight vector w explicitly. It can be shown that the weights are all positive and sum to 2 (the same properties also hold for Gauss quadrature weights, whose computation we discuss later in the chapter). From a practical point of view, this approach may be advantageous for integrating a collection of functions on a single Chebyshev grid. There is a classical formula for calculation of the weights with $O(n^2)$ operations [Davis & Rabinowitz 1984, Trefethen 2000], and it is also possible to compute the weights faster, in $O(n \log n)$ operations, using the FFT [Waldvogel 2006]. This fast algorithm is invoked by Chebfun when the command `chebpts` is called with two arguments, as we illustrate with $n+1 = 3$:

```
[nodes,weights] = chebpts(3)
```

```
nodes =
    -1
     0
     1
weights =
   0.333333333333333   1.333333333333333   0.333333333333333
```

By increasing 3 to one million we see the speed of Waldvogel's algorithm:

```
tic, [nodes,weights] = chebpts(1000000); toc
```

```
Elapsed time is 0.617872 seconds.
```

The other way to carry out Clenshaw–Curtis quadrature, simplest when just one or a small number of integrands are involved, is to use the FFT to transform the problem to coefficient space (see Chapter 3) at a cost of $O(n \log n)$ operations per integrand. (This idea was not proposed by Clenshaw and Curtis, who wrote before the rediscovery of the FFT in 1965, but by Morven Gentleman a few years later [Gentleman 1972a, 1972b].) To see how this works, we observe that the integral of the Chebyshev polynomial T_k from -1 to 1 is zero if k is odd and

$$\int_{-1}^{1} T_k(x)\,dx = \frac{2}{1-k^2} \tag{19.6}$$

if k is even (Exercise 19.9). This gives us the following theorem, the basis of the FFT realization of Clenshaw–Curtis quadrature:

Theorem 19.2: Integral of a Chebyshev series. *The integral of a degree n polynomial expressed as a Chebyshev series is*

$$\int_{-1}^{1} \sum_{k=0}^{n} c_k T_k(x)\,dx \;=\; \sum_{k=0,\,k\,\text{even}}^{n} \frac{2c_k}{1-k^2}.$$

Proof. Follows from (19.6). ∎

Chebfun applies Theorem 19.2 every time one types `sum(f)`. Chebyshev coefficients of f are computed by the FFT using `chebpoly`, and then they are summed with the factors $2/(1-k^2)$.

By combining (19.6) with Theorems 8.1 and 19.1, we can now write down a theorem about the geometric convergence of Clenshaw–Curtis and Gauss quadrature for analytic integrands. For Gauss quadrature, this estimate is due to Rabinowitz [1969], and the extension to Clenshaw–Curtis can be found in [Trefethen 2008]. This result is fundamental and very important. *For analytic integrands, the Gauss and Clenshaw–Curtis formulas converge geometrically.* Every numerical analysis textbook should state this fact.

Theorem 19.3: Quadrature formulas for analytic integrands. *Let a function f analytic in $[-1,1]$ be analytically continuable to the open ρ-ellipse E_ρ, where it satisfies $|f(z)| \le M$ for some M. Then $(n+1)$-point Clenshaw–Curtis quadrature with $n \ge 2$ applied to f satisfies*

$$|I - I_n| \le \frac{64}{15}\frac{M\rho^{1-n}}{\rho^2-1} \tag{19.7}$$

and $(n+1)$-point Gauss quadrature with $n \ge 1$ satisfies

$$|I - I_n| \le \frac{64}{15}\frac{M\rho^{-2n}}{\rho^2-1}. \tag{19.8}$$

The factor ρ^{1-n} in (19.7) can be improved to ρ^{-n} if n is even, and the factor $64/15$ can be improved to $144/35$ if $n \ge 4$ in (19.7) or $n \ge 2$ in (19.8).

Proof. If the constants $64/15$ are increased to 8 and $\rho^2 - 1$ is reduced to $\rho - 1$, these conclusions can be obtained as corollaries of Theorem 8.2 by noting that the error in integrating f will be the same as the error in integrating $f - p^*$.

To get the sharper results stated, we use an additional fact: both Gauss and Clenshaw–Curtis formulas get the right answer when integrating an odd function, namely zero. In particular the error is zero in integration of $T_k(x)$ for any odd k. Now by Theorem 19.1, Gauss quadrature is exact through the term of degree $2n+1$ in the Chebyshev expansion of f. Since odd terms do not contribute, we see that the error in integrating f by $(n+1)$-point Gauss quadrature will thus be the error in integrating

$$a_{2n+2}T_{2n+2}(x) + a_{2n+4}T_{2n+4}(x) + \dots,$$

a series in which the smallest index that appears is at least 4. Now by (19.6), the true integral of T_k for $k \ge 4$ is at most $2/15$. When T_k is integrated over $[-1,1]$ by the Gauss quadrature formula, the result will be at most 2 since the weights are positive and add up to 2. Thus the error in integrating each T_k is at most $2 + 2/15 = 32/15$. Combining this estimate with the bound $|a_k| \le 2M\rho^{-k}$ of Theorem 8.1 gives (19.8). The argument for (19.7) is analogous. For the improvement from $64/15$ to $144/35$, see Exercise 19.6. ∎

Just as Theorem 19.3 follows from the results of Chapter 8 for analytic integrands, there is an analogous result for differentiable integrands based on the results of Chapter 7.

Theorem 19.4: Quadrature formulas for differentiable integrands. *For an integer $\nu \ge 1$, let f have an absolutely continuous $(\nu-1)$st derivative $f^{(\nu-1)}$ on $[-1,1]$ and a νth derivative $f^{(\nu)}$ of bounded variation V. Then $(n+1)$-point Clenshaw–Curtis quadrature applied to f satisfies*

$$|I - I_n| \le \frac{32}{15}\frac{V}{\pi\nu(n-\nu)^\nu} \tag{19.9}$$

for $n > \nu$ and $(n+1)$-point Gauss quadrature satisfies

$$|I - I_n| \le \frac{32}{15}\frac{V}{\pi\nu(n-2\nu-1)^{2\nu+1}} \tag{19.10}$$

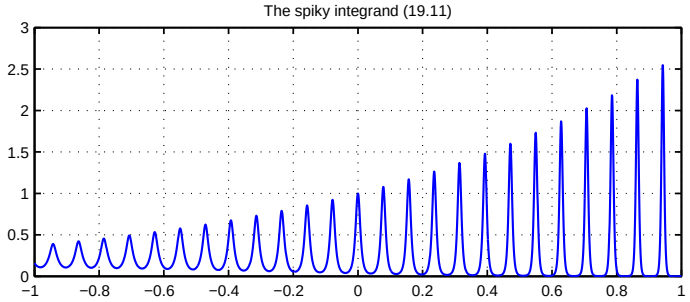
for $n > 2\nu + 1$.

Proof. Like the previous proof, but now based on Theorem 7.2. ∎

Here is a numerical example, the integration of the function (18.1) with a sequence of spikes:

$$I = \int_{-1}^{1} e^x \left[\operatorname{sech}(4\sin(40x))\right]^{\exp(x)}\,dx \tag{19.11}$$

```
ff = @(x) exp(x).*sech(4*sin(40*x)).^exp(x);
f = ff(x);
clf, plot(f), grid on, title('The spiky integrand (19.11)')
```



The corresponding chebfun is not exactly short:

```
length(f)
```

```
ans = 3521
```

Nevertheless, Chebfun computes its integral to 15 digits of accuracy in a fraction of a second:

```
sum(f)
```

```
ans = 0.543384000907901
```

Now let us look at Gauss quadrature. The nodes for the $n+1$-point Gauss formula are the roots of the Legendre polynomial $L_{n+1}(x)$. A good method for computing these numbers is implicit in Theorem 18.1 and the comment after it. According to that theorem, the roots of a polynomial expressed as a Chebyshev series are equal to the eigenvalues of a colleague matrix whose structure is tridiagonal apart from a nonzero final row. If the Chebyshev series reduces to the single polynomial T_{n+1}, the matrix reduces to tridiagonal without the extra row. Similarly the roots of a polynomial expressed as a series in Legendre polynomials are the eigenvalues of a comrade matrix, which is again tridiagonal except for a final row, and for the roots of L_{n+1} itself, the matrix reduces to tridiagonal. When symmetrized, this matrix is called a **Jacobi matrix** (Exercise 19.10). The classic numerical algorithm for implementing Gauss quadrature formulas comes from Golub and Welsch in 1969, who showed that the weights as well as the nodes can be obtained by solving the eigenvalue problem for this Jacobi matrix [Golub & Welsch 1969]. The Golub–Welsch algorithm can be coded in six lines of Matlab (see `gauss.m` in [Trefethen 2000]), and the operation count is in principle $O(n^2)$, though $O(n^3)$ in the simple implementation since Matlab does not offer a command to exploit the tridiagonal structure.

For larger values of n, there is a much faster alternative due to Glaser, Liu, and Rokhlin, based on numerical solution of certain linear ordinary differential equations [Glaser, Liu & Rokhlin 2007]. The operation count now shrinks dramatically to $O(n)$. The results of the Glaser–Liu–Rokhlin algorithm are available in Chebfun when the `legpts` command is called with two output arguments. Following the illustration of Clenshaw–Curtis quadrature earlier, here are nodes and weights for Gauss quadrature with $n+1=3$:

```
[nodes,weights] = legpts(3)
```

```
nodes =
  -0.774596669241484
                   0
   0.774596669241484
weights =
   0.555555555555555   0.888888888888889   0.555555555555555
```

And here is the time for one million points — much slower than for Clenshaw–Curtis quadrature, but still doable.

```
tic, [nodes,weights] = legpts(1000000); toc
```

```
Elapsed time is 28.109859 seconds.
```

For example, here is the integral of $\exp(-100x^2)$ computed by n-point Gauss quadrature for various values of n. We write `w*gg(s)` rather than `w'*gg(s)` since w as returned by `legpts` is a row vector, not a column vector.

```
gg = @(x) exp(-100*x.^2);
for n = 20:20:80
  tic, [s,w] = legpts(n+1);
  I = w*gg(s); t = toc;
  fprintf('n = %3d,  I = %16.14f,  time = %6.4f\n',n,I,t)
end
```

```
n =  20,  I = 0.18088674900834,  time = 0.0024
n =  40,  I = 0.17724541037977,  time = 0.0007
n =  60,  I = 0.17724538509055,  time = 0.0011
n =  80,  I = 0.17724538509055,  time = 0.0099
```

For the more difficult integral (19.11), bigger values of n are required. Nevertheless the computing times remain very short.

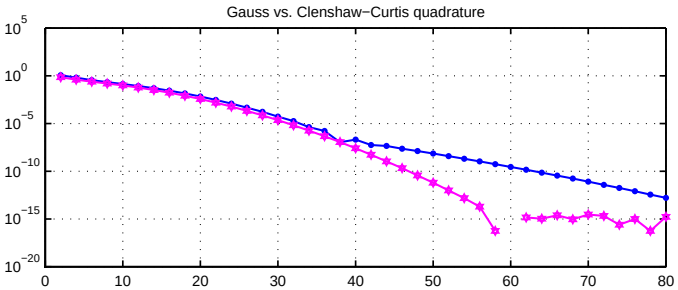
```
for n = 500:500:2000
  tic
  [s,w] = legpts(n+1);
  I = w*ff(s); t = toc;
  fprintf('n = %4d,  I = %16.14f,  time = %6.4f\n',n,I,t)
end
```

```
n =  500,  I = 0.54339275810622,  time = 0.0174
n = 1000,  I = 0.54338400182558,  time = 0.0303
n = 1500,  I = 0.54338400090784,  time = 0.0452
n = 2000,  I = 0.54338400090790,  time = 0.0578
```

Gauss quadrature has not often been employed for numbers of nodes in the thousands, because with traditional algorithms the computations are too expensive. It is clear from this experiment that the Glaser–Liu–Rokhlin algorithm makes such computations feasible after all.

So is Gauss quadrature the formula of choice? In particular, how does it compare with Clenshaw–Curtis quadrature as $n \to \infty$? As mentioned above, the traditional expectation, based on Theorem 19.1 and seemingly supported by Theorems 19.3 and 19.4, is that Gauss should converge twice as fast as Clenshaw–Curtis. However, numerical experiments show that the truth is not so simple. We begin with the easy integrand $\exp(-100x^2)$ just considered.

```
I = sum(chebfun(gg));
errcc = []; errgauss = [];
nn = 2:2:80;
for n = nn
   Icc = sum(chebfun(gg,n+1));
   errcc = [errcc abs(I-Icc)];
   [s,w] = legpts(n+1);
   Igauss = w*gg(s);
   errgauss = [errgauss abs(I-Igauss)];
end
MS = 'markersize';
hold off, semilogy(nn,errcc,'.-',MS,10), grid on
hold on, semilogy(nn,errgauss,'h-m',MS,4), grid on
title('Gauss vs. Clenshaw-Curtis quadrature')
```

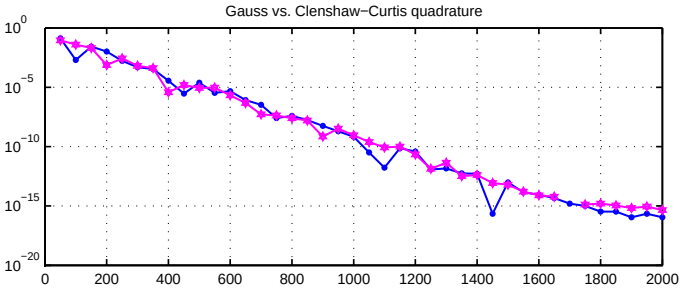


This behavior is typical: for smaller values of n, Clenshaw–Curtis (dots) and Gauss quadrature (stars) have similar accuracy, not a difference of a factor of 2. This effect was pointed out by Clenshaw and Curtis in their original paper

[1960]. Only at a sufficiently large value of n, if the integrand is analytic, does a kink appear in the Clenshaw–Curtis convergence curve, whose further convergence is then about half as slow as before. An explanation of this effect based on ideas of rational approximation is given in Figures 4–6 of [Trefethen 2008], and another explanation based on aliasing can be derived from Theorems 4.2 and 19.2 and goes back to O'Hara and Smith [1968] (Exercise 19.5). For a full analysis, see [Weideman & Trefethen 2007].

Here is a similar comparison for the harder integral (19.11):

```
I = sum(f);
errcc = []; errgauss = []; tcc = []; tgauss = [];
nn = 50:50:2000;
for n = nn
   tic, Icc = sum(chebfun(ff,n+1)); t = toc;
   tcc = [tcc t]; errcc = [errcc abs(I-Icc)];
   tic, [s,w] = legpts(n+1); t = toc;
   Igauss = w*ff(s);
   tgauss = [tgauss t]; errgauss = [errgauss abs(I-Igauss)];
end
hold off, semilogy(nn,errcc,'.-',MS,10), grid on
hold on, semilogy(nn,errgauss,'h-m',MS,4)
title('Gauss vs. Clenshaw-Curtis quadrature')
```



This time, for the values of n under study, the kink does not appear at all. Clenshaw–Curtis has approximately the same accuracy as Gauss throughout, and in particular, it obtains the correct integral to machine precision by around $n = 1800$, which is about half the length of the chebfun, `length(f)`, reported earlier! This is typical of Clenshaw–Curtis quadrature: just as with Gauss quadrature, the quadrature value often converges about twice as fast as the underlying polynomial approximation, even though Theorems 19.1, 19.3, and 19.4 give no hint of such behavior.

There is a theorem that substantiates this effect. The following result, whose proof we shall not give, comes from [Trefethen 2008].

Theorem 19.5: Clenshaw–Curtis quadrature for differentiable integrands. *Under the hypotheses of Theorem* 19.4*, the same conclusion* (19.10) *also holds for* $(n+1)$*-point Clenshaw–Curtis quadrature:*

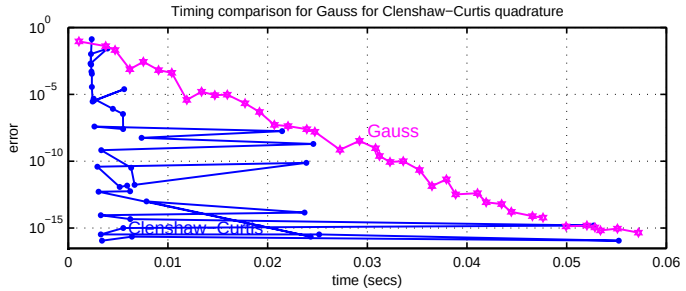
$$|I - I_n| \le \frac{32}{15} \frac{V}{\pi\nu(n-2\nu-1)^{2\nu+1}}. \tag{19.12}$$

The only difference is that this bound applies for all sufficiently large n *(depending on* ν *but not* f*) rather than for* $n > 2\nu + 1$*.*

Proof. See [Trefethen 2008]. Here, the definition of V is somewhat different from the one in [Trefethen 2008], but this does not affect the argument leading to (19.12). ∎

In the **for** loop of the experiment above, we stored times as well as values. This enables us to plot accuracy as a function of computing time, showing that Gauss quadrature, at least in the Chebfun implementation, is much the slower of the two methods.

```
hold off, semilogy(tcc,errcc,'.-',MS,10)
hold on, semilogy(tgauss,errgauss,'h-m',MS,4), grid on, ylim([3e-17,1])
a = axis;
text(mean(a(1:2)),2e-8,'Gauss',CO,'m')
text(a(1)+.1*(a(2)-a(1)),1e-15,'Clenshaw-Curtis',CO,'b')
xlabel('time (secs)'), ylabel error
title('Timing comparison for Gauss for Clenshaw-Curtis quadrature')
```



All in all, though Gauss quadrature is more celebrated than Clenshaw–Curtis, and certainly has some beautiful properties, it is not clear how often it is superior in practice.

For an extensive survey of many aspects of Gauss quadrature, see [Gautschi 1981], and for general information about numerical integration, see [Davis & Rabinowitz 1984]. In practical applications it is common to use adaptive formulas of low or moderate order rather than letting n increase toward ∞, though Chebfun is an exception to this pattern.

As mentioned earlier, both Gauss and Clenshaw–Curtis quadrature grids can be improved by a factor approaching $\pi/2$ by the introduction of a change of variables, taking us beyond the realm of polynomial approximations. These ideas are discussed in Chapter 22.

We close this chapter by mentioning an elegant application of Gauss quadrature nodes and weights pointed out by Wang [2010].

Theorem 19.6: Barycentric weights for Legendre points. *Let the numbers* $\lambda_0, \dots, \lambda_k$ *be defined by*

$$\lambda_k = (-1)^k \sqrt{(1-x_k^2) w_k}, \tag{19.13}$$

where $\{x_k\}$ *and* $\{w_k\}$ *are the nodes and weights for* $(n+1)$*-point Gauss quadrature. If these numbers are taken as weights in the barycentric formula* (5.11)*, they yield the polynomial interpolant through Legendre points.*

Proof. See [Wang 2010]. ∎

In view of the Glaser–Liu–Rokhlin algorithm for Gauss quadrature, this theorem implies that polynomial interpolants in Legendre points, like Chebyshev points, can be evaluated in $O(n)$ operations.

[To be added: (1) Reference on the invention of the $O(n^2)$ `clencurt` formula mentioned at the beginning. (2) Give the aliasing explanation of Theorem 19.5. (3) Say something about Newton–Cotes quadrature and the proof of divergence by Polya 1933. (4) Mention Evans and Kythe & Schäferkotter. (5) Mention Fejér quadrature. (6) Mention `hermpoly` and `lagpoly`. (7) Give the fast algorithm for C–C nodes and weights. (8) Is [Wang2010] really the first to do Theorem 19.6? (9) Mention Gauss-Chebyshev and other Gauss quadratures. For G-C, the weights are π/n, half that at ends. See Chawla 1968 and 1970, Math Comp and Computer J. (10) Reference on positivity of C-C and G weights. (11) If you compute expansion coeffs using Gauss quad, you must get exactly the expansion coeffs of the interpolant. (12) Say more about Glaser-Liu-Rokhlin—solves standard linear ODE for roots, then gets weights from K2AM (20). (13) Gauss converges if f is continuous: Stieltjes. (14) Make clear the old history (19th C) of geometric convergence for analytic integrands. (15) Review the proof of Theorem 18.3. Does the comment in the proof apply to Gauss as well as C-C? (16) Example with a chebpts loop analogous to that with the legpts loop.]

SUMMARY OF CHAPTER 19. *Clenshaw–Curtis quadrature is derived by interpolating a polynomial interpolant in Chebyshev points, and Gauss quadrature from Legendre points. The nodes and weights for both families can be computed quickly and accurately, even for millions of points. Though Guass has twice the polynomial order of accuracy of Clenshaw–Curtis, their rates of convergence are approximately the same for non-analytic integrands.*

Exercise 19.1. Riesz Representation Theorem. (a) Look up the Riesz Representation Theorem and write it down with a careful mathematical statement. (b) Show that the computation of an approximate integral I_n from $n+1$ samples of a function $f \in C[-1,1]$ by integrating the degree n polynomial interpolant through a fixed set of $n+1$ nodes in $[-1,1]$ is an example of the kind of linear functional to which this theorem applies, provided we work in a finite-dimensional space rather than all of $C[-1,1]$. (c) In what sense is the Riesz Representation Theorem significantly more general than is needed for this particular application to quadrature?

Exercise 19.2. `quad`, `quadl`, `quadgk`. Evaluate (19.11) with Matlab's `quad`, `quadl`, and `quadgk` commands. As a function of the specified precision, what is the actual accuracy obtained and how long does the computation take? How do these results compare with Chebfun `sum`?

Exercise 19.3. Gauss quadrature and Hermite interpolation. [to be written]

Exercise 19.4. Quadrature weights. (a) Use chebfun to illustrate the identity (19.4) for Clenshaw–Curtis quadrature in the case $n = 20$, $k = 7$. (b) Same for Gauss quadrature.

Exercise 19.5. Accuracy of Clenshaw–Curtis quadrature. (a) Using theorems of Chapters 4 and 19, derive an exact expression for the error in Clenshaw–Curtis quadrature applied to the function $f(x) = T_k(x)$ for $k > n$. (b) [to be continued. See eqs (9) and (9') of Gentleman [1972a].]

Exercise 19.6. Sharpening Theorem 19.3. Suppose we assume $n \geq 2$ instead of $n \geq 1$ in the Gauss quadrature bound of Theorem 19.3. Show why the constant $64/15$ improves to $144/35$. What is this actual "constant" as a function of n?

Exercise 19.7. Rates of convergence for particular integrands. [To be written. Fresnel integral? Gamma function?]

Exercise 19.8. Clenshaw–Curtis applied to Chebyshev polynomials. [Exercise to be written about these algebraically small errors.]

Exercise 19.9. Integral of a Chebyshev polynomial. Derive the formula (19.6) for the integral of $T_k(x)$ with k even. [Hint: Following the proof of Theorem 3.1, replace $T_k(x)dx$ by $(z^k + z^{-k})(dx/dz)dz$.]

Exercise 19.10. Golub–Welsch algorithm. [To be written.]

20. Carathéodory–Fejér approximation

We have seen that Chebyshev interpolants are near-best approximations in the sense that they come within a factor of at most $O(\log n)$ of best approximations, usually even closer. For most applications, this is all one could ask for. But there is another kind of near-best approximations that are so close to best that for smooth functions, they are often indistinguishable from best approximations to machine precision on a computer. These are **CF (Carathéodory–Fejér) approximations**, introduced by Gutknecht and Trefethen [1982]. Earlier related ideas were proposed in [Darlington 1970, Elliott 1973, Lam 1972, Talbot 1976], and the theoretical basis goes back to the early 20th century [Carathéodory & Fejér 1911, Schur 1918].[7]

Before explaining the mathematics of CF approximants, let us illustrate the remarkable degree of near-optimality they sometimes achieve. Here is the optimal ∞-norm error in approximation of $f(x) = e^x$ on $[-1,1]$ by a polynomial of degree 2:

```
x = chebfun('x'); format long
f = exp(x); n = 2;
pbest = remez(f,n);
errbest = norm(f-pbest,inf)
```

```
errbest =
   0.045017388402819
```

Here is the corresponding error for CF approximation computed by the Chebfun `cf` command:

```
pcf = cf(f,n);
errcf = norm(f-pcf,inf)
```

```
errcf =
   0.045017388414604
```

These two numbers agree to an extraordinary 9 significant digits. Comparing the best and CF polynomials directly to one another, we confirm that they are almost the same:

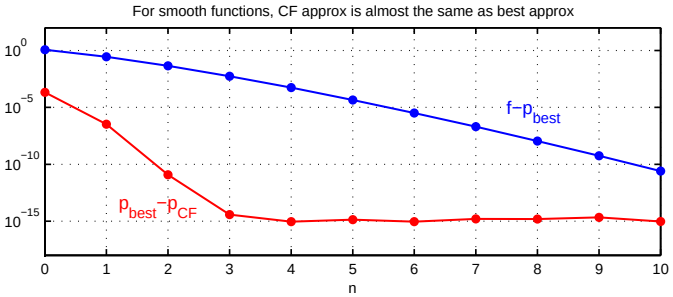
```
norm(pbest-pcf,inf)
```

```
ans = 1.178523945100096e-11
```

[7] Logically, this chapter could have appeared earlier, perhaps just after Chapter 10. We have deferred it to this point of the book, however, since the material is relatively difficult and none of the later chapters depend on it.

That was for degree $n = 2$, and the near-optimality of the CF approximants grows stronger as n increases. Let us explore the dependence on n. On a semilog plot, the upper curve in the next figure shows the accuracy of the best polynomial as an approximation to $f(x)$, while the lower curve shows the accuracy of the CF polynomial as an approximation to the best polynomial. The two errors are of entirely different orders, and for $n > 3$, the CF and best polynomials are indistinguishable in floating point arithmetic.

```
nn = 0:10; err1 = []; err2 = [];
for n = nn
    pbest = remez(f,n);
    err1 = [err1 norm(f-pbest,inf)];
    pcf = cf(f,n);
    err2 = [err2 norm(pbest-pcf,inf)];
end
hold off, semilogy(nn,err1,'.-'), grid on
hold on, semilogy(nn,err2,'.-r')
text(7.5,2e-6,'f-p_{best}',CO,'b',FS,10)
text(1.2,1e-14,'p_{best}-p_{CF}',CO,'r',FS,10)
ylim([1e-18,1e2]), xlabel n
title(['For smooth functions, ' ...
     'CF approx is almost the same as best approx'])
```

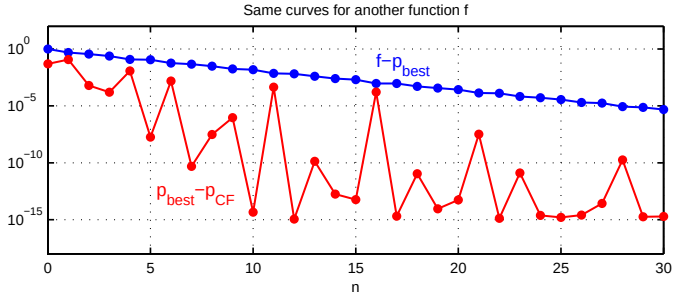


Here is the same experiment repeated for $f(x) = \tanh(4(x - 0.3))$.

```
f = tanh(4*(x-.3));
nn = 0:30; err1 = []; err2 = [];
for n = nn
    pbest = remez(f,n);
    err1 = [err1 norm(f-pbest,inf)];
    pcf = cf(f,n);
    err2 = [err2 norm(pbest-pcf,inf)];
end
hold off, semilogy(nn,err1,'.-'), grid on
hold on, semilogy(nn,err2,'.-r')
```



```
text(16,2e-2,'f-p_{best}',CO,'b',FS,10)
text(5.3,1e-13,'p_{best}-p_{CF}',CO,'r',FS,10)
ylim([1e-18,1e2]), xlabel n
title('Same curves for another function f')
```



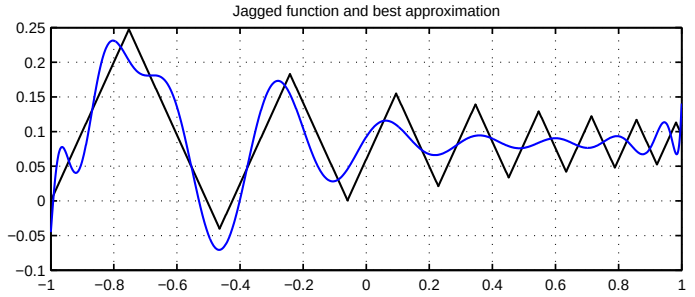
Again we see that `pbest−pcf` is much smaller than `f−pbest`, implying that the CF approximant is for practical purposes essentially optimal. (Concerning the erratic oscillations, see Exercise 20.3.) Yet it is far easier to compute:

```
tic, remez(f,20); tbest = toc
tic, cf(f,20); tcf = toc
```

```
tbest =
   0.126213000000000
tcf =
   0.009344000000000
```

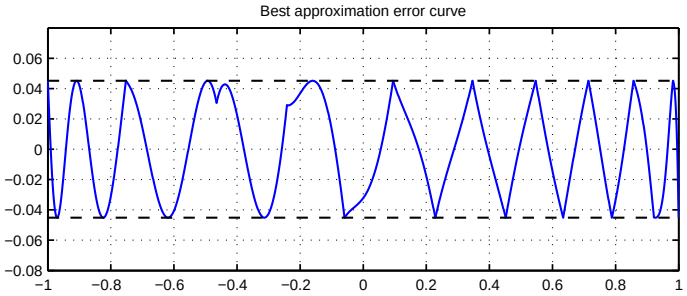
Turning to a non-smooth function, here again is the jagged example from Chapter 10 with its best approximation of degree 20:

```
f = cumsum(sign(sin(20*exp(x))));
hold off, plot(f,'k'), grid on
tic, [pbest,err] = remez(f,20); tbest = toc;
hold on, plot(pbest)
title('Jagged function and best approximation')
```



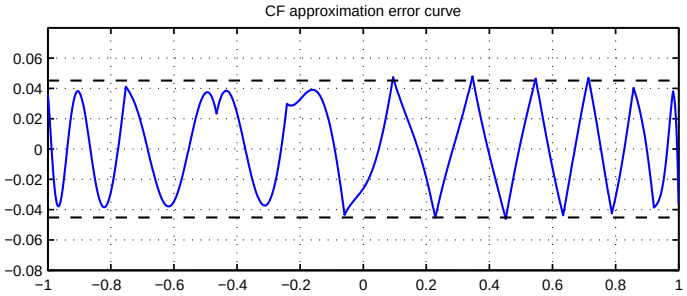
We saw the error curve before:

```
hold off, plot(f-pbest), grid on, hold on, axis([-1 1 -.08 .08])
plot([-1 1],err*[1 1],'--k'), plot([-1,1],-err*[1 1],'--k')
title('Best approximation error curve')
```



In CF approximation, we must start from a polynomial, not a jagged function. As a rule of thumb, truncating the Chebyshev series at 5 times the degree of the desired approximation is usually pretty safe. Here is what we get:

```
f100 = chebfun(f,100);
tic, pcf = cf(f100,20); tcf = toc;
hold off, plot(f-pcf), grid on, hold on, axis([-1 1 -.08 .08])
plot([-1 1],err*[1 1],'--k'), plot([-1,1],-err*[1 1],'--k')
title('CF approximation error curve')
```



Evidently the error falls short of optimality by just a few percent. Yet again the computation is much faster:

```
tbest
```

```
tbest =
   1.505368000000000
```

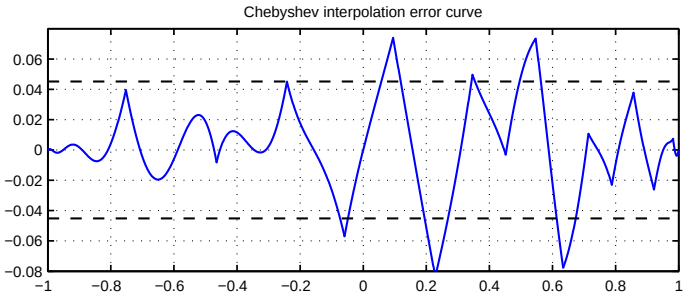


```
tcf
```

```
tcf =
   0.007593000000000
```

Here for comparison is the error in Chebyshev interpolation.

```
pinterp = chebfun(f,21);
hold off, plot(f-pinterp), grid on, hold on, axis([-1 1 -.08 .08])
plot([-1 1],err*[1 1],'--k'), plot([-1,1],-err*[1 1],'--k')
title('Chebyshev interpolation error curve')
```



The time has come to describe what CF approximation is all about. We shall see that the hallmark of this method is the use of eigenvalues and eigenvectors (or singular values and singular vectors) of a Hankel matrix of Chebyshev coefficients.

We start with a real function f on $[-1,1]$, which we want to approximate by a polynomial of degree $n \geq 0$. Following Theorem 3.1, we assume that f is Lipschitz continuous, so it has an absolutely convergent Chebyshev series

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x).$$

Since our aim is polynomial approximation, it is no loss of generality to simplify matters by supposing that $a_0 = a_1 = \cdots = a_n = 0$, so that the Chebyshev series of f begins at the term T_{n+1}. For technical simplicity, let us further suppose that the series is a finite one, ending at the term T_N for some $N \geq n+1$. Then f has the Chebyshev series

$$f(x) = \sum_{k=n+1}^{N} a_k T_k(x).$$

We now transplant f to a function F on the unit circle in the complex z-plane by defining $F(z) = F(z^{-1}) = f(x)$ for $|z| = 1$, where $x = \operatorname{Re} z = (z + z^{-1})/2$.

As in the proof of Theorem 3.1, this gives us a formula for F as a Laurent polynomial,

$$F(z) = \frac{1}{2} \sum_{k=n+1}^{N} a_k (z^k + z^{-k}).$$

We can divide F into two parts, $F(z) = G(z) + G(z^{-1})$, with

$$G(z) = \frac{1}{2} \sum_{k=n+1}^{N} a_k z^k.$$

The function G is called the **analytic part** of F, since it can be analytically continued to an analytic function in $|z| \le 1$. Similarly $G(z^{-1})$ is the **coanalytic part** of F, analytic for $1 \le |z| \le \infty$.

Now we ask the following question: what is the best approximation $\tilde{P}$ to G on the unit circle of the form

$$\tilde{P}(z) = \frac{1}{2} \sum_{k=-\infty}^{n} b_k z^k, \tag{20.1}$$

where the series converges for all z with $1 \le |z| < \infty$? In other words, $\tilde{P}$ must be analytic in the exterior of the unit disk apart from a pole of order at most n at $z = \infty$. This is the problem that Carathéodory and Fejér solved, and the solution is elegant. First of all, $\tilde{P}$ exists, and it is unique. Secondly, $G - \tilde{P}$ maps the unit circle onto a perfect circle that winds counterclockwise around the origin a number of times: the winding number is at least $n + 1$. Third, as shown by Schur a few years after Carathéodory and Fejér [Schur 1918], $\tilde{P}$ can be constructed explicitly by solving a certain matrix singular value problem. Let H denote the $(N-n) \times (N-n)$ real symmetric matrix of Chebyshev coefficients arranged like this,

$$H = \begin{pmatrix} a_{n+1} & a_{n+2} & \cdots & a_N \\ a_{n+2} & & & \\ \vdots & & & \\ a_N & & & \end{pmatrix}, \tag{20.2}$$

where the entries in the lower-right triangle are zero. A matrix with this structure, constant along diagonals so that a_{ij} depends only on $i + j$, is called a **Hankel matrix**. Let λ be the largest eigenvalue of H in absolute value, let $u = (u_0, u_1, \ldots, u_{N-n-1})^T$ be a corresponding real eigenvector, and define

$$u(z) = u_0 + u_1 z + \cdots + u_{N-n-1} z^{N-n-1}.$$

Here is the theorem due to Carathéodory and Fejér and Schur.

Theorem 20.1: Carathéodory–Fejér–Schur theorem. *The approximation problem described above has a unique solution $\tilde{P}$, and it is given by the error formula*

$$(G - \tilde{P})(z) = \lambda z^{n+1} \frac{u(z)}{\overline{u(z)}}. \tag{20.3}$$

The function $G - \tilde{P}$ maps the unit circle to a circle of radius $|\lambda|$ and winding number $\ge n+1$, and if $|\lambda| > |\mu|$ for all other eigenvalues μ, the winding number is exactly $n + 1$.

Proof. The result is due to Carathéodory and Fejér [1911] and Schur [1918]. See Theorem 1.1 of [Gutknecht & Trefethen 1982] and Theorem 4 of [Hayashi, Trefethen & Gutknecht 1990]. ∎

Theorem 20.1 is a mathematical assertion about the approximation of a function G on the unit circle by an infinite series. We use this result to construct the polynomial CF approximant as follows. Since $G - \tilde{P}$ maps the unit circle to a circle of winding number $\ge n + 1$, its real part

$$(G - \tilde{P})(z) + (G - \tilde{P})(z^{-1})$$

maps $[-1, 1]$ to an equiscillating curve with at least $n+2$ extreme points. Thus the function

$$\tilde{p}(x) = \tilde{P}(z) + \tilde{P}(z^{-1})$$

yields the equioscillatory behavior that characterizes a best approximation polynomial of degree n to $f(x)$ on $[-1, 1]$ (Theorem 10.1). Unfortunately, $\tilde{p}(x)$ is not a polynomial of degree n. However, it will generally be very close to one. The function $\tilde{P}$ will normally have Laurent series coefficients b_k that decay as $k \to -\infty$. We truncate these at degree $-n$ to define

$$P_{\text{CF}}(z) = \frac{1}{2} \sum_{k=-n}^{n} b_k z^k,$$

with real part (times 2)

$$p_{\text{CF}}(x) = P_{\text{CF}}(z) + P_{\text{CF}}(z^{-1}) = \frac{1}{2} \sum_{k=-n}^{n} (b_k + b_{-k}) z^k.$$

If the truncated terms are small, $f - p_{\text{CF}}$ maps $[-1, 1]$ to a curve that comes very close to equioscillation with $\ge n + 2$ extrema, and thus p_{CF} is close to optimal.

For more details on real polynomial CF approximation, with numerical examples, see [Gutknecht & Trefethen 1982], [Trefethen 1983], and [Hayashi, Trefethen & Gutknecht 1990].

Our experiments in the opening pages of this chapter showed that CF approximants can be exceedingly close to best. The truncation described above gives an idea of how this happens. In the simplest case, suppose f is an analytic function

on $[-1,1]$. Then by Theorem 8.1, its Chebyshev coefficients decrease geometrically, and let us suppose that this happens smoothly at a rate $a_k = O(\rho^k)$. Then roughly speaking, the dominant degree $n+1$ term of f is of order ρ^{-n-1}, and the terms $b_n, b_{n-1}, \ldots, b_{-n}$ are of orders $\rho^{-n-2}, \rho^{-n-3}, \ldots, \rho^{-3n-2}$. This suggests that the truncation in going from $\tilde{p}$ to $p_{\rm CF}$ will introduce an error of order ρ^{-3n-3}. This is usually a very small number, and in particular, much smaller than the error $\|f - p^*\|$ of order ρ^{-n-1}.

In fact, the actual order of accuracy for polynomial CF approximation is one order higher, ρ^{-3n-4} rather than ρ^{-3n-3}. (The reason is that the first truncated term is a multiple of T_{3n+3}, the same Chebyshev polynomial that dominates the error $f-p^*$ itself, and so it is not until the second truncated term, T_{3n+4}, that the equioscillation is broken.) On the other hand, to go from this rough argument to a precise theorem is not so easy, because in fact, Chebyshev series need not decay smoothly (Exericse 20.3). Here we quote without proof a theorem from [Gutknecht & Trefethen 1982].

Theorem 20.2: Accuracy of polynomial CF approximation. *For any fixed $m \geq 0$, let f have a Lipschitz continuous $(3m+3)$rd derivative on $[-1,1]$ with a nonzero $(m+1)$st derivative at $x = 0$, and for each $s \in (0,1]$, let p^* and $p_{\rm CF}$ be the best and the CF approximations of degree m to $f(sx)$ on $[-1,1]$, respectively. Then as $s \to 0$,*

$$\|f - p^*\| = O(s^{m+1}), \quad \neq O(s^{m+2}) \tag{20.4}$$

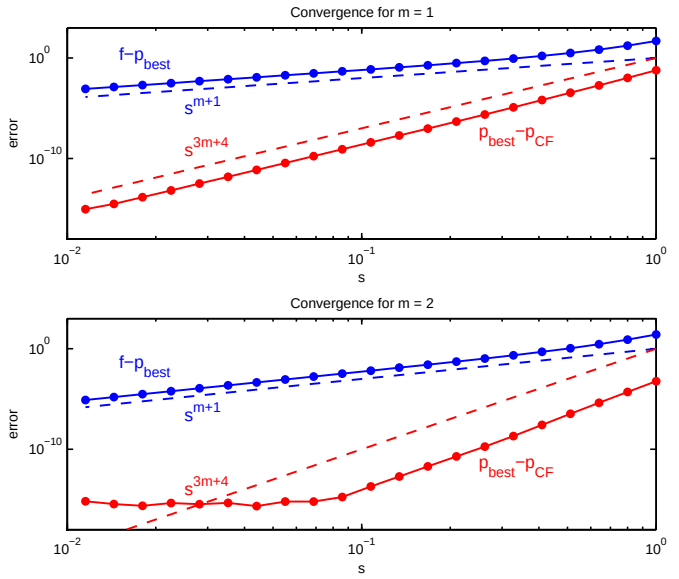
and

$$\|p_{\rm CF} - p^*\| = O(s^{3m+4}). \tag{20.5}$$

Proof. See Theorem 3.4 of [Gutknecht & Trefethen 1982]. ∎

We can verify this result numerically. The two plots below display norms for $m = 1$ and $m = 2$ in the case of the function $f(x) = e^{5x}$.

```
ff = @(x) exp(5*x);
for m = 1:2
  ss = .8.^(0:20); errfp = []; errpp = [];
  for s = ss
    f = chebfun(@(x) ff(s*x));
    pbest = remez(f,m); pcf = cf(f,m);
    errfp = [errfp norm(f-pbest,inf)];
    errpp = [errpp norm(pcf-pbest,inf)];
  end
  hold off, loglog(ss,errfp,'.-')
  hold on, loglog(ss,errpp,'.-r')
  loglog(ss,ss.^(m+1),'--');
  s = 0.025; text(s,.1*s^(m+1)/4,'s^{m+1}',CO,'b',FS,10)
  loglog(ss,ss.^(3*m+4),'--r')
  text(s,.02*s^(3*m+4)*1e4,'s^{3m+4}',CO,'r',FS,10)
  text(.015,.01+(2-m)*.5,'f-p_{best}',CO,'b',FS,10)
  text(.25,1e-12+(2-m)*1e-8,'p_{best}-p_{CF}',CO,'r',FS,10)
  axis([1e-2 1 1e-18 1e3])
  xlabel s, ylabel error
  title(['Convergence for m = ' int2str(m)])
  snapnow
end
```



In this chapter we have considered CF approximation in its simplest context of approximation of one polynomial f of degree N by another polynomial $p_{\rm CF}$ of degree n. In fact, the method is much more general. So long as f has an absolutely convergent Chebyshev series, which is implied for example if it is Lipschitz continuous, then Theorem 20.1 still applies [Hayashi, Trefethen & Gutknecht 1990]. Now H is an infinite matrix which can be shown to represent a compact operator on ℓ^2 or ℓ^1, its dominant eigenvector is an infinite vector, and $u(z)$ is defined by an infinite series. The error curve is still a continuous function of winding number at least $n+1$.

Another generalization is to approximation by rational functions rather than polynomials. Everything goes through in close analogy to what has been written here, and now the other eigenvalues of the Hankel matrix come into play. The theoretical underpinnings of rational CF approximation can be found in papers of Takagi [1924], Adamjan, Arov and Krein [1971], and Trefethen and Gutknecht [1983], as well as the article by Hayashi, Trefethen and Gutknecht cited above. Quite apart from theory, one can compute these approximations readily by the

Chebfun `cf` command using capabilities introduced by Joris van Deun. For details and examples see [Van Deun & Trefethen 2010].

[To be added: (1) Systems theory and Glover.]

SUMMARY OF CHAPTER 20. *Carathéodory–Fejér approximation constructs near-minimax approximations of a function $f \in C[-1,1]$ from the singular values and vectors of a Hankel matrix of Chebyshev coefficients. If f is smooth, CF approximants are often indistinguishable in machine precision from true best approximants.*

Exercise 20.1. Approximating the jagged function. Four of the figures of this chapter concerned approximations of degree 20 to a jagged function. (a) How do the L^2 norms of the best and CF approximations compare? (b) The CF approximation was based on truncation of the Chebyshev series at term $N = 100$. How does the ∞-norm of the error vary with N? (c) Draw a conclusion from this exploration: is the imperfect equioscillation of the error curve in the figure given in the text for this function mostly to the fact that CF approximation is not best approximation, or to the fact that $N < \infty$?

Exercise 20.2. Complex approximation on the unit disk. (a) Suppose f is an analytic function on the closed unit disk and p is a polynomial of degree n. Prove that p is a best approximation to f in the ∞-norm on the disk $|z| \le 1$ if and only if it is a best approximation on the circle $|z| = 1$. (b) Look up Rouché's theorem and write down a careful statement, citing your source. (c) Suppose f is an analytic function in the closed unit disk and p is a polynomial of degree n such that $f - p$ maps the unit circle to a circle of winding number at least $n+1$. Prove that p is a best approximation to f on the unit disk. (In fact it is unique, though this is not obvious.)

Exercise 20.3. Irregularity of CF approximation. The second figure of this chapter showed quite irregular dependence of $\|p_{\rm CF} - p^*\|$ on the degree n for the function $f(x) = \tanh(4(x - 0.3))$. In particular, $n = 15$ and $n = 16$ give very different results. Following the derivation of $p_{\text{tiny CF}}$ in the text, investigate this difference numerically. (a) For $n = 15$, how do the coefficients $|b_k|$ depend on k, and how big are the truncated terms in going from $\tilde{p}$ to $p_{\rm CF}$? (b) Same for $k = 16$.

21. Spectral methods

Theorem 8.2 described the geometric convergence of Chebyshev truncations and interpolants for an analytic function f defined on $[-1,1]$. For such a function, it is not just the polynomials that converge geometrically, but also their derivatives. The following theorem makes this precise. An early publication containing a result along these lines is [Tadmor 1986].

Theorem 21.1: Geometric convergence of derivatives. *Let a function f analytic in $[-1,1]$ be analytically continuable to the closed ρ-ellipse $\overline{E}_\rho$ for some $\rho > 1$. Then for any $\nu \ge 0$, the νth derivatives of the Chebyshev truncations f_n and interpolants p_n satisfy as $n \to \infty$*

$$\|f^{(\nu)} - f_n^{(\nu)}\| = O(\rho^{-n}), \quad \|f^{(\nu)} - p_n^{(\nu)}\| = O(\rho^{-n}). \tag{21.1}$$

Proof. Here is an outline, to be filled in in Exercise 21.1. If f is analytic in the closed ρ-ellipse, it is also analytic and bounded in the open $\tilde{\rho}$-ellipse for some $\tilde{\rho}$ with $\tilde{\rho} > \rho$. From Theorem 8.1 it follows that the Chebyshev coefficients satisfy $a_k = O(\tilde{\rho}^{-k})$. The bounds (21.1) follow by differentiating the Chebyshev series for $f^{(\nu)} - f_n^{(\nu)}$ and $f^{(\nu)} - p_n^{(\nu)}$ term by term. The differentiations introduce powers of n, since T_n' is of size $O(n^2)$ on $[-1,1]$, for example, but since $n^\alpha \tilde{\rho}^{-n} = O(\rho^{-n})$ as $n \to \infty$ for any fixed α, we still get $O(\rho^{-n})$ convergence for any fixed ν. ∎

The phenomenon captured in Theorems 8.2 and 21.1 is a general one in complex analysis. When a bound holds for an analytic function, there is a good chance that a similar bound holds for its derivatives too. The ultimate reason is that both function and derivative can be related to Cauchy integrals, and indeed, an alternative proof of Theorem 21.1 can be based on the Hermite integral formula (Exercise 21.10).

The present chapter is a very practical one, devoted to outlining some of the wide-ranging consequences of Theorem 21.1 for scientific computing: the whole field of **spectral methods** for solving differential equations. Spectral methods are noted for achieving **spectral accuracy**, which means accuracy that is limited not by the order of the numerical discretization, but only by the smoothness of the function being approximated. This is in contrast to a traditional finite difference or finite element method, which might achieve just $O((\Delta x)^2)$ or $O((\Delta x)^4)$ accuracy as $\Delta x \to 0$, say, where Δx is a grid spacing, even when the function being approximated is C^∞ or analytic. For a leisurely introduction to spectral methods on Chebyshev grids, see [Trefethen 2000].

We now drop $\{f_n\}$ and focus on **spectral collocation methods**, based on point values and polynomial interpolants, as opposed to **spectral Galerkin methods** based on integrals.

The fundamental tool of spectral collocation methods is the notion of a **differentiation matrix**. If p is a polynomial of degree n, it is determined by its values on the $(n+1)$-point Chebyshev grid in $[-1,1]$. The derivative p', a polynomial of degree $n-1$, is determined by its values on the same grid. The spectral differentiation matrix associated with this grid is the $(n+1) \times (n+1)$ matrix that represents the linear map from the vector of values of p on the grid to the vector of values of p'.

For example, the function $\sin(x)$ can be represented to machine precision by a Chebyshev interpolant p on a grid of 14 points:

```
p = sin(x);
length(p)

ans = 14
```

Suppose we wish to calculate the values of p' on the same grid. In Chebfun we can write

```
pp = diff(p);
x14 = chebpts(14);
pp14 = pp(x14)

pp14 =
   0.540302305868163
   0.564522388819887
   0.632936510563863
   0.732703188872980
   0.842943722651217
   0.937783753082982
   0.992744245701781
   0.992744245701781
   0.937783753082982
   0.842943722651217
   0.732703188872979
   0.632936510563863
   0.564522388819890
   0.540302305868169
```

But we can also get our hands on the differentiation matrix explicitly, with these commands:

```
[d,x] = domain([-1 1]);
D = diff(d);
D14 = D(14);
```

If the matrix `D14` is multiplied by the vector `p(x14)`, the result is the same vector `pp14` of sampled derivatives, up to rounding errors:

```
norm(pp14-D14*p(x14))

ans = 2.216084139546628e-14
```

Above, we put a semicolon after `D(14)` to avoid printing a 14×14 matrix. To give the idea while using up a little less space, here are the 3×3 and 5×5 Chebyshev differentiation matrices on $[-1, 1]$:

```
format short
D(3)

ans =
   -1.5000    2.0000   -0.5000
   -0.5000         0    0.5000
    0.5000   -2.0000    1.5000

D(5)

ans =
   -5.5000    6.8284   -2.0000    1.1716   -0.5000
   -1.7071    0.7071    1.4142   -0.7071    0.2929
    0.5000   -1.4142         0    1.4142   -0.5000
   -0.2929    0.7071   -1.4142   -0.7071    1.7071
    0.5000   -1.1716    2.0000   -6.8284    5.5000
```


Formulas for the entries of Chebyshev differentiation matrices were first published by Gottlieb, Hussaini & Orszag [1984], and recurrence relations for computing them fast and stably were given by Welfert [1997], based on earlier work by Fornberg [1988]. Welfert's paper in turn led to the influential MATLAB Differentiation Matrix Suite by Weideman and Reddy [2000].

There is no need to stop at the first derivative. Here is the 5×5 Chebyshev matrix corresponding to the second derivative on $[-1, 1]$:

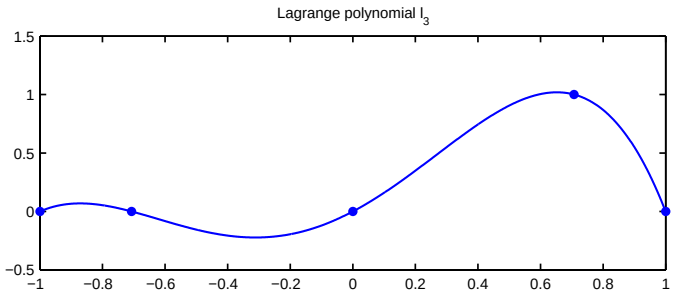
```
D2 = diff(d,2);
D2(5)

ans =
   17.0000  -28.4853   18.0000  -11.5147    5.0000
    9.2426  -14.0000    6.0000   -2.0000    0.7574
   -1.0000    4.0000   -6.0000    4.0000   -1.0000
    0.7574   -2.0000    6.0000  -14.0000    9.2426
    5.0000  -11.5147   18.0000  -28.4853   17.0000
```

Yes, `D2(5)` is the square of `D(5)`:

```
norm(D2(5)-(D(5))^2)

ans = 5.5939e-15
```

The entries of this matrix can be interpreted as follows. The jth column ($0 \le j \le n$) contains the second derivatives of the Lagrange polynomial $\ell_j(x)$ evaluated at grid points $x_0, \ldots, x_n$. That is, its (i, j) entry (with indexing from 0 to n) is $\ell_j''(x_i)$. (We have seen Lagrange polynomials in Chapters 5, 9 and 15.) For example, here is the Lagrange polynomial supported at x_3:

```
p3 = chebfun([0 0 0 1 0]);
clf, plot(p3,'.-')
title('Lagrange polynomial l_3')
```



Its second derivatives at the grid points are the values in the fourth column of the matrix $D(5)$ just shown:

```
p3pp = diff(p3,2);
x5 = chebpts(5);
p3pp(x5)
```

```
ans =
  -11.5147
   -2.0000
    4.0000
  -14.0000
  -28.4853
```

In Chebfun, an object like `D` or `D2` is called a **linop**. A linop is not a matrix, but rather a prescription for how to construct matrices of arbitrary order. (The computer science term for the process of filling such prescriptions is *lazy evaluation*.) If D is applied to an integer argument, the matrix of that dimension is produced,

```
size(D(33))
```

```
ans =
    33    33
```

If D is applied to a chebfun, it has the effect appropriate to the length of that chebfun:

```
f = sin(7*x).*exp(x).*tan(x);
norm(diff(f)-D*f)
```

```
ans = 0
```

Algebraic operations have been overloaded in Chebfun so that one can construct differential operators by combining these operations. For example, here is the linop corresponding to the map $L : u \mapsto u'' + u' + 100u$ on $[-1, 1]$:


```
L = diff(d,2) + diff(d) + 100;
```

An equivalent formulation, making explicit reference to the overloaded identity operator, would be

```
L = diff(d,2) + diff(d) + 100*eye(d);
```

Here is the 5×5 realization of this operator:

```
L(5)
```

```
ans =
  111.5000  -21.6569   16.0000  -10.3431    4.5000
    7.5355   86.7071    7.4142   -2.7071    1.0503
   -0.5000    2.5858   94.0000    5.4142   -1.5000
    0.4645   -1.2929    4.5858   85.2929   10.9497
    5.5000  -12.6863   20.0000  -35.3137  122.5000
```

We can illustrate its use by applying it to the chebfun for e^x:

```
f = exp(x);
Lf = L*f;
Lfexact = 102.*exp(x);
norm(Lf-Lfexact)
```

```
ans = 1.6795e-13
```

Now we come at last to spectral methods proper. If we just wanted to apply differential operators to functions, we would not need matrices. To solve a differential equation, however, we need to invert the process of applying a differential operator. We want to find a function u satisfying certain boundary conditions such that Lu is equal to a prescribed function f. This is where the matrices come in, for matrices can be inverted.

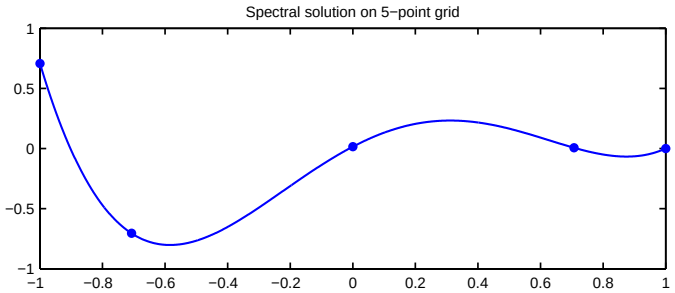
Suppose we ask, for example, what function u satisfies $u'' + u' + 100u = x$ on $[-1, 1]$ with boundary conditions $u(-1) = u(1) = 0$? The matrix realization above was in the absence of boundary conditions. Now we need to impose them, and the standard way of doing this is to modify one or more initial or final rows of the matrix, one row for each boundary condition (see Chapters 7 and 13 of [Trefethen 2000]). For Dirichlet boundary conditions, we change the first and last rows to correspond to rows of the identity:

```
L.bc = 'dirichlet';
L(5)
```

```
ans =
   50.1147   50.2700   -0.5000    0.1941   -0.0788
   -0.5000    2.5858   94.0000    5.4142   -1.5000
   -0.1147    0.2656   -0.5000   43.2703   57.0788
    1.0000         0         0         0         0
         0         0         0         0    1.0000
```

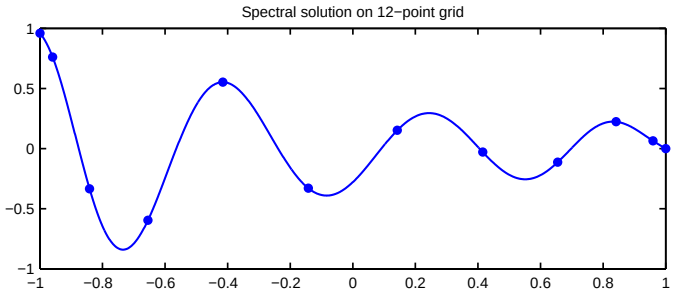
We can now use exactly this matrix to solve the ODE approximately with a 5×5 spectral discretization. The right-hand side of the matrix problem will be the vector of x sampled at the Chebyshev points — except that the first and last components of the vector will be changed to the appropriate Dirichlet values at x_0 and x_n, which are zero by default.

```
x5 = chebpts(5); x5([1 end]) = 0;
u5 = L(5)\x5;
plot(chebfun(u5),'.-')
title('Spectral solution on 5-point grid')
```



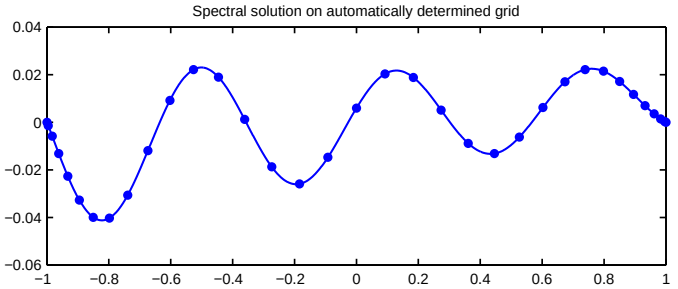
We have just computed our first solution of a boundary value problem with a spectral method. From the picture it is not evident whether the result is close to correct or not. In fact it is not, as increasing the resolution reveals:

```
x12 = chebpts(12); x12([1 end]) = 0;
u12 = L(12)\x12;
plot(chebfun(u12),'.-')
title('Spectral solution on 12-point grid')
```



This curve, as it happens, is begining to get close to the true solution. How fine a grid do we need to reach approximately machine precision? In Chebfun, the appropriate grid is determined automatically when one solves the problem without specifying dimensions, still with the backslash command:


```
u = L\x;
plot(u,'.-')
title('Spectral solution on automatically determined grid')
```



To get this result, Chebfun has solved matrix problems of size 9, 17, 33 and so on until its convergence criteria are satisfied. The final length is

```
length(u)
```

```
ans = 35
```

and we can verify that the accuracy is good:

```
norm(L*u-x)
```

```
ans = 1.0859e-13
```

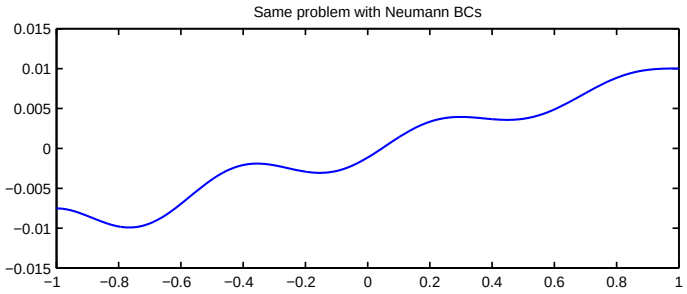
Of course, homogeneous Dirichlet conditions at both ends are only the simplest of innumerable possible boundary conditions for a boundary value problem. For a full account of how various boundary conditions can be specified in Chebfun, and how one can solve coupled systems of equations, see `help linop` and `help linop/and`. We give here just one more example. To solve the same ODE with homogeneous Neumann boundary conditions (i.e. $u'(-1) = u'(1) = 0$), the first and last rows get replaced by the corresponding rows of the first derivative matrix:

```
L.bc = 'neumann';
format short
L(5)
```

```
ans =
   50.1147   50.2700   -0.5000    0.1941   -0.0788
   -0.5000    2.5858   94.0000    5.4142   -1.5000
   -0.1147    0.2656   -0.5000   43.2703   57.0788
   -5.5000    6.8284   -2.0000    1.1716   -0.5000
    0.5000   -1.1716    2.0000   -6.8284    5.5000
```

Here is the solution, now plotted without dots:

```
u = L\x;
plot(u), ylim([-0.015 0.015])
title('Same problem with Neumann BCs')
```

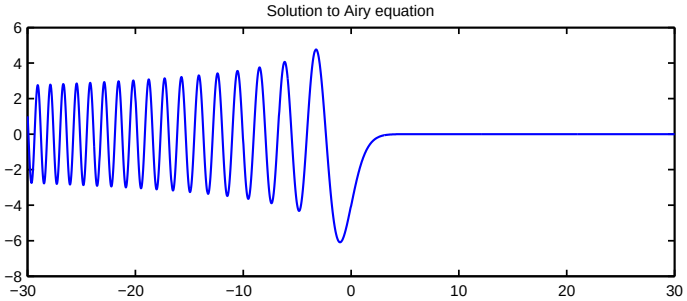


Spectral methods also solve problems with smooth variable coefficients. For example, suppose we wish to solve the Airy equation boundary value problem

$$u'' - xu = 0, \quad x \in [-30, 30],\ x(-30) = 1,\ x(30) = 0.$$

The variable coefficient corresponds to a **multiplier operator** $u \mapsto xu$, realized in Chebfun by an overloaded `diag` command. Here is the solution:

```
[d,x] = domain(-30,30);
L = diff(d,2) - diag(x);
L.lbc = 1; L.rbc = 0;
u = L\0;
plot(u)
title('Solution to Airy equation')
```



Spectral methods are good for nonlinear problems, too. Here one would normally use a Newton iteration or some variant. Chebfun allows nonlinear equations (and boundary conditions) to be prescribed in what is called a **chebop**,

specified via anonymous functions of the dependent variable. For example, the equation

$$\theta'' + \sin(\theta) = 0, \quad \theta \in [0, 6]$$

describes a nonlinear pendulum situated at height

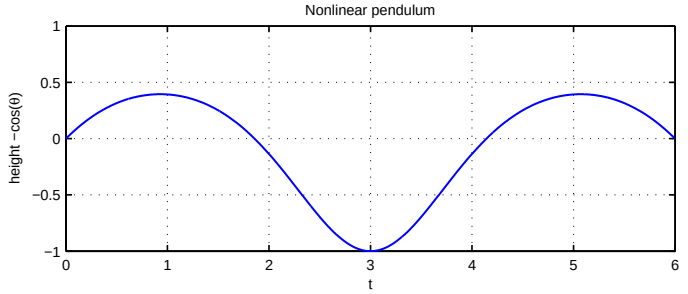
$$h = -\cos(\theta) \in [-1, 1].$$

If we prescribe boundary conditions

$$u(0) = -\pi/2, \quad u(6) = \pi/2,$$

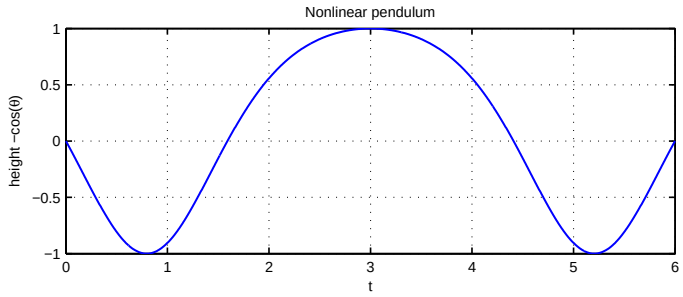
we can solve the system numerically with Chebfun like this. The backslash command is used again in this nonlinear context, though we are very far now from Matlab's original notion of solving a square system of linear equations.

```
[d,t,N] = domain(0,6);
N.op = @(theta) diff(theta,2) + sin(theta);
N.lbc = -pi/2; N.rbc = pi/2;
theta = N\0;
plot(-cos(theta)), grid on, ylim([-1 1])
title('Nonlinear pendulum')
xlabel t, ylabel('height -cos(\theta)')
```



This solution corresponds to the pendulum first going up above height 0 for a time, then swinging over to the other side, where it again goes above height 0. On the other hand suppose we change the right boundary condition to $5\pi/2$. Then another solution appears, corresponding to the pendulum swinging once around the top:

```
N.lbc = -pi/2; N.rbc = 5*pi/2;
theta = N\0;
plot(-cos(theta)), grid on, ylim([-1 1])
title('Nonlinear pendulum')
xlabel t, ylabel('height -cos(\theta)')
```



These solutions are not unique; see Exercise 21.9.

To compute solutions of nonlinear differential equations, Chebfun uses variants of Newton's method implemented for continuous functions rather than discrete vectors. The required "Jacobian matrices" are actually Fréchet derivative operators, which are constructed by a process of automatic differentiation. These facilities are due to Ásgeir Birkisson and Toby Driscoll.

This is a book about approximation theory, and we began this chapter with a fine approximation result, a theorem about the $O(\rho^{-n})$ accuracy of derivatives. It would be good if this theorem implied that spectral methods converge to analytic solutions at the rate $O(\rho^{-n})$, but it does not. Theorem 21.1 ensures that if u is an analytic solution to a boundary value problem $Lu = f$, then the Chebyshev interpolants to Lu would converge geometrically to f as $n \to \infty$. In spectral computations, however, we don't have the exact solution available to discretize, but must approximate it by solving matrix problems. One can hope that the approximations will converge at the expected rate, and indeed they do under many circumstances, but proving this requires further arguments, which we shall not discuss here.

Some of the ideas behind spectral methods are as old as Fourier and Chebyshev expansions, and many people contributed in the early years of computers including Lanczos, Elliott, Fox, and Clenshaw. But it was their application to the partial differential equations of fluid mechanics by Orszag beginning around 1970 that made these methods famous, and it was Orszag whose coined the term "spectral methods" [Orszag 1971a & 1971b]. Spectral methods divide into Fourier methods, for periodic problems, and Chebyshev and related methods, for nonperiodic problems. As always in this book we have emphasized the nonperiodic case, which is less obvious even though at bottom, mathematically, it is much the same. In applications, Fourier and Chebyshev are often found mixed together. For example, a 3D cylindrical geometry may be discretized by a nonperiodic Chebyshev grid for the radial variable, a periodic Fourier grid for the circumferential variable, and another periodic grid serving as an approximation to an ideal infinite Fourier grid for the longitudinal variable.

For details of the spectral methods incorporated in Chebfun, see [Driscoll, Bornemann & Trefethen 2008] for the linear case and [Birkisson & Driscoll 2010] for the nonlinear case. For information about spectral methods in general, see textbooks and monographs such as [Boyd 2001], [Fornber 1996], [Trefethen 2000] and [Canuto, Hussaini, Quarteroni and Zang 2006].

[To be added: (1) Tadmor says look up Sobolev inequality in Canuto and Quarteroni 1981. (2) Give barycentric formula for derivatives. (3) Give slick formula for entries of differentiation matrix. (4) Look up tau method in Lanczos Applied Analysis book. (5) Cheb pts for nonlinear DEs: Clenshaw and Norton 1963, Computer J, also Norton, Comp J 7. Integral eqs: Elliott 1963 Comp J 6. Linear diffl eqs: Clenshaw, The numer soln of linear diffl eqs in Cheb series, Proc Camb Phil Soc 53 (1957), 134–149. (6) Legendre diff matries: Berrut says see Bellman/Kashef/Casti JCP 1972. (7) Modify text for the rectangular differentiation matrices of Chebfun Version 4.]

SUMMARY OF CHAPTER 21. *Spectral collocation methods are numerical algorithms for solving differential equations based on polynomial or trigonometric interpolants. For problems with analytic solutions, they typically converge geometrically as the grid is refined.*

Exercise 21.1. Proof of Theorem 21.1. Write down a careful proof of Theorem 21.1 as a corollary of Theorems 3.1 and 8.1. Be sure to state precisely what properties of the Chebyshev polynomials $\{T_k\}$ your proof depends on.

Exercise 21.2. Differentation matrices. (a) The text displayed the 3×3 matrix $D(3)$. Derive the entries of this matrix analytically. (b) Also displayed was the 5×5 matrix $D2(5)$. Derive the entries of the middle column of this matrix analytically.

Exercise 21.3. Linear boundary value problems. Solve the following linear ODE boundary value problems numerically with Chebfun. In each case plot the solution and report the value of u at the midpoint of the interval and the length of the chebfun representing u.
(a) $0.001u'' + xu' - u = \exp(-10x^2)$, $x \in [-1,1]$, $u(-1) = 2$, $u(1) = 1$.
(b) $0.001u'' + (1-x^2)u = 1$, $x \in [-5,5]$, $u(-5) = 0$, $u(5) = 0$.
(c) $0.001u'' + \sin(x)u = 1$, $x \in [-10,10]$, $u(-10) = 0$, $u'(10) = 0$.

Exercise 21.4. Nonlinear boundary value problems. Find a solution numerically to each of the following nonlinear ODE boundary value problems. In each case plot the solution and report the value $u(0)$ at the midpoint of the interval.
(a) $0.05u'' + (u')^2 - u = 1$, $x \in [0,1]$, $u(0) = 2$, $u(1) = 1$.
(b) $0.03u'' - uu' - u = 0$, $x \in [-1,1]$, $u(-1) = 1$, $u(1) = 2$.

Exercise 21.5. Convergence with n. The text solved the boundary value problem $u'' + u' + 100u = x$ on $[-1,1]$ with boundary conditions $u(-1) = u(1) = 0$ for grid parameters $n+1 = 5$, 12, and 35. Perform a numerical study of the ∞-norm error of the solution as a function of n, and comment on the results.

Exercise 21.6. Bessel equation. [to be written]

Exercise 21.7. Rectangular differentiation matrices. [to be written]

Exercise 21.8. eigs. [to be written]

Exercise 21.9. Nonunique solutions. (a) For each of the two nonlinear pendulum problems solved at the end of the chapter, figure out on paper exactly how many solutions there must be. (You can use physical reasoning, or phase plane analysis.) (b) Find them numerically with Chebfun by using initial guesses of the form `N.guess = f(theta)` to start the iteration. Report the maximum heights $-\cos(\theta)$ of the pendulum in all cases, and the time(s) at which these heights are reached.

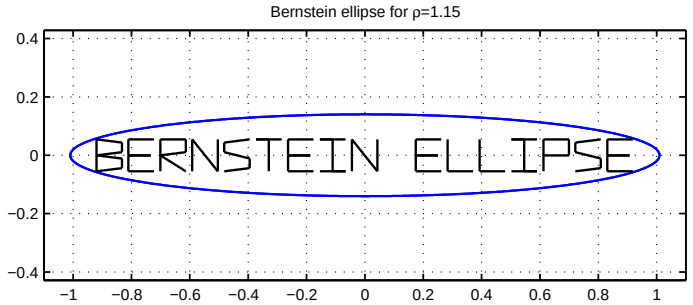
Exercise 21.10. Proof by Hermite integral formula.

22. Linear approximations: beyond polynomials

Several times in the previous chapters, we have hinted that polynomials are not optimal functions for linear approximation. (Nonlinear approximations are another matter and will make their appearance in the next chapter.) It is now time to explain these hints and introduce alternative approximations that may be up to $\pi/2$ times more efficient. One reason the alternatives are valuable is that they have practical advantages in some applications, especially for spectral methods in more than one space dimension. An equally important reason is that they push us to think more deeply about what it means to approximate a function and what may or may not be special about polynomials. The ideas of this chapter originate in [Hale & Trefethen 2008]. Related ideas are the basis of work on sinc function numerical methods [Stenger 1993 & 2010], tanh and double exponential or tanh-sinh quadrature [Sag & Szekeres 1964, Takahasi & Mori 1974, Mori & Sugihara 2001], and the transformed-grid spectral methods introduced by Kosloff and Tal-Ezer [1993].

Recall from Chapter 8 that if f is analytic on $[-1,1]$, then to investigate its polynomial approximations, we ask how large a Bernstein ellipse f can be analytically continued to with foci ± 1. We parametrize such an ellipse by the sum of its semimajor and semiminor axis lengths, a quantity denoted by $\rho > 1$. Here for example is the ellipse E_ρ with $\rho = 1.15$. The words "Bernstein ellipse" written inside will help in a moment to visualize a conformal map. (Mathematically, these words are a piecewise linear complex function of a real variable constructed by the Chebfun `scribble` command.)

```
w = exp(2i*pi*x);
z = @(rho) (rho*w+(rho*w).^(-1))/2;
clf, plot(z(1.15)), xlim([-1.1,1.1]), axis equal, grid on
title('Bernstein ellipse for \rho=1.15')
f = .01-.055i+.93*scribble('Bernstein ellipse');
hold on, plot(f,'k',LW,1.2)
```

Bernstein ellipses are unavoidable if one works with polynomial interpolants, but from the user's point of view, they have an unfortunate property: they are thicker in the middle than near the ends! For a function f to be analytic in the region just shown, its Taylor series about a point $x \approx 0$ must have radius of convergence 0.15 or more. For $x \approx \pm 1$, on the other hand, a radius of convergence of 0.05 or less is sufficient. Thus the smoothness requirement on f is nonuniform, and this is not an artifact of the analysis. Polynomials of a given degree really can resolve rougher behavior of a function f near the endpoints than in the middle. This phenomenon turns up in one form of another whenever approximation theorists seek sharp results about polynomial approximation, whether f is analytic or not. See for example [Timan 1951], [Lorentz 1986], and [Ditzian & Totik 1987].

Of course, there are some functions that have most of their complexity near ± 1, and for these, the nonuniform approximation power of polynomials may be an advantage. For example, functions of this kind arise in fluid mechanics problems with boundary layers. More often, however, the nonuniform approximation power of polynomials is a disadvantage from a practical point of view, as well as being a complication conceptually. If only those ellipses had constant width for all $x \in [-1,1]$!

As soon as one frames the difficulty in this way, a possibility for a solution suggests itself. The idea is to change variables by means of a function that conformally maps ellipses, approximately at least, to straight-sided ε-neighborhoods of $[-1,1]$, while mapping $[-1,1]$ to itself. To explore this idea we shall use the variable x for the domain where f is defined and introduce a new variable s for the parameter domain, where the Chebyshev points and ellipses live. Our conformal map will be $x = g(s)$, and we shall approximate a function $f(x)$ on $[-1,1]$ by $p(g^{-1}(x)) = p(s)$, where p is a polynomial. Equivalently, we shall approximate $f(g(s))$ on $[-1,1]$ by a polynomial. In the remainder of this chapter we explore the consequences of this idea, considering just one fixed example of a map g,

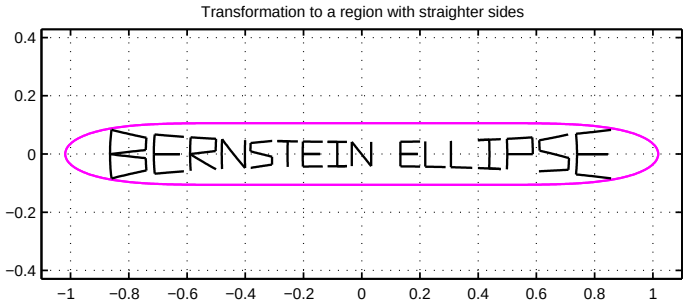
$$g(s) = \frac{1}{53089}(40320s + 6720s^3 + 3024s^5 + 1800s^7 + 1225s^9) \qquad (22.1)$$

```
g = chebfun(@(s) (40320*s+6720*s.^3+3024*s.^5+ ...
                          1800*s.^7+1225*s.^9)/53089);
```

See [Hale & Trefethen 2008] for an explanation of where this choice of g comes from and an investigation of other possibilities, some of which (notably a conformal map onto an infinite strip) come closer to realizing the maximum possible improvement by a factor of $\pi/2$. See also Exercises 22.2 and 22.3.

To begin the discussion, let us look at how g transforms ellipses about $[-1,1]$. Here is a plot of $g(E_{1.15})$, the transformed version of the ellipse shown earlier. Notice the much straighter sides.

```
hold off, plot(g(z(1.15)),'m')
xlim([-1.1,1.1]), axis equal, grid on
title('Transformation to a region with straighter sides')
hold on, plot(g(f),'k',LW,1.2)
```



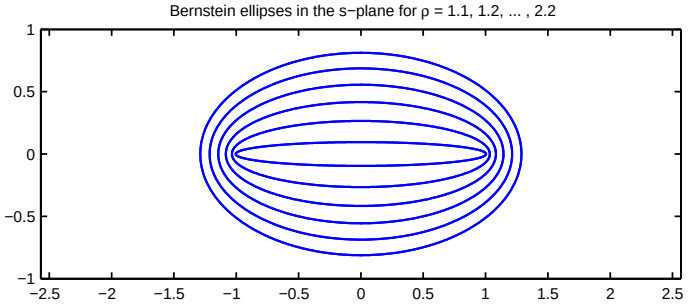
Following [Hale & Trefethen 2008], we call g a **sausage map** and $g(E_{1.15})$ a **sausage region**. The crucial property is that for most of its length, the sausage is narrower than the ellipse, as the distorted "Bernstein ellipse" label makes clear. The ellipse has half-width approximately $\rho - 1$, which is about 32% more than the half-width $0.76\,(\rho - 1)$ of the sausage:

```
format short
ellipse_width = max(imag(z(1.1)))
sausage_width = max(imag(g(z(1.1))))
ratio = ellipse_width/sausage_width
```

```
ellipse_width =
    0.0955
sausage_width =
    0.0724
ratio =
    1.3187
```

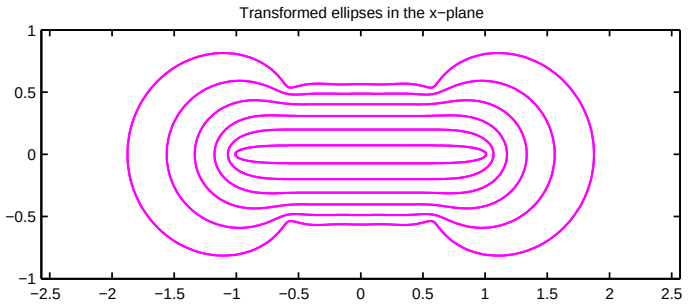

We can learn more by looking at a family of ellipses. Following Chapter 8, here is a plot of E_ρ for $\rho = 1, 1.2, \ldots, 2.2$:

```
w = exp(2i*pi*x);
hold off
for rho = 1.1:0.2:2.2
    plot((rho*w+(rho*w).^(-1))/2), hold on
end
ylim([-1 1]), axis equal
title(['Bernstein ellipses in the s-plane'...
       ' for \rho = 1.1, 1.2, ... , 2.2'])
```



Here is the corresponding figure for the images $g(E_\rho)$:

```
hold off
for rho = 1.1:0.2:2.2
    plot(g((rho*w+(rho*w).^(-1))/2),'m'), hold on
end
ylim([-1 1]), axis equal
title('Transformed ellipses in the x-plane')
```

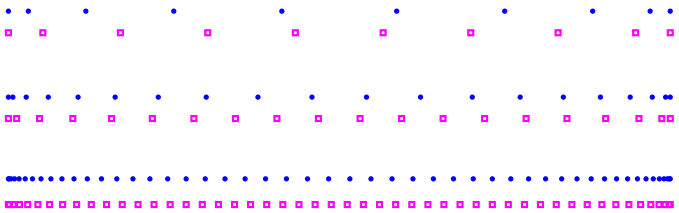


It is clear that near $[-1,1]$, the transformed ellipses are narrower and more uniform in shape than the ellipses, but further away, their behavior is more

irregular. We shall see something of the implications of these shapes as we explore the uses of this map.

Chapter 2 considered polynomial interpolants in Chebyshev points $\{s_k\}$. With the transformation g, f is interpolated by transformed polynomials $p(g^{-1}(x))$ in the points $\{g(s_k)\}$. We illustrate the difference between Chebyshev and transformed Chebyshev points by adapting a code segment from Chapter 17. The squares show the transformed points.

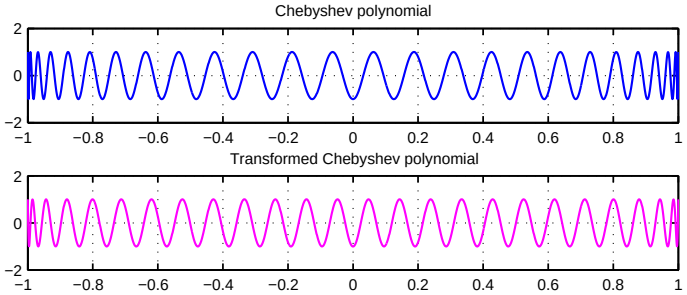
```
ss = chebpts(10);
clf, plot(ss,.9,'.b',MS,8), hold on, plot(g(ss),.8,'sm',MS,3)
ss = chebpts(20);
plot(ss,.5,'.b',MS,8), plot(g(ss),.4,'sm',MS,3)
ss = chebpts(50);
plot(ss,.12,'.b',MS,8), plot(g(ss),0,'sm',MS,3)
axis([-1 1 -.1 1.1]), axis off
```



Note that the squares are more evenly distributed than the dots, and in particular, they are denser in the middle, providing finer resolution.

Chapter 3 considered Chebyshev polynomials and series. We adapt another code segment from Chapter 17 to illustrate how a Chebyshev polynomial $T_n(x)$ compares to the corresponding transformed polynomial $T_n(g^{-1}(x))$. For this we need the inverse map g^{-1}.

```
gi = inv(g);
T50 = chebpoly(50); subplot(2,1,1), plot(T50), axis([-1 1 -2 2])
title('Chebyshev polynomial')
grid on, subplot(2,1,2)
plot(T50(gi),'m'), axis([-1 1 -2 2])
grid on, title('Transformed Chebyshev polynomial')
```

Notice that the lower curves are more like uniform sine waves than the upper ones.

Theorem 3.1 summarized some basic facts about Chebyshev series, and these carry over immediately to a theorem for transformed Chebyshev series. The theorem as stated assumes g is analytic, though in fact, continuous differentiability would be enough.

Theorem 22.1: Transformed Chebyshev series. *Let g be an analytic function on $[-1,1]$ mapping $[-1,1]$ to itself with $g'(s) > 0$. Then if f is Lipschitz continuous on $[-1,1]$, it has a unique representation as an absolutely convergent series*

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(g^{-1}(x)), \tag{22.2}$$

and the coefficients are given for $k \geq 1$ by the formula

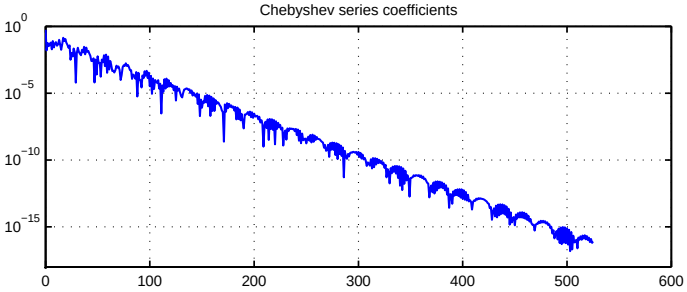
$$a_k = \frac{2}{\pi} \int_{-1}^{1} \frac{f(g(s))T_k(s)}{\sqrt{1-s^2}} ds, \tag{22.3}$$

and for $k = 0$ by the same formula with the factor $2/\pi$ changed to $1/\pi$.

Proof. This is a straightforward consequence of Theorem 3.1. ∎

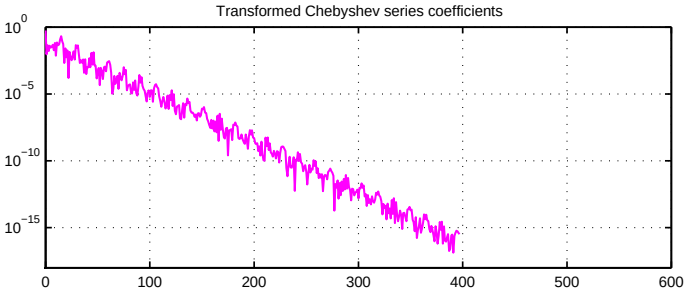
For many functions f, the transformed series are about 30% more efficient than the originals. For example, Chebyshev interpolation of $(2 + \cos(20x + 1))^{-1}$ requires about 520 terms for 15-digit accuracy:

```
f = 1./(2+cos(20*x+1));
clf, chebpolyplot(f), grid on, axis([0 600 1e-18 1])
title('Chebyshev series coefficients')
```



For the transformed interpolants the figure is closer to 400:

```
chebpolyplot(f(g),'m'), grid on, axis([0 600 1e-18 1])
title('Transformed Chebyshev series coefficients')
```



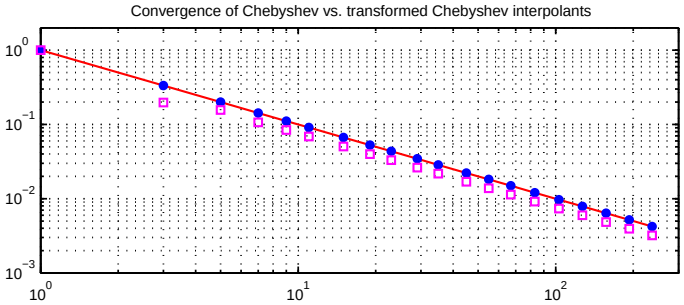
Chapter 7 considered convergence for differentiable functions. Theorem 7.2 can readily be restated for the transformed context — see Exercise 22.1. For a numerical illustration, here is a repetition of the experiment from Chapter 7 involving $f(x) = |x|$. On the loglog scale, the transformed approximants run parallel to the same line as the Chebyshev interpolants, but lower.

```
f = abs(x); fg = f(g);
nn = 2*round(2.^(0:.3:7))-1;
ee = 0*nn; ee2 = 0*nn;
for j = 1:length(nn)
    n = nn(j);
    fn = chebfun(f,n+1); ee(j) = norm(f-fn,inf);
    fn2 = chebfun(fg,n+1); ee2(j) = norm(fg-fn2,inf);
end
hold off, loglog(nn,1./nn,'r')
grid on, axis([1 300 1e-3 2])
hold on, loglog(nn,ee,'.'), loglog(nn,ee2,'sm',MS,5)
ratio = ee(end-4:end)./ee2(end-4:end)
title(['Convergence of Chebyshev vs. '...
```



```
    'transformed Chebyshev interpolants'])
```

```
ratio =
    1.3167    1.3167    1.3167    1.3167    1.3167
```



Chapter 8 considered convergence for analytic functions. Here is the transformed equivalent of Theorems 8.1 and 8.2.

Theorem 22.2: Transformed coefficients of analytic functions. *For given $\rho > 1$, let g and f be analytic functions on $[-1,1]$ that can be analytically continued to E_ρ and $g(E_\rho)$, respectively, with $|f(z)| \le M$ for $z \in g(E_\rho)$. Then the transformed Chebyshev coefficients of Theorem* 22.1 *satisfy*

$$|a_k| \le 2M\rho^{-n}, \tag{22.4}$$

the truncated transformed series satisfy

$$\|f - p_n(g^{-1}(x))\| \le \frac{2M\rho^{-n}}{\rho - 1}, \tag{22.5}$$

and the transformed Chebyshev interpolants satisfy

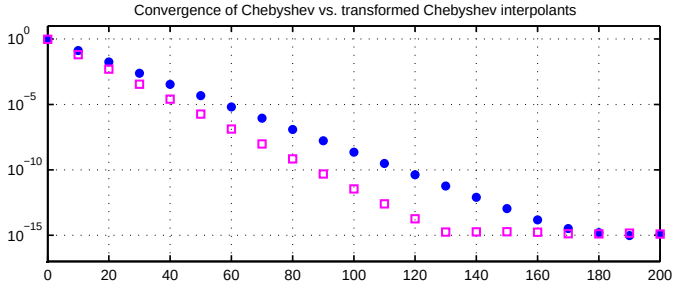
$$\|f - p_n(g^{-1}(x))\| \le \frac{4M\rho^{-n}}{\rho - 1}. \tag{22.6}$$

Proof. These results follow from Theorems 8.2 and 22.1. ∎

Here is a repetition of the Chapter 8 experiment for the Runge function, now with squares to show the transformed approximants.

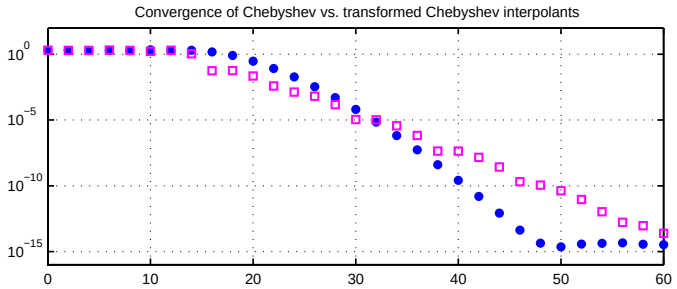
```
f = 1./(1+25*x.^2); fg = f(g);
nn = 0:10:200;
ee = 0*nn; ee2 = 0:nn;
for j = 1:length(nn)
    n = nn(j);
    fn = chebfun(f,n+1); ee(j) = norm(f-fn,inf);
```

```
    fn2 = chebfun(fg,n+1); ee2(j) = norm(fg-fn2,inf);
end
hold off, semilogy(nn,ee,'.')
hold on, semilogy(nn,ee2,'sm',MS,5)
grid on, axis([0 200 1e-17 10])
title(['Convergence of Chebyshev vs. '...
       'transformed Chebyshev interpolants'])
```



The speedup is clear. On the other hand, here is a repetition of the experiment with $\cos(20x)$.

```
f = cos(20*x); fg = f(g);
nn = 0:2:60;
ee = 0*nn; ee2 = 0:nn;
for j = 1:length(nn)
    n = nn(j);
    fn = chebfun(f,n+1); ee(j) = norm(f-fn,inf);
    fn2 = chebfun(fg,n+1); ee2(j) = norm(fg-fn2,inf);
end
hold off, semilogy(nn,ee,'.')
hold on, semilogy(nn,ee2,'sm',MS,5)
grid on, axis([0 60 1e-16 100])
title(['Convergence of Chebyshev vs. '...
       'transformed Chebyshev interpolants'])
```

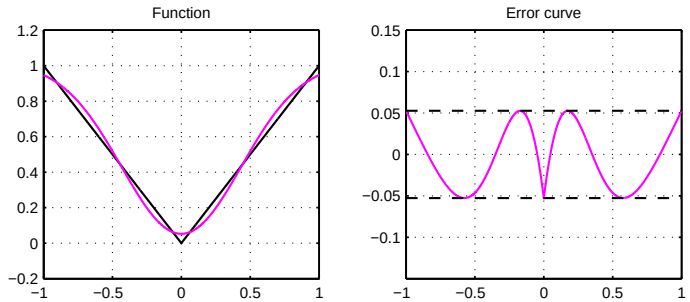


Now the result is ambiguous: the transformed method starts out ahead, but the standard Chebyshev method wins eventually. The explanation can be found in the nested ellipses E_ρ and their images plotted earlier. The function $\cos(20x)$ is entire, and for larger n, the Chebyshev points take good advantage of its analyticity well away from $[-1,1]$. The transformed points do not do as well. (The advantage of the transformation becomes decisive again if we change $\cos(20x)$ to $\cos(100x)$.)

We can see similar effects if we look at best approximations. For a non-smooth function like $|x|$, transformed polynomials typically approximate better than true ones. The following figures should be compared with those of Chapter 10, and the variable `ratio` quantifies the degree of improvement.

```
f = abs(x);
subplot(1,2,1), hold off, plot(f,'k'), grid on
fg = f(g);
[p,err] = remez(fg,4);
hold on, plot(p(gi),'m'), axis([-1 1 -.2 1.2])
title Function, subplot(1,2,2), hold off
plot(g,f-p(gi),'m'), grid on, hold on, axis([-1 1 -.15 .15])
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
[p2,err2] = remez(f,4); ratio = err2/err, title('Error curve')
```

```
ratio =
    1.2847
```

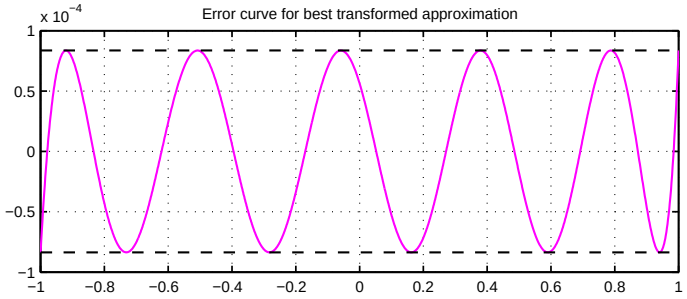


On the other hand for a gentle entire function like $\exp(x)$, pure polynomials converge very fast and transformed polynomials cannot compete. The following error curve is seven orders of magnitude bigger than that of Chapter 10.

```
f = exp(x);
fg = f(g);
[p,err] = remez(fg,10);
clf, plot(g,fg-p,'m'), grid on, hold on
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
```

```
[p2,err2] = remez(f,10); ratio = err2/err
xlim([-1 1])
title('Error curve for best transformed approximation')
```

```
ratio =
   2.9938e-07
```



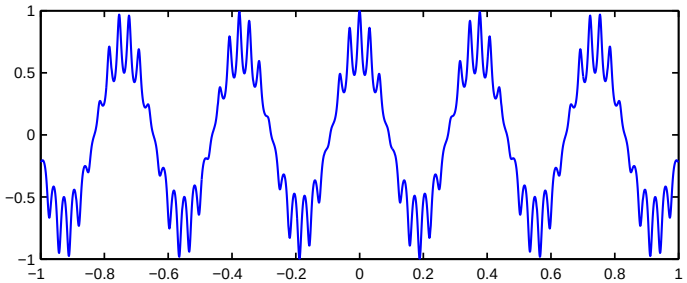
Our final application of transformed polynomial approximants is the one that is the subject of the original paper [Hale & Trefethen 2008]: quadrature. As described in Chapter 19, standard quadrature formulas are based on the idea of integrating a function numerically by interpolating it by a polynomial, then integrating the interpolant. This is the basis of all the well-known quadrature formulas, including Gauss, Newton–Cotes, Simpson, and Clenshaw–Curtis. But why should quadrature formulas be based on polynomials? This is not a question often encountered in the quadrature literature. Some of the explanation surely has to do with custom going back centuries, before the appearance of computers, when the algebraic simplicity of polynomials would have been a telling advantage. If one had to give a mathematical answer with still some validity today, it would probably be that a polynomial formula is optimal if the order is fixed while the grid size is decreased to zero. If the order increases to ∞, however, polynomial formulas are in no sense optimal.

In particular, a "transformed Gauss" quadrature formula can be obtained by applying Gauss quadrature to the integral on the right in the formula

$$\int_{-1}^{1} f(x) = \int_{-1}^{1} f(g(s))g'(s)ds. \tag{22.7}$$

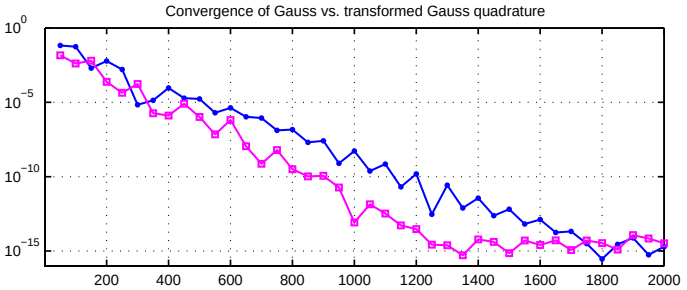
To illustrate this transplanted quadrature idea we pick a wiggly function,

```
f = cos(17*x)./(1+sin(100*x).^2);
clf, plot(f)
```

Here is a code in which `I` represents Gauss quadrature and `I2` is transformed Gauss quadrature — and we see that the dots decrease about 30% more slowly than the squares.

```
gp = diff(g);
Iexact = sum(f);
err = []; err2 = [];
nn = 50:50:2000;
for n = nn
   [s,w] = legpts(n);
   I = w*f(s); err = [err abs(I-Iexact)];
   I2 = w*(f(g(s)).*gp(s)); err2 = [err2 abs(I2-Iexact)];
end
hold off, semilogy(nn,err,'.-',MS,9), grid on
hold on, semilogy(nn,err2,'s-m',MS,4), axis([1 2000 1e-16 1])
title('Convergence of Gauss vs. transformed Gauss quadrature')
```



We emphasize: in the end a quadrature formula is just a quadrature formula, as specified in (18.3):

$$I_n = \sum_{k=0}^{n} w_k f(x_k). \tag{22.8}$$

Gauss leads to one choice of nodes and weights, Clenshaw–Curtis leads to another, transplanted Gauss leads to a third, transplanted Clenshaw–Curtis to a

fourth. Regardless of what concepts may have been employed in the derivation, in the end the quadrature formula is just a linear combination of function values, and the transformed formulas usually outperform the classical ones. For example, in [Hale & Trefethen 2008] it is proved that the transformed Gauss formulas based on mapping $E_{1.1}$ to an infinite strip converges 50% faster than Gauss quadrature for the class of functions analytic in the ε-neighborhood of $[-1,1]$, for any $\varepsilon < 0.05$.

This chapter has shown that polynomials are not the only effective general linear class of approximants for general functions f on an interval and indeed are often suboptimal. There is much more that can be said on this subject. For example, there is the matter of how the mapping g was derived and what other maps might be useful; an influential family of maps was introduced by Kosloff and Tal-Ezer [1993]. Another topic we have not discussed is the application to spectral methods, Kosloff and Tal-Ezer's motivation, and it is here that transformations of variables are perhaps most important in practice. Finally, there is the idea of using the map g for rational functions rather than polynomials. The last two ideas have been combined powerfully in Tee's adaptive rational spectral collocation method based on adaptively determined conformal maps [Tee & Trefethen 2006, Hale & Tee 2009].

[To be added: (1) Read Timan 1951. (2) Explain the connection of sausages to Taylor series for $(2/\pi)\sin^{-1}(s)$. (3) Clarify 32% and half-width 0.76. (4) Nearly-equispaced grids.]

SUMMARY OF CHAPTER 22. *Though many numerical methods are based on polynomial approximations of a function $f \in C[-1,1]$, such approximations are not optimal in any natural sense, for polynomials have higher resolution near the endpoints of the interval than near the middle. By a conformal transplantation one can derive approximations that are up to $\pi/2$ times more efficient.*

Exercise 22.1. A challenging integrand. Repeat the Gauss vs. transformed Gauss quadrature experiment for the "challenging integrand" (17.14). By approximately what percentage is Gauss slower than transformed Gauss for this function? How do you account for this behavior?

Exercise 22.2. Chebfun 'map'. Chebfun contains a `'map'` parameter which enables one to explore some of the ideas of this chapter in an automatic fashion (see `help chebfun/maps` for information). To illustrate this, construct `f = 1./(1+25*x.^2)` with both `x = chebfun('x')` as usual and also `x = chebfun('x','map',{'sausage',9})`. How do the `chebpolyplot` results compare? (b) What if the parameter 9 is varied to $1, 3, 5, \ldots 15$? (This is the degree of the expansion in (22.1).)

Exercise 22.3. Strip maps. [to be written, based on `'map'`.]

Exercise 22.4. Sausage maps of different orders. [To be written.]

Exercise 22.4. Transplanted Clenshaw–Curtis quadrature. [To be written.]

23. Nonlinear approximations: why rational functions?

Up to now, this book has been about polynomials, or in the last chapter, their transplants. The rest of the book is about rational functions, which have been a mainstay of approximation theory from the beginning. Why do rational approximations occupy such a large place in the approximation theory literature? Polynomials are familiar and comfortable, but rational functions seem complicated and specialized. Is their position in approximation theory justified, or is it an artifact of history, perhaps a holdover from the pre-computer era? In this chapter we attempt to answer these questions, and in doing so we shall find ourselves considering the broader question of what the uses are of the whole subject of approximation theory.

I think the answer is this. Although rational functions indeed became an established part of approximation theory long before computers and many of the associated practical applications, their place in the subject is deserved. Their importance stems from a conjunction of two facts. On the one hand, rational functions are more powerful than polynomials at approximating functions *near singularities* and on *unbounded domains*. On the other hand, for various reasons related for example to partial fraction decompositions, they are easier to work with than their nonlinearity might suggest — indeed, sometimes no more complicated than polynomials.

A rational function is the ratio of two polynomials, and in particular, given $m \ge 0$ and $n \ge 0$, we say that r is a rational function of **type (m,n)** if it can be written as a quotient p_m/q_n with $p_m \in P_m$ and $q_n \in P_n$. The set of all rational functions of type (m,n) is denoted by R_{mn}, and any $r \in R_{mn}$ can be written in the form

$$r(z) = \sum_{k=0}^{m} a_k z^k \Big/ \sum_{k=0}^{n} b_k z^k \tag{23.1}$$

for some real or complex coefficients $\{a_k\}$ and $\{b_k\}$. The degrees need not be exact, i.e., there is no requirement in general that a_m or b_n must be nonzero. Nor do we necessarily require that the numerator and denominator are relatively prime, that is, that they have no common zeros.

Suppose, however, that for some nonzero $r \in R_{mn}$, we choose a representation with relatively prime numerator and denominator. Define $\mu \le m$ to be the index of the highest degree nonzero numerator coefficient and similarly $\nu \le n$ for the denominator, and further normalize the coefficients by requiring $b_\nu = 1$.

Then we can write

$$r(z) = \sum_{k=0}^{\mu} a_k z^k \Big/ \sum_{k=0}^{\nu} b_k z^k \ , \quad a_\mu \neq 0, \ b_\nu = 1. \tag{23.2}$$

In this case r has exactly μ finite zeros and ν finite poles (counted with multiplicity): we say that r is of **exact type** (μ, ν). (If r is identically zero, it has exact type $(-\infty, 0)$.) If $\mu > \nu$, it has a pole at $z = \infty$ of order $\mu - \nu$, and if $\nu > \mu$ it has a zero at $z = \infty$ of order $\nu - \mu$. Basic properties of rational functions are described in books of complex analysis such as [Ahlfors 1953, Henrici 1974, Markushevich 1985].

These representations highlight the nonlinearity of rational functions, but a different perspective is reached when we represent them by **partial fractions**. (An excellent general reference on this subject is Chapter 7 of [Henrici 1974].) In the simplest situation, consider

$$r(z) = \sum_{k=1}^{n} \frac{c_k}{z - \zeta_k}, \tag{23.3}$$

where $\{\zeta_k\}$ are distinct real or complex numbers. For any coefficients $\{c_k\}$, this is a rational function of type $(n-1, n)$, and if the coefficients are nonzero, then r is of exactly this type. The number c_k is the **residue** of r at ζ_k. This representation highlights the linear aspects of rational functions. For example, whereas computing the integral of r written in the form p/q looks daunting, in the partial fraction representation we have simply

$$\int^z r(s)ds = C + \sum_{k=1}^{n} c_k \log(z - \zeta_k). \tag{23.4}$$

In applications, it is interesting how often a formula like this turns out to be crucial in making a rational function useful.

The partial fraction form (23.3) does not apply to all rational functions. One limitation is that it always represents a rational function of exact type $(\nu - 1, \nu)$ for some ν (assuming r is not identically zero). Another is that it does not represent all functions of exact type $(\nu - 1, \nu)$, since it cannot account for poles of multiplicity greater than 1. The following theorem gives a partial fraction representation for the general case.

Theorem 23.1. Partial fraction representation. *Given $m, n \geq 0$, let $r \in R_{mn}$ be arbitrary. Then r has a unique representation in the form*

$$r(z) = p_0(z) + \sum_{k=1}^{\mu} p_k((z - \zeta_k)^{-1}), \tag{23.5}$$

where p_0 is a polynomial of exact degree ν_0 for some $\nu_0 \leq m$ (unless $p = 0$) and $\{p_k\}$, $1 \leq k \leq \mu$, are polynomials of exact degrees $\nu_k \geq 1$ with $\sum_{k=1}^{\mu} \nu_k \leq n$.

Proof. See [ref?]. ∎

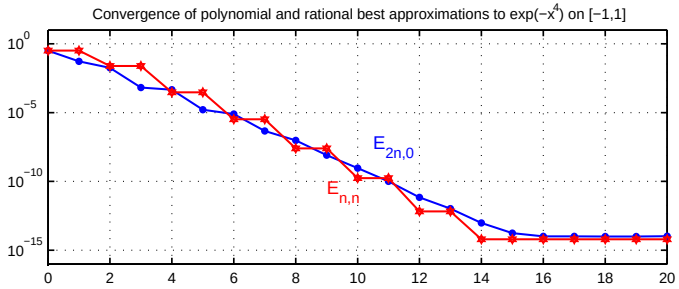
The function p_0 is the **polynomial part** of r, and $p_k((z-\zeta_k)^{-1})$ is its **principal part** at ζ_k.

This is all we shall say for the moment about the mathematics of rational functions. Let us now turn to the main subject of this chapter, the discussion of why these functions are useful in approximation theory and approximation practice.

The right place to start is with a cautionary observation. Rational functions are not always better than polynomials! Indeed, consider the most basic of all situations, in which f is a function analytic in a ρ-ellipse E_ρ for some $\rho > 1$. For such a function, by Theorem 8.2, polynomial approximations will converge at the rate $O(\rho^{-n})$. It turns out that a typical convergence rate for type (n, n) rational functions is $O(\rho^{-2n})$. So, doubling the number of parameters to be determined sometimes just approximately doubles the convergence rate. (In fact, sometimes it does not increase the convergence rate at all [Szabados 1970].) For applications of this kind, rational functions may outperform polynomials, but usually by a rather modest factor.

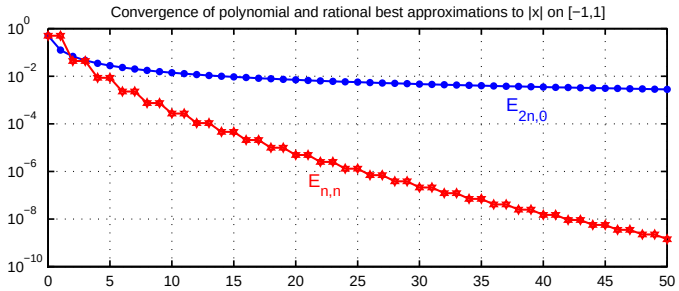
For example, here are a pair of curves showing $\|f - p^*_{2n}\|$ (dots) and $\|f - r^*_{nn}\|$ (stars) as functions of n for $f(x) = \exp(-x^4)$, where p^*_{2n} and r^*_{nn} are the best approximations to f in P_{2n} and R_{nn}, respectively. (We shall discuss rational best approximation and the Remez algorithm for computing them in Chapter 30.) Both curves decrease geometrically, and there is not much difference between them. [This code is a kluge based on `cf`, pending extension of the Chebfun `remez` command to more robust rational approximation.]

```
f = exp(-x.^4);
warning off
nn = 0:20; errp = []; errr = [];
for n = nn
  p2n = remez(f,2*n); errp = [errp norm(f-p2n,inf)];
  [p,q,foo] = cf(f,n,n); rnn = p./q; errr = [errr norm(f-rnn,inf)];
end
clf, semilogy(nn,errp,'.-',MS,12), grid on, ylim([1e-16 10])
hold on, semilogy(nn,errr,'h-r',MS,4)
text(10.5,2e-8,'E_{2n,0}',FS,10,CO,'b')
text(9,1e-11,'E_{n,n}',FS,10,CO,'r')
title(['Convergence of polynomial and rational '...
       'best approximations to exp(-x^4) on [-1,1]'])
```



What makes rational functions important is that, in contrast to this example, there are many problems where one wants to operate near singularities, or on unbounded domains. For these problems, rational approximations may converge much faster than polynomials. For example, here is an experiment like the last one, but with $f(x) = |x|$. For this function, a type (n, n) rational approximant with $n = 150$ gives 16-digit accuracy, whereas polynomial approximants would need $n = 10^{15}$ to do so well. [This code is another kluge.]

```
f = abs(x);
xx = linspace(-1,1,1000);
nn = 0:50; errp = [];
errr = [.5 4.37e-2 8.50e-3 2.28e-3 7.37e-4 2.69e-4 1.07e-4 ...
        4.60e-5 2.09e-5 9.89e-6 4.88e-6 2.49e-6 1.30e-6 ...
        6.3*exp(-pi*sqrt(26:2:max(nn)))];
errr = kron(errr,[1 1]); errr(end) = [];
for n = nn
  p2n = remez(f,2*n); errp = [errp norm(f(xx)-p2n(xx),inf)];
end
hold off, semilogy(nn,errp,'.-',MS,12), grid on
hold on, semilogy(nn,errr,'h-r',MS,4)
text(37,3e-4,'E_{2n,0}',FS,10,CO,'b')
text(21,2e-7,'E_{n,n}',FS,10,CO,'r')
title(['Convergence of polynomial and rational '...
       'best approximations to |x| on [-1,1]'])
```



The approximation of $|x|$ by rational functions is one of the "two famous problems" to be considered in the next chapter. In 1964 Donald Newman proved that whereas polynomial approximants to $|x|$ converge just at the rate $O(n^{-1})$, for rational approximants the rate is $\exp(-C\sqrt{n})$ with $C > 1$ [Newman 1964]. This result rigorously established the possibility of an exponential difference in effectiveness of the two types of approximations.

The rest of this chapter is devoted to an outline of twelve applications in which rational approximations are useful. In most of these examples, there is a singularity or unbounded domain in the picture. The exceptions are applications #1 and #7, where rational functions outperform polynomials less decisively.

1. Elementary and special functions. Classically, approximation theory brings to mind the problem of designing subroutines for computers to evaluate elementary functions, like $\sin x$, and special functions, like Airy or Bessel functions. For some of these applications, especially when the number of digits of accuracy required is known in advance, rational approximations prove to be the best choice. A classic project in this line is the SPECFUN software package [Cody 1993], descendent of the earlier FUNPACK [Cody 1975], which uses rational best approximations to evaluate Bessel functions, error functions, gamma functions and exponential integrals to 18 digits of accuracy. For many years a driving force behind these software products and a great expert on the matter of practical rational approximations was W. J. Cody at the Argonne National Laboratory; Cody's version of the rational Remez algorithm is described in [Cody, Fraser & Hart 1968]. For a presentation of some of the state of the art in the early 21st century, see [Muller 2006].

2. Digital filters. In electrical engineering, the construction of low-pass, high-pass, and other digital filters often involves approximation of functions with jumps. (For these problems the approximation domain is usually the unit circle in the complex plane.) Jumps amount to singularities on or near the domain of approximation, and Theorem 8.3 implies that polynomials have no chance of rapid convergence for such functions. As Newman's theorem would lead us to expect, rational approximations sometimes do much better. Engineers use the term FIR (Finite Impulse Response) for polynomial filters and IIR (Infinite Impulse Response) in the rational case [Oppenheim, Schafer & Buck 1999].

3. Extrapolation of sequences and series. The mathematical sciences are full of problems of extrapolation. For example, one might be interested in $\lim_{h\to 0} f(h)$, where $f(h)$ is a quantity computed numerically on a grid of spacing h. For such a problem, f is often analytic at $h = 0$, in which case *Richardson extrapolation,* based on interpolating the data by a polynomial, may be beautifully effective. On the other hand, suppose we want to evaluate $\lim_{n\to\infty} a_n$ for a sequence $\{a_n\}$. We can regard this problem too as $\lim_{h\to 0} f(h)$ with the definition $f(1/n) = a_n$, but now, in many applications, $f(h)$ will not be analytic at $h = 0$ and Richardson extrapolation will be ineffective. The more powerful extrapolation methods that

have been developed for such problems, such as Aitken extrapolation and the eta algorithm, are mostly based on rational approximations. See Chapter 26, "Extrapolation of sequences and series".

4. Determination of poles. Suppose a function f is analytic on $[a,b]$ and has some real or complex poles nearby whose positions and residues are of interest. Classic examples of such problems arise in the study of phase transitions in condensed matter physics. If we approximate f by polynomials on $[a,b]$, then by Theorem 8.3, the convergence fails outside a ρ-ellipse of analyticity, so not much information about poles can be obtained. If we approximate by rational functions, exponential convergence to some of the poles can often be achieved. Specifically, a good strategy is to consider the poles of r_{mn} for moderate values of n, where r_{mn} is a rational approximant to f obtained by Padé or Chebyshev–Padé approximation or rational interpolation or least-squares. See Chapter 31, "Determination of poles and analytic continuation".

5. Analytic continuation. If f is analytic on $[a,b]$, then in many applications it can be analytically continued, in theory, to the rest of the complex plane, apart from exceptional points and curves in the form of poles, other singularities, and branch cuts. Computing such continuations numerically, however, is a difficult problem. One could try approximating f by a polynomial, but this approach will be useless outside a Bernstein ellipse of analyticity. Rational functions, by contrast, may be effective for continuation much further out. Again see Chapter 31, "Determination of poles and analytic continuation".

6. Eigenvalues and eigenvectors of matrices. Suppose we want to compute an eigenvector of a matrix A. One approach, the *power method,* is to pick a starting vector x and compute $\lim_{n\to\infty} A^n x$, but the convergence of this polynomial-based idea is very slow in general. A much faster method, *inverse iteration*, is based on rational approximations: find an approximation μ to some eigenvalue λ and compute $\lim_{n\to\infty} (A-\mu I)^{-n}x$. The convergence gets faster the closer μ is to the singularity λ, and exploitation of this effect leads to the spectacularly effective QR algorithm for matrix eigenvalues and eigenvectors [Francis 1961]. Experts in numerical linear algebra do not usually think about rational approximations when discussing inverse iteration or the QR algorithm, but such approximations come explicitly to the fore in the analysis of extensions such as shift-and-invert Arnoldi or rational Krylov iteration [Güttel 2010].

7. Exponential of a matrix. A famous paper in numerical analysis is "Nineteen dubious ways to compute the exponential of a matrix", by Moler and Van Loan in 1978, reprinted in expanded form 25 years later [Moler & Van Loan 2003]. These authors compared many algorithms for computing e^A and reached the conclusion that the most effective was a scaling-and-squaring method based on Padé approximation [Ward 1977]. Here, first A is scaled so that its norm is on the order of 1. Then e^A is approximated by $r(A)$, where r is a type (n,n) Padé approximant to e^z. This is an example where rational approximations

outperform polynomials not decisively but by a more or less constant factor. A key point is that a type (n,n) approximant can be computed with little more effort than a type $(n,0)$ approximant, because the work is dominated by computing the powers $A^2, A^3, \ldots, A^n$, and once these are known for the numerator, they can be reused for the denominator. This approach is used by the matrix exponential program `expm` in Matlab, which for many years was based on type $(6,6)$ Padé approximation. A more careful analysis of the scaling-and-squaring algorithm was later provided by Higham [2009], who concluded that a better choice was type $(13,13)$, and the `expm` code was adjusted accordingly in Matlab Version 8. In [Higham & Al-Mohy 2010, Appendix A] the authors conclude that Padé approximants are up to 23% more efficient than Taylor polynomials in this application.

8. Model reduction and optimal control. A major topic in numerical linear algebra and control theory is the approximation of complicated input-output systems by simpler ones for more efficient computation. Via the Laplace transform, problems of this kind (in the case of continuous as opposed to discrete time) can in many cases be reduced to problems of approximation on the imaginary axis in the complex plane. The unbounded domain makes rational approximations a natural choice, and in fortunate cases, a system with hundreds of thousands of degrees of freedom may be reduced to a model with just dozens or hundreds. One set of methods for such problems goes by the name of H^∞ approximation, based on results by Adamjan, Arov and Krein [1971] and Glover [1984] that are related to the CF approximation method discussed in Chapter 20. For more information see [Antoulas 2005, Zhou, Doyle & Glover 1996].

9. Numerical solution of stiff PDEs. The Laplace operator Δ on a spatial domain Ω with Dirichlet boundary conditions has an infinite set of negative real eigenvalues diverging to $-\infty$. To solve the heat equation $\partial u/\partial t = \Delta u$ numerically on Ω with initial data $u(x,0) = u_0$, one would like to be able to compute the matrix exponential product $e^{tA}v_0$, where A is a matrix discretization of Δ and v_0 is a discretization of u_0. The wide range of eigenvalues makes such a problem "stiff", posing challenges for numerical methods. One method for coping with stiffness is to find a rational function $r(x)$ that approximates e^x accurately on $(-\infty,0]$, hence in particular at all of the eigenvalues of A, and then to compute $r(tA)v_0$. Polynomials cannot approximate a bounded function on an infinite interval, but rational functions can. This problem of rational approximation of e^x on $(-\infty,0]$ goes back to Cody, Meinardus & Varga [1969], whose "1/9 conjecture", eventually settled by Gonchar and Rakhmanov [1986], is the other famous problem considered in the next chapter. Generalizations have become important in scientific computing in recent years in the design of *exponential integrators* for the fast numerical solution of stiff nonlinear ordinary and partial differential equations [Hochbruck & Ostermann 2010, Kassam & Trefethen 2005, Schmelzer & Trefethen 2007].

10. Quadrature formulas. As we have seen in Chapter 19, a quadrature for-

mula approximates an integral $I = \int_a^b f(x)dx$ by a finite linear combination $I_n = \sum_{k=0}^n w_k f(x_k)$. If the weights w_k are interpreted as residues of a rational function $r(z)$ with poles at the nodes x_k, then by estimation of a Cauchy integral over a contour Γ enclosing $[a, b]$ in the complex plane, one can show that the error in I is bounded in terms of the size of f in the region enclosed by Γ times the error in approximation of the analytic function $\log((z+1)/(z-1))$ by r over the same region. So every quadrature formula is connected with a rational approximation problem. In fact, Gauss's original derivation of the $(n+1)$-point Gauss quadrature formula on $[-1, 1]$ was based on exactly this connection: he used type $(n, n+1)$ Padé approximation of $\log((z+1)/(z-1))$ at $z = \infty$ [Gauss 1814]. See Chapter 29, "Rational approximation and quadrature".

11. Adaptive spectral methods for PDEs. The barycentric interpolation formula has the form of a rational function that reduces to a polynomial for a special choice of weights (Chapter 5). Regardless of the choice of weights, however, one still gets an interpolant, and in some applications there is no compelling reason to force the interpolant to be a polynomial. This opens up the possibility of much more flexible rational interpolants, which have the particular advantage of not being so sensitive to the distribution of the interpolation points. These ideas originate with Salzer [1981] and Schneider and Werner [1986], building on earlier work as far back as Jacobi [1846], and were later developed by Berrut and Mittelmann [1997] and Floater and Hormann [2007]. For ordinary and partial differential equations, they form the basis of adaptive spectral methods for solving problems whose solutions have singularities close to the region of approximation [Tee & Trefethen 2006, Hale & Tee 2009].

12. One-way wave equations. Our final application became well known in the 1970s and 1980s [Halpern & Trefethen 1988]. The usual wave equation permits energy propagation in all directions, but there are applications where one would like to restrict to half the permitted angles, a 180° range. For example, this idea is useful in underwater acoustics [Tappert 1977], in geophysical migration [Claerbout 1985], and in the design of absorbing boundary conditions for numerical simulations [Lindman 1975, Engquist & Majda 1977]. How can we define a system that behaves like $u_{tt} = u_{xx} + u_{yy}$ for leftgoing waves, say, with negative x-component of velocity, while not propagating rightgoing waves? (The subscripts represent partial derivatives.) A Fourier transform shows that the dispersion relation of such a system should be $\xi = \omega\sqrt{1-s^2}$, where $s = \eta/\omega$ and ω, ξ, η are the dual variables to t, x, y. Only the positive branch of the square root should be present, making this system a *pseudodifferential operator.* However, a rational approximation $\sqrt{1-s^2} \approx r(s)$ simplifies this to a differential equation. For example, the type $(2, 2)$ Padé approximation $r(s) = (1 - \frac{3}{4}s^2)/(1 - \frac{1}{4}s^2)$ leads to the PDE $u_{xtt} - \frac{1}{4}u_{xyy} = u_{ttt} - \frac{3}{4}u_{tyy}$, sometimes known as the "45° equation" because it has high accuracy approximately for angles up to 45°.

We have now examined a list of twelve applications. In concluding this chapter I would like to consider what light these may shed on the biggest question of

all, namely, what is the use of approximation theory?

To see some possible views, let us go back to 1901. That was the year of Runge's important paper (Chapter 13), whose title was[8]

"On empirical functions and interpolation between equidistant ordinates."

In reading this today, one is struck by the word "empirical". The empirical theme is echoed in the opening sentence:

The relationship between two measurable quantities can, strictly speaking, not be found by observation.

Runge goes on to mention "observations" six times more in the opening paragraph. It would seem that his motivation is the processing of scientific data: interpolation in the traditional sense of evaluating a function at points lying between those at which it is listed in a table.

The next year, 1902, brought another landmark of approximation theory: Kirchberger's PhD thesis under Hilbert in Göttingen, which included the first statement and proof of the equioscillation theorem for polynomial approximation (Theorem 10.1). Here is the first paragraph of Kirchberger's paper a year later [1903], which sets forth a clear motivation for approximation theory. Perhaps we may imagine that this was also Hilbert's view of the subject.[9]

The notion of a function entails the assumption that a numerical value of the function can be calculated for any value of the independent variable. But since the only operations that can really be carried out numerically are the four elementary operations of addition, subtraction, multiplication and division, or strictly speaking only the first three of these, it follows that we are really only masters of more general functions insofar as we can replace them by rational functions, that is, represent them approximately. This highlights the great significance of approximation problems for the whole of mathematics and the special role of approximation by polynomials and rational functions. Indeed, for numer-

[8] Title: "Über empirische Funktionen und die Interpolation zwischen äquidistanten Ordinaten." First sentence: "Die Abhängigkeit zwischen zwei messbaren Grössen kann, strenge genommen, durch Beobachtung überhaupt nicht gefunden werden."

[9] "Mit dem Begriff der Funktion ist das Postulat der numerischen Berechnung der Funktionswerte für irgendwelche Werte der unabhängigen Variabeln gegeben. Da aber die vier elementaren Spezies der Addition, Subtraktion, Multiplikation und Division, oder streng genommen nur die erste drei derselben, die einzigen numerisch ausführbaren Rechnungsarten, alle andern aber nur insoweit durchführbar sind, als sie sich auf diese zurückführen lassen, so folgt hieraus, daß wir sämtlichen Funktionen nur insoweit numerisch beherrschen, als sie sich durch rationale Funktionen ersetzen, d. h. angenähert darstellen lassen. Hieraus erhellt die große Bedeutung der Annäherungsprobleme für die gesamte Mathematik und die ausgezeichnete Stellung, die die Probleme der Annäherung durch rationale order ganze rationale Funktionen einnehmen. In der Tat setzt, wenigstens für die numerische Berechnung, jede Annäherung durch andere, z. B. trigonometrische, Funktionen die annäherungsweise Ersetzbarkeit dieser Funktionen durch rationale voraus."

ical calculation at least, any use of other approximations such as trigonometric functions presupposes that these can in turn be approximated by rational functions.

Updated to 2011, we may say that Kirchberger's justification of approximation theory is all about *machine arithmetic.* Approximation by polynomials and rational functions is important, he is saying, because ultimately computers can only carry out polynomial and rational operations.

Both Runge's emphasis on data and Kirchberger's emphasis on arithmetic capture aspects of approximation theory that remain valid today. In particular, Kirchberger's paragraph seems a remarkably clear statement of a justification of approximation theory that in a certain philosophical sense seems almost unarguable (although the line between "primitive" operations like + and "derived" ones like $\sin(\cdot)$ is not always so clear on actual computers, with their multiple levels of hardware, software and microcode). The same argument is often seen nowadays.

Nevertheless I do not think data analysis or machine arithmetic get at the heart of why approximation theory is important and interesting. In fact I don't think Runge's words even capture the truth of why *he* was interested in the subject! (He becomes more of a mathematician in the second half of his paper.) What these observations miss is the importance of *algorithms.*

Let us look again at the list of applications. Kirchberger's motivation could be said to be on target for #1 and #2 (evaluation of functions, digital filters), and Runge's for #3, #4, and #5 (extrapolation, determination of poles, analytic continuation). But the remaining seven items need to be accounted for in other ways. It is noteworthy that applications #6 to #9 all involve matrices, sometimes of very large dimension (eigenvalues and eigenvectors, exponentials of matrices, model reduction, stiff PDEs). Applications #9 to #12 all involve integrals and differential equations (stiff PDEs, quadrature, adaptive spectral methods, one-way wave equations). In most of these problems we seem a long way from scalars x and $r(x)$: the polynomial and rational operations are applied to matrices and operators.

Chebfun provides another interesting data point (for polynomials rather than rational functions). Chebfun is built on a century of developments in polynomial interpolation and approximation, and it makes it possible to work with univariate functions numerically in almost unlimited ways. A particularly important Chebfun capability is finding roots of a function $f(x)$, which enables many further operations like computing maxima, absolute values, and 1-norms. Chebfun finds the roots by the algorithm proposed by Good [1961] and Boyd 2002]: approximate f by polynomial interpolants, then find roots of the polynomials by computing eigenvalues of colleague matrices (Chapter 18). This is as powerful an application of approximation theory as one could ask for, but it

has little to do with data analysis or machine arithmetic.

Why are polynomial and rational approximations interesting? Not because $r(x)$ is easier to evaluate than $\exp(x)$, but because $r(A)$ is easier to evaluate than $\exp(A)$, and $r(\partial/\partial x)$ is easier to evaluate than $\exp(\partial/\partial x)$! Not because we can *evaluate* $p(x)$, but because we can *find its roots*!

[To be added: (1) Say something about the fundamental matter of stability and implicitness, even of ODE formulas. (2) Mention the confusing fact that in model reduction, the function to be approximated is often rational. (3) Connect applications 7 and 9 better. (4) Fix up the kluge codes.]

SUMMARY OF CHAPTER 23. *Rational functions are more powerful than polynomials for approximating functions with singularities or on unbounded integrals. This is the source of their importance in approximation theory and approximation practice.*

Exercise 23.1. Examples of partial fractions. Express the following functions in partial fraction form: (a) $x^3/(1-x)$ (b) $x/(x^2-4)$, (c) $x^2/(x^2-4)^2$, (d) $(1-x^3)/(1+x^2)$.

Exercise 23.2. Uses of partial fractions. (a) Express the function $r(x) = (x(x-1)(x-2))^{-1}$ in partial fractions. (b) What is its integral from 1 to t? (c) What is the value of the infinite sum $r(1) + r(2) + r(3) + \cdots$?

Exercise 23.3. Another infinite sum. (a) Based on numerical experiments, conjecture a value of the infinite sum $1/(1\cdot 3\cdot 5) + 2/(3\cdot 5\cdot 7) + 3/(5\cdot 7\cdot 9) + \cdots$. (b) Verify your conjecture with partial fractions.

Exercise 23.4. A trigonometric identity. Verify the identity $1/(1\cdot 3\cdot 5) - 1/(7\cdot 9\cdot 11) + 1/(13\cdot 15\cdot 17) - \cdots = \pi/48$.

Exercise 23.5. Polynomial vs. rational experiments. Produce plots comparing $E_{2n,0}(f)$ and $E_{n,n}(f)$ for the following functions f defined on $[-1,1]$: (a) $\log(1+x^2)$, (b) $\tanh(5x)$, (c) $\exp(x)/(2-x)$.

24. Rational best approximation

Chapter 10 considered best or "minimax" approximation by polynomials, that is, approximation in the ∞-norm, where optimality is characterized by an equioscillating error curve. This chapter presents analogous results for approximation by rational functions. Much remains the same, but a crucial new feature is the appearance of a number known as the *defect* in the equioscillation condition, which leads to the phenomenon of square blocks of degenerate entries in the "Walsh table" of best approximations. This complication adds a fascinating new ingredient to the theory, but it is a complication with destructive consequences in terms of the fragility of rational approximations and the difficulty of computing them numerically. An antidote to some such difficulties may be the

use of algorithms based on weighted linearized least-squares, a theme we shall take up in Chapter 26.

Another new feature in rational approximation is that we must now be careful to distinguish real and complex situations, because of a curious phenomenon: best rational approximations to real functions are in general complex, and as a corollary, nonunique. This effect is intriguing, but it has little relevance to practical approximation, so for the most part we shall restrict our attention to approximations in the space R_{mn}^{real} consisting of functions in R_{mn} with real coefficients.

We will first state the main theorem, then give some examples, and then present a proof. To begin the discussion, we must define the defect. Suppose $r \in R_{mn}$, that is, r is a rational function of type (m,n). As discussed in the last chapter, this means that r can be written as a fraction p/q in lowest terms with p and q having exact degrees $\mu \le m$ and $\nu \le n$. The **defect** d of r in R_{mn} is the number between 0 and n defined by

$$d = \min\{m-\mu, n-\nu\} \ge 0. \tag{24.1}$$

Note that d is a measure of how far *both* the numerator and the denominator degrees fall short of their maximum allowed values. Thus $(1-x^2)/(1+x^2)$, for example, has defect 0 in R_{22} or R_{23} and defect 1 in R^{33}.

A special case to be noted is the situation in which $r = 0$, that is, r is identically zero. Recall that in this case we defined $\mu = -\infty$ and $\nu = 0$, so that r is said to have exact type $(-\infty, 0)$. The definition (24.1) remains in force in this case, so if $r = 0$, we say that r has defect $d = n$ in R_{mn}, regardless of m and n.

The reason why defects matter has to do with the counting of zeros. Suppose $r = p/q \in R_{mn}$ has exact type (μ,ν) and $\tilde{r} = \tilde{p}/\tilde{q}$ is another function in R_{mn}. Then we have

$$r - \tilde{r} = \frac{p}{q} - \frac{\tilde{p}}{\tilde{q}} = \frac{p\tilde{q} - \tilde{p}q}{q\tilde{q}},$$

a rational function of type $(\max\{\mu+n, m+\nu\}, n+\nu)$. By (24.1), this implies that $r-\tilde{r}$ is of type $(m+n-d, 2n-d)$. Thus $r-\tilde{r}$ can have at most $m+n-d$ zeros, and this zero count is a key to equioscillation and uniqueness results.

Here is our main theorem. Existence was first proved by de la Vallée Poussin [1911] and by Walsh [1931]. The equioscillation idea goes back to Chebyshev [1859].

Theorem 24.1: Equioscillation characterization of best approximants. *A real function $f \in C[-1,1]$ has a unique best approximation $r^* \in R_{mn}^{\text{real}}$, and a function $r \in R_{mn}^{\text{real}}$ is equal to r^* if and only if $f-r$ equioscillates between at least $m+n+2-d$ extreme points, where d is the defect of r in R_{mn}.*

"Equioscillation" here is defined just as in Chapter 10. For $f-r$ to equioscillate in k points means that there exists a set of numbers $-1 \le x_1 < \cdots < x_k \le 1$ such that

$$f(x_j) - r(x_j) = (-1)^{j+i}\|f-r\|, \qquad 1 \le j \le k$$

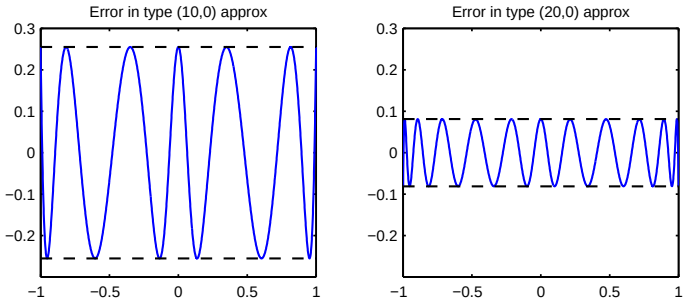
with $i = 0$ or 1. Here and throughout this chapter, $\|\cdot\|$ is the supremum norm.

We now give some examples. To begin with, here is a function with a spike at $x = 0$:

```
f = exp(-100*x.^2);
```

Polynomial approximations of this function converge rather slowly. For example, it takes $n = 20$ to achieve one digit of accuracy:

```
[p,err] = remez(f,10);
subplot(1,2,1), hold off, plot(f-p), hold on
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
title('Error in type (10,0) approx'), ylim(.3*[-1 1])
[p,err] = remez(f,20);
subplot(1,2,2), hold off, plot(f-p), hold on
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
title('Error in type (20,0) approx'), ylim(.3*[-1 1])
```

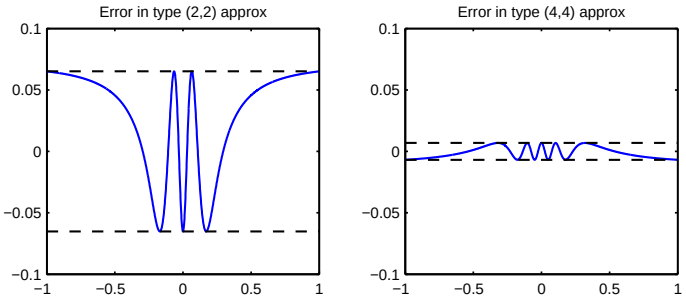


Notice that the extreme points of these error curves are distributed all across $[-1,1]$, even though the challenging part of the function would appear to be in the middle. As discussed in Chapter 10, this is typical of polynomial best approximations.

If we switch to rational approximations, which can also be computed by Chebfun's `remez` command, the accuracy improves. Here we see error curves for approximations of types $(2,2)$ and $(4,4)$, with much smaller errors although the degrees are low. Note that most of the extreme points are now localized in the middle.

```
[p,q,rh,err] = remez(f,2,2);
```

```
subplot(1,2,1), hold off, plot(f-p./q), hold on
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
title('Error in type (2,2) approx'), ylim(.1*[-1 1])
[p,q,rh,err] = remez(f,4,4);
subplot(1,2,2), hold off, plot(f-p./q), hold on
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
title('Error in type (4,4) approx'), ylim(.1*[-1 1])
```

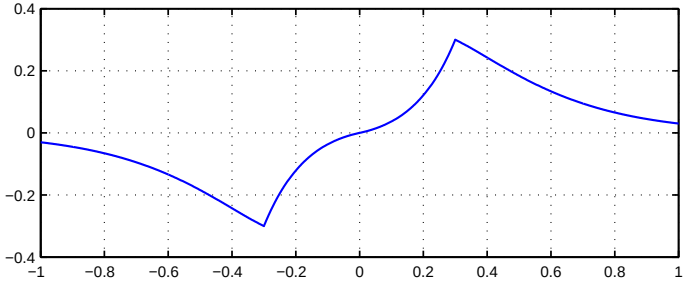


The error curves just plotted provide good examples of the role of the defect in the characterization of best approximants. The function f is even, and so are its best approximations (Exercise 24.1). Thus we expect that the type $(2,2)$, $(3,2)$, $(2,3)$ and $(3,3)$ best approximations will all be the same function, a rational function of exact type $(2,2)$ whose error curve has 7 points of equioscillation. For $(m,n) = (2,2)$, the defect is 0 and there is one more equioscillation point than the minimum $m+n+2-d = 6$. For $(m,n) = (3,2)$ or $(2,3)$, the defect is 0 and the number of equiscillation points is exactly the minimum $m+n+2-d$. For $(m,n) = (3,3)$, the defect is 1 and the number of equiscillation points is again exactly the minimum $m+n+2-d$.

Similarly, the error curve in the plot on the right, with 11 extrema, indicates that this rational function is a best approximation not only of type $(4,4)$ but also of types $(5,4)$, $(4,5)$, and $(5,5)$.

Here is another example, an odd function:

```
f = x.*exp(-5*abs(abs(x)-.3));
clf, plot(f), grid on, ylim(.4*[-1 1])
```

If we look for a best approximation of type $(4,5)$, we find that the numerator has exact degree 3:

```
[p,q,rh,err] = remez(f,4,4);
format short, chebpoly(p)
```

```
ans =
    0.0169   -0.0000    0.0575   -0.0000
```

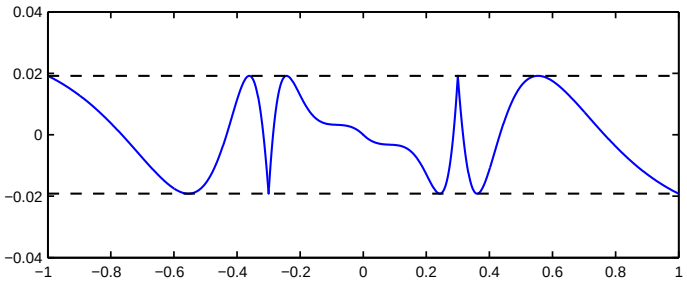
and the denominator has exact degree 4:

```
chebpoly(q)
```

```
ans =
    0.2146   -0.0000    0.7435   -0.0000    0.5493
```

The defect is 1, so there must be at least $4+5+2-1 = 10$ extreme points in the error curve. In fact, there are exactly 10:

```
plot(f-p./q), hold on, ylim(.04*[-1 1])
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
```



We conclude that r is the best approximation of types $(4,4), (4,5), (3,4)$ and $(3,5)$.

Let us now turn to the proof of Theorem 24.1. For polynomial approximations, our analogous theorem was Theorem 10.1, whose proof proceeded in four steps:

1. *Existence proof via compactness.*
2. *Equioscillation ⇒ optimality.*
3. *Optimality ⇒ equisoscillation.*
4. *Uniqueness proof via equioscillation.*

For rational functions, we shall follow the same sequence. The main novelty is in step 1, where compactness must be applied in a subtler way.

Part 1 of proof: Existence via compactness. For polynomial approximation, in Chapter 10, we noted that $\|f-p\|$ is a continuous function on P_n, and since one candidate approximation was the zero polynomial, it was enough to look in the bounded subset $\{p \in P_n : \|f-p\| \le \|f\|\}$. Since this set was compact, the minimum was attained.

For rational functions, $\|f-r\|$ is again a continuous function on R_{mn}, and again it is enough to look in the bounded subset $\{r \in R_{mn} : \|f-r\| \le \|f\|\}$, or more simply, the larger bounded set $\{r \in R_{mn} : \|r\| \le 2\|f\|\}$. The difficulty is that bounded sets of rational functions are not in general compact. To illustrate this fact, consider the family of functions

$$r_\varepsilon(x) = \frac{x^3+\varepsilon}{x^2+\varepsilon}, \tag{24.2}$$

where $\varepsilon > 0$ is a parameter. For each ε, $r_\varepsilon(x)$ is a continuous function on $[-1,1]$. As $\varepsilon \to 0$, however, r_ε behaves discontinuously:

$$\lim_{\varepsilon\to 0} r_\varepsilon(x) = \begin{cases} 1 & x = 0, \\ x & x \ne 0. \end{cases}$$

So we cannot find a limit function r_0 by taking a limit as $\varepsilon \to 0$. What saves us, however, is that the spaces of numerators and denominators are both compact, so we can argue that they separately approach limits p_0 and q_0, which in this example would be x^3 and x^2. We then define a limiting rational function by $r_0 = p_0/q_0$ and argue by continuity that it has desirable properties. This kind of reasoning is spelled out in greater generality in [Walsh 1931].

Suppose then that $\{r_k\}$ is a sequence of functions in R_{mn}^{real} with $\|r_k\| \le 2\|f\|$ and

$$\lim_{k\to\infty} \|f-r_k\| = E = \inf_{r\in R_{mn}^{\text{real}}} \|f-r\|.$$

Write each r_k in the form p_k/q_k with $p_k \in P_m$, $q_k \in P_n$, $q_k(x) \ne 0$ for all $x \in [-1,1]$, and $\|q_k\| = 1$, hence $\|p_k\| \le \|q_k\|\|r_k\| \le 2\|f\|$. Since $\{p_k\}$ and $\{q_k\}$ lie in compact sets, we may assume by passing to a subsequence if necessary that $p_k \to p^*$ and $q_k \to q^*$ for some $p^* \in P_m$ and $q^* \in P_n$. Since $\|q_k\| = 1$ for each k, $\|q^*\| = 1$ too, and thus q^* is not identically zero but has at most a finite set of zeros on $[-1,1]$. Now define $r^* = p^*/q^* \in R_{mn}^{\text{real}}$. For all $x \in [-1,1]$ except perhaps the zeros of q^*, $|f(x)-r^*(x)| = \lim_{k\to\infty}|f(x)-r_k(x)| \le E$. By

continuity, the same must hold for all $x \in [-1,1]$, with p^* having zeros in $[-1,1]$ wherever q^* does. Thus r^* is a best approximation to f. ∎

Part 2 of proof: Equioscillation ⇒ optimality. Suppose $f-r$ takes equal extreme values with alternating signs at $m+n+2-d$ points $x_0 < x_1 < \cdots < x_{m+n+1-d}$, and suppose $\|f-\tilde r\| < \|f-r\|$ for some $\tilde r \in R_{mn}^{\text{real}}$. Then $r-\tilde r$ must take nonzero values with alternating signs at the equioscillation points, implying that it must take the value zero in at least $m+n+1-d$ points in-between. However, as observed above, $r-\tilde r$ is of type $(m+n-d, 2n-d)$. Thus it cannot have $m+n+1-d$ zeros unless it is identically zero, a contradiction. ∎

Part 3 of proof: Optimality ⇒ equisoscillation. Suppose $f-r$ equioscillates at fewer than $m+n+2-d$ points, and set $E = \|f-r\|$. Without loss of generality suppose the leftmost extremum is one where $f-r$ takes the value $-E$. Then there are numbers $-1 < x_1 < \cdots < x_k < 1$ with $k \le m+n-d$ and $\varepsilon > 0$ such that $(f-r)(x) < E-\varepsilon$ for $x \in [-1,x_1] \cup [x_2,x_3] \cup [x_4,x_5] \cup \cdots$ and $(f-r)(x) > -E+\varepsilon$ for $x \in [x_1,x_2] \cup [x_3,x_4] \cup \cdots$. Let r be written in the form p/q, where p has degree $\mu \le m-d$ and q has degree $\nu \le n-d$, with p and q having no roots in common. The proof now consists of showing that r can be perturbed to a function $\tilde r = (p+\delta p)/(q+\delta q) \in R_{mn}$ with the properties that $\|\tilde r - r\| < \varepsilon$ and $\tilde r - r$ is strictly negative for $x \in (-1,x_1) \cup (x_2,x_3) \cup (x_4,x_5) \cup \cdots$ and strictly positive for $x \in (x_1,x_2) \cup (x_3,x_4) \cup \cdots$. Such a function $\tilde r$ will have error less than E throughout the whole interval $[-1,1]$. We calculate

$$\frac{p+\delta p}{q+\delta q} = \frac{(p+\delta p)(q-\delta q)}{q^2} + O(\|\delta q\|^2)$$

and therefore

$$\tilde r - r = \frac{q\delta p - p\delta q}{q^2} + O(\|\delta p\|\|\delta q\| + \|\delta q\|^2).$$

We are done if we can show that δp and δq can be chosen so that $q\delta p - p\delta q$ is a nonzero polynomial of degree exactly k with roots $x_1, \ldots, x_k$. This can be shown by the Fredholm alternative of linear algebra. The map from the $(m+n+2)$-dimensional set of choices of δp and δq to the $(m+n+1-d)$-dimensional space of polynomials $q\delta p - p\delta q$ is linear. To show the map is surjective, it is enough to show that its kernel has dimension $d+1$ but no more. Suppose then that $q\delta p - p\delta q$ is zero, that is, $q\delta p = p\delta q$. Then since p and q have no roots in common, all the roots of p must be roots of δp and all the roots of q must be roots of δq. In other words we must have $\delta p = gp$ and $\delta q = gq$ for some polynomial g. Since δp has degree no greater than m and δq has degree no greater than n, g can have degree no greater than d. The set of polynomials of degree d has dimension $d+1$, so we are done. ∎

Part 4 of proof: Uniqueness via equioscillation. Finally, to prove uniqueness, suppose r is a best approximation whose error curve equioscillates between extreme points at $x_0 < x_1 < \cdots < x_{m+n+1-d}$, and suppose $\|f-\tilde r\| \le \|f-r\|$ for some $\tilde r \in R_{mn}^{\text{real}}$. Then (without loss of generality) $(r-\tilde r)(x)$ must be ≤ 0 at

$x_0, x_2, x_4, \ldots$ and ≥ 0 at $x_1, x_3, x_5, \ldots$. This implies that $r - \tilde{r}$ has roots in each of the $m+n+1-d$ closed intervals $[x_0, x_1], \ldots, [x_{m+n-d}, x_{m+n+1-d}]$, and since $r - \tilde{r}$ is a rational function of type $(m+n-d, 2n-d)$, the same must hold for its numerator polynomial. We wish to conclude that its numerator polynomial has at least $m+n+1-d$ roots in total, counted with multiplicity, implying that $r = \tilde{r}$. The argument for this is the same as given in the proof of Theorem 10.1. ∎

We have now finished the substantial mathematics. It is time to look at some of the consequences.

One of the recurring themes in the subject of rational approxmation is the phenomenon of *square blocks in the Walsh table.* Suppose that a real function $f \in C[-1,1]$ is given, and consider the set of all of its real rational best approximations of type (m,n) for various $m, n \geq 0$. We can imagine these laid out in an array, with m along the horizontal and n along the vertical. This array is called the **Walsh table** for f [Walsh 1934].

Generically, all the entries in the Walsh table for a given f will be distinct, and in this case we say that f is **normal**. Sometimes, however, certain entries in the table may be repeated, and in fact this is a frequent occurrence because it happens whenever f is even or odd. If f is even, then for any nonegative integers j and k, all of its rational approximations of types $(2j, 2k)$, $(2j+1, 2k)$, $(2j, 2k+1)$ and $(2j+1, 2k+1)$ must be the same. Similarly, if f is odd, then all of its approximations of types $(2j+1, 2k)$, $(2j+2, 2k)$, $(2j+1, 2k+1)$ and $(2j+2, 2k+1)$ must be the same. We have already seen a number of examples.

More generally, repeated entries or "degeneracies" in the Walsh table may take complicated forms. Nevertheless the equioscillation condition imposes quite a bit of structure on the chaos. Degeneracies always appear precisely in a pattern of square blocks. The following statement of this result is taken from [Trefethen 1984], where a discussion of various aspects of this and related problems can be found. We shall return to the subject of square blocks in Chapter 27, on Padé approximation.

Theorem 24.2: Square blocks in the Walsh table. *The Walsh table of best real rational approximants to a real rational function $f \in C[-1,1]$ breaks into precisely square blocks containing identical entries. (If f is rational, one of these will be infinite in extent.) The only exception is that if an entry $r = 0$ appears in the table, then it fills all of the columns to the left of some fixed index $m = m_0$.*

Proof. Given a nonrational function f, let $r \neq 0$ be a best approximation in $R_{\mu\nu}^{\text{real}}$ of exact type (μ, ν). (The cases of rational f or $r = 0$ can be handled separately.) By Theorem 24.1, the number of equioscillation points of $f - r$ is $\mu + \nu + 2 + k$ for some integer $k \geq 0$. We note that r is an approximation to f

in R_{mn}^{real} for any $m \geq \mu$ and $n \geq \nu$, and the defect is $\min\{m-\mu, n-\nu\}$. Thus by Theorem 24.1, r is the best approximation to f precisely for those values of (m,n) satisfying $m \geq \mu$, $n \geq \nu$, and $\mu+\nu+2+k \geq m+n+2-\min\{m-\mu, n-\nu\}$. The latter condition simplifies to $n \leq \nu + k$ and $m \leq \mu + k$, showing that r is the best approximation to f precisely in the square block $\mu \leq m \leq \mu + k$, $\nu \leq n \leq \nu + k$. ∎

Within a square block in the Walsh table, the defect d is equal to zero precisely in the first column and the first row. An approximation with $d = 0$ is sometimes said to be **nondegenerate**. It can have more points of equioscillation than the generic number $m+n+2$, but never fewer.

As mentioned above, the theory of equioscillation and degeneracies is very appealing mathematically. As an example we note a result due to Werner [1964], in completion of earlier work of Maehly and Witzgall: the type (m,n) *best approximation operator*, which maps functions f to their best approximations r_{mn}^*, is continuous at f with respect to the supremum norm if and only if $f \in R_{mn}$ or the corresponding function r_{mn}^* is nondegenerate. As pointed out in [Trefethen 1984], the essential reason for this effect is that if a function r^* is the best approximation to f in a nontrivial square block, then a small perturbation $f \to \tilde{f}$ might fracture that block into pieces of size 1×1. If (m,n) corresponds to a degenerate position in the block, with $d > 0$, then the best approximation $\tilde{r}^*$ for such an $\tilde{f}$ would need to have a higher equioscillation number than that of r^* for f, requiring $\tilde{r}^*$ to be far from r^* if $\|f - r^*\|$ is positive.

These complications hint at some of the practical difficulties of rational approximation. For example, the Remez algorithm is based on explicit manipulation of equioscillation sets, known as extremal sets. If the number of extremal points is not known a priori, it is plausible that one may expect numerical difficulties in certain circumstances. Indeed this is the case, and so far as I am aware, no implementation of the Remez algorithm for rational approximation, including Chebfun's, can be called fully robust. Other methods may have better prospects.

We finish by returning to the matter of best *complex* approximations to real functions. Nonuniqueness of certain complex rational approximations was pointed out by Walsh in the 1930s. Later Lungu [1971] noticed, following a suggestion of Gonchar, that the nonuniqueness can be seen even for approximation of a real function f on $[-1,1]$, with examples as simple as type $(1,1)$ approximation of $|x|$. (Exercise 24.3 gives another proof that there must exist such examples.) These observations were rediscovered independently by Saff and Varga [1978a]. Ruttan [1981] showed that complex best approximations are always better than real ones in the strict lower-right triangle of a square block, that is, when a type (m,n) best approximation equioscillates in no more than $m+n+1$ points. Trefethen and Gutknecht [1983] showed that for every (m,n) with $n \geq m+3$, examples exist where the ratio of the optimal complex and real errors is arbitrarily small. Levin, Ruttan and Varga showed that the minimal ratio is exactly

1/3 for $n = m + 2$ and exactly 1/2 for $1 \le n \le m + 1$ [Ruttan & Varga 1989]. None of this has much to do with practical approximation, but it is fascinating.

SUMMARY OF CHAPTER 24. *Any real function $f \in C[-1,1]$ has a unique best approximation $r^* \in R_{mn}^{\text{real}}$ with respect to the ∞-norm, and r^* is characterized by having an error curve that equioscillates in at least $m+n+2-d$ extreme points, where d is the defect of r in R_{mn}. In the Walsh table of all best approximations to f indexed by m and n, repeated entries, if any, lie in exactly square blocks.*

Exercise 24.1. Approximating even functions. Prove that if a real function $f \in C[-1,1]$ is even, then its best approximations of all types (m,n) are even.

Exercise 24.2. Approximating the Gaussian. The first figures of this chapter considered lower degree polynomial and rational approximations of $\exp(-100x^2)$ on $[-1,1]$. Make a plot of the errors in approximations of types $(n,0)$ and (n,n), now taking n as high as you can. (You may find that the CF command takes you farther than REMEZ.) How do the polynomial and rational approximations compare?

Exercise 24.3. A quick proof of nonuniqueness. (a) Suppose a real function $f \in C[-1,1]$ takes both the values 1 and -1. Prove that no real rational function $r \in R_{0n}^{\text{real}}$, for any n, can have $\|f - r\| < 1$. (b) On the other hand, show that for any $\varepsilon > 0$, there is a complex rational function $r \in R_{0n}$ for some n with $\|f - r\| < \varepsilon$. (Hint: perturb f by an imaginary constant and consider its reciprocal.) (c) Conclude that type $(0,n)$ complex rational best approximations in $C[-1,1]$ are nonunique in general for large enough n.

Exercise 24.4. A function with a spike. Plot chebfuns of the function (24.2) for $\varepsilon = 1, 0.1, \dots, 10^{-6}$ and determine the polynomial degree $n(\varepsilon)$ of the chebfun in each case. What is the observed asymptotic behavior of $n(\varepsilon)$ as $\varepsilon \to 0$? How accurately can you explain this observation based on the theory of Chapter 8?

Exercise 24.5. de la Vallée Poussin lower bound. Suppose an approximation $r \in R_{mn}^{\text{real}}$ to $f \in C[-1,1]$ approximately equioscillates in the sense that there are points $-1 \le s_0 < s_1 < \cdots < s_{m+n+1-d} \le 1$ at which $f - r$ alternates in sign with $|f(s_j) - r(s_j)| \ge \varepsilon$ for some $\varepsilon > 0$, where d is the defect of r in R_{mn}. Show that the best approximation $r^* \in R_{mn}^{\text{real}}$ satisfies $\|f - r^*\| \ge \varepsilon$.

25. Two famous problems

In this chapter we discuss two problems of rational approximation that have been the focus of special attention over the years: approximation of $|x|$ on $[-1,1]$, a prototype of approximation of non-smooth functions, and approximation of e^x on $(-\infty, 0]$, a prototype of approximation on unbounded domains. Both stories go back many decades and feature initial theorems, later conjectures based on numerical experiments, and eventual proofs of the conjectures based on mathematical methods related to potential theory. We shall not present

the proofs of the sharpest results, but we shall show that the essential rates of approximation can be achieved by using the trick that appears several times in this book: if a function $f(x)$ can be written as an integral with respect to a variable s, then an approximation $r(x)$ in partial fractions form is obtained by applying a quadrature formula (19.3) to the integral.

The problem of approximation of $|x|$ on $[-1,1]$ starts at the beginning of the 20th century, when polynomial approximations of this function were of interest to Lebesgue, de la Vallée Poussin, Jackson, and Bernstein. This was an era when the fundamental results of approximability were being developed, and $|x|$ served as a function from which many other results could be derived. Bernstein's prize-winning article on the subject ran for 57 pages [Bernstein 1912c]. Among other things, Bernstein proved that in best polynomial approximation of $|x|$ as $n \to \infty$, the errors decrease inverse-linearly but no faster, that is, at the rate $O(n^{-1})$ but not $o(n^{-1})$.

Why inverse-linearly? This is an example of the fundamental fact of approximation theory which we mentioned first in Chapter 7: the close connection between the smoothness of a function and its rate of approximation. The function $f(x) = |x|$ has a derivative of bounded variation $V = 2$ on $[-1,1]$, so by Theorem 7.2, its Chebyshev truncations $\{f_n\}$ satisfy

$$\|f - f_n\| \le \frac{4}{\pi(n-1)}$$

for $n \ge 2$, and its Chebyshev interpolants $\{p_n\}$ satisfy the same bound with 4 replaced by 8. Thus approximations to $|x|$ converge at least at the rate $O(n^{-1})$. What Bernstein showed is that the rate is in fact no better than this: no approximations to $|x|$ can beat Chebyshev truncation or interpolation by more than a constant factor. Or to put it another way, convergence of polynomial approximants to a function f at a rate faster than $O(n^{-1})$ implies that f is in some sense smoother than $|x|$. Such results in the direction *approximability* $\Longrightarrow$ *smoothness* go by the general name of *Bernstein theorems*. In this book we have presented one result of this kind: Theorem 8.3, asserting that geometric convergence implies analyticity.

It is hard not to be curious about the constants. Bernstein in fact proved in [Bernstein 1914b] that there exists a number β such that the best approximation errors satisfy

$$E_n(|x|) \sim \frac{\beta}{n} \tag{25.1}$$

as $n \to \infty$, and he obtained the bound

$$0.278 < \beta < 0.286.$$

(Theorem 7.2 gives $\beta \le 4/\pi \approx 1.27$.) He noted that $1/2\sqrt{\pi} \approx 0.28209\ldots$ falls in this range, a value which became known as *Bernstein's conjecture*. Seventy

years later, Varga and Carpenter [1985] investigated the problem numerically to great accuracy and found that Bernstein's conjecture was false: the true value is

$$\beta \approx 0.28016949902386913303643649\ldots.$$

(Of course the difference between 0.282 and 0.280 would have not the slightest practical importance.) Along with this numerical result, which was based on Richardson extrapolation, Varga and Carpenter established the rigorous bounds

$$0.2801685460 < \beta < 0.2801733791. \tag{25.2}$$

For example, here are the values of $nE_n(|x|)$ for $n = 1, 2, 4, \ldots, 64$, showing quadratic convergence to the limit value. A comparison with the much more accurate Table 2.1 of [Varga & Carpenter 1985] indicates that the Chebfun results are accurate in all but the last digit or two.

```
f = abs(x);
limit = 0.280169499023869133;
for n = 2.^(0:6)
  [p,err] = remez(f,n);
  ss = 'n = %3d   n*err = %16.14f   n*err-limit = %10.2e\n';
  fprintf(ss,n,n*err,n*err-limit)
end
```

```
n =   1   n*err = 0.50000000000000   n*err-limit =   2.20e-01
n =   2   n*err = 0.25000000000000   n*err-limit =  -3.02e-02
n =   4   n*err = 0.27048359711114   n*err-limit =  -9.69e-03
n =   8   n*err = 0.27751782467506   n*err-limit =  -2.65e-03
n =  16   n*err = 0.27948883759454   n*err-limit =  -6.81e-04
n =  32   n*err = 0.27999815195641   n*err-limit =  -1.71e-04
n =  64   n*err = 0.28012658713999   n*err-limit =  -4.29e-05
```

Now all this is for polynomial approximation. What about rational approximation? As mentioned in Chapter 23, the dramatic discovery here came from Donald Newman, fifty years after Bernstein: best rational approximants to $|x|$ converge "root-exponentially". Newman's bounds were these:

$$\frac{1}{2}e^{-9\sqrt{n}} \le E_{nn}(|x|) \le 3e^{-\sqrt{n}}. \tag{25.3}$$

We have already seen in the second plot of Chapter 23 what a big speed-up this is as compared with (25.1). For approximating non-smooth functions, rational functions may be far more powerful than polynomials.

Again mathematicians could not resist trying to sharpen the constants. First Vyacheslavov [1975] found that the correct exponent is midway between Newman's bounds of 1 and 9: it is π. Then Varga, Ruttan and Carpenter [1993] performed computations with a version of the Remez algorithm to 200 decimal places, leading to numerical evidence for the conjecture

$$E_{nn} \sim 8e^{-\pi\sqrt{n}}$$

as $n \to \infty$. Soon afterwards this result was proved by Stahl [1993]. Later Stahl generalized the result to approximation of x^α on $[0, 1]$ for any $\alpha > 0$ [Stahl 2003].

The following theorem summarizes the results we have mentioned.

Theorem 25.1. Approximation of $|x|$ on $[-1, 1]$. *The errors in best polynomial and rational approximation of $|x|$ on $[-1, 1]$ satisfy*

$$E_{n0}(|x|) \sim \frac{\beta}{n}, \quad \beta = 0.2801\ldots \tag{25.4}$$

and

$$E_{nn}(|x|) \sim 8e^{-\pi\sqrt{n}} \tag{25.5}$$

as $n \to \infty$.

Proof. Equation (25.4) is due to Varga and Carpenter [1985] and (25.5) is due to Stahl [1993]. ∎

Why can rational approximations of $|x|$ achieve $O(C^{-\sqrt{n}})$ accuracy? The crucial fact is that the poles of r can be chosen to cluster near the singular point $x = 0$. In particular, a good choice is to make the poles approach 0 geometrically, for each fixed n, with a geometric factor depending on $\sqrt{n}$.

Here is a derivation of a rational approximation that achieves the right root-exponential convergence. (Arguments like this have been made by Stenger in various publications; see for example [Stenger 1986].) We start from the identity

$$\frac{1}{|x|} = \frac{2}{\pi}\int_0^\infty \frac{dt}{t^2 + x^2},$$

which is derived in calculus courses. Multiplying by x^2 gives

$$|x| = \frac{2x^2}{\pi}\int_0^\infty \frac{dt}{t^2 + x^2}. \tag{25.6}$$

(This formula is perhaps due to Roberts [1971], though the essence of the matter dates to Zolotarev in the 1870s.) The change of variables $t = e^s$, $dt = e^s ds$ converts this to

$$|x| = \frac{2x^2}{\pi}\int_{-\infty}^\infty \frac{e^s ds}{e^{2s} + x^2}, \tag{25.7}$$

which is an attractive integral to work with because the integrand decays exponentially as $|s| \to \infty$. We now get a rational approximation of $|x|$ by approximating this integral by the trapezoid rule with node spacing $h > 0$:

$$r(x) = \frac{2hx^2}{\pi} \sum_{k=-(n-2)/4}^{(n-2)/4} \frac{e^{kh}}{e^{2kh} + x^2}. \tag{25.8}$$

Here n is a positive even number, and there are $n/2$ terms in the sum, so $r(x)$ is a rational function of x of type (n, n). There are two sources of error that make $r(x)$ differ from $|x|$. The fact that the sum has been terminated at a limit $n < \infty$ introduces an error on the order of $e^{-nh/4}$, and the finite step size $h > 0$ introduces an error on the order of $e^{-\pi^2/h}$. (The integrand is analytic in the strip around the real s-axis of half-width $a = \pi/2$, correponding to a convergence rate $e^{-2\pi a/h}$.) Balancing these sources of error suggests the condition $e^{-nh/4} \approx e^{-\pi^2/h}$, that is,

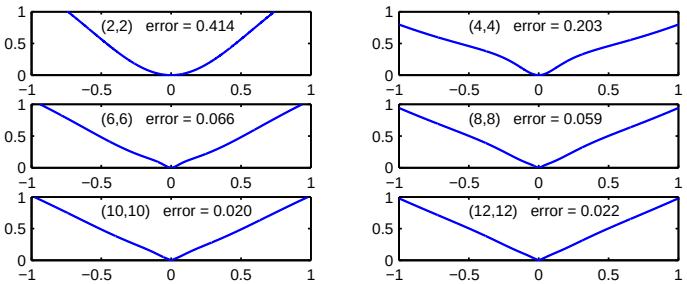
$$h \approx 2\pi/\sqrt{n}, \tag{25.9}$$

with error of order

$$e^{-(\pi/2)\sqrt{n}}. \tag{25.10}$$

We can see these approximations with an experiment.

```
for n = 2:2:12
  r = 0*x;
  h = 2*pi/sqrt(n);
  for k = -(n-2)/4:(n-2)/4
    r = r + exp(k*h)./(exp(2*k*h)+x.^2);
  end
  r = (2*h/pi)*x.^2.*r;
  subplot(3,2,n/2), plot(r), ylim([0 1])
  err = norm(f-r,inf);
  ss = sprintf('(%1d,%1d)   error = %5.3f',n,n,err);
  text(-.5,.78,ss,FS,8)
end
```



The poles of (25.8)–(25.9) in the x-plane lie at

$$\pm i e^{2\pi k/\sqrt{n}}. \tag{25.11}$$

Here are these numbers (those in the upper half-plane) for the six approximations plotted above, showing the wide range of amplitudes associated with the exponential spacing.

```
disp('Poles of rational approximants to |x|:')
for n = 2:2:12
  h = 2*pi/sqrt(n);
  k = -(n-2)/4:(n-2)/4;
  y = exp(k*h);
  fprintf('%8.2ei  ',y), disp(' ')
end
```

```
Poles of rational approximants to |x|:
1.00e+00i
2.08e-01i  4.81e+00i
7.69e-02i  1.00e+00i  1.30e+01i
3.57e-02i  3.29e-01i  3.04e+00i  2.80e+01i
1.88e-02i  1.37e-01i  1.00e+00i  7.29e+00i  5.32e+01i
1.07e-02i  6.58e-02i  4.04e-01i  2.48e+00i  1.52e+01i  9.32e+01i
```

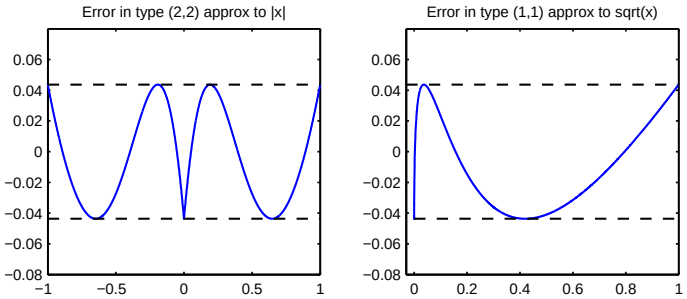
The approximations aren't optimal, but they are close. The convergence rate (25.10) as $n \to \infty$ is one-quarter the optimal rate (25.5) in the sense that we need 4 times as large a value of n to achieve a certain accuracy in (25.10) as in (25.5).

Above, we computed errors for best polynomial approximations to $|x|$ with the Chebfun command `remez`. In the rational case, `remez` does not succeed in computing best approximations beyond a certain low order. This difficulty is related to the exponential spacing of the oscillations of $f - r^*$ near $x = 0$.

It is worth noting that the problem of approximating $|x|$ on $[-1, 1]$ is equivalent to certain other approximation problems. If $r(x)$ is a type (m, n) approximation to $|x|$ on $[-1, 1]$, then normally r will be an even function of x and m and n can be taken to be even too. Thus $r(x) = \tilde{r}(x^2)$, where $\tilde{r}$ is a rational function of type $(m/2, n/2)$. Since $\tilde{r}(x^2)$ approximates $|x|$ for $x \in [-1, 1]$, $\tilde{r}(x)$ approximates $\sqrt{x}$ for $x \in [0, 1]$. This reasoning holds for any approximations, and in particular, by counting equioscillations one finds that best type (m, n) approximation of $|x|$ on $[-1, 1]$ is equivalent to best type $(m/2, n/2)$ approximation of $\sqrt{x}$ on $[0, 1]$. The following pair of plots illustrates this equivalence. Notice that the error curves are the same apart from the scaling of the x-axis.

```
f = abs(x);
[p,q,rh,err] = remez(f,2,2); clf
```

```
subplot(1,2,1), plot(f-p./q), hold on
ylim(.08*[-1 1])
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
title('Error in type (2,2) approx to |x|')
f = chebfun('sqrt(x)',[0,1],'splitting','on');
[p,q,rh,err] = remez(f,1,1);
subplot(1,2,2), plot(f-p./q), hold on
axis([-.03 1 .08*[-1 1]])
plot([-.03 1],err*[1 1],'--k'), plot([0 1],-err*[1 1],'--k')
title('Error in type (1,1) approx to sqrt(x)')
```



For applications in scientific computing, the approximation of $\sqrt{x}$ on an interval $[a, b]$ is particularly interesting because of the case in which x is a matrix A with eigenvalues in $[a, b]$, which might come from discretizing a differential operator. Rational approximations of the square root lead to powerful algorithms for evaluating $A^{1/2}v$ for vectors v, as described in [Hale, Higham & Trefethen 2008] and [Higham 2008].

We now turn to the second of the famous problems of this chapter: approximation of e^x on $(-\infty, 0]$. This problem was introduced in a paper of Cody, Meinardus, and Varga [1969], which drew attention to the connection of such approximations with the numerical solution of partial differential equations, since a rational approximation can be used to compute the exponential of a matrix arising from a numerical discretization [Moler & Van Loan 2003].[10] Curiously, despite that good motivation from applied mathematics, the influence of this paper was mainly in theoretical approximation theory for quite a few decades, until computers and numerical linear algebra had advanced to the point where it became more practical to take advantage of algorithms based on rational functions.

[10]The Cody–Meinardus–Varga paper was important in my life. As a graduate student in the Numerical Analysis Group at Stanford, I happened to come across it one evening around 1980 in a pile of Gene Golub's discarded reprints — "help yourself". Its mix of theory and numerical caluclations appealed to me intensely and led to my computation of the constant 9.28903... a few years later [Trefethen and Gutknecht 1983].

The first thing we may note about approximation of e^x on $(-\infty, 0]$ is that polynomials cannot do the job at all. Since any non-constant polynomial $p(x)$ diverges to $\pm\infty$ as $x \to -\infty$, the only polynomials that can approximate e^x with finite error on $(-\infty, 0]$ are constants, so the minimax error can never be less than $1/2$.

Inverse-polynomials of the form $1/p_n(x)$, however, can be chosen to converge geometrically. This makes sense when you consider that e^x on $(-\infty, 0]$ is the same as $1/e^x$ for $x \in [0, \infty)$. Cody, Meinardus and Varga noted that to achieve geometric convergence, it is enough to consider $1/p_n(x)$, where p_n is the degree-n truncation of the Taylor series for e^x. They showed that these approximations converge at a rate $O(2^{-n})$, and then they improved this rate to $O(2.298^{-n})$ by a shift of origin. It was later proved by Schönhage [1973] that the optimal rate for inverse-polynomials is $O(3^{-n})$.

Since $1/p_n(x)$ is a rational function of type (n, n), these observations tell us that best rational type (n, n) approximations to e^x on $(-\infty, 0]$ converge at least geometrically. Newman [1974] proved that the convergence is no faster than geometric. What is the optimal rate? With twice as many parameters to work with as with inverse-polynomials, one might guess that it should be $O(9^{-n})$, and this idea became known in the 1970s as the "1/9 conjecture". In fact, the optimal convergence rate turned out to be $O(H^n)$ with $H \approx 1/9.28903$, a number now known as *Halphen's constant*, equal to the unique positive root of the equation

$$h(s) = \sum_{k=1}^{\infty} \frac{ks^n}{1-(-s)^n} = \frac{1}{8}. \tag{25.12}$$

This number was conjectured numerically based on Carathéodory–Fejér singular values by Trefethen and Gutknecht [1983], verified to many digits by high-precision Remes algorithms by Carpenter, Ruttan and Varga [1984], conjectured to have the exact value associated with a certain problem of elliptic functions treated by Halphen [1886] by Magnus via the Carathéodory–Fejér method [1985], and then proved using quite different methods of potential theory by Gonchar and Rakhmanov [1989]. This work represents a fascinating and important line of investigation in approximation theory, and for a summary of many of the ideas with generalizations to related problems, a good place to start is [Stahl & Schmelzer 2009]. Presentations of some of the potential theory underlying results in this area can be found in [Stahl & Totik 1992] and [Saff & Totik 1997].

Following the idea presented earlier for $|x|$ on $[-1, 1]$, it is interesting to see what can be achieved for this problem by the trapezoid rule approximation of a contour integral. Here is a derivation of a rational approximation that achieves the rate $O((2.849\ldots)^{-n})$, adapted from [Weideman & Trefethen 2007]; such approximations are discussed more generally in [Trefethen, Weideman & Schmelzer 2006]. We begin with a Laplace transform identity that is easily

proved by residue calculus,

$$e^x = \frac{1}{2\pi i} \int \frac{e^t dt}{t - x}$$

for $x \in (-\infty, 0]$, where the integral is over any contour in the complex plane that starts at $-\infty$ below the t-axis, circles around $t = 0$, and finishes at $-\infty$ above the t-axis. Choosing the contour to be a parabola, we convert this to an integral over the real s-axis by the change of variables

$$t = (is + a)^2, \quad dt = 2i(is + a)ds$$

for some constant $a > 0$, which gives

$$e^x = \frac{1}{\pi} \int \frac{e^{(is+a)^2}(is + a)ds}{(is + a)^2 - x}. \tag{25.13}$$

As in (25.8), we now approximate this integral by the trapezoid rule with node spacing $h > 0$:

$$r(x) = \frac{h}{\pi} \sum_{k=-(n-1)/2}^{(n-1)/2} \frac{e^{(ikh+a)^2}(ikh + a)}{(ikh + a)^2 - x}. \tag{25.14}$$

Here n is a positive even number, and since x rather than x^2 appears in each term we now take n terms in the sum rather than $n/2$ as in (25.8) to make $r(x)$ a rational function of x of type (n, n).

This time, the integral has square-exponential rather than just exponential decay as $s \to \infty$, so choosing $h = O(1/\sqrt{n})$ is enough to make the errors from endpoint truncation exponentially small. We also have the parameter a to play with. By taking $a = O(\sqrt{n})$, we can make the errors due to grid spacing exponentially small too, and in this fashion we can achieve geometric convergence. More precisely, the choices

$$a = \sqrt{\frac{\pi n}{24}}, \quad h = \sqrt{\frac{3\pi}{2n}} \tag{25.15}$$

lead to the convergence rate

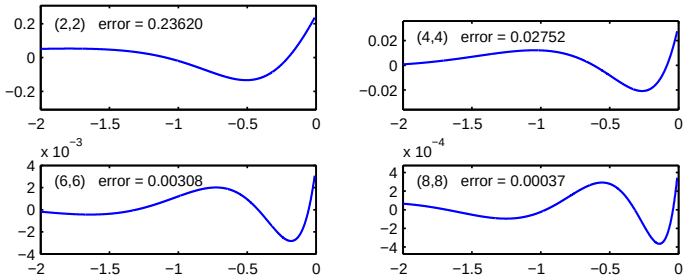
$$\|f - r_{nn}\| = O(e^{-\pi n/3}) \approx O((2.849\ldots)^{-n}). \tag{25.16}$$

As before, we can see these approximations with an experiment, this time plotting $f - r$ rather than r itself.

```
x = chebfun('x',[-2,-.01]);
f = exp(x);
for n = 2:2:8
  r = 0*x;
  h = sqrt(3*pi/(2*n));
```



```
  a = sqrt(pi*n/24);
  for k = -(n-1)/2:(n-1)/2
    r = r + exp((1i*k*h+a)^2)*(1i*k*h+a)./((1i*k*h+a)^2-x);
  end
  r = (h/pi)*real(r);
  subplot(2,2,n/2), plot(f-r)
  err = norm(f-r,inf);
  ss = sprintf('(%1d,%1d)   error = %7.5f',n,n,err);
  axis([-2,0,1.3*err*[-1 1]])
  text(-1.9,.85*err,ss,FS,8)
end
```



Let us summarize these results with a theorem, which goes further to include the precise leading-order asymptotic behavior of the best approximation errors as conjectured by Magnus [1994] and proved by Aptekarev [2002].

Theorem 25.2. Approximation of e^x on $(-\infty, 0]$. *The errors in best type* $(0, n)$ *and* (n, n) *rational approximation of* $\exp(x)$ *on* $(-\infty, 0]$ *satisfy*

$$\lim_{n\to\infty} E_{0n}^{1/n} = \frac{1}{3} \tag{25.17}$$

and

$$E_{nn} \sim 2H^{n+1/2}, \quad H = 1/9.2890254919208\ldots \tag{25.18}$$

as $n \to \infty$.

Proof. Equation (25.17) is due to Schönhage [1973] and (25.18) to Aptekarev [2002], extending the earlier result on nth root asymptotics and the constant H by Gonchar and Rakhmanov [1989]. ∎

We finish this chapter by showing that the numerical computation of these best approximants is surprisingly easily. The crucial matter is to note that the change of variables

$$x = a\frac{s - 1}{s + 1}, \qquad s = \frac{a + x}{a - x} \tag{25.19}$$

where a is a positive parameter, maps the negative real axis $(-\infty, 0]$ in x to the interval $(-1, 1]$ in s. Since the mapping is a rational function of type $(1, 1)$,

it transplants a rational function of type (n,n) in s or x to a rational function of type (n,n) in the other variable. In particular, for the approximation of $f(x) = e^x$ on $(-\infty, 0]$, let us define

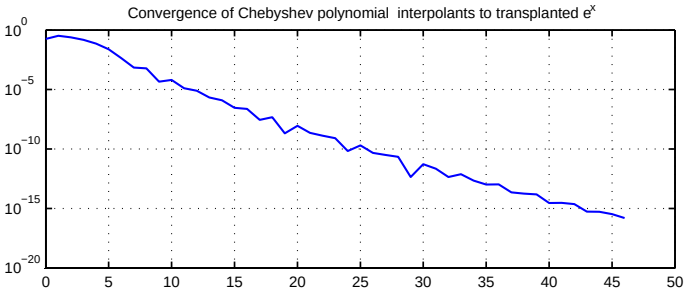
$$F(s) = e^{a(s-1)/(s+1)}, \quad s \in (-1,1]. \tag{25.20}$$

A good choice of the parameter is $a = 9$, which has an important effect for numerical computation in improving the conditioning of the approximation problem. We now find we have a function that can be approximated to machine precision by a Chebyshev interpolating polynomial $p(s)$ of degree less than 50:

```
s = chebfun('s',[-1,1]);
F = exp(9*(s-1)./(s+1));
length(f)
ans = 15
```

The Chebyshev series of F decreases at a good exponential rate:

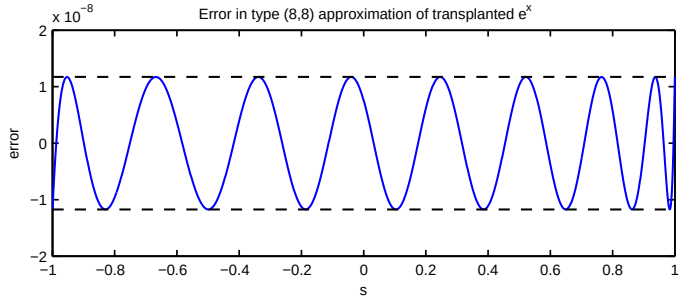
```
clf, chebpolyplot(F), grid on
title(['Convergence of Chebyshev polynomial' ...
       '  interpolants to transplanted e^x'])
```



This gives us yet another way to compute rational approximations to e^x on $(-\infty, 0]$: truncate this Chebyshev series in s, then transplant by (25.19) to get rational functions in x.

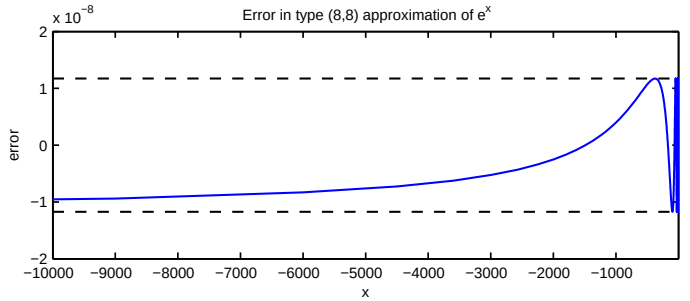
Alternatively, we can get true best approximations from (25.19) by applying the Chebfun REMEZ command. Here for example is the error for the best approximation of type $(8,8)$ plotted in the s variable, showing 18 points of equioscillation.

```
[P,Q,RH,err] = remez(F,8,8); R = P./Q;
hold off, plot(F-R), hold on
plot([-1 1],err*[1 1],'--k'), plot([-1 1],-err*[1 1],'--k')
xlabel s, ylabel error, ylim(2e-8*[-1,1])
title(['Error in type (8,8) approximation'...
       ' of transplanted e^x'])
```

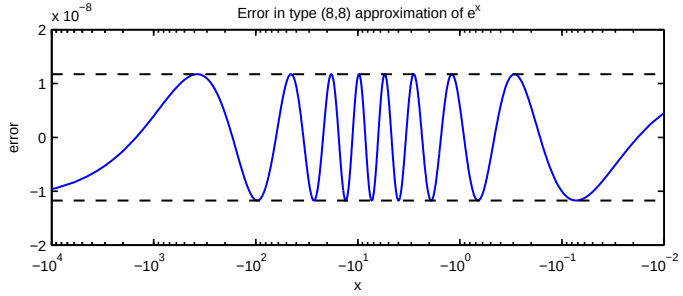
If we plot the same curve in the x variable, it's hard to see much because of the varying scale:

```
s1 = -.999; s2 = .999;
s = chebfun('s',[s1 s2]);
x = 9*(s-1)./(s+1);
hold off, plot(x,F{s1,s2}-R{s1,s2}), hold on
xx = [-1e4 -1e-2];
plot(xx,err*[1,1],'--k'), plot(xx,-err*[1,1],'--k')
xlim(xx)
xlabel x, ylabel error, ylim(2e-8*[-1,1])
title('Error in type (8,8) approximation of e^x')
```



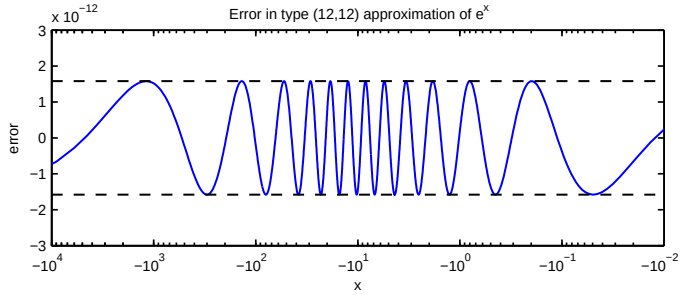
Putting the x axis on a log scale, however, makes the plot informative again:

```
hold off, semilogx(x,F{s1,s2}-R{s1,s2}), hold on
semilogx(xx,err*[1,1],'--k'), plot(xx,-err*[1,1],'--k')
xlim(xx)
xlabel x, ylabel error, ylim(2e-8*[-1,1])
title('Error in type (8,8) approximation of e^x')
```



Here is the analogous plot for type $(12, 12)$ approximation:

```
[P,Q,RH,err] = remez(F,12,12); R = P./Q;
hold off, semilogx(x,F{s1,s2}-R{s1,s2}), hold on
plot(xx,err*[1,1],'--k'), plot(xx,-err*[1,1],'--k')
xlim(xx)
xlabel x, ylabel error, ylim(3e-12*[-1,1])
title('Error in type (12,12) approximation of e^x')
```



These plots are modeled after [Trefethen, Weideman & Schmelzer 2006], where it is shown that Carathéodory–Fejér approximation is equally effective and even faster than the Remes algorithm at computing these approximations.

[To be added: (1) A hint of Bernstein's argument. (2) Ganelius and Green's functions? (3) n-width?]

SUMMARY OF CHAPTER 25. *Two problems involving rational functions have attracted special attention, highlighting the power of rational approximations near singularities and on unbounded domains. For approximating $|x|$ on $[-1, 1]$, best rational functions converge root-exponentially whereas polynomials converge linearly. For approximating e^x on $(-\infty, 0]$, best rational functions converge geometrically whereas polynomials do not converge at all. Both rates of approximation can be achieved by constructing partial fractions from trapezoid rule approximations to certain integrals.*

Exercise 25.1. [Richardson extrapolation of Bernstein data.]

Exercise 25.2. [Newman points.]

Exercise 25.3. Newton iteration for $|x|$. (This problem has roots in [Roberts 1971].) (a) Let x be a number, and suppose we want to solve the equation $r^2 = x^2$ for the unknown r using Newton iteration. Show that the iteration formula is $r^{(k+1)} = ((r^{(k)})^2 + x^2)/2r^{(k)}$. (b) If the initial guess is $r^{(0)} = 1$, then for $k \ge 1$, what is the smallest n for which the rational function $r^{(k)}(x)$ is of type (n, n)? (c) Use Chebfun to compute and plot the approximations $r^{(0)}(x), ..., r^{(5)}(x)$ on the interval $[-1, 1]$. What is the sup-norm error $\||x| - r^{(k)}(x)\|$, and where is it attained? (d) What rate of convergence does this correspond to for $\||x| - r^{(k)}(x)\|$ as a function of n? How does this compare with the optimal rate given by Theorem 25.1? (e) Make a semilog plot of $|\,|x| - r^{(5)}(x)|$ as a function of $x \in [-1, 1]$ and comment further on the nature of these rational approximations.

Exercise 25.4. An elementary argument for e^x on $(-\infty, 0]$. A degree n polynomial $p(s)$ on $[-1, 1]$ can be transplanted to a type (n, n) rational function $r(x)$ on $(-\infty, 0]$ by the map (25.19). Combine this observation with Theorem 8.2 to show that type (n, n) approximants to e^x on $(-\infty, 0]$ exist with accuracy $O(\exp(-Cn^{-2/3}))$ for some $C > 0$ as $n \to \infty$.

Exercise 25.5. Computing Halphen's constant. Write a short Chebfun program that computes Halphen's constant to 10 or more digits based on the condition (25.12).

Exercise 25.6. Computing Halphen's constant via elliptic functions.

Exercise 25.7. Best approximation errors for e^x. (a) Using REMEZ and the change of variables (25.20), compute best approximation errors in type (n, n) approximation of e^x on $(-\infty, 0]$ for $n = 0, 1, \dots, 13$. Plot the results on a log scale and compare them with estimates from the asymptotic formula (25.18). Also on a log scale, plot the difference between the estimates and the true errors, and comment on the results. (b) Repeat the computation with CF instead of REMEZ. This time, plot the different between the CF and true errors on a log scale, and comment on the results.

Exercise 25.8. Approximation in the complex plane. It is stated in [Stahl & Schmelzer 2009] that the poles of best type (n, n) approximations to e^x on $(-\infty, 0]$ move off to ∞ as $n \to \infty$, and the convergence at nth-root rate governed by $h \approx 1/9.28903$ applies on any compact set in the complex plane. With this result in mind, produce contour plots in the complex z-plane for the errors $|e^z - r_{nn}(z)|$ for the approximations (25.14)–(25.15) with $n = 2, 4, 6, 8, 10$. Do you think these approximations converge on all compact sets in the plane?

26. Rational interpolation and least-squares

For polynomials, we have emphasized that although best approximations with their equioscillating error curves are fascinating, Chebyshev interpolants or truncations are just as good for most applications and simpler to compute since the problem is linear. The same is true of rational functions. Best rational approximations are fascinating, but for practical purposes, it is usually a better idea to use rational interpolants, and again an important part of the problem is linear

since one can multiply through by the denominator.

But there is a big difference. Rational interpolation problems are not entirely linear, and unlike polynomial interpolation problems, they suffer from both nonexistence and discontinuous dependence on data in some settings. To use rational interpolants effectively, one must formulate the problem in a way that bypasses such effects. The method we shall recommend for this, here and in the next two chapters, makes use of the singular value decomposition (SVD) and the generalization of the linearized interpolation problem to one of least-squares fitting. This approach originates in [Pachón, Gonnet & van Deun 2011] and [Gonnet, Pachón & Trefethen 2011]. The literature of rational interpolation goes back to Cauchy [1821] and Jacobi [1846], but most of it is rather far from computational practice.

Here is an example to illustrate the difficulties. Suppose we seek a rational function $r \in R_{11}$ satisfying the conditions

$$r(-1) = 2, \quad r(0) = 1, \quad r(1) = 2. \tag{26.1}$$

Since a function in R_{11} is determined by three parameters, the count appears right for this problem to be solvable. In fact, however, there is no solution, and one can prove this by showing that if a function in R_{11} takes equal values at two points, it must be a constant (Exercise 26.1). We conclude: solutions to rational interpolation problems do not always exist.

Let us modify the problem and seek a function $r \in R_{11}$ satisfying the conditions

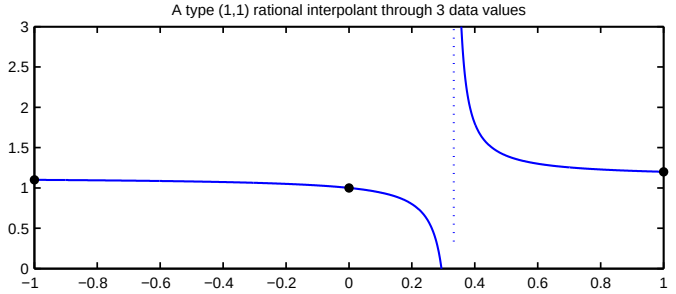
$$r(-1) = 1 + \varepsilon, \quad r(0) = 1, \quad r(1) = 1 + 2\varepsilon, \tag{26.2}$$

where ε is a parameter. Now there is a solution for any ε, namely

$$r(z) = 1 + \frac{\frac{4}{3}\varepsilon x}{x - \frac{1}{3}}. \tag{26.3}$$

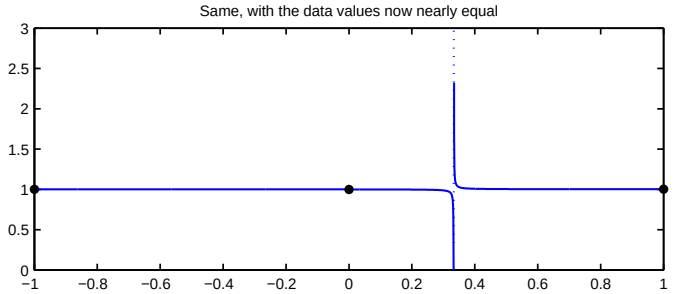
However, this is not quite the smooth interpolant one might have hoped for. Here is the picture for $\varepsilon = 0.1$:

```
r = @(ep) 1 + (4/3)*ep*x./(x-(1/3));
ep = 0.1;
hold off, plot(r(ep)), ylim([0 3])
hold on, plot([-1 0 1],[1+ep 1 1+2*ep],'.k')
title('A type (1,1) rational interpolant through 3 data values')
```

And here it is for $\varepsilon = .001$:

```
ep = 0.001;
hold off, plot(r(ep)), ylim([0 3])
hold on, plot([-1 0 1],[1+ep 1 1+2*ep],'.k')
title('Same, with the data values now nearly equal')
```



Looking back at the formula (26.3), we see that for any nonzero value of ε, this function has a pole at $x = 1/3$. When ε is small, the effect of the pole is quite localized, and we may confirm this by calculating that the residue is $(4/3)\varepsilon$. Another way to interpret the local effect of the pole is to note that r has a zero at a distance just $O(\varepsilon)$ from the pole:

$$\text{pole: } x = \tfrac{1}{3}, \qquad \text{zero: } x = \tfrac{1}{3}/(1 - \tfrac{4}{3}\varepsilon).$$

For $|x - \frac{1}{3}| \gg \varepsilon$, the pole and the zero will effectively cancel. This example shows that even when a rational interpolation problem has a unique solution, the problem may be ill-posed in the sense that the solution depends discontinuously on the data. For $\varepsilon = 0$, (26.3) reduces to the constant $r = 1$, whereas for any nonzero ε there is a pole, though it seems to have little to do with approximating the data. Such poles are often called **spurious poles**. Since a spurious pole is typically associated with a nearby zero that approximately cancels its effect further away, another term is **Froissart doublet**, named after the physicist

Marcel Froissart, or we may say that the function has a **spurious pole-zero pair**.

Here is an example somewhat closer to practical approximation. Define

```
f = cos(exp(x));
```

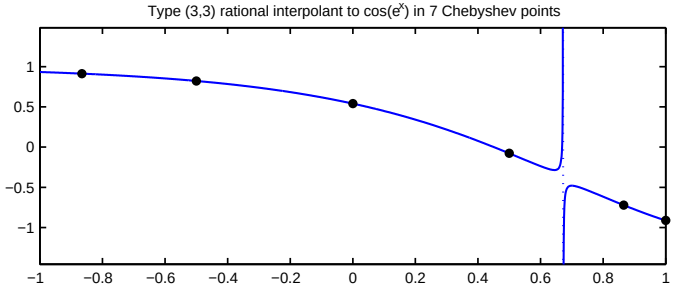
and suppose we want to construct rational interpolants of type (n, n) to f based on samples at $2n + 1$ Chebyshev points in $[-1, 1]$. Chebfun has a command `ratinterp` that will do this, and here a is a table of the maximum errors obtained by `ratinterp` for $n = 1, 2, \ldots, 6$:

```
disp('    (n,n)       Error ')
for n = 1:6
  [p,q] = ratinterp(f,n,n);
  err = norm(f-p./q,inf);
  fprintf('    (%1d,%1d)     %7.2e\n',n,n,err)
end
```

```
    (n,n)       Error
    (1,1)     2.46e-01
    (2,2)     7.32e-03
    (3,3)        Inf
    (4,4)     6.11e-06
    (5,5)     4.16e-07
    (6,6)     6.19e-09
```

We seem to have very fast convergence, but what has gone wrong with the type $(3, 3)$ approximant? A plot reveals that the problem is a spurious pole:

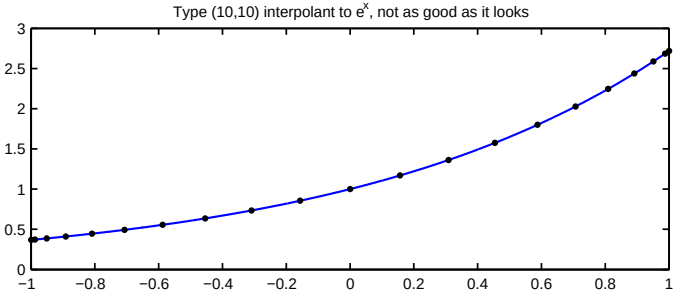
```
[p,q] = ratinterp(f,3,3);
hold off, plot(p./q), hold on
xx = chebpts(7); plot(xx,f(xx),'.k')
title(['Type (3,3) rational interpolant ' ...
       'to cos(e^x) in 7 Chebyshev points'])
```



One might suspect that this artifact has something to do with rounding errors on a computer, but it is not so. The spurious pole is in the mathematics, with residue equal to about -0.0013.

In other examples, on the other hand, spurious poles do indeed arise from rounding errors. In fact, they appear very commonly when one aims for approximations with accuracy close to machine precision. Here, for example, is what happens when `ratinterp` is called upon to compute the interpolant of type $(10, 10)$ of e^x in 21 Chebyshev points:

```
[p,q] = ratinterp(exp(x),10,10);
hold off, plot(p./q), hold on
xx = chebpts(21); plot(xx,exp(xx),'.k',MS,10)
title(['Type (10,10) interpolant to e^x, ' ...
       'not as good as it looks'])
```



The picture looks fine, but that is only because Chebfun has failed to detect that p/q has a spurious pole-zero pair:

```
spurious_zero = roots(p)
spurious_pole = roots(q)
```

```
spurious_zero =
  -0.652038909870924
spurious_pole =
  -0.652038909870924
```

The pole and zero differ at the level of rounding errors:

```
separation = spurious_pole - spurious_zero
```

```
separation =
     4.440892098500626e-16
```

The proper response to this problem is not to strive to compute in exact arithmetic, which would leave us with a terribly ill-conditioned problem and in any

case with spurious poles of the mathematically valid sort exemplified earlier. Instead, we must adjust the formulation of the rational interpolation problem so as to make it more robust. In this last example, it seems clear that a good algorithm should be sensible enough to cancel the pole and zero and return a function of exact type $(9,9)$ instead of $(10,10)$. We now show how this can be done systematically with the SVD.

At this point, we shall change settings. Logically, we would now proceed to develop a robust rational interpolation strategy on $[-1,1]$. However, that route would require us to combine new ideas related to robustness with the complexities of Chebyshev points, Chebyshev polynomials, and rational barycentric interpolation formulas. Instead, now and for the rest of the book we shall move from the real interval $[-1,1]$ to the unit disk and switch variable names from x to z. This will make the presentation simpler, and it fits with the fact that many applications of rational interpolants and approximants involve complex variables.

Specifically, here is the problem addressed in the remainder of this chapter, following [Gonnet, Pachón & Trefethen 2011]. Suppose f is a function defined on the unit circle in the complex plane and we consider its values $f(z_j)$ at the $(N+1)$st roots of unity for some $N \ge 0$,

$$z_j = e^{2\pi ij/(N+1)}, \quad 0 \le j \le N.$$

Using this information, how can we construct good approximations $r \in R_{mn}$? We assume for the moment that m, n and N are related by $N = m+n$. The parameter count is then right for an interpolant $r = p/q$ satisfying

$$\frac{p(z_j)}{q(z_j)} = f(z_j), \quad 0 \le j \le N, \tag{26.4}$$

but as we have seen, such a function does not always exist.

Our first step towards greater robustness will be to linearize the problem and seek polynomials $p \in P_m$ and $q \in P_n$ such that

$$p(z_j) = f(z_j)q(z_j), \quad 0 \le j \le N. \tag{26.5}$$

By itself, this set of equations isn't very useful, because it has the trivial solution $p = q = 0$. Some kind of normalization is needed, and for this we introduce the representations

$$p(z) = \sum_{k=0}^{m} p_k z^k, \qquad q(z) = \sum_{k=0}^{n} q_k z^k$$

with

$$\mathbf{p} = (p_0, \dots, p_m)^T, \qquad \mathbf{q} = (q_0, \dots, q_n)^T.$$

Our normalization will be the condition

$$\|\mathbf{q}\| = 1, \tag{26.6}$$

where $\|\cdot\|$ is the standard 2-norm on vectors,

$$\|\mathbf{q}\| = \left(\sum_{k=0}^{n} |q_k|^2 \right)^{1/2},$$

and similarly for vectors of dimensions other than $n+1$. Our linearized rational interpolation problem consists of solving the two equations (26.5)–(26.6).

We turn this into a matrix problem as follows. Given an arbitrary vector $\mathbf{q}$, there is a corresponding polynomial $q \in P_n$, which we may evaluate at the $(N+1)$st roots of unity $\{z_j\}$. Multiplying by the values $f(z_j)$ gives a set of $N+1$ numbers $f(z_j)q(z_j)$. There is a unique polynomial $\hat{p} \in P_N$ that interpolates these data,

$$\hat{p}(z_j) = f(z_j)q(z_j), \quad 0 \le j \le N.$$

Let $\hat{p}$ be written as

$$\hat{p}(z) = \sum_{k=0}^{N} \hat{p}_k z^k, \quad \hat{\mathbf{p}} = (\hat{p}_0, \dots, \hat{p}_N)^T.$$

Then $\hat{\mathbf{p}}$ is a linear function of $\mathbf{q}$, and we may accordingly express it as the product

$$\hat{\mathbf{p}} = \hat{Z}\mathbf{q},$$

where $\hat{Z}$ is a rectangular matrix of dimensions $(N+1) \times (n+1)$ depending on f. It can be shown that $\hat{Z}$ is a Toeplitz matrix with entries given by the discrete Laurent or Fourier coefficients

$$z_{jk} = \frac{1}{N+1} \sum_{\ell=0}^{N} z_\ell^{k-j} f(z_\ell). \tag{26.7}$$

And now we can solve (26.5)–(26.6). Let $\tilde{Z}$ be the $n \times (n+1)$ matrix consisting of the last n rows of $\hat{Z}$. Since $\tilde{Z}$ has more columns than rows, it has a nontrivial null vector, and for $\mathbf{q}$ we take any such null vector normalized to length 1:

$$\tilde{Z}\mathbf{q} = 0, \quad \|\mathbf{q}\| = 1. \tag{26.8}$$

The corresponding vector $\hat{\mathbf{p}} = \hat{Z}\mathbf{q}$ is equal to zero in positions $m+1$ through N, and we take $\mathbf{p}$ to be the remaining, initial portion of $\hat{\mathbf{p}}$: $p_j = \hat{p}_j$, $0 \le j \le m$. In matrix form we can write this as

$$\mathbf{p} = Z\mathbf{q}, \tag{26.9}$$

where Z is the $(m+1) \times (n+1)$ matrix consisting of the first $m+1$ rows of $\hat{Z}$. Equations (26.8)–(26.9) constitute a solution to (26.5)–(26.6).

In a numerical implementation of the algorithm just described, the operations should properly be combined into a Matlab function, but for the sake of in-line

presentation, we shall achieve the necessary effect with a string of anonymous functions.

The first step is to construct the Toeplitz matrix $\hat{Z}$ using Matlab's `fft` command. The `real` command below eliminates imaginary parts at the level of rounding errors, and would need to be removed for a function f that was not real on the real axis.

```
fj = @(f,N) f(exp(2i*pi*(0:N)'/(N+1)));
extract = @(A,I,J) A(I,J);
column = @(f,N) real(fft(fj(f,N)))/(N+1);
row = @(f,n,N) extract(column(f,N),[1 N+1:-1:N+2-n],1);
Zhat = @(f,n,N) toeplitz(column(f,N),row(f,n,N));
```

Next we extract the submatrices $\tilde{Z}$ and Z:

```
Ztilde = @(f,m,n,N) extract(Zhat(f,n,N),m+2:N+1,:);
Z = @(f,m,n,N) extract(Zhat(f,n,N),1:m+1,:);
```

Finally we compute the vector $\mathbf{q}$ using Matlab's `null` command, which makes use of the SVD, and multiply by Z to get $\mathbf{p}$:

```
q = @(f,m,n,N) null(Ztilde(f,m,n,N));
p = @(f,m,n,N) Z(f,m,n,N)*q(f,m,n,N);
```

For example, here are the coefficients of the type $(2,2)$ interpolant to e^z in the 5th roots of unity:

```
f = @(z) exp(z);
m = 2; n = 2; N = m+n;
pp = p(f,m,n,N)
qq = q(f,m,n,N)
```

```
pp =
  -0.893131422200046
  -0.446418130422149
  -0.074390723603151
qq =
  -0.891891822763679
   0.446093473426966
  -0.074361209330862
```

The zeros lie in the left half-plane and the poles in the right half-plane:

```
rzeros = roots(flipud(pp))
rpoles = roots(flipud(qq))
```



```
rzeros =
 -3.000495954331878 + 1.732909565613550i
 -3.000495954331878 - 1.732909565613550i
rpoles =
  2.999503890813022 + 1.731191260767684i
  2.999503890813022 - 1.731191260767684i
```

Here are the values of the interpolant at $z = 0$ and $z = 2$, which one can see are not too far from e^0 and e^2:

```
r = @(z) polyval(flipud(pp),z)./polyval(flipud(qq),z);
approximation = r([0 2])
exact = exp([0 2])
```

```
approximation =
   1.001389854021227   7.011719966971134
exact =
   1.000000000000000   7.389056098930650
```

Now let us take stock. We have derived an algorithm for computing rational interpolants based on the linearized formula (26.5), but we have not yet dealt with spurious poles. Indeed, the solution developed so far has neither uniqueness nor continuous dependence on data. It is time to take our second step toward greater robustness, again relying on the SVD.

An example will illustrate what needs to be done. Suppose that instead of a type $(2,2)$ interpolant to e^z in 5 points, we want a type $(10,10)$ interpolant in 21 points. (This is like the type $(10,10)$ interpolant computed earlier, but now in roots of unity rather than Chebyshev points.) Here is what we find:

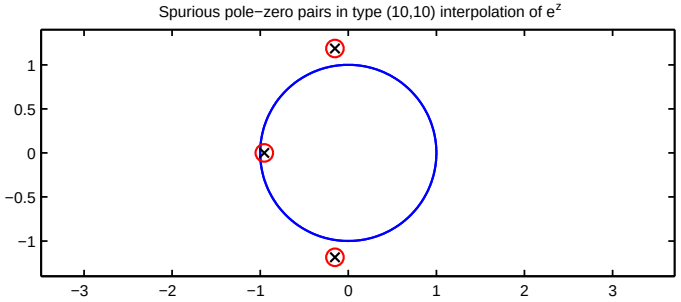
```
m = 10; n = 10; N = m+n;
format short
pp = p(f,m,n,N)
qq = q(f,m,n,N)
```

```
pp =
    0.7083    0.0888    0.5542   -0.4282
    1.2484    0.5251    0.3191    0.2516
    1.1840    0.5173   -0.7445   -0.0644
    0.9629   -0.5332   -0.8487   -0.0012
    0.3525   -0.3230   -0.3190    0.0156
    0.0725   -0.0785   -0.0653    0.0052
    0.0095   -0.0112   -0.0085    0.0008
    0.0008   -0.0010   -0.0007    0.0001
    0.0000   -0.0001   -0.0000    0.0000
    0.0000   -0.0000   -0.0000    0.0000
    0.0000   -0.0000   -0.0000    0.0000
```

```
qq =
    0.7083    0.0888    0.5542   -0.4282
    0.5401    0.4363   -0.2351    0.6798
    0.2898    0.0366   -0.7864   -0.5301
    0.2850   -0.8028   -0.0371    0.2604
   -0.1970    0.3850    0.1274   -0.0751
    0.0503   -0.0871   -0.0379    0.0137
   -0.0073    0.0119    0.0059   -0.0017
    0.0007   -0.0011   -0.0006    0.0001
   -0.0000    0.0001    0.0000   -0.0000
    0.0000   -0.0000   -0.0000    0.0000
   -0.0000    0.0000    0.0000   -0.0000
```

Instead of the expected vectors $\mathbf{p}$ and $\mathbf{q}$, we have matrices of dimension 11×4, and the reason is, $\tilde{Z}$ has a nullspace of dimension 4. This would not be true in exact arithmetic, but it is true in 16-digit floating-point. If we construct an interpolant from one of these vectors, it will have three spurious pole-zero pairs. Here is an illustration, showing that the spurious poles (crosses) and zeros (cricles) are near the unit circle, which is typical. The other seven non-spurious poles and zeros have moduli about ten times larger.

```
rpoles = roots(flipud(pp(:,1)));
rzeros = roots(flipud(qq(:,1)));
hold off, plot(exp(2i*pi*x))
ylim([-1.4 1.4]), axis equal, hold on
plot(rpoles,'xk',MS,7)
plot(rzeros,'or',MS,9)
title(['Spurious pole-zero pairs in type ' ...
       '(10,10) interpolation of e^z'])
```



Having spotted the problem, we can fix it as follows. If $\tilde{Z}$ has rank $n-d$ for some $d \geq 1$, then it has a nullspace of dimension $d+1$. (We intentionally use the same letter d as was used to denote the defect in the Chapter 24.) There must exist a vector $\mathbf{q}$ in this nullspace whose final d entries are zero. We could do some linear algebra to construct this vector, but a simpler approach is to

reduce m and n by d and N by $2d$ and compute the interpolant again. Here is a function for computing d with the help of Matlab's `rank` command, which is based on the SVD. The tolerance 10^{-12} ensures that contributions close to machine precision are discarded.

```
d = @(f,m,n,N) n-rank(Ztilde(f,m,n,N),1e-12);
```

We redefine `q` and `p` to use this information:

```
q = @(f,m,n,N,d) null(Ztilde(f,m-d,n-d,N-2*d));
p = @(f,m,n,N,d) Z(f,m-d,n-d,N-2*d)*q(f,m,n,N,d);
```

Our example now gives vectors instead of matrices, with no spurious poles.

```
pp = p(f,m,n,N,d(f,m,n,N)); qq = q(f,m,n,N,d(f,m,n,N));
format long
disp('           pp                  qq'), disp([pp qq])
```

```
          pp                qq
  -0.889761508243745  -0.889761508243590
  -0.444881276261385   0.444880231982283
  -0.101109523963195  -0.101109001823663
  -0.013481293296605   0.013481177243185
  -0.001123443568854  -0.001123429053771
  -0.000056172338565   0.000056171300325
  -0.000001337441819  -0.000001337407096
```

This type $(7,7)$ rational function approximates e^z to approximately machine precision in the unit disk. To verify this, we write a function `error` that measures the maximum of $|f(z)-r(z)|$ over 1000 random points in the disk:

```
r = @(z) polyval(flipud(pp),z)./polyval(flipud(qq),z);
z = sqrt(rand(1000,1)).*exp(2i*pi*rand(1000,1));
error = @(f,r) norm(f(z)-r(z),inf);
error(f,r)
```

```
ans = 8.999729433362549e-13
```

Mathematically, in exact arithmetic, the trick of reducing m and n by d restores uniqueness and continuous dependence on data, making the rational interpolation problem well-posed. On a computer, we do the same but rely on finite tolerances to remove contributions from singular values close to machine epsilon. A much more careful version of this algorithm can be found in the Matlab code `ratdisk` presented in [Gonnet, Pachón & Trefethen 2011].

We conclude this chapter by taking our third step towards robustness. So far, we have spoken only of interpolation, where the number of data values exactly matches the number of parameters in the fit. In some approximation problems,

however, it may be better to have more data than parameters and perform a least-squares fit. This is one of those situations, and in particular, a least-squares formulation will reduce the likelihood of obtaining poles in the region near the unit circle where one is hoping for good approximation. This is why we have included the parameter N throughout the derivation of the last six pages. We will now consider the situation $N > m + n$. Typicaly choices for practical applications might be $N = 2(m + n)$ or $N = 4(m + n)$.

Given a vector $\mathbf{q}$ and corresponding function q, we have already defined $\|\mathbf{q}\|$ as the usual 2-norm. For the function q, let us now define

$$\|q\|_N = (N+1)^{-1/2} \sum_{k=0}^{N} |q(z_j)|^2,$$

a weighted 2-norm of the values of $q(z)$ over the unit circle. So long as $N \geq n$, the two norms are equal:

$$\|q\|_N = \|\mathbf{q}\|.$$

The norm $\|\cdot\|_N$, however, applies to any function, not just a polynomial. In particular, our linearized least-squares rational approximation problem is this generalization of (26.5)–(26.6):

$$\|p - fq\|_N = \text{minimum}, \quad \|q\|_N = 1. \tag{26.10}$$

The algorithm we have derived for interpolation solves this problem too. What changes is that the matrix $\tilde{Z}$, of dimension $(N - m) \times (n + 1)$, may no longer have a null vector. If its singular values are $\sigma_1 \geq \cdots \geq \sigma_{n+1} \geq 0$, then the minimum error will be

$$\|p - fq\|_N = \sigma_{n+1},$$

which may be positive or zero. If $\sigma_n > \sigma_{n+1}$, $\mathbf{q}$ is obtained from the corresponding singular vector and that is all there is to it. If

$$\sigma_{n-d} > \sigma_{n-d+1} = \cdots = \sigma_{n+1}$$

for some $d \geq 1$, then the minimum singular space is of dimension $d + 1$, and as before, we reduce m and n by d. The parameter N can be left unchanged, so f does not need to be evaluated at any new points.

For example, let f be the function

```
f = @(z) log(1.44-z.^2);
```

with branch points at ± 1.2, and suppose we want a type $(40, 40)$ least-squares approximant with $N = 400$. The approximation delivered by the SVD algorithm comes out with exact type $(18, 18)$:

```
m = 40; n = 40; N = 400;
pp = p(f,m,n,N,d(f,m,n,N)); qq = q(f,m,n,N,d(f,m,n,N));
mu = length(pp)-1; nu = length(qq)-1;
fprintf('    mu = %2d    nu = %2d\n',mu,nu)
```



```
    mu = 18    nu = 18
```

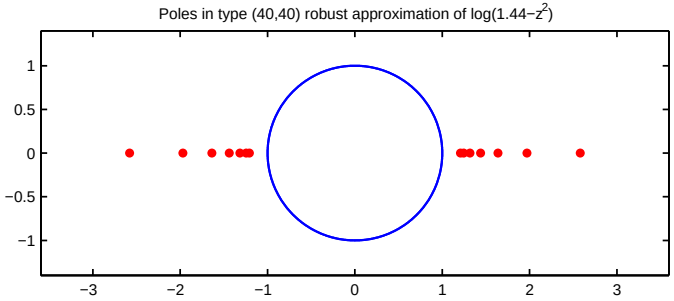
The accuracy in the unit disk is good (Exercise 26.4):

```
r = @(z) polyval(flipud(pp),z)./polyval(flipud(qq),z);
error(f,r)
```

```
ans = 4.218427953398217e-12
```

Here are the poles:

```
rpoles = roots(flipud(qq));
hold off, plot(exp(2i*pi*x))
ylim([-1.4 1.4]), axis equal, hold on
plot(rpoles+1e-10i,'.r',MS,14)
title(['Poles in type (40,40) robust ' ...
       'approximation of log(1.44-z^2)'])
```

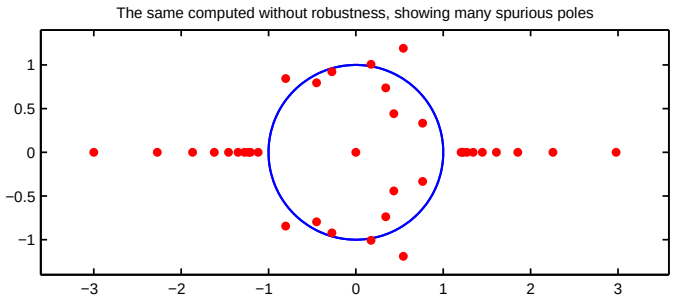


For comparison, suppose we revert to the original definitions of the anonymous functions `p` and `q`, with no removal of negligible singular values:

```
q = @(f,m,n,N) null(Ztilde(f,m,n,N));
p = @(f,m,n,N) Z(f,m,n,N)*q(f,m,n,N);
```

Now the computation comes out with exact type $(40, 40)$, and half the poles are spurious:

```
m = 40; n = 40; N = 400;
pp = p(f,m,n,N); pp = pp(:,end);
qq = q(f,m,n,N); qq = qq(:,end);
rpoles = roots(flipud(qq));
hold off, plot(exp(2i*pi*x))
ylim([-1.4 1.4]), axis equal, hold on
plot(rpoles+1e-10i,'.r',MS,14)
title(['The same computed without robustness, ' ...
       'showing many spurious poles'])
```



The error looks excellent,

```
r = @(z) polyval(flipud(pp),z)./polyval(flipud(qq),z);
error(f,r)
```

```
ans = 2.775556849639900e-14
```

but it is not so good in fact. Because of the spurious poles, the maximum error in the unit disk is actually infinite, but this has gone undetected at the 1000 random sample points used by the `error` command.

SUMMARY OF CHAPTER 26. *Generically, there exists a unique type (m,n) rational interpolant through $m+n+1$ data points, but such interpolants do not always exist, depend discontinuously on the data, and exhibit spurious pole-zero pairs both in exact arithmetic and even more commonly in floating point. Such interpolants can be computed by solving a linear algebra problem involving a Toeplitz matrix of discrete Fourier coefficients. Uniqueness, continuous dependence, and avoidance of spurious poles can be achieved by reducing m and n when the minimal singular value of this matrix is multiple.*

Exercise 26.1. Nonexistence of certain interpolants. Show that if a function in R_{11} takes equal values at two points, it must be a constant.

Exercise 26.2. An invalid argument. We saw that the type $(3,3)$ interpolant to $\cos(e^x)$ in 7 Chebyshev points has a pole near $x=0.6$. What is the flaw in the following argument? (Spell it out carefully, don't just give a word or two.) The interpolant through these 7 data values can be regarded as a combination of cardinal functions, i.e., type $(3,3)$ rational interpolants through Kronecker delta functions supported at each of the data points. If the sum has a pole at x_0, then one of the cardinal interpolants must have a pole at x_0. So type $(3,3)$ rational interpolants to almost every set of data at these 7 points will have a pole at exactly the same place.

Exercise 26.3. Explicit example of degeneracy. [The type $(1,1)$ example from the beginning of the chapter.]

Exercise 26.4. Rational vs. polynomial approximation. The final computational example of this chapter considered type (n,n) rational approximation of $f(z)=\log(1.44-z^2)$ with $n=40$, which was reduced to $n=18$ by the robust algorithm. For degree $2n$ polynomial approximation, one would expect accuracy of order $O(\rho^{-2n})$ where ρ is the radius of convergence of the Taylor series of f at $z=0$. How large would n need to be for this figure to be comparable to the observed accuracy of 10^{-11}?

27. Padé approximation

[Not yet written]

28. Extrapolation of sequences and analytic continuation

[Not yet written]

References

Each reference is followed by a note highlighting a contribution of that publication that is relevant to this book. These notes are by no means exhaustive; in most cases the references include other significant contributions too. Papers listed by authors such as Chebyshev, Gauss, Jacobi, and Weierstrass can also be found in their collected works.

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