## CHAPTER

## 8



## Approximation Theory

## Introduction

Hooke's law states that when a force is applied to a spring constructed of uniform material, the length of the spring is a linear function of that force. We can write the linear function as $F(l)=k(l-E)$, where $F(l)$ represents the force required to stretch the spring $l$ units, the constant $E$ represents the length of the spring with no force applied, and the constant $k$ is the spring constant.



Suppose we want to determine the spring constant for a spring that has initial length 5.3 in . We apply forces of 2,4 , and 6 lb to the spring and find that its length increases to 7.0 , 9.4 , and 12.3 in., respectively. A quick examination shows that the points $(0,5.3),(2,7.0)$, $(4,9.4)$, and $(6,12.3)$ do not quite lie in a straight line. Although we could use a random pair of these data points to approximate the spring constant, it would seem more reasonable to find the line that best approximates all the data points to determine the constant. This type of approximation will be considered in this chapter, and this spring application can be found in Exercise 7 of Section 8.1.

Approximation theory involves two general types of problems. One problem arises when a function is given explicitly, but we wish to find a "simpler" type of function, such as a polynomial, to approximate values of the given function. The other problem in approximation theory is concerned with fitting functions to given data and finding the "best" function in a certain class to represent the data.

Both problems have been touched upon in Chapter 3. The $n$th Taylor polynomial about the number $x_{0}$ is an excellent approximation to an $(n+1)$-times differentiable function $f$ in a small neighborhood of $x_{0}$. The Lagrange interpolating polynomials, or, more generally, osculatory polynomials, were discussed both as approximating polynomials and as polynomials to fit certain data. Cubic splines were also discussed in that chapter. In this chapter, limitations to these techniques are considered, and other avenues of approach are discussed.

### 8.1 Discrete Least Squares Approximation

Table 8.1

| $x_{i}$ | $y_{i}$ | $x_{i}$ | $y_{i}$ |
| :---: | :---: | :---: | :---: |
| 1 | 1.3 | 6 | 8.8 |
| 2 | 3.5 | 7 | 10.1 |
| 3 | 4.2 | 8 | 12.5 |
| 4 | 5.0 | 9 | 13.0 |
| 5 | 7.0 | 10 | 15.6 |

Consider the problem of estimating the values of a function at nontabulated points, given the experimental data in Table 8.1.

Figure 8.1 shows a graph of the values in Table 8.1. From this graph, it appears that the actual relationship between $x$ and $y$ is linear. The likely reason that no line precisely fits the data is because of errors in the data. So it is unreasonable to require that the approximating function agree exactly with the data. In fact, such a function would introduce oscillations that were not originally present. For example, the graph of the ninth-degree interpolating polynomial shown in unconstrained mode for the data in Table 8.1 is obtained in Maple using the commands
$p:=\operatorname{interp}([1,2,3,4,5,6,7,8,9,10],[1.3,3.5,4.2,5.0,7.0,8.8,10.1,12.5,13.0,15.6], x):$ $\operatorname{plot}(p, x=1 . .10)$


The plot obtained (with the data points added) is shown in Figure 8.2.

Figure 8.2

This polynomial is clearly a poor predictor of information between a number of the data points. A better approach would be to find the "best" (in some sense) approximating line, even if it does not agree precisely with the data at any point.

Let $a_{1} x_{i}+a_{0}$ denote the $i$ th value on the approximating line and $y_{i}$ be the $i$ th given $y$-value. We assume throughout that the independent variables, the $x_{i}$, are exact, it is the dependent variables, the $y_{i}$, that are suspect. This is a reasonable assumption in most experimental situations.

The problem of finding the equation of the best linear approximation in the absolute sense requires that values of $a_{0}$ and $a_{1}$ be found to minimize

$$
E_{\infty}\left(a_{0}, a_{1}\right)=\max _{1 \leq i \leq 10}\left\{\left|y_{i}-\left(a_{1} x_{i}+a_{0}\right)\right|\right\} .
$$

This is commonly called a minimax problem and cannot be handled by elementary techniques.

Another approach to determining the best linear approximation involves finding values of $a_{0}$ and $a_{1}$ to minimize

$$
E_{1}\left(a_{0}, a_{1}\right)=\sum_{i=1}^{10}\left|y_{i}-\left(a_{1} x_{i}+a_{0}\right)\right| .
$$

This quantity is called the absolute deviation. To minimize a function of two variables, we need to set its partial derivatives to zero and simultaneously solve the resulting equations. In the case of the absolute deviation, we need to find $a_{0}$ and $a_{1}$ with

$$
0=\frac{\partial}{\partial a_{0}} \sum_{i=1}^{10}\left|y_{i}-\left(a_{1} x_{i}+a_{0}\right)\right| \quad \text { and } \quad 0=\frac{\partial}{\partial a_{1}} \sum_{i=1}^{10}\left|y_{i}-\left(a_{1} x_{i}+a_{0}\right)\right|
$$

The problem is that the absolute-value function is not differentiable at zero, and we might not be able to find solutions to this pair of equations.

## Linear Least Squares

The least squares approach to this problem involves determining the best approximating line when the error involved is the sum of the squares of the differences between the $y$-values on the approximating line and the given $y$-values. Hence, constants $a_{0}$ and $a_{1}$ must be found that minimize the least squares error:

$$
E_{2}\left(a_{0}, a_{1}\right)=\sum_{i=1}^{10}\left[y_{i}-\left(a_{1} x_{i}+a_{0}\right)\right]^{2}
$$

The least squares method is the most convenient procedure for determining best linear approximations, but there are also important theoretical considerations that favor it. The minimax approach generally assigns too much weight to a bit of data that is badly in error, whereas the absolute deviation method does not give sufficient weight to a point that is considerably out of line with the approximation. The least squares approach puts substantially more weight on a point that is out of line with the rest of the data, but will not permit that point to completely dominate the approximation. An additional reason for considering the least squares approach involves the study of the statistical distribution of error. (See [Lar], pp. 463-481.)

The general problem of fitting the best least squares line to a collection of data $\left\{\left(x_{i}, y_{i}\right)\right\}_{i=1}^{m}$ involves minimizing the total error,

$$
E \equiv E_{2}\left(a_{0}, a_{1}\right)=\sum_{i=1}^{m}\left[y_{i}-\left(a_{1} x_{i}+a_{0}\right)\right]^{2},
$$

The word normal as used here implies perpendicular. The normal equations are obtained by finding perpendicular directions to a multidimensional surface.
with respect to the parameters $a_{0}$ and $a_{1}$. For a minimum to occur, we need both

$$
\frac{\partial E}{\partial a_{0}}=0 \quad \text { and } \quad \frac{\partial E}{\partial a_{1}}=0,
$$

that is,

$$
0=\frac{\partial}{\partial a_{0}} \sum_{i=1}^{m}\left[\left(y_{i}-\left(a_{1} x_{i}-a_{0}\right)\right]^{2}=2 \sum_{i=1}^{m}\left(y_{i}-a_{1} x_{i}-a_{0}\right)(-1)\right.
$$

and

$$
0=\frac{\partial}{\partial a_{1}} \sum_{i=1}^{m}\left[y_{i}-\left(a_{1} x_{i}+a_{0}\right)\right]^{2}=2 \sum_{i=1}^{m}\left(y_{i}-a_{1} x_{i}-a_{0}\right)\left(-x_{i}\right) .
$$

These equations simplify to the normal equations:

$$
a_{0} \cdot m+a_{1} \sum_{i=1}^{m} x_{i}=\sum_{i=1}^{m} y_{i} \quad \text { and } \quad a_{0} \sum_{i=1}^{m} x_{i}+a_{1} \sum_{i=1}^{m} x_{i}^{2}=\sum_{i=1}^{m} x_{i} y_{i} .
$$

The solution to this system of equations is

$$
\begin{equation*}
a_{0}=\frac{\sum_{i=1}^{m} x_{i}^{2} \sum_{i=1}^{m} y_{i}-\sum_{i=1}^{m} x_{i} y_{i} \sum_{i=1}^{m} x_{i}}{m\left(\sum_{i=1}^{m} x_{i}^{2}\right)-\left(\sum_{i=1}^{m} x_{i}\right)^{2}} \tag{8.1}
\end{equation*}
$$

and

$$
\begin{equation*}
a_{1}=\frac{m \sum_{i=1}^{m} x_{i} y_{i}-\sum_{i=1}^{m} x_{i} \sum_{i=1}^{m} y_{i}}{m\left(\sum_{i=1}^{m} x_{i}^{2}\right)-\left(\sum_{i=1}^{m} x_{i}\right)^{2}} . \tag{8.2}
\end{equation*}
$$

Example 1 Find the least squares line approximating the data in Table 8.1.
Solution We first extend the table to include $x_{i}^{2}$ and $x_{i} y_{i}$ and sum the columns. This is shown in Table 8.2.

Table 8.2

| $x_{i}$ | $y_{i}$ | $x_{i}^{2}$ | $x_{i} y_{i}$ | $P\left(x_{i}\right)=1.538 x_{i}-0.360$ |
| ---: | ---: | ---: | ---: | :---: |
| 1 | 1.3 | 1 | 1.3 | 1.18 |
| 2 | 3.5 | 4 | 7.0 | 2.72 |
| 3 | 4.2 | 9 | 12.6 | 4.25 |
| 4 | 5.0 | 16 | 20.0 | 5.79 |
| 5 | 7.0 | 25 | 35.0 | 7.33 |
| 6 | 8.8 | 36 | 52.8 | 8.87 |
| 7 | 10.1 | 49 | 70.7 | 10.41 |
| 8 | 12.5 | 64 | 100.0 | 11.94 |
| 9 | 13.0 | 81 | 117.0 | 13.48 |
| 10 | 15.6 | 100 | 156.0 | 15.02 |
| 55 | 81.0 | 385 | 572.4 | $E=\sum_{i=1}^{10}\left(y_{i}-P\left(x_{i}\right)\right)^{2} \approx 2.34$ |

The normal equations (8.1) and (8.2) imply that

$$
a_{0}=\frac{385(81)-55(572.4)}{10(385)-(55)^{2}}=-0.360
$$

and

$$
a_{1}=\frac{10(572.4)-55(81)}{10(385)-(55)^{2}}=1.538
$$

so $P(x)=1.538 x-0.360$. The graph of this line and the data points are shown in Figure 8.3. The approximate values given by the least squares technique at the data points are in Table 8.2.

## Figure 8.3



## Polynomial Least Squares

The general problem of approximating a set of data, $\left\{\left(x_{i}, y_{i}\right) \mid i=1,2, \ldots, m\right\}$, with an algebraic polynomial

$$
P_{n}(x)=a_{n} x^{n}+a_{n-1} x^{n-1}+\cdots+a_{1} x+a_{0}
$$

of degree $n<m-1$, using the least squares procedure is handled similarly. We choose the constants $a_{0}, a_{1}, \ldots, a_{n}$ to minimize the least squares error $E=E_{2}\left(a_{0}, a_{1}, \ldots, a_{n}\right)$, where

$$
\begin{aligned}
E & =\sum_{i=1}^{m}\left(y_{i}-P_{n}\left(x_{i}\right)\right)^{2} \\
& =\sum_{i=1}^{m} y_{i}^{2}-2 \sum_{i=1}^{m} P_{n}\left(x_{i}\right) y_{i}+\sum_{i=1}^{m}\left(P_{n}\left(x_{i}\right)\right)^{2}
\end{aligned}
$$

$$
\begin{aligned}
& =\sum_{i=1}^{m} y_{i}^{2}-2 \sum_{i=1}^{m}\left(\sum_{j=0}^{n} a_{j} x_{i}^{j}\right) y_{i}+\sum_{i=1}^{m}\left(\sum_{j=0}^{n} a_{j} x_{i}^{j}\right)^{2} \\
& =\sum_{i=1}^{m} y_{i}^{2}-2 \sum_{j=0}^{n} a_{j}\left(\sum_{i=1}^{m} y_{i} x_{i}^{j}\right)+\sum_{j=0}^{n} \sum_{k=0}^{n} a_{j} a_{k}\left(\sum_{i=1}^{m} x_{i}^{j+k}\right)
\end{aligned}
$$

As in the linear case, for $E$ to be minimized it is necessary that $\partial E / \partial a_{j}=0$, for each $j=0,1, \ldots, n$. Thus, for each $j$, we must have

$$
0=\frac{\partial E}{\partial a_{j}}=-2 \sum_{i=1}^{m} y_{i} x_{i}^{j}+2 \sum_{k=0}^{n} a_{k} \sum_{i=1}^{m} x_{i}^{j+k}
$$

This gives $n+1$ normal equations in the $n+1$ unknowns $a_{j}$. These are

$$
\begin{equation*}
\sum_{k=0}^{n} a_{k} \sum_{i=1}^{m} x_{i}^{j+k}=\sum_{i=1}^{m} y_{i} x_{i}^{j}, \quad \text { for each } j=0,1, \ldots, n \tag{8.3}
\end{equation*}
$$

It is helpful to write the equations as follows:

$$
\begin{array}{r}
a_{0} \sum_{i=1}^{m} x_{i}^{0}+a_{1} \sum_{i=1}^{m} x_{i}^{1}+a_{2} \sum_{i=1}^{m} x_{i}^{2}+\cdots+a_{n} \sum_{i=1}^{m} x_{i}^{n}=\sum_{i=1}^{m} y_{i} x_{i}^{0}, \\
a_{0} \sum_{i=1}^{m} x_{i}^{1}+a_{1} \sum_{i=1}^{m} x_{i}^{2}+a_{2} \sum_{i=1}^{m} x_{i}^{3}+\cdots+a_{n} \sum_{i=1}^{m} x_{i}^{n+1}=\sum_{i=1}^{m} y_{i} x_{i}^{1}, \\
\\
\vdots \\
a_{0} \sum_{i=1}^{m} x_{i}^{n}+a_{1} \sum_{i=1}^{m} x_{i}^{n+1}+a_{2} \sum_{i=1}^{m} x_{i}^{n+2}+\cdots+a_{n} \sum_{i=1}^{m} x_{i}^{2 n}=\sum_{i=1}^{m} y_{i} x_{i}^{n} .
\end{array}
$$

These normal equations have a unique solution provided that the $x_{i}$ are distinct (see Exercise 14).

Example 2 Fit the data in Table 8.3 with the discrete least squares polynomial of degree at most 2 .
Solution For this problem, $n=2, m=5$, and the three normal equations are

Table 8.3

| $i$ | $x_{i}$ | $y_{i}$ |
| :---: | :---: | :---: |
| 1 | 0 | 1.0000 |
| 2 | 0.25 | 1.2840 |
| 3 | 0.50 | 1.6487 |
| 4 | 0.75 | 2.1170 |
| 5 | 1.00 | 2.7183 |

$$
\begin{aligned}
5 a_{0}+2.5 a_{1}+1.875 a_{2} & =8.7680 \\
2.5 a_{0}+1.875 a_{1}+1.5625 a_{2} & =5.4514 \\
1.875 a_{0}+1.5625 a_{1}+1.3828 a_{2} & =4.4015
\end{aligned}
$$

To solve this system using Maple, we first define the equations
$e q 1:=5 a 0+2.5 a 1+1.875 a 2=8.7680:$
$e q 2:=2.5 a 0+1.875 a 1+1.5625 a 2=5.4514:$
$e q 3:=1.875 a 0+1.5625 a 1+1.3828 a 2=4.4015$
and then solve the system with
solve( $\{e q 1, e q 2, e q 3\},\{a 0, a 1, a 2\})$
This gives

$$
\left\{a_{0}=1.005075519, \quad a_{1}=0.8646758482, \quad a_{2}=.8431641518\right\}
$$

Thus the least squares polynomial of degree 2 fitting the data in Table 8.3 is

$$
P_{2}(x)=1.0051+0.86468 x+0.84316 x^{2}
$$

whose graph is shown in Figure 8.4. At the given values of $x_{i}$ we have the approximations shown in Table 8.4.

Figure 8.4


Table 8.4

| $i$ | 1 | 2 | 3 | 4 | 5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $x_{i}$ | 0 | 0.25 | 0.50 | 0.75 | 1.00 |
| $y_{i}$ | 1.0000 | 1.2840 | 1.6487 | 2.1170 | 2.7183 |
| $P\left(x_{i}\right)$ | 1.0051 | 1.2740 | 1.6482 | 2.1279 | 2.7129 |
| $y_{i}-P\left(x_{i}\right)$ | -0.0051 | 0.0100 | 0.0004 | -0.0109 | 0.0054 |

The total error,

$$
E=\sum_{i=1}^{5}\left(y_{i}-P\left(x_{i}\right)\right)^{2}=2.74 \times 10^{-4}
$$

is the least that can be obtained by using a polynomial of degree at most 2 .

Maple has a function called LinearFit within the Statistics package which can be used to compute the discrete least squares approximations. To compute the approximation in Example 2 we first load the package and define the data

$$
\text { with }(\text { Statistics }): \text { xvals }:=\operatorname{Vector}([0,0.25,0.5,0.75,1]): \text { yvals }:=\operatorname{Vector}([1,1.284,1.6487,
$$ 2.117, 2.7183]):

To define the least squares polynomial for this data we enter the command $P:=x \rightarrow \operatorname{LinearFit}\left(\left[1, x, x^{2}\right], x v a l s, y v a l s, x\right): P(x)$

Maple returns a result which rounded to 5 decimal places is

$$
1.00514+0.86418 x+0.84366 x^{2}
$$

The approximation at a specific value, for example at $x=1.7$, is found with $P(1.7)$

$$
4.91242
$$

At times it is appropriate to assume that the data are exponentially related. This requires the approximating function to be of the form

$$
\begin{equation*}
y=b e^{a x} \tag{8.4}
\end{equation*}
$$

or

$$
\begin{equation*}
y=b x^{a} \tag{8.5}
\end{equation*}
$$

for some constants $a$ and $b$. The difficulty with applying the least squares procedure in a situation of this type comes from attempting to minimize

$$
E=\sum_{i=1}^{m}\left(y_{i}-b e^{a x_{i}}\right)^{2}, \quad \text { in the case of Eq. (8.4), }
$$

or

$$
E=\sum_{i=1}^{m}\left(y_{i}-b x_{i}^{a}\right)^{2}, \quad \text { in the case of Eq. (8.5). }
$$

The normal equations associated with these procedures are obtained from either

$$
0=\frac{\partial E}{\partial b}=2 \sum_{i=1}^{m}\left(y_{i}-b e^{a x_{i}}\right)\left(-e^{a x_{i}}\right)
$$

and

$$
0=\frac{\partial E}{\partial a}=2 \sum_{i=1}^{m}\left(y_{i}-b e^{a x_{i}}\right)\left(-b x_{i} e^{a x_{i}}\right), \quad \text { in the case of Eq. (8.4); }
$$

or

$$
0=\frac{\partial E}{\partial b}=2 \sum_{i=1}^{m}\left(y_{i}-b x_{i}^{a}\right)\left(-x_{i}^{a}\right)
$$

and

$$
0=\frac{\partial E}{\partial a}=2 \sum_{i=1}^{m}\left(y_{i}-b x_{i}^{a}\right)\left(-b\left(\ln x_{i}\right) x_{i}^{a}\right), \quad \text { in the case of Eq. (8.5). }
$$

No exact solution to either of these systems in $a$ and $b$ can generally be found.
The method that is commonly used when the data are suspected to be exponentially related is to consider the logarithm of the approximating equation:

$$
\ln y=\ln b+a x, \quad \text { in the case of Eq. (8.4), }
$$

and

$$
\ln y=\ln b+a \ln x, \quad \text { in the case of Eq. (8.5). }
$$

In either case, a linear problem now appears, and solutions for $\ln b$ and $a$ can be obtained by appropriately modifying the normal equations (8.1) and (8.2).

However, the approximation obtained in this manner is not the least squares approximation for the original problem, and this approximation can in some cases differ significantly from the least squares approximation to the original problem. The application in Exercise 13 describes such a problem. This application will be reconsidered as Exercise 11 in Section 10.3, where the exact solution to the exponential least squares problem is approximated by using methods suitable for solving nonlinear systems of equations.

Illustration Consider the collection of data in the first three columns of Table 8.5.

Table 8.5

| $i$ | $x_{i}$ | $y_{i}$ | $\ln y_{i}$ | $x_{i}^{2}$ | $x_{i} \ln y_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 1.00 | 5.10 | 1.629 | 1.0000 | 1.629 |
| 2 | 1.25 | 5.79 | 1.756 | 1.5625 | 2.195 |
| 3 | 1.50 | 6.53 | 1.876 | 2.2500 | 2.814 |
| 4 | 1.75 | 7.45 | 2.008 | 3.0625 | 3.514 |
| 5 | 2.00 | 8.46 | 2.135 | 4.0000 | 4.270 |
|  | 7.50 |  | 9.404 | 11.875 | 14.422 |

If $x_{i}$ is graphed with $\ln y_{i}$, the data appear to have a linear relation, so it is reasonable to assume an approximation of the form

$$
y=b e^{a x}, \quad \text { which implies that } \quad \ln y=\ln b+a x
$$

Extending the table and summing the appropriate columns gives the remaining data in Table 8.5.

Using the normal equations (8.1) and (8.2),

$$
a=\frac{(5)(14.422)-(7.5)(9.404)}{(5)(11.875)-(7.5)^{2}}=0.5056
$$

and

$$
\ln b=\frac{(11.875)(9.404)-(14.422)(7.5)}{(5)(11.875)-(7.5)^{2}}=1.122
$$

With $\ln b=1.122$ we have $b=e^{1.122}=3.071$, and the approximation assumes the form

$$
y=3.071 e^{0.5056 x}
$$

At the data points this gives the values in Table 8.6. (See Figure 8.5.)

Table 8.6

| $i$ | $x_{i}$ | $y_{i}$ | $3.071 e^{0.5056 x_{i}}$ | $\left\|y_{i}-3.071 e^{0.5056 x_{i}}\right\|$ |
| :---: | :---: | :---: | :---: | :---: |
| 1 | 1.00 | 5.10 | 5.09 | 0.01 |
| 2 | 1.25 | 5.79 | 5.78 | 0.01 |
| 3 | 1.50 | 6.53 | 6.56 | 0.03 |
| 4 | 1.75 | 7.45 | 7.44 | 0.01 |
| 5 | 2.00 | 8.46 | 8.44 | 0.02 |

Figure 8.5


Exponential and other nonlinear discrete least squares approximations can be obtain in the Statistics package by using the commands ExponentialFit and NonlinearFit.

For example, the approximation in the Illustration can be obtained by first defining the data with
$X:=\operatorname{Vector}([1,1.25,1.5,1.75,2]): Y:=\operatorname{Vector}([5.1,5.79,6.53,7.45,8.46]):$
and then issuing the command
ExponentialFit $(X, Y, x)$
gives the result, rounded to 5 decimal places,

$$
3.07249 e^{0.50572 x}
$$

If instead the NonlinearFit command is issued, the approximation produced uses methods of Chapter 10 for solving a system of nonlinear equations. The approximation that Maple gives in this case is

$$
3.06658(1.66023)^{x} \approx 3.06658 e^{0.50695}
$$

## EXERCISE SET 8.1

1. Compute the linear least squares polynomial for the data of Example 2.
2. Compute the least squares polynomial of degree 2 for the data of Example 1, and compare the total error $E$ for the two polynomials.
3. Find the least squares polynomials of degrees 1,2 , and 3 for the data in the following table. Compute the error $E$ in each case. Graph the data and the polynomials.

| $x_{i}$ | 1.0 | 1.1 | 1.3 | 1.5 | 1.9 | 2.1 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $y_{i}$ | 1.84 | 1.96 | 2.21 | 2.45 | 2.94 | 3.18 |

4. Find the least squares polynomials of degrees 1,2 , and 3 for the data in the following table. Compute the error $E$ in each case. Graph the data and the polynomials.

| $x_{i}$ | 0 | 0.15 | 0.31 | 0.5 | 0.6 | 0.75 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $y_{i}$ | 1.0 | 1.004 | 1.031 | 1.117 | 1.223 | 1.422 |

5. Given the data:

| $x_{i}$ | 4.0 | 4.2 | 4.5 | 4.7 | 5.1 | 5.5 | 5.9 | 6.3 | 6.8 | 7.1 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $y_{i}$ | 102.56 | 113.18 | 130.11 | 142.05 | 167.53 | 195.14 | 224.87 | 256.73 | 299.50 | 326.72 |

a. Construct the least squares polynomial of degree 1 , and compute the error.
b. Construct the least squares polynomial of degree 2 , and compute the error.
c. Construct the least squares polynomial of degree 3, and compute the error.
d. Construct the least squares approximation of the form $b e^{a x}$, and compute the error.
e. Construct the least squares approximation of the form $b x^{a}$, and compute the error.
6. Repeat Exercise 5 for the following data.

| $x_{i}$ | 0.2 | 0.3 | 0.6 | 0.9 | 1.1 | 1.3 | 1.4 | 1.6 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $y_{i}$ | 0.050446 | 0.098426 | 0.33277 | 0.72660 | 1.0972 | 1.5697 | 1.8487 | 2.5015 |

7. In the lead example of this chapter, an experiment was described to determine the spring constant $k$ in Hooke's law:

$$
F(l)=k(l-E) .
$$

The function $F$ is the force required to stretch the spring $l$ units, where the constant $E=5.3 \mathrm{in}$. is the length of the unstretched spring.
a. Suppose measurements are made of the length $l$, in inches, for applied weights $F(l)$, in pounds, as given in the following table.

| $F(l)$ | $l$ |
| :---: | ---: |
| 2 | 7.0 |
| 4 | 9.4 |
| 6 | 12.3 |

Find the least squares approximation for $k$.
b. Additional measurements are made, giving more data:

| $F(l)$ | $l$ |
| ---: | ---: |
| 3 | 8.3 |
| 5 | 11.3 |
| 8 | 14.4 |
| 10 | 15.9 |

Compute the new least squares approximation for $k$. Which of (a) or (b) best fits the total experimental data?
8. The following list contains homework grades and the final-examination grades for 30 numerical analysis students. Find the equation of the least squares line for this data, and use this line to determine the homework grade required to predict minimal A $(90 \%)$ and $\mathrm{D}(60 \%)$ grades on the final.

| Homework | Final | Homework | Final |
| :---: | :---: | :---: | ---: |
| 302 | 45 | 323 | 83 |
| 325 | 72 | 337 | 99 |
| 285 | 54 | 337 | 70 |
| 339 | 54 | 304 | 62 |
| 334 | 79 | 319 | 66 |
| 322 | 65 | 234 | 51 |
| 331 | 99 | 337 | 53 |
| 279 | 63 | 351 | 100 |
| 316 | 65 | 339 | 67 |
| 347 | 99 | 343 | 83 |
| 343 | 83 | 314 | 42 |
| 290 | 74 | 344 | 79 |
| 326 | 76 | 185 | 59 |
| 233 | 57 | 340 | 75 |
| 254 | 45 | 316 | 45 |

9. The following table lists the college grade-point averages of 20 mathematics and computer science majors, together with the scores that these students received on the mathematics portion of the ACT (American College Testing Program) test while in high school. Plot these data, and find the equation of the least squares line for this data.

| ACT <br> score | Grade-point <br> average | ACT <br> score | Grade-point <br> average |
| :---: | :---: | :---: | :---: |
| 28 | 3.84 | 29 | 3.75 |
| 25 | 3.21 | 28 | 3.65 |
| 28 | 3.23 | 27 | 3.87 |
| 27 | 3.63 | 29 | 3.75 |
| 28 | 3.75 | 21 | 1.66 |
| 33 | 3.20 | 28 | 3.12 |
| 28 | 3.41 | 28 | 2.96 |
| 29 | 3.38 | 26 | 2.92 |
| 23 | 3.53 | 30 | 3.10 |
| 27 | 2.03 | 24 | 2.81 |

10. The following set of data, presented to the Senate Antitrust Subcommittee, shows the comparative crash-survivability characteristics of cars in various classes. Find the least squares line that approximates these data. (The table shows the percent of accident-involved vehicles in which the most severe injury was fatal or serious.)

| Type | Average <br> Weight | Percent <br> Occurrence |
| :--- | :---: | :---: |
| 1. Domestic luxury regular | 4800 lb | 3.1 |
| 2. Domestic intermediate regular | 3700 lb | 4.0 |
| 3. Domestic economy regular | 3400 lb | 5.2 |
| 4. Domestic compact | 2800 lb | 6.4 |
| 5. Foreign compact | 1900 lb | 9.6 |

11. To determine a relationship between the number of fish and the number of species of fish in samples taken for a portion of the Great Barrier Reef, P. Sale and R. Dybdahl [SD] fit a linear least squares polynomial to the following collection of data, which were collected in samples over a 2 -year period. Let $x$ be the number of fish in the sample and $y$ be the number of species in the sample.

| $x$ | $y$ | $x$ | $y$ | $x$ | $y$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 13 | 11 | 29 | 12 | 60 | 14 |
| 15 | 10 | 30 | 14 | 62 | 21 |
| 16 | 11 | 31 | 16 | 64 | 21 |
| 21 | 12 | 36 | 17 | 70 | 24 |
| 22 | 12 | 40 | 13 | 72 | 17 |
| 23 | 13 | 42 | 14 | 100 | 23 |
| 25 | 13 | 55 | 22 | 130 | 34 |

Determine the linear least squares polynomial for these data.
12. To determine a functional relationship between the attenuation coefficient and the thickness of a sample of taconite, V. P. Singh [Si] fits a collection of data by using a linear least squares polynomial. The following collection of data is taken from a graph in that paper. Find the linear least squares polynomial fitting these data.

| Thickness $(\mathrm{cm})$ | Attenuation coefficient $(\mathrm{dB} / \mathrm{cm})$ |
| :---: | :---: |
| 0.040 | 26.5 |
| 0.041 | 28.1 |
| 0.055 | 25.2 |
| 0.056 | 26.0 |
| 0.062 | 24.0 |
| 0.071 | 25.0 |
| 0.071 | 26.4 |
| 0.078 | 27.2 |
| 0.082 | 25.6 |
| 0.090 | 25.0 |
| 0.092 | 26.8 |
| 0.100 | 24.8 |
| 0.105 | 27.0 |
| 0.120 | 25.0 |
| 0.123 | 27.3 |
| 0.130 | 26.9 |
| 0.140 | 26.2 |

13. In a paper dealing with the efficiency of energy utilization of the larvae of the modest sphinx moth (Pachysphinx modesta), L. Schroeder [Schr1] used the following data to determine a relation between $W$, the live weight of the larvae in grams, and $R$, the oxygen consumption of the larvae in milliliters/hour. For biological reasons, it is assumed that a relationship in the form of $R=b W^{a}$ exists between $W$ and $R$.
a. Find the logarithmic linear least squares polynomial by using

$$
\ln R=\ln b+a \ln W
$$

b. Compute the error associated with the approximation in part (a):

$$
E=\sum_{i=1}^{37}\left(R_{i}-b W_{i}^{a}\right)^{2}
$$

c. Modify the logarithmic least squares equation in part (a) by adding the quadratic term $c\left(\ln W_{i}\right)^{2}$, and determine the logarithmic quadratic least squares polynomial.
d. Determine the formula for and compute the error associated with the approximation in part (c).

| $W$ | $R$ | $W$ | $R$ | $W$ | $R$ | $W$ | $R$ | $W$ | $R$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0.017 | 0.154 | 0.025 | 0.23 | 0.020 | 0.181 | 0.020 | 0.180 | 0.025 | 0.234 |
| 0.087 | 0.296 | 0.111 | 0.357 | 0.085 | 0.260 | 0.119 | 0.299 | 0.233 | 0.537 |
| 0.174 | 0.363 | 0.211 | 0.366 | 0.171 | 0.334 | 0.210 | 0.428 | 0.783 | 1.47 |
| 1.11 | 0.531 | 0.999 | 0.771 | 1.29 | 0.87 | 1.32 | 1.15 | 1.35 | 2.48 |
| 1.74 | 2.23 | 3.02 | 2.01 | 3.04 | 3.59 | 3.34 | 2.83 | 1.69 | 1.44 |
| 4.09 | 3.58 | 4.28 | 3.28 | 4.29 | 3.40 | 5.48 | 4.15 | 2.75 | 1.84 |
| 5.45 | 3.52 | 4.58 | 2.96 | 5.30 | 3.88 |  |  | 4.83 | 4.66 |
| 5.96 | 2.40 | 4.68 | 5.10 |  |  |  |  | 5.53 | 6.94 |

14. Show that the normal equations (8.3) resulting from discrete least squares approximation yield a symmetric and nonsingular matrix and hence have a unique solution. [Hint: Let $A=\left(a_{i j}\right)$, where

$$
a_{i j}=\sum_{k=1}^{m} x_{k}^{i+j-2}
$$

and $x_{1}, x_{2}, \ldots, x_{m}$ are distinct with $n<m-1$. Suppose $A$ is singular and that $\mathbf{c} \neq \mathbf{0}$ is such that $\mathbf{c}^{t} A \mathbf{c}=0$. Show that the $n$ th-degree polynomial whose coefficients are the coordinates of $\mathbf{c}$ has more than $n$ roots, and use this to establish a contradiction.]

### 8.2 Orthogonal Polynomials and Least Squares Approximation

The previous section considered the problem of least squares approximation to fit a collection of data. The other approximation problem mentioned in the introduction concerns the approximation of functions.

Suppose $f \in C[a, b]$ and that a polynomial $P_{n}(x)$ of degree at most $n$ is required that will minimize the error

$$
\int_{a}^{b}\left[f(x)-P_{n}(x)\right]^{2} d x
$$

To determine a least squares approximating polynomial; that is, a polynomial to minimize this expression, let

$$
P_{n}(x)=a_{n} x^{n}+a_{n-1} x^{n-1}+\cdots+a_{1} x+a_{0}=\sum_{k=0}^{n} a_{k} x^{k}
$$

and define, as shown in Figure 8.6,

$$
E \equiv E_{2}\left(a_{0}, a_{1}, \ldots, a_{n}\right)=\int_{a}^{b}\left(f(x)-\sum_{k=0}^{n} a_{k} x^{k}\right)^{2} d x
$$

The problem is to find real coefficients $a_{0}, a_{1}, \ldots, a_{n}$ that will minimize $E$. A necessary condition for the numbers $a_{0}, a_{1}, \ldots, a_{n}$ to minimize $E$ is that

$$
\frac{\partial E}{\partial a_{j}}=0, \quad \text { for each } j=0,1, \ldots, n
$$

Figure 8.6


Since

$$
E=\int_{a}^{b}[f(x)]^{2} d x-2 \sum_{k=0}^{n} a_{k} \int_{a}^{b} x^{k} f(x) d x+\int_{a}^{b}\left(\sum_{k=0}^{n} a_{k} x^{k}\right)^{2} d x
$$

we have

$$
\frac{\partial E}{\partial a_{j}}=-2 \int_{a}^{b} x^{j} f(x) d x+2 \sum_{k=0}^{n} a_{k} \int_{a}^{b} x^{j+k} d x
$$

Hence, to find $P_{n}(x)$, the $(n+1)$ linear normal equations

$$
\begin{equation*}
\sum_{k=0}^{n} a_{k} \int_{a}^{b} x^{j+k} d x=\int_{a}^{b} x^{j} f(x) d x, \quad \text { for each } j=0,1, \ldots, n \tag{8.6}
\end{equation*}
$$

must be solved for the $(n+1)$ unknowns $a_{j}$. The normal equations always have a unique solution provided that $f \in C[a, b]$. (See Exercise 15.)

Example 1 Find the least squares approximating polynomial of degree 2 for the function $f(x)=\sin \pi x$ on the interval $[0,1]$.

Solution The normal equations for $P_{2}(x)=a_{2} x^{2}+a_{1} x+a_{0}$ are

$$
\begin{array}{r}
a_{0} \int_{0}^{1} 1 d x+a_{1} \int_{0}^{1} x d x+a_{2} \int_{0}^{1} x^{2} d x=\int_{0}^{1} \sin \pi x d x \\
a_{0} \int_{0}^{1} x d x+a_{1} \int_{0}^{1} x^{2} d x+a_{2} \int_{0}^{1} x^{3} d x=\int_{0}^{1} x \sin \pi x d x \\
a_{0} \int_{0}^{1} x^{2} d x+a_{1} \int_{0}^{1} x^{3} d x+a_{2} \int_{0}^{1} x^{4} d x=\int_{0}^{1} x^{2} \sin \pi x d x .
\end{array}
$$

Performing the integration yields

$$
a_{0}+\frac{1}{2} a_{1}+\frac{1}{3} a_{2}=\frac{2}{\pi}, \quad \frac{1}{2} a_{0}+\frac{1}{3} a_{1}+\frac{1}{4} a_{2}=\frac{1}{\pi}, \quad \frac{1}{3} a_{0}+\frac{1}{4} a_{1}+\frac{1}{5} a_{2}=\frac{\pi^{2}-4}{\pi^{3}} .
$$

These three equations in three unknowns can be solved to obtain

$$
a_{0}=\frac{12 \pi^{2}-120}{\pi^{3}} \approx-0.050465 \text { and } a_{1}=-a_{2}=\frac{720-60 \pi^{2}}{\pi^{3}} \approx 4.12251
$$

Consequently, the least squares polynomial approximation of degree 2 for $f(x)=\sin \pi x$ on $[0,1]$ is $P_{2}(x)=-4.12251 x^{2}+4.12251 x-0.050465$. (See Figure 8.7.)

Figure 8.7


Example 1 illustrates a difficulty in obtaining a least squares polynomial approximation. An $(n+1) \times(n+1)$ linear system for the unknowns $a_{0}, \ldots, a_{n}$ must be solved, and the coefficients in the linear system are of the form

$$
\int_{a}^{b} x^{j+k} d x=\frac{b^{j+k+1}-a^{j+k+1}}{j+k+1}
$$

a linear system that does not have an easily computed numerical solution. The matrix in the linear system is known as a Hilbert matrix, which is a classic example for demonstrating round-off error difficulties. (See Exercise 11 of Section 7.5.)

Another disadvantage is similar to the situation that occurred when the Lagrange polynomials were first introduced in Section 3.1. The calculations that were performed in obtaining the best $n$ th-degree polynomial, $P_{n}(x)$, do not lessen the amount of work required to obtain $P_{n+1}(x)$, the polynomial of next higher degree.

## Linearly Independent Functions

A different technique to obtain least squares approximations will now be considered. This turns out to be computationally efficient, and once $P_{n}(x)$ is known, it is easy to determine $P_{n+1}(x)$. To facilitate the discussion, we need some new concepts.

Definition 8.1 The set of functions $\left\{\phi_{0}, \ldots, \phi_{n}\right\}$ is said to be linearly independent on $[a, b]$ if, whenever

$$
c_{0} \phi_{0}(x)+c_{1} \phi_{1}(x)+\cdots+c_{n} \phi_{n}(x)=0, \quad \text { for all } x \in[a, b],
$$

we have $c_{0}=c_{1}=\cdots=c_{n}=0$. Otherwise the set of functions is said to be linearly dependent.

Theorem 8.2 Suppose that, for each $j=0,1, \ldots, n, \phi_{j}(x)$ is a polynomial of degree $j$. Then $\left\{\phi_{0}, \ldots, \phi_{n}\right\}$ is linearly independent on any interval $[a, b]$.

Proof Let $c_{0}, \ldots, c_{n}$ be real numbers for which

$$
P(x)=c_{0} \phi_{0}(x)+c_{1} \phi_{1}(x)+\cdots+c_{n} \phi_{n}(x)=0, \quad \text { for all } x \in[a, b] .
$$

The polynomial $P(x)$ vanishes on $[a, b]$, so it must be the zero polynomial, and the coefficients of all the powers of $x$ are zero. In particular, the coefficient of $x^{n}$ is zero. But $c_{n} \phi_{n}(x)$ is the only term in $P(x)$ that contains $x^{n}$, so we must have $c_{n}=0$. Hence

$$
P(x)=\sum_{j=0}^{n-1} c_{j} \phi_{j}(x)
$$

In this representation of $P(x)$, the only term that contains a power of $x^{n-1}$ is $c_{n-1} \phi_{n-1}(x)$, so this term must also be zero and

$$
P(x)=\sum_{j=0}^{n-2} c_{j} \phi_{j}(x)
$$

In like manner, the remaining constants $c_{n-2}, c_{n-3}, \ldots, c_{1}, c_{0}$ are all zero, which implies that $\left\{\phi_{0}, \phi_{1}, \ldots, \phi_{n}\right\}$ is linearly independent on $[a, b]$.

Example 2 Let $\phi_{0}(x)=2, \phi_{1}(x)=x-3$, and $\phi_{2}(x)=x^{2}+2 x+7$, and $Q(x)=a_{0}+a_{1} x+a_{2} x^{2}$. Show that there exist constants $c_{0}, c_{1}$, and $c_{2}$ such that $Q(x)=c_{0} \phi_{0}(x)+c_{1} \phi_{1}(x)+c_{2} \phi_{2}(x)$.

Solution By Theorem 8.2, $\left\{\phi_{0}, \phi_{1}, \phi_{2}\right\}$ is linearly independent on any interval $[a, b]$. First note that

$$
1=\frac{1}{2} \phi_{0}(x), \quad x=\phi_{1}(x)+3=\phi_{1}(x)+\frac{3}{2} \phi_{0}(x),
$$

and

$$
\begin{aligned}
x^{2} & =\phi_{2}(x)-2 x-7=\phi_{2}(x)-2\left[\phi_{1}(x)+\frac{3}{2} \phi_{0}(x)\right]-7\left[\frac{1}{2} \phi_{0}(x)\right] \\
& =\phi_{2}(x)-2 \phi_{1}(x)-\frac{13}{2} \phi_{0}(x) .
\end{aligned}
$$

Hence

$$
\begin{aligned}
Q(x) & =a_{0}\left[\frac{1}{2} \phi_{0}(x)\right]+a_{1}\left[\phi_{1}(x)+\frac{3}{2} \phi_{0}(x)\right]+a_{2}\left[\phi_{2}(x)-2 \phi_{1}(x)-\frac{13}{2} \phi_{0}(x)\right] \\
& =\left(\frac{1}{2} a_{0}+\frac{3}{2} a_{1}-\frac{13}{2} a_{2}\right) \phi_{0}(x)+\left[a_{1}-2 a_{2}\right] \phi_{1}(x)+a_{2} \phi_{2}(x) .
\end{aligned}
$$

The situation illustrated in Example 2 holds in a much more general setting. Let $\prod_{n}$ denote the set of all polynomials of degree at most $\boldsymbol{n}$. The following result is used extensively in many applications of linear algebra. Its proof is considered in Exercise 13.

Theorem 8.3 Suppose that $\left\{\phi_{0}(x), \phi_{1}(x), \ldots, \phi_{n}(x)\right\}$ is a collection of linearly independent polynomials in $\prod_{n}$. Then any polynomial in $\prod_{n}$ can be written uniquely as a linear combination of $\phi_{0}(x)$, $\phi_{1}(x), \ldots, \phi_{n}(x)$.

## Orthogonal Functions

To discuss general function approximation requires the introduction of the notions of weight functions and orthogonality.

Definition 8.4 An integrable function $w$ is called a weight function on the interval $I$ if $w(x) \geq 0$, for all $x$ in $I$, but $w(x) \not \equiv 0$ on any subinterval of $I$.

The purpose of a weight function is to assign varying degrees of importance to approximations on certain portions of the interval. For example, the weight function

$$
w(x)=\frac{1}{\sqrt{1-x^{2}}}
$$

places less emphasis near the center of the interval $(-1,1)$ and more emphasis when $|x|$ is near 1 (see Figure 8.8). This weight function is used in the next section.

Suppose $\left\{\phi_{0}, \phi_{1}, \ldots, \phi_{n}\right\}$ is a set of linearly independent functions on $[a, b]$ and $w$ is a weight function for $[a, b]$. Given $f \in C[a, b]$, we seek a linear combination

$$
P(x)=\sum_{k=0}^{n} a_{k} \phi_{k}(x)
$$

to minimize the error

$$
E=E\left(a_{0}, \ldots, a_{n}\right)=\int_{a}^{b} w(x)\left[f(x)-\sum_{k=0}^{n} a_{k} \phi_{k}(x)\right]^{2} d x .
$$

This problem reduces to the situation considered at the beginning of this section in the special case when $w(x) \equiv 1$ and $\phi_{k}(x)=x^{k}$, for each $k=0,1, \ldots, n$.

The normal equations associated with this problem are derived from the fact that for each $j=0,1, \ldots, n$,

$$
0=\frac{\partial E}{\partial a_{j}}=2 \int_{a}^{b} w(x)\left[f(x)-\sum_{k=0}^{n} a_{k} \phi_{k}(x)\right] \phi_{j}(x) d x .
$$

The system of normal equations can be written

$$
\int_{a}^{b} w(x) f(x) \phi_{j}(x) d x=\sum_{k=0}^{n} a_{k} \int_{a}^{b} w(x) \phi_{k}(x) \phi_{j}(x) d x, \quad \text { for } j=0,1, \ldots, n .
$$

If the functions $\phi_{0}, \phi_{1}, \ldots, \phi_{n}$ can be chosen so that

$$
\int_{a}^{b} w(x) \phi_{k}(x) \phi_{j}(x) d x= \begin{cases}0, & \text { when } j \neq k  \tag{8.7}\\ \alpha_{j}>0, & \text { when } j=k\end{cases}
$$

then the normal equations will reduce to

$$
\int_{a}^{b} w(x) f(x) \phi_{j}(x) d x=a_{j} \int_{a}^{b} w(x)\left[\phi_{j}(x)\right]^{2} d x=a_{j} \alpha_{j}
$$

for each $j=0,1, \ldots, n$. These are easily solved to give

$$
a_{j}=\frac{1}{\alpha_{j}} \int_{a}^{b} w(x) f(x) \phi_{j}(x) d x
$$

Hence the least squares approximation problem is greatly simplified when the functions $\phi_{0}, \phi_{1}, \ldots, \phi_{n}$ are chosen to satisfy the orthogonality condition in Eq. (8.7). The remainder of this section is devoted to studying collections of this type.

Definition $8.5\left\{\phi_{0}, \phi_{1}, \ldots, \phi_{n}\right\}$ is said to be an orthogonal set of functions for the interval $[a, b]$ with respect to the weight function $w$ if

$$
\int_{a}^{b} w(x) \phi_{k}(x) \phi_{j}(x) d x= \begin{cases}0, & \text { when } j \neq k \\ \alpha_{j}>0, & \text { when } j=k\end{cases}
$$

If, in addition, $\alpha_{j}=1$ for each $j=0,1, \ldots, n$, the set is said to be orthonormal.

This definition, together with the remarks preceding it, produces the following theorem.
Theorem 8.6 If $\left\{\phi_{0}, \ldots, \phi_{n}\right\}$ is an orthogonal set of functions on an interval $[a, b]$ with respect to the weight function $w$, then the least squares approximation to $f$ on $[a, b]$ with respect to $w$ is

$$
P(x)=\sum_{j=0}^{n} a_{j} \phi_{j}(x)
$$

where, for each $j=0,1, \ldots, n$,

$$
a_{j}=\frac{\int_{a}^{b} w(x) \phi_{j}(x) f(x) d x}{\int_{a}^{b} w(x)\left[\phi_{j}(x)\right]^{2} d x}=\frac{1}{\alpha_{j}} \int_{a}^{b} w(x) \phi_{j}(x) f(x) d x
$$

Although Definition 8.5 and Theorem 8.6 allow for broad classes of orthogonal functions, we will consider only orthogonal sets of polynomials. The next theorem, which is based on the Gram-Schmidt process, describes how to construct orthogonal polynomials on $[a, b]$ with respect to a weight function $w$.

Theorem 8.7 The set of polynomial functions $\left\{\phi_{0}, \phi_{1}, \ldots, \phi_{n}\right\}$ defined in the following way is orthogonal on $[a, b]$ with respect to the weight function $w$.

$$
\phi_{0}(x) \equiv 1, \quad \phi_{1}(x)=x-B_{1}, \quad \text { for each } x \text { in }[a, b],
$$

where

$$
B_{1}=\frac{\int_{a}^{b} x w(x)\left[\phi_{0}(x)\right]^{2} d x}{\int_{a}^{b} w(x)\left[\phi_{0}(x)\right]^{2} d x}
$$

and when $k \geq 2$,

$$
\phi_{k}(x)=\left(x-B_{k}\right) \phi_{k-1}(x)-C_{k} \phi_{k-2}(x), \quad \text { for each } x \text { in }[a, b],
$$

where

$$
B_{k}=\frac{\int_{a}^{b} x w(x)\left[\phi_{k-1}(x)\right]^{2} d x}{\int_{a}^{b} w(x)\left[\phi_{k-1}(x)\right]^{2} d x}
$$

and

$$
C_{k}=\frac{\int_{a}^{b} x w(x) \phi_{k-1}(x) \phi_{k-2}(x) d x}{\int_{a}^{b} w(x)\left[\phi_{k-2}(x)\right]^{2} d x}
$$

Theorem 8.7 provides a recursive procedure for constructing a set of orthogonal polynomials. The proof of this theorem follows by applying mathematical induction to the degree of the polynomial $\phi_{n}(x)$.

Corollary 8.8 For any $n>0$, the set of polynomial functions $\left\{\phi_{0}, \ldots, \phi_{n}\right\}$ given in Theorem 8.7 is linearly independent on $[a, b]$ and

$$
\int_{a}^{b} w(x) \phi_{n}(x) Q_{k}(x) d x=0
$$

for any polynomial $Q_{k}(x)$ of degree $k<n$.

Proof For each $k=0,1, \ldots, n, \phi_{k}(x)$ is a polynomial of degree $k$. So Theorem 8.2 implies that $\left\{\phi_{0}, \ldots, \phi_{n}\right\}$ is a linearly independent set.

Let $Q_{k}(x)$ be a polynomial of degree $k<n$. By Theorem 8.3 there exist numbers $c_{0}, \ldots, c_{k}$ such that

$$
Q_{k}(x)=\sum_{j=0}^{k} c_{j} \phi_{j}(x)
$$

Because $\phi_{n}$ is orthogonal to $\phi_{j}$ for each $j=0,1, \ldots, k$ we have

$$
\int_{a}^{b} w(x) Q_{k}(x) \phi_{n}(x) d x=\sum_{j=0}^{k} c_{j} \int_{a}^{b} w(x) \phi_{j}(x) \phi_{n}(x) d x=\sum_{j=0}^{k} c_{j} \cdot 0=0
$$

The set of Legendre polynomials, $\left\{P_{n}(x)\right\}$, is orthogonal on $[-1,1]$ with respect to the weight function $w(x) \equiv 1$. The classical definition of the Legendre polynomials requires that $P_{n}(1)=1$ for each $n$, and a recursive relation is used to generate the polynomials when $n \geq 2$. This normalization will not be needed in our discussion, and the least squares approximating polynomials generated in either case are essentially the same.

Using the Gram-Schmidt process with $P_{0}(x) \equiv 1$ gives

$$
B_{1}=\frac{\int_{-1}^{1} x d x}{\int_{-1}^{1} d x}=0 \quad \text { and } \quad P_{1}(x)=\left(x-B_{1}\right) P_{0}(x)=x
$$

Also,

$$
B_{2}=\frac{\int_{-1}^{1} x^{3} d x}{\int_{-1}^{1} x^{2} d x}=0 \quad \text { and } \quad C_{2}=\frac{\int_{-1}^{1} x^{2} d x}{\int_{-1}^{1} 1 d x}=\frac{1}{3}
$$

so

$$
P_{2}(x)=\left(x-B_{2}\right) P_{1}(x)-C_{2} P_{0}(x)=(x-0) x-\frac{1}{3} \cdot 1=x^{2}-\frac{1}{3}
$$

The higher-degree Legendre polynomials shown in Figure 8.9 are derived in the same manner. Although the integration can be tedious, it is not difficult with a Computer Algebra System.

Figure 8.9


For example, the Maple command int is used to compute the integrals $B_{3}$ and $C_{3}$ :
$B 3:=\frac{\operatorname{int}\left(x\left(x^{2}-\frac{1}{3}\right)^{2}, x=-1 . .1\right)}{\operatorname{int}\left(\left(x^{2}-\frac{1}{3}\right)^{2}, x=-1 . .1\right)} ; \quad C 3:=\frac{\operatorname{int}\left(x\left(x^{2}-\frac{1}{3}\right), x=-1 . .1\right)}{\operatorname{int}\left(x^{2}, x=-1 . .1\right)}$

$$
\begin{gathered}
0 \\
\frac{4}{15}
\end{gathered}
$$

Thus

$$
P_{3}(x)=x P_{2}(x)-\frac{4}{15} P_{1}(x)=x^{3}-\frac{1}{3} x-\frac{4}{15} x=x^{3}-\frac{3}{5} x .
$$

The next two Legendre polynomials are

$$
P_{4}(x)=x^{4}-\frac{6}{7} x^{2}+\frac{3}{35} \quad \text { and } \quad P_{5}(x)=x^{5}-\frac{10}{9} x^{3}+\frac{5}{21} x .
$$

The Legendre polynomials were introduced in Section 4.7, where their roots, given on page 232, were used as the nodes in Gaussian quadrature.

## EXERCISE SET 8.2

1. Find the linear least squares polynomial approximation to $f(x)$ on the indicated interval if
a. $\quad f(x)=x^{2}+3 x+2, \quad[0,1]$;
b. $\quad f(x)=x^{3}, \quad[0,2]$;
c. $\quad f(x)=\frac{1}{x}, \quad[1,3]$;
d. $\quad f(x)=e^{x}, \quad[0,2]$;
e. $\quad f(x)=\frac{1}{2} \cos x+\frac{1}{3} \sin 2 x, \quad[0,1]$;
f. $\quad f(x)=x \ln x, \quad[1,3]$.
2. Find the linear least squares polynomial approximation on the interval $[-1,1]$ for the following functions.
a. $\quad f(x)=x^{2}-2 x+3$
b. $\quad f(x)=x^{3}$
c. $\quad f(x)=\frac{1}{x+2}$
d. $f(x)=e^{x}$
e. $f(x)=\frac{1}{2} \cos x+\frac{1}{3} \sin 2 x$
f. $\quad f(x)=\ln (x+2)$
3. Find the least squares polynomial approximation of degree two to the functions and intervals in Exercise 1.
4. Find the least squares polynomial approximation of degree 2 on the interval $[-1,1]$ for the functions in Exercise 3.
5. Compute the error $E$ for the approximations in Exercise 3.
6. Compute the error $E$ for the approximations in Exercise 4.
7. Use the Gram-Schmidt process to construct $\phi_{0}(x), \phi_{1}(x), \phi_{2}(x)$, and $\phi_{3}(x)$ for the following intervals.
a. $[0,1]$
b. $[0,2]$
c. $[1,3]$
8. Repeat Exercise 1 using the results of Exercise 7.
9. Obtain the least squares approximation polynomial of degree 3 for the functions in Exercise 1 using the results of Exercise 7.
10. Repeat Exercise 3 using the results of Exercise 7.
11. Use the Gram-Schmidt procedure to calculate $L_{1}, L_{2}$, and $L_{3}$, where $\left\{L_{0}(x), L_{1}(x), L_{2}(x), L_{3}(x)\right\}$ is an orthogonal set of polynomials on $(0, \infty)$ with respect to the weight functions $w(x)=e^{-x}$ and $L_{0}(x) \equiv 1$. The polynomials obtained from this procedure are called the Laguerre polynomials.
12. Use the Laguerre polynomials calculated in Exercise 11 to compute the least squares polynomials of degree one, two, and three on the interval $(0, \infty)$ with respect to the weight function $w(x)=e^{-x}$ for the following functions:
a. $\quad f(x)=x^{2}$
b. $\quad f(x)=e^{-x}$
c. $\quad f(x)=x^{3}$
d. $\quad f(x)=e^{-2 x}$
13. Suppose $\left\{\phi_{0}, \phi_{1}, \ldots, \phi_{n}\right\}$ is any linearly independent set in $\prod_{n}$. Show that for any element $Q \in \prod_{n}$, there exist unique constants $c_{0}, c_{1}, \ldots, c_{n}$, such that

$$
Q(x)=\sum_{k=0}^{n} c_{k} \phi_{k}(x) .
$$

14. Show that if $\left\{\phi_{0}, \phi_{1}, \ldots, \phi_{n}\right\}$ is an orthogonal set of functions on $[a, b]$ with respect to the weight function $w$, then $\left\{\phi_{0}, \phi_{1}, \ldots, \phi_{n}\right\}$ is a linearly independent set.
15. Show that the normal equations (8.6) have a unique solution. [Hint: Show that the only solution for the function $f(x) \equiv 0$ is $a_{j}=0, j=0,1, \ldots, n$. Multiply Eq. (8.6) by $a_{j}$, and sum over all $j$. Interchange the integral sign and the summation sign to obtain $\int_{a}^{b}[P(x)]^{2} d x=0$. Thus, $P(x) \equiv 0$, so $a_{j}=0$, for $j=0, \ldots, n$. Hence, the coefficient matrix is nonsingular, and there is a unique solution to Eq. (8.6).]

### 8.3 Chebyshev Polynomials and Economization of Power Series

The Chebyshev polynomials $\left\{T_{n}(x)\right\}$ are orthogonal on $(-1,1)$ with respect to the weight function $w(x)=\left(1-x^{2}\right)^{-1 / 2}$. Although they can be derived by the method in the previous

Pafnuty Lvovich Chebyshev (1821-1894) did exceptional mathematical work in many areas, including applied mathematics, number theory, approximation theory, and probability. In 1852 he traveled from St. Petersburg to visit mathematicians in France, England, and Germany. Lagrange and Legendre had studied individual sets of orthogonal polynomials, but Chebyshev was the first to see the important consequences of studying the theory in general. He developed the Chebyshev polynomials to study least squares approximation and probability, then applied his results to interpolation, approximate quadrature, and other areas.
section, it is easier to give their definition and then show that they satisfy the required orthogonality properties.

For $x \in[-1,1]$, define

$$
\begin{equation*}
T_{n}(x)=\cos [n \arccos x], \quad \text { for each } n \geq 0 . \tag{8.8}
\end{equation*}
$$

It might not be obvious from this definition that for each $n, T_{n}(x)$ is a polynomial in $x$, but we will now show this. First note that

$$
T_{0}(x)=\cos 0=1 \quad \text { and } \quad T_{1}(x)=\cos (\arccos x)=x .
$$

For $n \geq 1$, we introduce the substitution $\theta=\arccos x$ to change this equation to

$$
T_{n}(\theta(x)) \equiv T_{n}(\theta)=\cos (n \theta), \quad \text { where } \theta \in[0, \pi]
$$

A recurrence relation is derived by noting that

$$
T_{n+1}(\theta)=\cos (n+1) \theta=\cos \theta \cos (n \theta)-\sin \theta \sin (n \theta)
$$

and

$$
T_{n-1}(\theta)=\cos (n-1) \theta=\cos \theta \cos (n \theta)+\sin \theta \sin (n \theta)
$$

Adding these equations gives

$$
T_{n+1}(\theta)=2 \cos \theta \cos (n \theta)-T_{n-1}(\theta)
$$

Returning to the variable $x=\cos \theta$, we have, for $n \geq 1$,

$$
T_{n+1}(x)=2 x \cos (n \arccos x)-T_{n-1}(x),
$$

that is,

$$
\begin{equation*}
T_{n+1}(x)=2 x T_{n}(x)-T_{n-1}(x) . \tag{8.9}
\end{equation*}
$$

Because $T_{0}(x)=1$ and $T_{1}(x)=x$, the recurrence relation implies that the next three Chebyshev polynomials are

$$
\begin{aligned}
& T_{2}(x)=2 x T_{1}(x)-T_{0}(x)=2 x^{2}-1 \\
& T_{3}(x)=2 x T_{2}(x)-T_{1}(x)=4 x^{3}-3 x
\end{aligned}
$$

and

$$
T_{4}(x)=2 x T_{3}(x)-T_{2}(x)=8 x^{4}-8 x^{2}+1
$$

The recurrence relation also implies that when $n \geq 1, T_{n}(x)$ is a polynomial of degree $n$ with leading coefficient $2^{n-1}$. The graphs of $T_{1}, T_{2}, T_{3}$, and $T_{4}$ are shown in Figure 8.10.

Figure 8.10


To show the orthogonality of the Chebyshev polynomials with respect to the weight function $w(x)=\left(1-x^{2}\right)^{-1 / 2}$, consider

$$
\int_{-1}^{1} \frac{T_{n}(x) T_{m}(x)}{\sqrt{1-x^{2}}} d x=\int_{-1}^{1} \frac{\cos (n \arccos x) \cos (m \arccos x)}{\sqrt{1-x^{2}}} d x
$$

Reintroducing the substitution $\theta=\arccos x$ gives

$$
d \theta=-\frac{1}{\sqrt{1-x^{2}}} d x
$$

and

$$
\int_{-1}^{1} \frac{T_{n}(x) T_{m}(x)}{\sqrt{1-x^{2}}} d x=-\int_{\pi}^{0} \cos (n \theta) \cos (m \theta) d \theta=\int_{0}^{\pi} \cos (n \theta) \cos (m \theta) d \theta
$$

Suppose $n \neq m$. Since

$$
\cos (n \theta) \cos (m \theta)=\frac{1}{2}[\cos (n+m) \theta+\cos (n-m) \theta]
$$

we have

$$
\begin{aligned}
\int_{-1}^{1} \frac{T_{n}(x) T_{m}(x)}{\sqrt{1-x^{2}}} d x & =\frac{1}{2} \int_{0}^{\pi} \cos ((n+m) \theta) d \theta+\frac{1}{2} \int_{0}^{\pi} \cos ((n-m) \theta) d \theta \\
& =\left[\frac{1}{2(n+m)} \sin ((n+m) \theta)+\frac{1}{2(n-m)} \sin ((n-m) \theta)\right]_{0}^{\pi}=0
\end{aligned}
$$

By a similar technique (see Exercise 9), we also have

$$
\begin{equation*}
\int_{-1}^{1} \frac{\left[T_{n}(x)\right]^{2}}{\sqrt{1-x^{2}}} d x=\frac{\pi}{2}, \quad \text { for each } n \geq 1 \tag{8.10}
\end{equation*}
$$

The Chebyshev polynomials are used to minimize approximation error. We will see how they are used to solve two problems of this type:

- an optimal placing of interpolating points to minimize the error in Lagrange interpolation;
- a means of reducing the degree of an approximating polynomial with minimal loss of accuracy.

The next result concerns the zeros and extreme points of $T_{n}(x)$.
Theorem 8.9 The Chebyshev polynomial $T_{n}(x)$ of degree $n \geq 1$ has $n$ simple zeros in $[-1,1]$ at

$$
\bar{x}_{k}=\cos \left(\frac{2 k-1}{2 n} \pi\right), \quad \text { for each } k=1,2, \ldots, n .
$$

Moreover, $T_{n}(x)$ assumes its absolute extrema at

$$
\bar{x}_{k}^{\prime}=\cos \left(\frac{k \pi}{n}\right) \quad \text { with } \quad T_{n}\left(\bar{x}_{k}^{\prime}\right)=(-1)^{k}, \quad \text { for each } \quad k=0,1, \ldots, n .
$$

## Proof Let

$$
\bar{x}_{k}=\cos \left(\frac{2 k-1}{2 n} \pi\right), \quad \text { for } k=1,2, \ldots, n .
$$

Then

$$
T_{n}\left(\bar{x}_{k}\right)=\cos \left(n \arccos \bar{x}_{k}\right)=\cos \left(n \arccos \left(\cos \left(\frac{2 k-1}{2 n} \pi\right)\right)\right)=\cos \left(\frac{2 k-1}{2} \pi\right)=0 .
$$

But the $\bar{x}_{k}$ are distinct (see Exercise 10) and $T_{n}(x)$ is a polynomial of degree $n$, so all the zeros of $T_{n}(x)$ must have this form.

To show the second statement, first note that

$$
T_{n}^{\prime}(x)=\frac{d}{d x}[\cos (n \arccos x)]=\frac{n \sin (n \arccos x)}{\sqrt{1-x^{2}}}
$$

and that, when $k=1,2, \ldots, n-1$,

$$
T_{n}^{\prime}\left(\bar{x}_{k}^{\prime}\right)=\frac{n \sin \left(n \arccos \left(\cos \left(\frac{k \pi}{n}\right)\right)\right)}{\sqrt{1-\left[\cos \left(\frac{k \pi}{n}\right)\right]^{2}}}=\frac{n \sin (k \pi)}{\sin \left(\frac{k \pi}{n}\right)}=0 .
$$

Since $T_{n}(x)$ is a polynomial of degree $n$, its derivative $T_{n}^{\prime}(x)$ is a polynomial of degree ( $n-1$ ), and all the zeros of $T_{n}^{\prime}(x)$ occur at these $n-1$ distinct points (that they are distinct is considered in Exercise 11). The only other possibilities for extrema of $T_{n}(x)$ occur at the endpoints of the interval $[-1,1]$; that is, at $\bar{x}_{0}^{\prime}=1$ and at $\bar{x}_{n}^{\prime}=-1$.

For any $k=0,1, \ldots, n$ we have

$$
T_{n}\left(\bar{x}_{k}^{\prime}\right)=\cos \left(n \arccos \left(\cos \left(\frac{k \pi}{n}\right)\right)\right)=\cos (k \pi)=(-1)^{k} .
$$

So a maximum occurs at each even value of $k$ and a minimum at each odd value. . . .
The monic (polynomials with leading coefficient 1) Chebyshev polynomials $\tilde{T}_{n}(x)$ are derived from the Chebyshev polynomials $T_{n}(x)$ by dividing by the leading coefficient $2^{n-1}$. Hence

$$
\begin{equation*}
\tilde{T}_{0}(x)=1 \quad \text { and } \quad \tilde{T}_{n}(x)=\frac{1}{2^{n-1}} T_{n}(x), \quad \text { for each } n \geq 1 \tag{8.11}
\end{equation*}
$$

The recurrence relationship satisfied by the Chebyshev polynomials implies that

$$
\begin{align*}
\tilde{T}_{2}(x) & =x \tilde{T}_{1}(x)-\frac{1}{2} \tilde{T}_{0}(x) \quad \text { and }  \tag{8.12}\\
\tilde{T}_{n+1}(x) & =x \tilde{T}_{n}(x)-\frac{1}{4} \tilde{T}_{n-1}(x), \quad \text { for each } n \geq 2
\end{align*}
$$

The graphs of $\tilde{T}_{1}, \tilde{T}_{2}, \tilde{T}_{3}, \tilde{T}_{4}$, and $\tilde{T}_{5}$ are shown in Figure 8.11.

Figure 8.11


Because $\tilde{T}_{n}(x)$ is just a multiple of $T_{n}(x)$, Theorem 8.9 implies that the zeros of $\tilde{T}_{n}(x)$ also occur at

$$
\bar{x}_{k}=\cos \left(\frac{2 k-1}{2 n} \pi\right), \quad \text { for each } k=1,2, \ldots, n
$$

and the extreme values of $\tilde{T}_{n}(x)$, for $n \geq 1$, occur at

$$
\begin{equation*}
\bar{x}_{k}^{\prime}=\cos \left(\frac{k \pi}{n}\right), \quad \text { with } \quad \tilde{T}_{n}\left(\bar{x}_{k}^{\prime}\right)=\frac{(-1)^{k}}{2^{n-1}}, \quad \text { for each } k=0,1,2, \ldots, n \tag{8.13}
\end{equation*}
$$

Let $\tilde{\prod}_{n}$ denote the set of all monic polynomials of degree $\boldsymbol{n}$. The relation expressed in Eq. (8.13) leads to an important minimization property that distinguishes $\tilde{T}_{n}(x)$ from the other members of $\widetilde{\prod}_{n}$.

Theorem 8.10 The polynomials of the form $\tilde{T}_{n}(x)$, when $n \geq 1$, have the property that

$$
\frac{1}{2^{n-1}}=\max _{x \in[-1,1]}\left|\tilde{T}_{n}(x)\right| \leq \max _{x \in[-1,1]}\left|P_{n}(x)\right|, \quad \text { for all } P_{n}(x) \in \widetilde{\prod}_{n}
$$

Moreover, equality occurs only if $P_{n} \equiv \tilde{T}_{n}$.

Proof Suppose that $P_{n}(x) \in \widetilde{\prod}_{n}$ and that

$$
\max _{x \in[-1,1]}\left|P_{n}(x)\right| \leq \frac{1}{2^{n-1}}=\max _{x \in[-1,1]}\left|\tilde{T}_{n}(x)\right| .
$$

Let $Q=\tilde{T}_{n}-P_{n}$. Then $\tilde{T}_{n}(x)$ and $P_{n}(x)$ are both monic polynomials of degree $n$, so $Q(x)$ is a polynomial of degree at most $(n-1)$. Moreover, at the $n+1$ extreme points $\bar{x}_{k}^{\prime}$ of $\tilde{T}_{n}(x)$, we have

$$
Q\left(\bar{x}_{k}^{\prime}\right)=\tilde{T}_{n}\left(\bar{x}_{k}^{\prime}\right)-P_{n}\left(\bar{x}_{k}^{\prime}\right)=\frac{(-1)^{k}}{2^{n-1}}-P_{n}\left(\bar{x}_{k}^{\prime}\right) .
$$

However

$$
\left|P_{n}\left(\bar{x}_{k}^{\prime}\right)\right| \leq \frac{1}{2^{n-1}}, \quad \text { for each } k=0,1, \ldots, n
$$

so we have

$$
Q\left(\bar{x}_{k}^{\prime}\right) \leq 0, \quad \text { when } k \text { is odd } \quad \text { and } \quad Q\left(\bar{x}_{k}^{\prime}\right) \geq 0, \quad \text { when } k \text { is even. }
$$

Since $Q$ is continuous, the Intermediate Value Theorem implies that for each $j=$ $0,1, \ldots, n-1$ the polynomial $Q(x)$ has at least one zero between $\bar{x}_{j}^{\prime}$ and $\bar{x}_{j+1}^{\prime}$. Thus, $Q$ has at least $n$ zeros in the interval $[-1,1]$. But the degree of $Q(x)$ is less than $n$, so $Q \equiv 0$. This implies that $P_{n} \equiv \tilde{T}_{n}$.

## Minimizing Lagrange Interpolation Error

Theorem 8.10 can be used to answer the question of where to place interpolating nodes to minimize the error in Lagrange interpolation. Theorem 3.3 on page 112 applied to the interval $[-1,1]$ states that, if $x_{0}, \ldots, x_{n}$ are distinct numbers in the interval $[-1,1]$ and if $f \in C^{n+1}[-1,1]$, then, for each $x \in[-1,1]$, a number $\xi(x)$ exists in $(-1,1)$ with

$$
f(x)-P(x)=\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\left(x-x_{0}\right)\left(x-x_{1}\right) \cdots\left(x-x_{n}\right)
$$

where $P(x)$ is the Lagrange interpolating polynomial. Generally, there is no control over $\xi(x)$, so to minimize the error by shrewd placement of the nodes $x_{0}, \ldots, x_{n}$, we choose $x_{0}, \ldots, x_{n}$ to minimize the quantity

$$
\left|\left(x-x_{0}\right)\left(x-x_{1}\right) \cdots\left(x-x_{n}\right)\right|
$$

throughout the interval $[-1,1]$.
Since $\left(x-x_{0}\right)\left(x-x_{1}\right) \cdots\left(x-x_{n}\right)$ is a monic polynomial of degree $(n+1)$, we have just seen that the minimum is obtained when

$$
\left(x-x_{0}\right)\left(x-x_{1}\right) \cdots\left(x-x_{n}\right)=\tilde{T}_{n+1}(x)
$$

The maximum value of $\left|\left(x-x_{0}\right)\left(x-x_{1}\right) \cdots\left(x-x_{n}\right)\right|$ is smallest when $x_{k}$ is chosen for each $k=0,1, \ldots, n$ to be the $(k+1)$ st zero of $\tilde{T}_{n+1}$. Hence we choose $x_{k}$ to be

$$
\bar{x}_{k+1}=\cos \left(\frac{2 k+1}{2(n+1)} \pi\right) .
$$

Because $\max _{x \in[-1,1]}\left|\tilde{T}_{n+1}(x)\right|=2^{-n}$, this also implies that

$$
\frac{1}{2^{n}}=\max _{x \in[-1,1]}\left|\left(x-\bar{x}_{1}\right) \cdots\left(x-\bar{x}_{n+1}\right)\right| \leq \max _{x \in[-1,1]}\left|\left(x-x_{0}\right) \cdots\left(x-x_{n}\right)\right|,
$$

for any choice of $x_{0}, x_{1}, \ldots, x_{n}$ in the interval $[-1,1]$. The next corollary follows from these observations.

Corollary 8.11 Suppose that $P(x)$ is the interpolating polynomial of degree at most $n$ with nodes at the zeros of $T_{n+1}(x)$. Then

$$
\max _{x \in[-1,1]}|f(x)-P(x)| \leq \frac{1}{2^{n}(n+1)!} \max _{x \in[-1,1]}\left|f^{(n+1)}(x)\right|, \quad \text { for each } f \in C^{n+1}[-1,1] .
$$

## Minimizing Approximation Error on Arbitrary Intervals

The technique for choosing points to minimize the interpolating error is extended to a general closed interval $[a, b]$ by using the change of variables

$$
\tilde{x}=\frac{1}{2}[(b-a) x+a+b]
$$

to transform the numbers $\bar{x}_{k}$ in the interval $[-1,1]$ into the corresponding number $\tilde{x}_{k}$ in the interval $[a, b]$, as shown in the next example.

Example 1 Let $f(x)=x e^{x}$ on [0, 1.5]. Compare the values given by the Lagrange polynomial with four equally-spaced nodes with those given by the Lagrange polynomial with nodes given by zeros of the fourth Chebyshev polynomial.
Solution The equally-spaced nodes $x_{0}=0, x_{1}=0.5, x_{2}=1$, and $x_{3}=1.5$ give

$$
\begin{aligned}
& L_{0}(x)=-1.3333 x^{3}+4.0000 x^{2}-3.6667 x+1 \\
& L_{1}(x)=4.0000 x^{3}-10.000 x^{2}+6.0000 x \\
& L_{2}(x)=-4.0000 x^{3}+8.0000 x^{2}-3.0000 x \\
& L_{3}(x)=1.3333 x^{3}-2.000 x^{2}+0.66667 x
\end{aligned}
$$

which produces the polynomial

$$
\begin{aligned}
P_{3}(x)= & L_{0}(x)(0)+L_{1}(x)\left(0.5 e^{0.5}\right)+L_{2}(x) e^{1}+L_{3}(x)\left(1.5 e^{1.5}\right)=1.3875 x^{3} \\
& +0.057570 x^{2}+1.2730 x
\end{aligned}
$$

For the second interpolating polynomial, we shift the zeros $\bar{x}_{k}=\cos ((2 k+1) / 8) \pi$, for $k=0,1,2,3$, of $\tilde{T}_{4}$ from $[-1,1]$ to [ $\left.0,1.5\right]$, using the linear transformation

$$
\tilde{x}_{k}=\frac{1}{2}\left[(1.5-0) \bar{x}_{k}+(1.5+0)\right]=0.75+0.75 \bar{x}_{k} .
$$

Because

$$
\begin{gathered}
\bar{x}_{0}=\cos \frac{\pi}{8}=0.92388, \quad \bar{x}_{1}=\cos \frac{3 \pi}{8}=0.38268, \\
\bar{x}_{2}=\cos \frac{5 \pi}{8}=-0.38268, \quad \text { and } \bar{x}_{4}=\cos \frac{7 \pi}{8}=-0.92388,
\end{gathered}
$$

we have

$$
\tilde{x}_{0}=1.44291, \quad \tilde{x}_{1}=1.03701, \quad \tilde{x}_{2}=0.46299, \quad \text { and } \quad \tilde{x}_{3}=0.05709
$$

The Lagrange coefficient polynomials for this set of nodes are

$$
\begin{aligned}
& \tilde{L}_{0}(x)=1.8142 x^{3}-2.8249 x^{2}+1.0264 x-0.049728 \\
& \tilde{L}_{1}(x)=-4.3799 x^{3}+8.5977 x^{2}-3.4026 x+0.16705 \\
& \tilde{L}_{2}(x)=4.3799 x^{3}-11.112 x^{2}+7.1738 x-0.37415 \\
& \tilde{L}_{3}(x)=-1.8142 x^{3}+5.3390 x^{2}-4.7976 x+1.2568
\end{aligned}
$$

The functional values required for these polynomials are given in the last two columns of Table 8.7. The interpolation polynomial of degree at most 3 is

$$
\tilde{P}_{3}(x)=1.3811 x^{3}+0.044652 x^{2}+1.3031 x-0.014352
$$

Table 8.7

| $x$ | $f(x)=x e^{x}$ | $\tilde{x}$ | $f(\tilde{x})=x e^{x}$ |
| :---: | :---: | :---: | :---: |
| $x_{0}=0.0$ | 0.00000 | $\tilde{x}_{0}=1.44291$ | 6.10783 |
| $x_{1}=0.5$ | 0.824361 | $\tilde{x}_{1}=1.03701$ | 2.92517 |
| $x_{2}=1.0$ | 2.71828 | $\tilde{x}_{2}=0.46299$ | 0.73560 |
| $x_{3}=1.5$ | 6.72253 | $\tilde{x}_{3}=0.05709$ | 0.060444 |

For comparison, Table 8.8 lists various values of $x$, together with the values of $f(x), P_{3}(x)$, and $\tilde{P}_{3}(x)$. It can be seen from this table that, although the error using $P_{3}(x)$ is less than using $\tilde{P}_{3}(x)$ near the middle of the table, the maximum error involved with using $\tilde{P}_{3}(x), 0.0180$, is considerably less than when using $P_{3}(x)$, which gives the error 0.0290 . (See Figure 8.12.)

Table 8.8

| $x$ | $f(x)=x e^{x}$ | $P_{3}(x)$ | $\left\|x e^{x}-P_{3}(x)\right\|$ | $\tilde{P}_{3}(x)$ | $\left\|x e^{x}-\tilde{P}_{3}(x)\right\|$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 0.15 | 0.1743 | 0.1969 | 0.0226 | 0.1868 | 0.0125 |
| 0.25 | 0.3210 | 0.3435 | 0.0225 | 0.3358 | 0.0148 |
| 0.35 | 0.4967 | 0.5121 | 0.0154 | 0.5064 | 0.0097 |
| 0.65 | 1.245 | 1.233 | 0.012 | 1.231 | 0.014 |
| 0.75 | 1.588 | 1.572 | 0.016 | 1.571 | 0.017 |
| 0.85 | 1.989 | 1.976 | 0.013 | 1.974 | 0.015 |
| 1.15 | 3.632 | 3.650 | 0.018 | 3.644 | 0.012 |
| 1.25 | 4.363 | 4.391 | 0.028 | 4.382 | 0.019 |
| 1.35 | 5.208 | 5.237 | 0.029 | 5.224 | 0.016 |

Figure 8.12


## Reducing the Degree of Approximating Polynomials

Chebyshev polynomials can also be used to reduce the degree of an approximating polynomial with a minimal loss of accuracy. Because the Chebyshev polynomials have a minimum maximum-absolute value that is spread uniformly on an interval, they can be used to reduce the degree of an approximation polynomial without exceeding the error tolerance.

Consider approximating an arbitrary $n$ th-degree polynomial

$$
P_{n}(x)=a_{n} x^{n}+a_{n-1} x^{n-1}+\cdots+a_{1} x+a_{0}
$$

on $[-1,1]$ with a polynomial of degree at most $n-1$. The object is to choose $P_{n-1}(x)$ in $\prod_{n-1}$ so that

$$
\max _{x \in[-1,1]}\left|P_{n}(x)-P_{n-1}(x)\right|
$$

is as small as possible.
We first note that $\left(P_{n}(x)-P_{n-1}(x)\right) / a_{n}$ is a monic polynomial of degree $n$, so applying Theorem 8.10 gives

$$
\max _{x \in[-1,1]}\left|\frac{1}{a_{n}}\left(P_{n}(x)-P_{n-1}(x)\right)\right| \geq \frac{1}{2^{n-1}} .
$$

Equality occurs precisely when

$$
\frac{1}{a_{n}}\left(P_{n}(x)-P_{n-1}(x)\right)=\tilde{T}_{n}(x)
$$

This means that we should choose

$$
P_{n-1}(x)=P_{n}(x)-a_{n} \tilde{T}_{n}(x)
$$

and with this choice we have the minimum value of

$$
\max _{x \in[-1,1]}\left|P_{n}(x)-P_{n-1}(x)\right|=\left|a_{n}\right| \max _{x \in[-1,1]}\left|\frac{1}{a_{n}}\left(P_{n}(x)-P_{n-1}(x)\right)\right|=\frac{\left|a_{n}\right|}{2^{n-1}}
$$

Illustration The function $f(x)=e^{x}$ is approximated on the interval $[-1,1]$ by the fourth Maclaurin polynomial

$$
P_{4}(x)=1+x+\frac{x^{2}}{2}+\frac{x^{3}}{6}+\frac{x^{4}}{24}
$$

which has truncation error

$$
\left|R_{4}(x)\right|=\frac{\left|f^{(5)}(\xi(x))\right|\left|x^{5}\right|}{120} \leq \frac{e}{120} \approx 0.023, \quad \text { for }-1 \leq x \leq 1
$$

Suppose that an error of 0.05 is tolerable and that we would like to reduce the degree of the approximating polynomial while staying within this bound.

The polynomial of degree 3 or less that best uniformly approximates $P_{4}(x)$ on $[-1,1]$ is

$$
\begin{aligned}
P_{3}(x)=P_{4}(x)-a_{4} \tilde{T}_{4}(x) & =1+x+\frac{x^{2}}{2}+\frac{x^{3}}{6}+\frac{x^{4}}{24}-\frac{1}{24}\left(x^{4}-x^{2}+\frac{1}{8}\right) \\
& =\frac{191}{192}+x+\frac{13}{24} x^{2}+\frac{1}{6} x^{3}
\end{aligned}
$$

With this choice, we have

$$
\left|P_{4}(x)-P_{3}(x)\right|=\left|a_{4} \tilde{T}_{4}(x)\right| \leq \frac{1}{24} \cdot \frac{1}{2^{3}}=\frac{1}{192} \leq 0.0053 .
$$

Adding this error bound to the bound for the Maclaurin truncation error gives

$$
0.023+0.0053=0.0283
$$

which is within the permissible error of 0.05 .
The polynomial of degree 2 or less that best uniformly approximates $P_{3}(x)$ on $[-1,1]$ is

$$
\begin{aligned}
P_{2}(x) & =P_{3}(x)-\frac{1}{6} \tilde{T}_{3}(x) \\
& =\frac{191}{192}+x+\frac{13}{24} x^{2}+\frac{1}{6} x^{3}-\frac{1}{6}\left(x^{3}-\frac{3}{4} x\right)=\frac{191}{192}+\frac{9}{8} x+\frac{13}{24} x^{2}
\end{aligned}
$$

However,

$$
\left|P_{3}(x)-P_{2}(x)\right|=\left|\frac{1}{6} \tilde{T}_{3}(x)\right|=\frac{1}{6}\left(\frac{1}{2}\right)^{2}=\frac{1}{24} \approx 0.042
$$

which—when added to the already accumulated error bound of 0.0283 -exceeds the tolerance of 0.05 . Consequently, the polynomial of least degree that best approximates $e^{x}$ on $[-1,1]$ with an error bound of less than 0.05 is

$$
P_{3}(x)=\frac{191}{192}+x+\frac{13}{24} x^{2}+\frac{1}{6} x^{3} .
$$

Table 8.9 lists the function and the approximating polynomials at various points in $[-1,1]$. Note that the tabulated entries for $P_{2}$ are well within the tolerance of 0.05 , even though the error bound for $P_{2}(x)$ exceeded the tolerance.

## Table 8.9

| $x$ | $e^{x}$ | $P_{4}(x)$ | $P_{3}(x)$ | $P_{2}(x)$ | $\left\|e^{x}-P_{2}(x)\right\|$ |
| ---: | :---: | :---: | :---: | :---: | :---: |
| -0.75 | 0.47237 | 0.47412 | 0.47917 | 0.45573 | 0.01664 |
| -0.25 | 0.77880 | 0.77881 | 0.77604 | 0.74740 | 0.03140 |
| 0.00 | 1.00000 | 1.00000 | 0.99479 | 0.99479 | 0.00521 |
| 0.25 | 1.28403 | 1.28402 | 1.28125 | 1.30990 | 0.02587 |
| 0.75 | 2.11700 | 2.11475 | 2.11979 | 2.14323 | 0.02623 |

## EXERCISE SET 8.3

1. Use the zeros of $\tilde{T}_{3}$ to construct an interpolating polynomial of degree 2 for the following functions on the interval $[-1,1]$.
a. $\quad f(x)=e^{x}$
b. $\quad f(x)=\sin x$
c. $\quad f(x)=\ln (x+2)$
d. $\quad f(x)=x^{4}$
2. Use the zeros of $\tilde{T}_{4}$ to construct an interpolating polynomial of degree 3 for the functions in Exercise 1.
3. Find a bound for the maximum error of the approximation in Exercise 1 on the interval $[-1,1]$.
4. Repeat Exercise 3 for the approximations computed in Exercise 3.
5. Use the zeros of $\tilde{T}_{3}$ and transformations of the given interval to construct an interpolating polynomial of degree 2 for the following functions.
a. $\quad f(x)=\frac{1}{x}, \quad[1,3]$
b. $\quad f(x)=e^{-x}, \quad[0,2]$
c. $\quad f(x)=\frac{1}{2} \cos x+\frac{1}{3} \sin 2 x, \quad[0,1]$
d. $\quad f(x)=x \ln x, \quad[1,3]$
6. Find the sixth Maclaurin polynomial for $x e^{x}$, and use Chebyshev economization to obtain a lesserdegree polynomial approximation while keeping the error less than 0.01 on $[-1,1]$.
7. Find the sixth Maclaurin polynomial for $\sin x$, and use Chebyshev economization to obtain a lesserdegree polynomial approximation while keeping the error less than 0.01 on $[-1,1]$.
8. Show that for any positive integers $i$ and $j$ with $i>j$, we have $T_{i}(x) T_{j}(x)=\frac{1}{2}\left[T_{i+j}(x)+T_{i-j}(x)\right]$.
9. Show that for each Chebyshev polynomial $T_{n}(x)$, we have

$$
\int_{-1}^{1} \frac{\left[T_{n}(x)\right]^{2}}{\sqrt{1-x^{2}}} d x=\frac{\pi}{2} .
$$

10. Show that for each $n$, the Chebyshev polynomial $T_{n}(x)$ has $n$ distinct zeros in $(-1,1)$.
11. Show that for each $n$, the derivative of the Chebyshev polynomial $T_{n}(x)$ has $n-1$ distinct zeros in $(-1,1)$.

### 8.4 Rationalfunction Approximation

The class of algebraic polynomials has some distinct advantages for use in approximation:

- There are a sufficient number of polynomials to approximate any continuous function on a closed interval to within an arbitrary tolerance;
- Polynomials are easily evaluated at arbitrary values; and
- The derivatives and integrals of polynomials exist and are easily determined.

The disadvantage of using polynomials for approximation is their tendency for oscillation. This often causes error bounds in polynomial approximation to significantly exceed the average approximation error, because error bounds are determined by the maximum approximation error. We now consider methods that spread the approximation error more evenly over the approximation interval. These techniques involve rational functions.

A rational function $r$ of degree $N$ has the form

$$
r(x)=\frac{p(x)}{q(x)}
$$

where $p(x)$ and $q(x)$ are polynomials whose degrees sum to $N$.
Every polynomial is a rational function (simply let $q(x) \equiv 1$ ), so approximation by rational functions gives results that are no worse than approximation by polynomials. However, rational functions whose numerator and denominator have the same or nearly the same degree often produce approximation results superior to polynomial methods for the same amount of computation effort. (This statement is based on the assumption that the amount of computation effort required for division is approximately the same as for multiplication.)

Rational functions have the added advantage of permitting efficient approximation of functions with infinite discontinuities near, but outside, the interval of approximation. Polynomial approximation is generally unacceptable in this situation.
and 5. Compare these results with those produced from the other Padé approximations of degree five.
a. $\quad n=0, m=5$
b. $\quad n=1, m=4$
c. $\quad n=3, m=2$
d. $\quad n=4, m=1$
8. Express the following rational functions in continued-fraction form:
a. $\frac{x^{2}+3 x+2}{x^{2}-x+1}$
b. $\frac{4 x^{2}+3 x-7}{2 x^{3}+x^{2}-x+5}$
c. $\frac{2 x^{3}-3 x^{2}+4 x-5}{x^{2}+2 x+4}$
d. $\frac{2 x^{3}+x^{2}-x+3}{3 x^{3}+2 x^{2}-x+1}$
9. Find all the Chebyshev rational approximations of degree 2 for $f(x)=e^{-x}$. Which give the best approximations to $f(x)=e^{-x}$ at $x=0.25,0.5$, and 1 ?
10. Find all the Chebyshev rational approximations of degree 3 for $f(x)=\cos x$. Which give the best approximations to $f(x)=\cos x$ at $x=\pi / 4$ and $\pi / 3$ ?
11. Find the Chebyshev rational approximation of degree 4 with $n=m=2$ for $f(x)=\sin x$. Compare the results at $x_{i}=0.1 i$, for $i=0,1,2,3,4,5$, from this approximation with those obtained in Exercise 5 using a sixth-degree Padé approximation.
12. Find all Chebyshev rational approximations of degree 5 for $f(x)=e^{x}$. Compare the results at $x_{i}=0.2 i$, for $i=1,2,3,4,5$, with those obtained in Exercises 3 and 4 .
13. To accurately approximate $f(x)=e^{x}$ for inclusion in a mathematical library, we first restrict the domain of $f$. Given a real number $x$, divide by $\ln \sqrt{10}$ to obtain the relation

$$
x=M \cdot \ln \sqrt{10}+s,
$$

where $M$ is an integer and $s$ is a real number satisfying $|s| \leq \frac{1}{2} \ln \sqrt{10}$.
a. Show that $e^{x}=e^{s} \cdot 10^{M / 2}$.
b. Construct a rational function approximation for $e^{s}$ using $n=m=3$. Estimate the error when $0 \leq|s| \leq \frac{1}{2} \ln \sqrt{10}$.
c. Design an implementation of $e^{x}$ using the results of part (a) and (b) and the approximations

$$
\frac{1}{\ln \sqrt{10}}=0.8685889638 \quad \text { and } \quad \sqrt{10}=3.162277660
$$

14. To accurately approximate $\sin x$ and $\cos x$ for inclusion in a mathematical library, we first restrict their domains. Given a real number $x$, divide by $\pi$ to obtain the relation

$$
|x|=M \pi+s, \quad \text { where } M \text { is an integer and }|s| \leq \frac{\pi}{2}
$$

a. Show that $\sin x=\operatorname{sgn}(x) \cdot(-1)^{M} \cdot \sin s$.
b. Construct a rational approximation to $\sin s$ using $n=m=4$. Estimate the error when $0 \leq|s| \leq$ $\pi / 2$.
c. Design an implementation of $\sin x$ using parts (a) and (b).
d. Repeat part (c) for $\cos x$ using the fact that $\cos x=\sin (x+\pi / 2)$.

### 8.5 Trigonometric Polynomial Approximation

The use of series of sine and cosine functions to represent arbitrary functions had its beginnings in the 1750 s with the study of the motion of a vibrating string. This problem was considered by Jean d'Alembert and then taken up by the foremost mathematician of the time, Leonhard Euler. But it was Daniel Bernoulli who first advocated the use of the infinite sums of sine and cosines as a solution to the problem, sums that we now know as Fourier series. In the early part of the 19th century, Jean Baptiste Joseph Fourier used these series to study the flow of heat and developed quite a complete theory of the subject.

During the late 17th and early 18th centuries, the Bernoulli family produced no less than 8 important mathematicians and physicists. Daniel Bernoulli's most important work involved the pressure, density, and velocity of fluid flow, which produced what is known as the Bernoulli principle.

Joseph Fourier (1768-1830)
published his theory of trigonometric series in Théorie analytique de la chaleur to solve the problem of steady state heat distribution in a solid.

The first observation in the development of Fourier series is that, for each positive integer $n$, the set of functions $\left\{\phi_{0}, \phi_{1}, \ldots, \phi_{2 n-1}\right\}$, where

$$
\begin{aligned}
& \phi_{0}(x)=\frac{1}{2} \\
& \phi_{k}(x)=\cos k x, \quad \text { for each } k=1,2, \ldots, n,
\end{aligned}
$$

and

$$
\phi_{n+k}(x)=\sin k x, \quad \text { for each } k=1,2, \ldots, n-1,
$$

is an orthogonal set on $[-\pi, \pi]$ with respect to $w(x) \equiv 1$. This orthogonality follows from the fact that for every integer $j$, the integrals of $\sin j x$ and $\cos j x$ over $[-\pi, \pi]$ are 0 , and we can rewrite products of sine and cosine functions as sums by using the three trigonometric identities

$$
\begin{align*}
\sin t_{1} \sin t_{2} & =\frac{1}{2}\left[\cos \left(t_{1}-t_{2}\right)-\cos \left(t_{1}+t_{2}\right)\right] \\
\cos t_{1} \cos t_{2} & =\frac{1}{2}\left[\cos \left(t_{1}-t_{2}\right)+\cos \left(t_{1}+t_{2}\right)\right]  \tag{8.19}\\
\sin t_{1} \cos t_{2} & =\frac{1}{2}\left[\sin \left(t_{1}-t_{2}\right)+\sin \left(t_{1}+t_{2}\right)\right]
\end{align*}
$$

## Orthogonal Trigonometric Polynomials

Let $\mathcal{T}_{n}$ denote the set of all linear combinations of the functions $\phi_{0}, \phi_{1}, \ldots, \phi_{2 n-1}$. This set is called the set of trigonometric polynomials of degree less than or equal to $n$. (Some sources also include an additional function in the set, $\phi_{2 n}(x)=\sin n x$.)

For a function $f \in C[-\pi, \pi]$, we want to find the continuous least squares approximation by functions in $\mathcal{T}_{n}$ in the form

$$
S_{n}(x)=\frac{a_{0}}{2}+a_{n} \cos n x+\sum_{k=1}^{n-1}\left(a_{k} \cos k x+b_{k} \sin k x\right)
$$

Since the set of functions $\left\{\phi_{0}, \phi_{1}, \ldots, \phi_{2 n-1}\right\}$ is orthogonal on $[-\pi, \pi]$ with respect to $w(x) \equiv 1$, it follows from Theorem 8.6 on page 515 and the equations in (8.19) that the appropriate selection of coefficients is

$$
\begin{equation*}
a_{k}=\frac{\int_{-\pi}^{\pi} f(x) \cos k x d x}{\int_{-\pi}^{\pi}(\cos k x)^{2} d x}=\frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos k x d x, \quad \text { for each } k=0,1,2, \ldots, n \tag{8.20}
\end{equation*}
$$

and

$$
\begin{equation*}
b_{k}=\frac{\int_{-\pi}^{\pi} f(x) \sin k x d x}{\int_{-\pi}^{\pi}(\sin k x)^{2} d x}=\frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin k x d x, \quad \text { for each } k=1,2, \ldots, n-1 \tag{8.21}
\end{equation*}
$$

The limit of $S_{n}(x)$ when $n \rightarrow \infty$ is called the Fourier series of $f$. Fourier series are used to describe the solution of various ordinary and partial-differential equations that occur in physical situations.

Example 1 Determine the trigonometric polynomial from $\mathcal{T}_{n}$ that approximates

$$
f(x)=|x|, \quad \text { for }-\pi<x<\pi .
$$

Solution We first need to find the coefficients

$$
\begin{aligned}
& a_{0}=\frac{1}{\pi} \int_{-\pi}^{\pi}|x| d x=-\frac{1}{\pi} \int_{-\pi}^{0} x d x+\frac{1}{\pi} \int_{0}^{\pi} x d x=\frac{2}{\pi} \int_{0}^{\pi} x d x=\pi \\
& a_{k}=\frac{1}{\pi} \int_{-\pi}^{\pi}|x| \cos k x d x=\frac{2}{\pi} \int_{0}^{\pi} x \cos k x d x=\frac{2}{\pi k^{2}}\left[(-1)^{k}-1\right]
\end{aligned}
$$

for each $k=1,2, \ldots, n$, and

$$
b_{k}=\frac{1}{\pi} \int_{-\pi}^{\pi}|x| \sin k x d x=0, \quad \text { for each } k=1,2, \ldots, n-1
$$

That the $b_{k}$ 's are all 0 follows from the fact that $g(x)=|x| \sin k x$ is an odd function for each $k$, and the integral of a continuous odd function over an interval of the form $[-a, a]$ is 0 . (See Exercises 13 and 14.) The trigonometric polynomial from $\mathcal{T}_{n}$ approximating $f$ is therefore,

$$
S_{n}(x)=\frac{\pi}{2}+\frac{2}{\pi} \sum_{k=1}^{n} \frac{(-1)^{k}-1}{k^{2}} \cos k x
$$

The first few trigonometric polynomials for $f(x)=|x|$ are shown in Figure 8.13.

Figure 8.13


The Fourier series for $f$ is

$$
S(x)=\lim _{n \rightarrow \infty} S_{n}(x)=\frac{\pi}{2}+\frac{2}{\pi} \sum_{k=1}^{\infty} \frac{(-1)^{k}-1}{k^{2}} \cos k x
$$

Since $|\cos k x| \leq 1$ for every $k$ and $x$, the series converges, and $S(x)$ exists for all real numbers $x$.

## Discrete Trigonometric Approximation

There is a discrete analog that is useful for the discrete least squares approximation and the interpolation of large amounts of data.

Suppose that a collection of $2 m$ paired data points $\left\{\left(x_{j}, y_{j}\right)\right\}_{j=0}^{2 m-1}$ is given, with the first elements in the pairs equally partitioning a closed interval. For convenience, we assume that the interval is $[-\pi, \pi]$, so, as shown in Figure 8.14,

$$
\begin{equation*}
x_{j}=-\pi+\left(\frac{j}{m}\right) \pi, \quad \text { for each } j=0,1, \ldots, 2 m-1 . \tag{8.22}
\end{equation*}
$$

If it is not $[-\pi, \pi]$, a simple linear transformation could be used to transform the data into this form.

Figure 8.14


The goal in the discrete case is to determine the trigonometric polynomial $S_{n}(x)$ in $\mathcal{T}_{n}$ that will minimize

$$
E\left(S_{n}\right)=\sum_{j=0}^{2 m-1}\left[y_{j}-S_{n}\left(x_{j}\right)\right]^{2}
$$

To do this we need to choose the constants $a_{0}, a_{1}, \ldots, a_{n}, b_{1}, b_{2}, \ldots, b_{n-1}$ to minimize

$$
\begin{equation*}
E\left(S_{n}\right)=\sum_{j=0}^{2 m-1}\left\{y_{j}-\left[\frac{a_{0}}{2}+a_{n} \cos n x_{j}+\sum_{k=1}^{n-1}\left(a_{k} \cos k x_{j}+b_{k} \sin k x_{j}\right)\right]\right\}^{2} \tag{8.23}
\end{equation*}
$$

The determination of the constants is simplified by the fact that the set $\left\{\phi_{0}, \phi_{1}, \ldots\right.$, $\left.\phi_{2 n-1}\right\}$ is orthogonal with respect to summation over the equally spaced points $\left\{x_{j}\right\}_{j=0}^{2 m-1}$ in $[-\pi, \pi]$. By this we mean that for each $k \neq l$,

$$
\begin{equation*}
\sum_{j=0}^{2 m-1} \phi_{k}\left(x_{j}\right) \phi_{l}\left(x_{j}\right)=0 . \tag{8.24}
\end{equation*}
$$

To show this orthogonality, we use the following lemma.

Lemma 8.12 Suppose that the integer $r$ is not a multiple of $2 m$. Then

- $\quad \sum_{j=0}^{2 m-1} \cos r x_{j}=0 \quad$ and $\quad \sum_{j=0}^{2 m-1} \sin r x_{j}=0$.

Moreover, if $r$ is not a multiple of $m$, then

- $\quad \sum_{j=0}^{2 m-1}\left(\cos r x_{j}\right)^{2}=m \quad$ and $\quad \sum_{j=0}^{2 m-1}\left(\sin r x_{j}\right)^{2}=m$.

Euler first used the symbol $i$ in 1794 to represent $\sqrt{-1}$ in his memoir De Formulis
Differentialibus Angularibus.

Proof Euler's Formula states that with $i^{2}=-1$, we have, for every real number $z$,

$$
\begin{equation*}
e^{i z}=\cos z+i \sin z \tag{8.25}
\end{equation*}
$$

Applying this result gives

$$
\sum_{j=0}^{2 m-1} \cos r x_{j}+i \sum_{j=0}^{2 m-1} \sin r x_{j}=\sum_{j=0}^{2 m-1}\left(\cos r x_{j}+i \sin r x_{j}\right)=\sum_{j=0}^{2 m-1} e^{i r x_{j}}
$$

But

$$
e^{i r x_{j}}=e^{i r(-\pi+j \pi / m)}=e^{-i r \pi} \cdot e^{i r j \pi / m}
$$

so

$$
\sum_{j=0}^{2 m-1} \cos r x_{j}+i \sum_{j=0}^{2 m-1} \sin r x_{j}=e^{-i r \pi} \sum_{j=0}^{2 m-1} e^{i r j \pi / m}
$$

Since $\sum_{j=0}^{2 m-1} e^{i r j \pi / m}$ is a geometric series with first term 1 and ratio $e^{i r \pi / m} \neq 1$, we have

$$
\sum_{j=0}^{2 m-1} e^{i r j \pi / m}=\frac{1-\left(e^{i r \pi / m}\right)^{2 m}}{1-e^{i r \pi / m}}=\frac{1-e^{2 i r \pi}}{1-e^{i r \pi / m}}
$$

But $e^{2 i r \pi}=\cos 2 r \pi+i \sin 2 r \pi=1$, so $1-e^{2 i r \pi}=0$ and

$$
\sum_{j=0}^{2 m-1} \cos r x_{j}+i \sum_{j=0}^{2 m-1} \sin r x_{j}=e^{-i r \pi} \sum_{j=0}^{2 m-1} e^{i r j \pi / m}=0
$$

This implies that both the real and imaginary parts are zero, so

$$
\sum_{j=0}^{2 m-1} \cos r x_{j}=0 \quad \text { and } \quad \sum_{j=0}^{2 m-1} \sin r x_{j}=0
$$

In addition, if $r$ is not a multiple of $m$, these sums imply that

$$
\sum_{j=0}^{2 m-1}\left(\cos r x_{j}\right)^{2}=\sum_{j=0}^{2 m-1} \frac{1}{2}\left(1+\cos 2 r x_{j}\right)=\frac{1}{2}\left[2 m+\sum_{j=0}^{2 m-1} \cos 2 r x_{j}\right]=\frac{1}{2}(2 m+0)=m
$$

and, similarly, that

$$
\sum_{j=0}^{2 m-1}\left(\sin r x_{j}\right)^{2}=\sum_{j=0}^{2 m-1} \frac{1}{2}\left(1-\cos 2 r x_{j}\right)=m
$$

We can now show the orthogonality stated in (8.24). Consider, for example, the case

$$
\sum_{j=0}^{2 m-1} \phi_{k}\left(x_{j}\right) \phi_{n+l}\left(x_{j}\right)=\sum_{j=0}^{2 m-1}\left(\cos k x_{j}\right)\left(\sin l x_{j}\right)
$$

Since

$$
\cos k x_{j} \sin l x_{j}=\frac{1}{2}\left[\sin (l+k) x_{j}+\sin (l-k) x_{j}\right]
$$

and $(l+k)$ and $(l-k)$ are both integers that are not multiples of $2 m$, Lemma 8.12 implies that

$$
\sum_{j=0}^{2 m-1}\left(\cos k x_{j}\right)\left(\sin l x_{j}\right)=\frac{1}{2}\left[\sum_{j=0}^{2 m-1} \sin (l+k) x_{j}+\sum_{j=0}^{2 m-1} \sin (l-k) x_{j}\right]=\frac{1}{2}(0+0)=0 .
$$

This technique is used to show that the orthogonality condition is satisfied for any pair of the functions and to produce the following result.

Theorem 8.13 The constants in the summation

$$
S_{n}(x)=\frac{a_{0}}{2}+a_{n} \cos n x+\sum_{k=1}^{n-1}\left(a_{k} \cos k x+b_{k} \sin k x\right)
$$

that minimize the least squares sum

$$
E\left(a_{0}, \ldots, a_{n}, b_{1}, \ldots, b_{n-1}\right)=\sum_{j=0}^{2 m-1}\left(y_{j}-S_{n}\left(x_{j}\right)\right)^{2}
$$

are

- $\quad a_{k}=\frac{1}{m} \sum_{j=0}^{2 m-1} y_{j} \cos k x_{j}, \quad$ for each $k=0,1, \ldots, n$,
and
- $\quad b_{k}=\frac{1}{m} \sum_{j=0}^{2 m-1} y_{j} \sin k x_{j}, \quad$ for each $k=1,2, \ldots, n-1$.

The theorem is proved by setting the partial derivatives of $E$ with respect to the $a_{k}$ 's and the $b_{k}$ 's to zero, as was done in Sections 8.1 and 8.2 , and applying the orthogonality to simplify the equations. For example,

$$
0=\frac{\partial E}{\partial b_{k}}=2 \sum_{j=0}^{2 m-1}\left[y_{j}-S_{n}\left(x_{j}\right)\right]\left(-\sin k x_{j}\right)
$$

so

$$
\begin{aligned}
0= & \sum_{j=0}^{2 m-1} y_{j} \sin k x_{j}-\sum_{j=0}^{2 m-1} S_{n}\left(x_{j}\right) \sin k x_{j} \\
= & \sum_{j=0}^{2 m-1} y_{j} \sin k x_{j}-\frac{a_{0}}{2} \sum_{j=0}^{2 m-1} \sin k x_{j}-a_{n} \sum_{j=0}^{2 m-1} \sin k x_{j} \cos n x_{j} \\
& -\sum_{l=1}^{n-1} a_{l} \sum_{j=0}^{2 m-1} \sin k x_{j} \cos l x_{j}-\sum_{\substack{l=1, l \neq k}}^{n-1} b_{l} \sum_{j=0}^{2 m-1} \sin k x_{j} \sin l x_{j}-b_{k} \sum_{j=0}^{2 m-1}\left(\sin k x_{j}\right)^{2} .
\end{aligned}
$$

The orthogonality implies that all but the first and last sums on the right side are zero, and Lemma 8.12 states the final sum is $m$. Hence

$$
0=\sum_{j=0}^{2 m-1} y_{j} \sin k x_{j}-m b_{k},
$$

which implies that

$$
b_{k}=\frac{1}{m} \sum_{j=0}^{2 m-1} y_{j} \sin k x_{j}
$$

The result for the $a_{k}$ 's is similar but need an additional step to determine $a_{0}$ (See Exercise 17.)

Example 2 Find $S_{2}(x)$, the discrete least squares trigonometric polynomial of degree 2 for $f(x)=$ $2 x^{2}-9$ when $x$ is in $[-\pi, \pi]$.

Solution We have $m=2(2)-1=3$, so the nodes are

$$
x_{j}=\pi+\frac{j}{m} \pi \quad \text { and } \quad y_{j}=f\left(x_{j}\right)=2 x_{j}^{2}-9, \quad \text { for } j=0,1,2,3,4,5
$$

The trigonometric polynomial is

$$
S_{2}(x)=\frac{1}{2} a_{0}+a_{2} \cos 2 x+\left(a_{1} \cos x+b_{1} \sin x\right)
$$

where

$$
a_{k}=\frac{1}{3} \sum_{j=0}^{5} y_{j} \cos k x_{j}, \text { for } k=0,1,2, \quad \text { and } \quad b_{1}=\frac{1}{3} \sum_{j=0}^{5} y_{j} \sin x_{j}
$$

The coefficients are

$$
\begin{aligned}
a_{0}= & \frac{1}{3}\left(f(-\pi)+f\left(-\frac{2 \pi}{3}\right)+f\left(-\frac{\pi}{3}\right) f(0)+f\left(\frac{\pi}{3}\right)+f\left(\frac{2 \pi}{3}\right)\right)=-4.10944566 \\
a_{1}= & \frac{1}{3}\left(f(-\pi) \cos (-\pi)+f\left(-\frac{2 \pi}{3}\right) \cos \left(-\frac{2 \pi}{3}\right)+f\left(-\frac{\pi}{3}\right) \cos \left(-\frac{\pi}{3}\right) f(0) \cos 0\right. \\
& \left.+f\left(\frac{\pi}{3}\right) \cos \left(\frac{\pi}{3}\right)+f\left(\frac{2 \pi}{3}\right) \cos \left(\frac{2 \pi}{3}\right)\right)=-8.77298169 \\
a_{2}= & \frac{1}{3}\left(f(-\pi) \cos (-2 \pi)+f\left(-\frac{2 \pi}{3}\right) \cos \left(-\frac{4 \pi}{3}\right)+f\left(-\frac{\pi}{3}\right) \cos \left(-\frac{2 \pi}{3}\right) f(0) \cos 0\right. \\
& \left.+f\left(\frac{\pi}{3}\right) \cos \left(\frac{2 \pi}{3}\right)+f\left(\frac{2 \pi}{3}\right) \cos \left(\frac{4 \pi}{3}\right)\right)=2.92432723
\end{aligned}
$$

and

$$
\begin{aligned}
b_{1}= & \frac{1}{3}\left(f(-\pi) \sin (-\pi)+f\left(-\frac{2 \pi}{3}\right) \sin \left(-\frac{\pi}{3}\right)+f\left(-\frac{\pi}{3}\right)\left(-\frac{\pi}{3}\right) f(0) \sin 0\right. \\
& \left.+f\left(\frac{\pi}{3}\right)\left(\frac{\pi}{3}\right)+f\left(\frac{2 \pi}{3}\right)\left(\frac{2 \pi}{3}\right)\right)=0
\end{aligned}
$$

Thus

$$
S_{2}(x)=\frac{1}{2}(-4.10944562)-8.77298169 \cos x+2.92432723 \cos 2 x
$$

Figure 8.15 shows $f(x)$ and the discrete least squares trigonometric polynomial $S_{2}(x)$.

Figure 8.15


The next example gives an illustration of finding a least-squares approximation for a function that is defined on a closed interval other than $[-\pi, \pi]$.

Example 3 Find the discrete least squares approximation $S_{3}(x)$ for

$$
f(x)=x^{4}-3 x^{3}+2 x^{2}-\tan x(x-2)
$$

using the data $\left\{\left(x_{j}, y_{j}\right)\right\}_{j=0}^{9}$, where $x_{j}=j / 5$ and $y_{j}=f\left(x_{j}\right)$.
Solution We first need the linear transformation from $[0,2]$ to $[-\pi, \pi]$ given by

$$
z_{j}=\pi\left(x_{j}-1\right) .
$$

Then the transformed data have the form

$$
\left\{\left(z_{j}, f\left(1+\frac{z_{j}}{\pi}\right)\right)\right\}_{j=0}^{9} .
$$

The least squares trigonometric polynomial is consequently,

$$
S_{3}(z)=\left[\frac{a_{0}}{2}+a_{3} \cos 3 z+\sum_{k=1}^{2}\left(a_{k} \cos k z+b_{k} \sin k z\right)\right],
$$

where

$$
a_{k}=\frac{1}{5} \sum_{j=0}^{9} f\left(1+\frac{z_{j}}{\pi}\right) \cos k z_{j}, \quad \text { for } k=0,1,2,3,
$$

and

$$
b_{k}=\frac{1}{5} \sum_{j=0}^{9} f\left(1+\frac{z_{j}}{\pi}\right) \sin k z_{j}, \quad \text { for } k=1,2
$$

Evaluating these sums produces the approximation

$$
\begin{aligned}
S_{3}(z)= & 0.76201+0.77177 \cos z+0.017423 \cos 2 z+0.0065673 \cos 3 z \\
& -0.38676 \sin z+0.047806 \sin 2 z
\end{aligned}
$$

and converting back to the variable $x$ gives

$$
\begin{aligned}
S_{3}(x)= & 0.76201+0.77177 \cos \pi(x-1)+0.017423 \cos 2 \pi(x-1) \\
& +0.0065673 \cos 3 \pi(x-1)-0.38676 \sin \pi(x-1)+0.047806 \sin 2 \pi(x-1)
\end{aligned}
$$

Table 8.12 lists values of $f(x)$ and $S_{3}(x)$.

Table 8.12

| $x$ | $f(x)$ | $S_{3}(x)$ | $\left\|f(x)-S_{3}(x)\right\|$ |
| :---: | ---: | ---: | ---: |
| 0.125 | 0.26440 | 0.24060 | $2.38 \times 10^{-2}$ |
| 0.375 | 0.84081 | 0.85154 | $1.07 \times 10^{-2}$ |
| 0.625 | 1.36150 | 1.36248 | $9.74 \times 10^{-4}$ |
| 0.875 | 1.61282 | 1.60406 | $8.75 \times 10^{-3}$ |
| 1.125 | 1.36672 | 1.37566 | $8.94 \times 10^{-3}$ |
| 1.375 | 0.71697 | 0.71545 | $1.52 \times 10^{-3}$ |
| 1.625 | 0.07909 | 0.06929 | $9.80 \times 10^{-3}$ |
| 1.875 | -0.14576 | -0.12302 | $2.27 \times 10^{-2}$ |

## EXERCISESET 8.5

1. Find the continuous least squares trigonometric polynomial $S_{2}(x)$ for $f(x)=x^{2}$ on $[-\pi, \pi]$.
2. Find the continuous least squares trigonometric polynomial $S_{n}(x)$ for $f(x)=x$ on $[-\pi, \pi]$.
3. Find the continuous least squares trigonometric polynomial $S_{3}(x)$ for $f(x)=e^{x}$ on $[-\pi, \pi]$.
4. Find the general continuous least squares trigonometric polynomial $S_{n}(x)$ for $f(x)=e^{x}$ on $[-\pi, \pi]$.
5. Find the general continuous least squares trigonometric polynomial $S_{n}(x)$ for

$$
f(x)= \begin{cases}0, & \text { if }-\pi<x \leq 0 \\ 1, & \text { if } 0<x<\pi\end{cases}
$$

6. Find the general continuous least squares trigonometric polynomial $S_{n}(x)$ in for

$$
f(x)= \begin{cases}-1, & \text { if }-\pi<x<0 \\ 1, & \text { if } 0 \leq x \leq \pi\end{cases}
$$

7. Determine the discrete least squares trigonometric polynomial $S_{n}(x)$ on the interval $[-\pi, \pi]$ for the following functions, using the given values of $m$ and $n$ :
a. $\quad f(x)=\cos 2 x, m=4, n=2$
b. $\quad f(x)=\cos 3 x, m=4, n=2$
c. $f(x)=\sin \frac{x}{2}+2 \cos \frac{x}{3}, m=6, n=3$
d. $f(x)=x^{2} \cos x, m=6, n=3$
8. Compute the error $E\left(S_{n}\right)$ for each of the functions in Exercise 7.
9. Determine the discrete least squares trigonometric polynomial $S_{3}(x)$, using $m=4$ for $f(x)=e^{x} \cos 2 x$ on the interval $[-\pi, \pi]$. Compute the error $E\left(S_{3}\right)$.
10. Repeat Exercise 9 using $m=8$. Compare the values of the approximating polynomials with the values of $f$ at the points $\xi_{j}=-\pi+0.2 j \pi$, for $0 \leq j \leq 10$. Which approximation is better?
11. Let $f(x)=2 \tan x-\sec 2 x$, for $2 \leq x \leq 4$. Determine the discrete least squares trigonometric polynomials $S_{n}(x)$, using the values of $n$ and $m$ as follows, and compute the error in each case.
a. $\quad n=3, \quad m=6$
b. $\quad n=4, \quad m=6$
12. a. Determine the discrete least squares trigonometric polynomial $S_{4}(x)$, using $m=16$, for $f(x)=$ $x^{2} \sin x$ on the interval $[0,1]$.
b. Compute $\int_{0}^{1} S_{4}(x) d x$.
c. Compare the integral in part (b) to $\int_{0}^{1} x^{2} \sin x d x$.
13. Show that for any continuous odd function $f$ defined on the interval $[-a, a]$, we have $\int_{-a}^{a} f(x) d x=0$.
14. Show that for any continuous even function $f$ defined on the interval $[-a, a]$, we have $\int_{-a}^{a} f(x) d x=$ $2 \int_{0}^{a} f(x) d x$.
15. Show that the functions $\phi_{0}(x)=1 / 2, \phi_{1}(x)=\cos x, \ldots, \phi_{n}(x)=\cos n x, \phi_{n+1}(x)=\sin x, \ldots$, $\phi_{2 n-1}(x)=\sin (n-1) x$ are orthogonal on $[-\pi, \pi]$ with respect to $w(x) \equiv 1$.
16. In Example 1 the Fourier series was determined for $f(x)=|x|$. Use this series and the assumption that it represents $f$ at zero to find the value of the convergent infinite series $\sum_{k=0}^{\infty}\left(1 /(2 k+1)^{2}\right)$.
17. Show that the form of the constants $a_{k}$ for $k=0, \ldots, n$ in Theorem 8.13 is correct as stated.

### 8.6 Fast Fourier Transforms

In the latter part of Section 8.5, we determined the form of the discrete least squares polynomial of degree $n$ on the $2 m$ data points $\left\{\left(x_{j}, y_{j}\right)\right\}_{j=0}^{2 m-1}$, where $x_{j}=-\pi+(j / m) \pi$, for each $j=0,1, \ldots, 2 m-1$.

The interpolatory trigonometric polynomial in $\mathcal{T}_{m}$ on these $2 m$ data points is nearly the same as the least squares polynomial. This is because the least squares trigonometric polynomial minimizes the error term

$$
E\left(S_{m}\right)=\sum_{j=0}^{2 m-1}\left(y_{j}-S_{m}\left(x_{j}\right)\right)^{2}
$$

and for the interpolatory trigonometric polynomial, this error is 0 , hence minimized, when the $S_{m}\left(x_{j}\right)=y_{j}$, for each $j=0,1, \ldots, 2 m-1$.

A modification is needed to the form of the polynomial, however, if we want the coefficients to assume the same form as in the least squares case. In Lemma 8.12 we found that if $r$ is not a multiple of $m$, then

$$
\sum_{j=0}^{2 m-1}\left(\cos r x_{j}\right)^{2}=m
$$

Interpolation requires computing instead

$$
\sum_{j=0}^{2 m-1}\left(\cos m x_{j}\right)^{2}
$$

which (see Exercise 8) has the value $2 m$. This requires the interpolatory polynomial to be written as

$$
\begin{equation*}
S_{m}(x)=\frac{a_{0}+a_{m} \cos m x}{2}+\sum_{k=1}^{m-1}\left(a_{k} \cos k x+b_{k} \sin k x\right) \tag{8.26}
\end{equation*}
$$

if we want the form of the constants $a_{k}$ and $b_{k}$ to agree with those of the discrete least squares polynomial; that is,

