

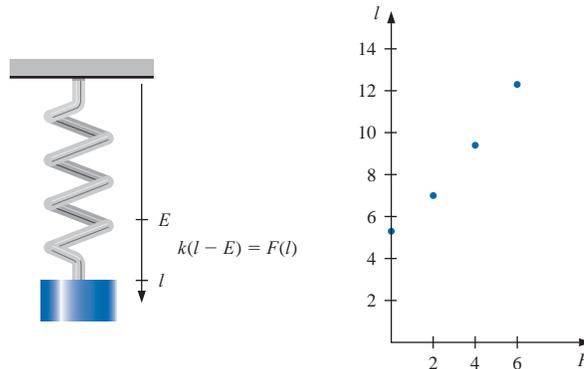
CHAPTER

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

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

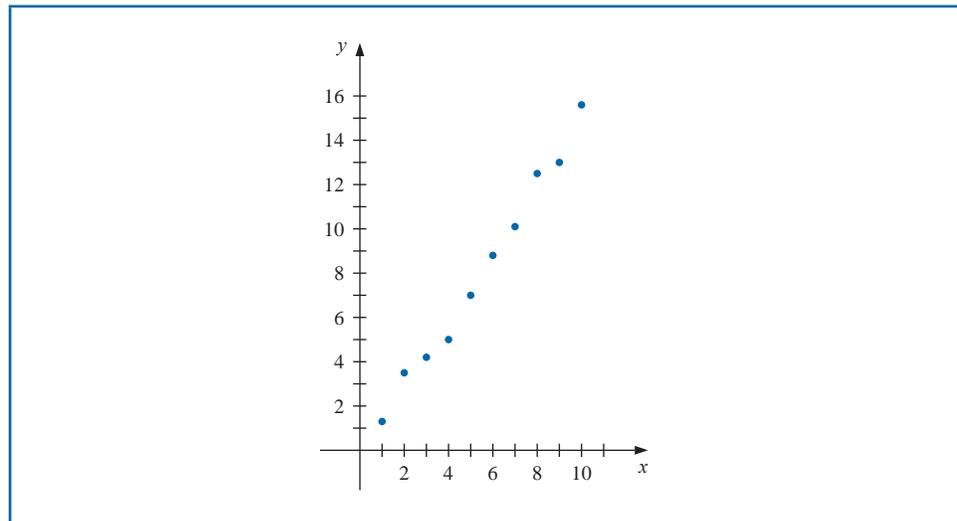
Table 8.1

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

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

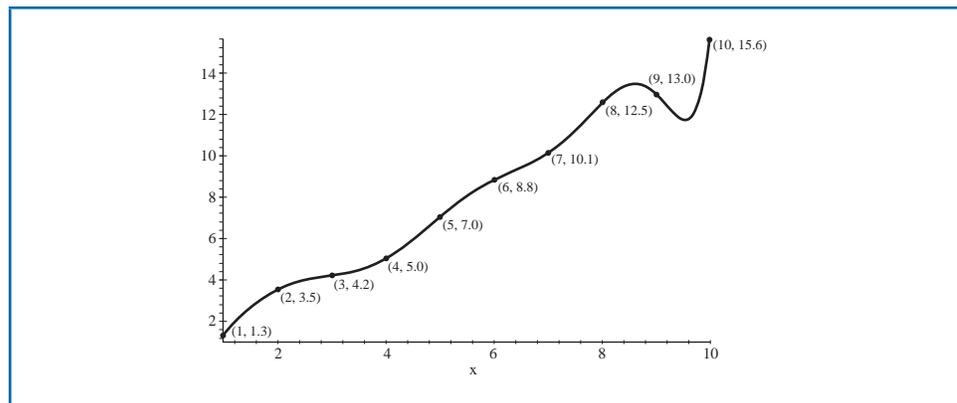
```
p := interp([1, 2, 3, 4, 5, 6, 7, 8, 9, 10], [1.3, 3.5, 4.2, 5.0, 7.0, 8.8, 10.1, 12.5, 13.0, 15.6], x);
plot(p, x = 1..10)
```

Figure 8.1



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 $a_1x_i + a_0$ 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

$$E_\infty(a_0, a_1) = \max_{1 \leq i \leq 10} \{|y_i - (a_1x_i + a_0)|\}.$$

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

$$E_1(a_0, a_1) = \sum_{i=1}^{10} |y_i - (a_1x_i + a_0)|.$$

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

$$0 = \frac{\partial}{\partial a_0} \sum_{i=1}^{10} |y_i - (a_1x_i + a_0)| \quad \text{and} \quad 0 = \frac{\partial}{\partial a_1} \sum_{i=1}^{10} |y_i - (a_1x_i + a_0)|.$$

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:

$$E_2(a_0, a_1) = \sum_{i=1}^{10} [y_i - (a_1x_i + a_0)]^2.$$

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 $\{(x_i, y_i)\}_{i=1}^m$ involves minimizing the total error,

$$E \equiv E_2(a_0, a_1) = \sum_{i=1}^m [y_i - (a_1x_i + a_0)]^2,$$

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,

$$0 = \frac{\partial}{\partial a_0} \sum_{i=1}^m [y_i - (a_1 x_i - a_0)]^2 = 2 \sum_{i=1}^m (y_i - a_1 x_i - a_0)(-1)$$

and

$$0 = \frac{\partial}{\partial a_1} \sum_{i=1}^m [y_i - (a_1 x_i + a_0)]^2 = 2 \sum_{i=1}^m (y_i - a_1 x_i - a_0)(-x_i).$$

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

$$a_0 = \frac{\sum_{i=1}^m x_i^2 \sum_{i=1}^m y_i - \sum_{i=1}^m x_i y_i \sum_{i=1}^m x_i}{m \left(\sum_{i=1}^m x_i^2 \right) - \left(\sum_{i=1}^m x_i \right)^2} \tag{8.1}$$

and

$$a_1 = \frac{m \sum_{i=1}^m x_i y_i - \sum_{i=1}^m x_i \sum_{i=1}^m y_i}{m \left(\sum_{i=1}^m x_i^2 \right) - \left(\sum_{i=1}^m x_i \right)^2}. \tag{8.2}$$

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	$x_i y_i$	$P(x_i) = 1.538x_i - 0.360$
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	$E = \sum_{i=1}^{10} (y_i - P(x_i))^2 \approx 2.34$

The word normal as used here implies perpendicular. The normal equations are obtained by finding perpendicular directions to a multidimensional surface.

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

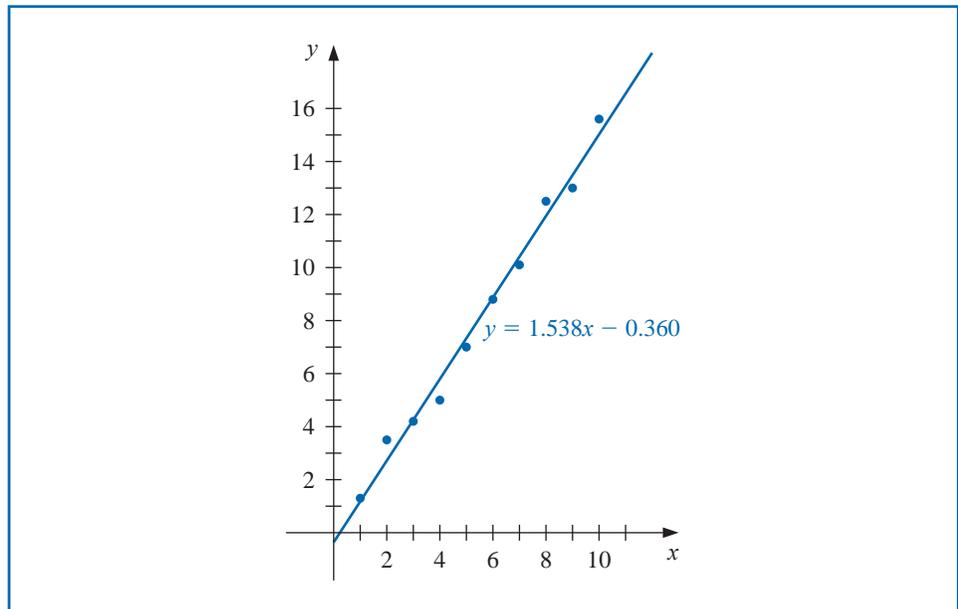
$$a_0 = \frac{385(81) - 55(572.4)}{10(385) - (55)^2} = -0.360$$

and

$$a_1 = \frac{10(572.4) - 55(81)}{10(385) - (55)^2} = 1.538,$$

so $P(x) = 1.538x - 0.360$. 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, $\{(x_i, y_i) \mid i = 1, 2, \dots, m\}$, with an algebraic polynomial

$$P_n(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0,$$

of degree $n < m - 1$, using the least squares procedure is handled similarly. We choose the constants a_0, a_1, \dots, a_n to minimize the least squares error $E = E_2(a_0, a_1, \dots, a_n)$, where

$$\begin{aligned} E &= \sum_{i=1}^m (y_i - P_n(x_i))^2 \\ &= \sum_{i=1}^m y_i^2 - 2 \sum_{i=1}^m P_n(x_i) y_i + \sum_{i=1}^m (P_n(x_i))^2 \end{aligned}$$

$$\begin{aligned} &= \sum_{i=1}^m y_i^2 - 2 \sum_{i=1}^m \left(\sum_{j=0}^n a_j x_i^j \right) y_i + \sum_{i=1}^m \left(\sum_{j=0}^n a_j x_i^j \right)^2 \\ &= \sum_{i=1}^m y_i^2 - 2 \sum_{j=0}^n a_j \left(\sum_{i=1}^m y_i x_i^j \right) + \sum_{j=0}^n \sum_{k=0}^n a_j a_k \left(\sum_{i=1}^m x_i^{j+k} \right). \end{aligned}$$

As in the linear case, for E to be minimized it is necessary that $\partial E / \partial a_j = 0$, for each $j = 0, 1, \dots, n$. 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

$$\sum_{k=0}^n a_k \sum_{i=1}^m x_i^{j+k} = \sum_{i=1}^m y_i x_i^j, \quad \text{for each } j = 0, 1, \dots, n. \tag{8.3}$$

It is helpful to write the equations as follows:

$$\begin{aligned} a_0 \sum_{i=1}^m x_i^0 + a_1 \sum_{i=1}^m x_i^1 + a_2 \sum_{i=1}^m x_i^2 + \cdots + a_n \sum_{i=1}^m x_i^n &= \sum_{i=1}^m y_i x_i^0, \\ a_0 \sum_{i=1}^m x_i^1 + a_1 \sum_{i=1}^m x_i^2 + a_2 \sum_{i=1}^m x_i^3 + \cdots + a_n \sum_{i=1}^m x_i^{n+1} &= \sum_{i=1}^m y_i x_i^1, \\ &\vdots \\ a_0 \sum_{i=1}^m x_i^n + a_1 \sum_{i=1}^m x_i^{n+1} + a_2 \sum_{i=1}^m x_i^{n+2} + \cdots + a_n \sum_{i=1}^m x_i^{2n} &= \sum_{i=1}^m y_i x_i^n. \end{aligned}$$

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

$$\begin{aligned} 5a_0 + 2.5a_1 + 1.875a_2 &= 8.7680, \\ 2.5a_0 + 1.875a_1 + 1.5625a_2 &= 5.4514, \\ 1.875a_0 + 1.5625a_1 + 1.3828a_2 &= 4.4015. \end{aligned}$$

To solve this system using Maple, we first define the equations

$$\begin{aligned} eq1 &:= 5a_0 + 2.5a_1 + 1.875a_2 = 8.7680: \\ eq2 &:= 2.5a_0 + 1.875a_1 + 1.5625a_2 = 5.4514: \\ eq3 &:= 1.875a_0 + 1.5625a_1 + 1.3828a_2 = 4.4015 \end{aligned}$$

and then solve the system with

$$\text{solve}(\{eq1, eq2, eq3\}, \{a_0, a_1, a_2\})$$

This gives

$$\{a_0 = 1.005075519, \quad a_1 = 0.8646758482, \quad a_2 = .8431641518\}$$

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

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

$$P_2(x) = 1.0051 + 0.86468x + 0.84316x^2,$$

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

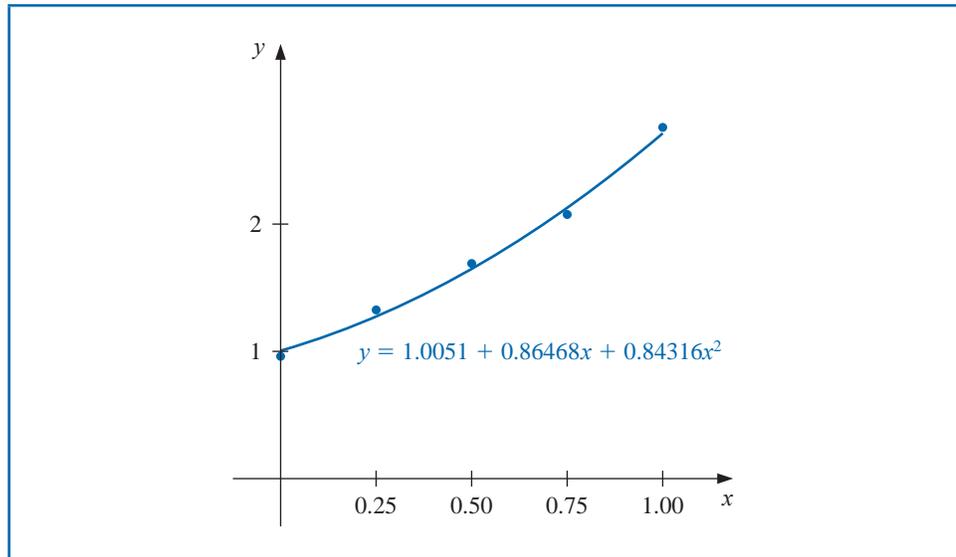


Table 8.4

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
$P(x_i)$	1.0051	1.2740	1.6482	2.1279	2.7129
$y_i - P(x_i)$	-0.0051	0.0100	0.0004	-0.0109	0.0054

The total error,

$$E = \sum_{i=1}^5 (y_i - P(x_i))^2 = 2.74 \times 10^{-4},$$

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

```
with(Statistics): xvals := Vector([0, 0.25, 0.5, 0.75, 1]): yvals := 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 → LinearFit([1, x, x^2], xvals, yvals, x): P(x)
```

Maple returns a result which rounded to 5 decimal places is

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

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

$$y = be^{ax} \quad (8.4)$$

or

$$y = bx^a, \quad (8.5)$$

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

$$E = \sum_{i=1}^m (y_i - be^{ax_i})^2, \quad \text{in the case of Eq. (8.4),}$$

or

$$E = \sum_{i=1}^m (y_i - bx_i^a)^2, \quad \text{in the case of Eq. (8.5).}$$

The normal equations associated with these procedures are obtained from either

$$0 = \frac{\partial E}{\partial b} = 2 \sum_{i=1}^m (y_i - be^{ax_i})(-e^{ax_i})$$

and

$$0 = \frac{\partial E}{\partial a} = 2 \sum_{i=1}^m (y_i - be^{ax_i})(-bx_i e^{ax_i}), \quad \text{in the case of Eq. (8.4);}$$

or

$$0 = \frac{\partial E}{\partial b} = 2 \sum_{i=1}^m (y_i - bx_i^a)(-x_i^a)$$

and

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

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:

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

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

$$y = be^{ax}, \quad \text{which implies that } \ln y = \ln b + ax.$$

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

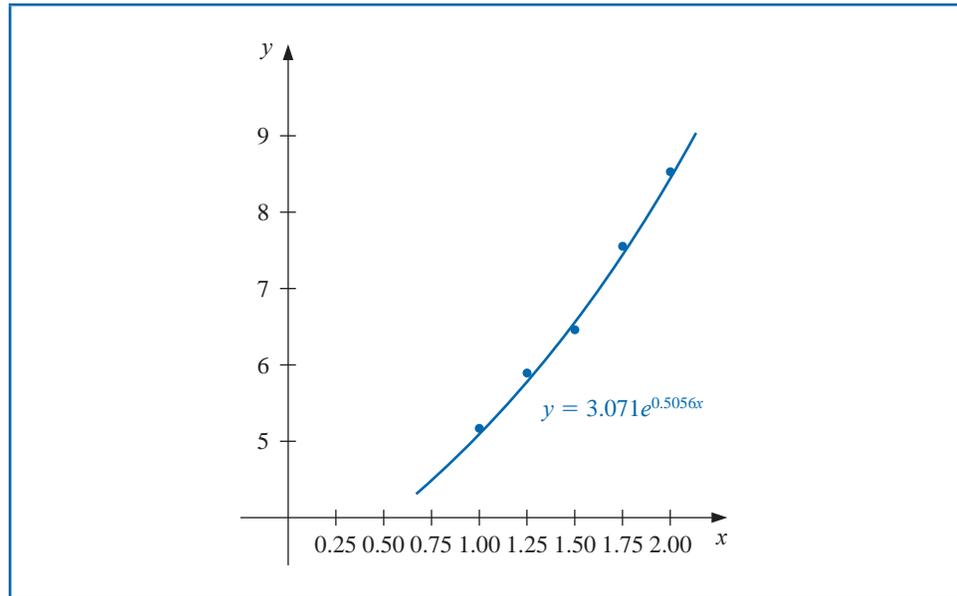
$$y = 3.071e^{0.5056x}.$$

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

Table 8.6

i	x_i	y_i	$3.071e^{0.5056x_i}$	$ y_i - 3.071e^{0.5056x_i} $
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 obtained 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 := Vector([1, 1.25, 1.5, 1.75, 2]): Y := 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,

$$3.07249e^{0.50572x}$$

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

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

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

- Construct the least squares polynomial of degree 1, and compute the error.
 - Construct the least squares polynomial of degree 2, and compute the error.
 - Construct the least squares polynomial of degree 3, and compute the error.
 - Construct the least squares approximation of the form be^{ax} , and compute the error.
 - Construct the least squares approximation of the form bx^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 $E = 5.3$ in. is the length of the unstretched spring.

- 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 .

- 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 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 score	Grade-point average	ACT score	Grade-point 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 Weight	Percent 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 (cm)	Attenuation coefficient (dB/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 $R = bW^a$ 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):

$$E = \sum_{i=1}^{37} (R_i - bW_i^a)^2.$$

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

<i>W</i>	<i>R</i>								
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 $A = (a_{ij})$, where

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

and x_1, x_2, \dots, 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

$$\int_a^b [f(x) - P_n(x)]^2 dx.$$

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

$$P_n(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0 = \sum_{k=0}^n a_k x^k,$$

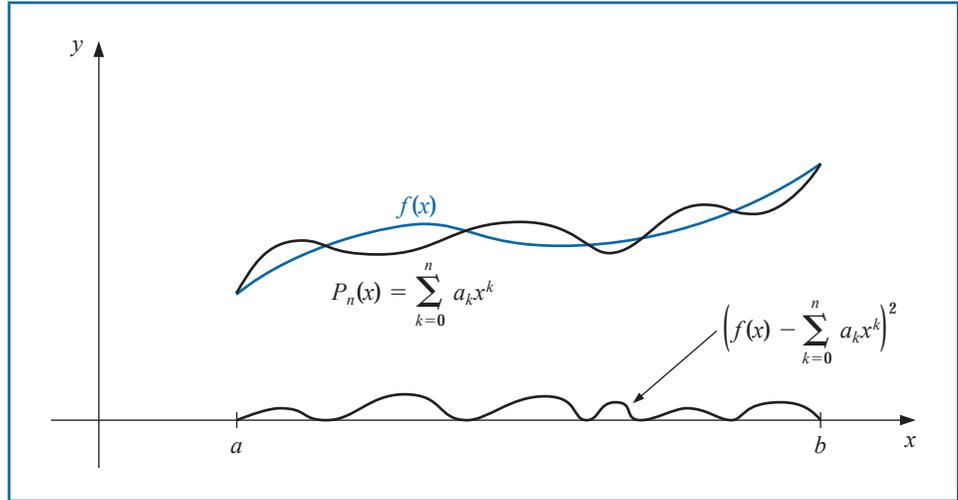
and define, as shown in Figure 8.6,

$$E \equiv E_2(a_0, a_1, \dots, a_n) = \int_a^b \left(f(x) - \sum_{k=0}^n a_k x^k \right)^2 dx.$$

The problem is to find real coefficients a_0, a_1, \dots, a_n that will minimize E . A necessary condition for the numbers a_0, a_1, \dots, a_n to minimize E is that

$$\frac{\partial E}{\partial a_j} = 0, \quad \text{for each } j = 0, 1, \dots, n.$$

Figure 8.6



Since

$$E = \int_a^b [f(x)]^2 dx - 2 \sum_{k=0}^n a_k \int_a^b x^k f(x) dx + \int_a^b \left(\sum_{k=0}^n a_k x^k \right)^2 dx,$$

we have

$$\frac{\partial E}{\partial a_j} = -2 \int_a^b x^j f(x) dx + 2 \sum_{k=0}^n a_k \int_a^b x^{j+k} dx.$$

Hence, to find $P_n(x)$, the $(n+1)$ linear **normal equations**

$$\sum_{k=0}^n a_k \int_a^b x^{j+k} dx = \int_a^b x^j f(x) dx, \quad \text{for each } j = 0, 1, \dots, n, \quad (8.6)$$

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

$$\begin{aligned} a_0 \int_0^1 1 dx + a_1 \int_0^1 x dx + a_2 \int_0^1 x^2 dx &= \int_0^1 \sin \pi x dx, \\ a_0 \int_0^1 x dx + a_1 \int_0^1 x^2 dx + a_2 \int_0^1 x^3 dx &= \int_0^1 x \sin \pi x dx, \\ a_0 \int_0^1 x^2 dx + a_1 \int_0^1 x^3 dx + a_2 \int_0^1 x^4 dx &= \int_0^1 x^2 \sin \pi x dx. \end{aligned}$$

Performing the integration yields

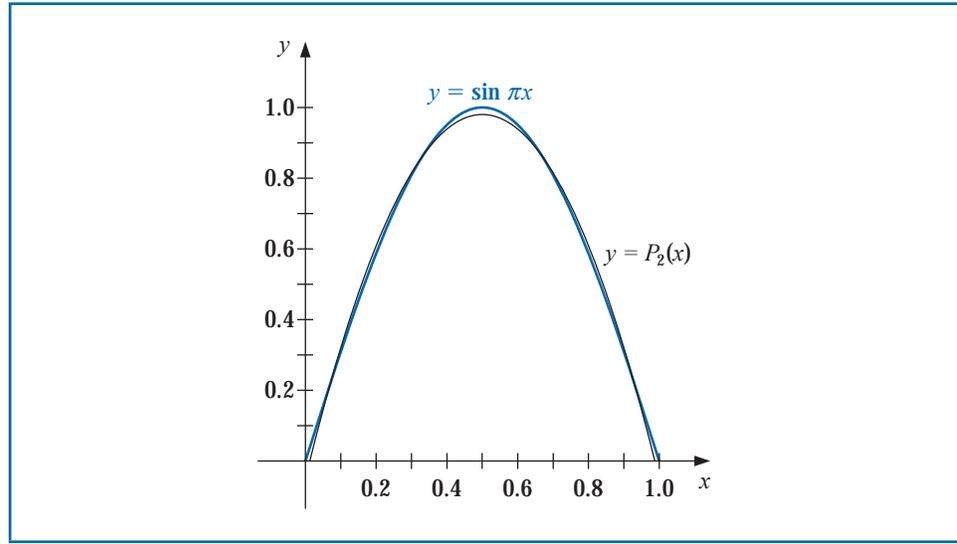
$$a_0 + \frac{1}{2}a_1 + \frac{1}{3}a_2 = \frac{2}{\pi}, \quad \frac{1}{2}a_0 + \frac{1}{3}a_1 + \frac{1}{4}a_2 = \frac{1}{\pi}, \quad \frac{1}{3}a_0 + \frac{1}{4}a_1 + \frac{1}{5}a_2 = \frac{\pi^2 - 4}{\pi^3}.$$

These three equations in three unknowns can be solved to obtain

$$a_0 = \frac{12\pi^2 - 120}{\pi^3} \approx -0.050465 \quad \text{and} \quad a_1 = -a_2 = \frac{720 - 60\pi^2}{\pi^3} \approx 4.12251.$$

Consequently, the least squares polynomial approximation of degree 2 for $f(x) = \sin \pi x$ on $[0, 1]$ is $P_2(x) = -4.12251x^2 + 4.12251x - 0.050465$. (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, \dots, a_n must be solved, and the coefficients in the linear system are of the form

$$\int_a^b x^{j+k} dx = \frac{b^{j+k+1} - a^{j+k+1}}{j+k+1},$$

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 $\{\phi_0, \dots, \phi_n\}$ is said to be **linearly independent** on $[a, b]$ if, whenever

$$c_0\phi_0(x) + c_1\phi_1(x) + \dots + c_n\phi_n(x) = 0, \quad \text{for all } x \in [a, b],$$

we have $c_0 = c_1 = \dots = c_n = 0$. Otherwise the set of functions is said to be **linearly dependent**. ■

David Hilbert (1862–1943) was the dominant mathematician at the turn of the 20th century. He is best remembered for giving a talk at the International Congress of Mathematicians in Paris in 1900 in which he posed 23 problems that he thought would be important for mathematicians in the next century.

Theorem 8.2 Suppose that, for each $j = 0, 1, \dots, n$, $\phi_j(x)$ is a polynomial of degree j . Then $\{\phi_0, \dots, \phi_n\}$ is linearly independent on any interval $[a, b]$. ■

Proof Let c_0, \dots, c_n be real numbers for which

$$P(x) = c_0\phi_0(x) + c_1\phi_1(x) + \dots + c_n\phi_n(x) = 0, \quad \text{for all } x \in [a, b].$$

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 $c_{n-2}, c_{n-3}, \dots, c_1, c_0$ are all zero, which implies that $\{\phi_0, \phi_1, \dots, \phi_n\}$ is linearly independent on $[a, b]$. ■ ■ ■

Example 2 Let $\phi_0(x) = 2$, $\phi_1(x) = x - 3$, and $\phi_2(x) = x^2 + 2x + 7$, and $Q(x) = a_0 + a_1x + a_2x^2$. 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, $\{\phi_0, \phi_1, \phi_2\}$ 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

$$\begin{aligned} x^2 &= \phi_2(x) - 2x - 7 = \phi_2(x) - 2\left[\phi_1(x) + \frac{3}{2}\phi_0(x)\right] - 7\left[\frac{1}{2}\phi_0(x)\right] \\ &= \phi_2(x) - 2\phi_1(x) - \frac{13}{2}\phi_0(x). \end{aligned}$$

Hence

$$\begin{aligned} Q(x) &= a_0\left[\frac{1}{2}\phi_0(x)\right] + a_1\left[\phi_1(x) + \frac{3}{2}\phi_0(x)\right] + a_2\left[\phi_2(x) - 2\phi_1(x) - \frac{13}{2}\phi_0(x)\right] \\ &= \left(\frac{1}{2}a_0 + \frac{3}{2}a_1 - \frac{13}{2}a_2\right)\phi_0(x) + [a_1 - 2a_2]\phi_1(x) + a_2\phi_2(x). \quad \blacksquare \end{aligned}$$

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 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 $\{\phi_0(x), \phi_1(x), \dots, \phi_n(x)\}$ 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 $\phi_0(x), \phi_1(x), \dots, \phi_n(x)$. ■

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 $w(x) \neq 0$ 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 $\{\phi_0, \phi_1, \dots, \phi_n\}$ 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

$$E = E(a_0, \dots, a_n) = \int_a^b w(x) \left[f(x) - \sum_{k=0}^n a_k \phi_k(x) \right]^2 dx.$$

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 $k = 0, 1, \dots, n$.

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

$$0 = \frac{\partial E}{\partial a_j} = 2 \int_a^b w(x) \left[f(x) - \sum_{k=0}^n a_k \phi_k(x) \right] \phi_j(x) dx.$$

The system of normal equations can be written

$$\int_a^b w(x) f(x) \phi_j(x) dx = \sum_{k=0}^n a_k \int_a^b w(x) \phi_k(x) \phi_j(x) dx, \quad \text{for } j = 0, 1, \dots, n.$$

If the functions $\phi_0, \phi_1, \dots, \phi_n$ can be chosen so that

$$\int_a^b w(x) \phi_k(x) \phi_j(x) dx = \begin{cases} 0, & \text{when } j \neq k, \\ \alpha_j > 0, & \text{when } j = k, \end{cases} \quad (8.7)$$

then the normal equations will reduce to

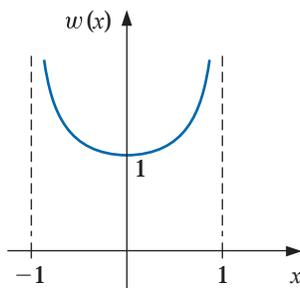
$$\int_a^b w(x) f(x) \phi_j(x) dx = a_j \int_a^b w(x) [\phi_j(x)]^2 dx = a_j \alpha_j,$$

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

$$a_j = \frac{1}{\alpha_j} \int_a^b w(x) f(x) \phi_j(x) dx.$$

Hence the least squares approximation problem is greatly simplified when the functions $\phi_0, \phi_1, \dots, \phi_n$ are chosen to satisfy the *orthogonality* condition in Eq. (8.7). The remainder of this section is devoted to studying collections of this type.

Figure 8.8



The word *orthogonal* means right-angled. So in a sense, orthogonal functions are perpendicular to one another.

Definition 8.5 $\{\phi_0, \phi_1, \dots, \phi_n\}$ is said to be an **orthogonal set of functions** for the interval $[a, b]$ with respect to the weight function w if

$$\int_a^b w(x)\phi_k(x)\phi_j(x) dx = \begin{cases} 0, & \text{when } j \neq k, \\ \alpha_j > 0, & \text{when } j = k. \end{cases}$$

If, in addition, $\alpha_j = 1$ for each $j = 0, 1, \dots, n$, the set is said to be **orthonormal**. ■

This definition, together with the remarks preceding it, produces the following theorem.

Theorem 8.6 If $\{\phi_0, \dots, \phi_n\}$ 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 $j = 0, 1, \dots, n$,

$$a_j = \frac{\int_a^b w(x)\phi_j(x)f(x) dx}{\int_a^b w(x)[\phi_j(x)]^2 dx} = \frac{1}{\alpha_j} \int_a^b w(x)\phi_j(x)f(x) dx. \quad \blacksquare$$

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 $\{\phi_0, \phi_1, \dots, \phi_n\}$ 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

$$B_1 = \frac{\int_a^b xw(x)[\phi_0(x)]^2 dx}{\int_a^b w(x)[\phi_0(x)]^2 dx},$$

and when $k \geq 2$,

$$\phi_k(x) = (x - B_k)\phi_{k-1}(x) - C_k\phi_{k-2}(x), \quad \text{for each } x \text{ in } [a, b],$$

where

$$B_k = \frac{\int_a^b xw(x)[\phi_{k-1}(x)]^2 dx}{\int_a^b w(x)[\phi_{k-1}(x)]^2 dx}$$

and

$$C_k = \frac{\int_a^b xw(x)\phi_{k-1}(x)\phi_{k-2}(x) dx}{\int_a^b w(x)[\phi_{k-2}(x)]^2 dx}. \quad \blacksquare$$

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 $\phi_n(x)$.

Erhard Schmidt (1876–1959) received his doctorate under the supervision of David Hilbert in 1905 for a problem involving integral equations. Schmidt published a paper in 1907 in which he gave what is now called the Gram-Schmidt process for constructing an orthonormal basis for a set of functions. This generalized results of Jorgen Pedersen Gram (1850–1916) who considered this problem when studying least squares. Laplace, however, presented a similar process much earlier than either Gram or Schmidt.

Corollary 8.8 For any $n > 0$, the set of polynomial functions $\{\phi_0, \dots, \phi_n\}$ given in Theorem 8.7 is linearly independent on $[a, b]$ and

$$\int_a^b w(x)\phi_n(x)Q_k(x) dx = 0,$$

for any polynomial $Q_k(x)$ of degree $k < n$. ■

Proof For each $k = 0, 1, \dots, n$, $\phi_k(x)$ is a polynomial of degree k . So Theorem 8.2 implies that $\{\phi_0, \dots, \phi_n\}$ 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, \dots, c_k such that

$$Q_k(x) = \sum_{j=0}^k c_j \phi_j(x).$$

Because ϕ_n is orthogonal to ϕ_j for each $j = 0, 1, \dots, k$ we have

$$\int_a^b w(x)Q_k(x)\phi_n(x) dx = \sum_{j=0}^k c_j \int_a^b w(x)\phi_j(x)\phi_n(x) dx = \sum_{j=0}^k c_j \cdot 0 = 0. \quad \blacksquare \blacksquare \blacksquare$$

Illustration The set of **Legendre polynomials**, $\{P_n(x)\}$, 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

$$B_1 = \frac{\int_{-1}^1 x dx}{\int_{-1}^1 dx} = 0 \quad \text{and} \quad P_1(x) = (x - B_1)P_0(x) = x.$$

Also,

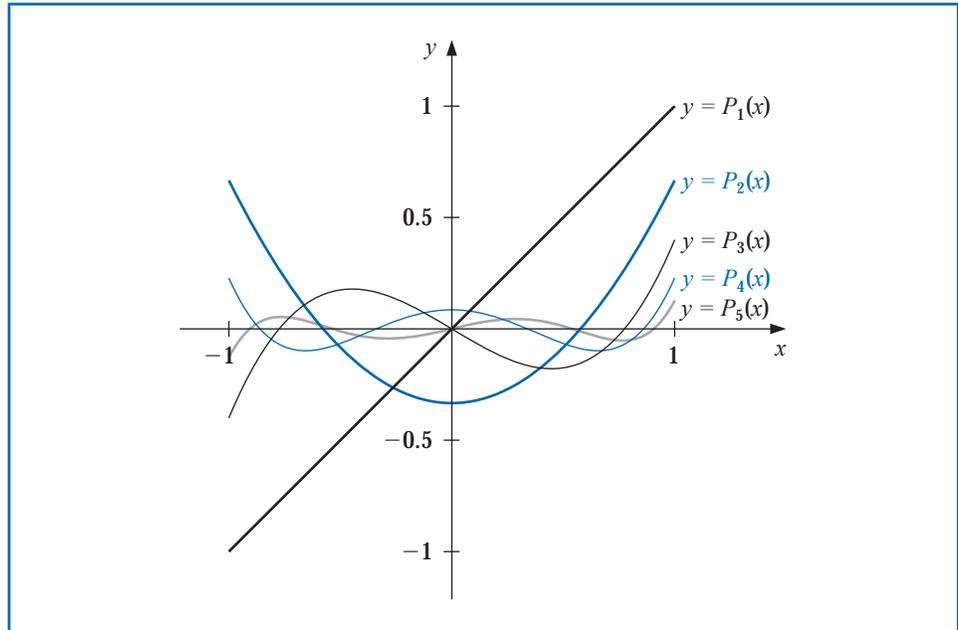
$$B_2 = \frac{\int_{-1}^1 x^3 dx}{\int_{-1}^1 x^2 dx} = 0 \quad \text{and} \quad C_2 = \frac{\int_{-1}^1 x^2 dx}{\int_{-1}^1 1 dx} = \frac{1}{3},$$

so

$$P_2(x) = (x - B_2)P_1(x) - C_2P_0(x) = (x - 0)x - \frac{1}{3} \cdot 1 = x^2 - \frac{1}{3}.$$

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 :

$$B_3 := \frac{\text{int}\left(x\left(x^2 - \frac{1}{3}\right)^2, x = -1..1\right)}{\text{int}\left(\left(x^2 - \frac{1}{3}\right)^2, x = -1..1\right)}; \quad C_3 := \frac{\text{int}\left(x\left(x^2 - \frac{1}{3}\right), x = -1..1\right)}{\text{int}\left(x^2, x = -1..1\right)}$$

$$\frac{0}{\frac{4}{15}}$$

Thus

$$P_3(x) = xP_2(x) - \frac{4}{15}P_1(x) = x^3 - \frac{1}{3}x - \frac{4}{15}x = x^3 - \frac{3}{5}x.$$

The next two Legendre polynomials are

$$P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35} \quad \text{and} \quad P_5(x) = x^5 - \frac{10}{9}x^3 + \frac{5}{21}x. \quad \square$$

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

- Find the linear least squares polynomial approximation to $f(x)$ on the indicated interval if
 - $f(x) = x^2 + 3x + 2$, $[0, 1]$;
 - $f(x) = x^3$, $[0, 2]$;
 - $f(x) = \frac{1}{x}$, $[1, 3]$;
 - $f(x) = e^x$, $[0, 2]$;
 - $f(x) = \frac{1}{2} \cos x + \frac{1}{3} \sin 2x$, $[0, 1]$;
 - $f(x) = x \ln x$, $[1, 3]$.
- Find the linear least squares polynomial approximation on the interval $[-1, 1]$ for the following functions.
 - $f(x) = x^2 - 2x + 3$
 - $f(x) = x^3$
 - $f(x) = \frac{1}{x+2}$
 - $f(x) = e^x$
 - $f(x) = \frac{1}{2} \cos x + \frac{1}{3} \sin 2x$
 - $f(x) = \ln(x+2)$
- Find the least squares polynomial approximation of degree two to the functions and intervals in Exercise 1.
- Find the least squares polynomial approximation of degree 2 on the interval $[-1, 1]$ for the functions in Exercise 3.
- Compute the error E for the approximations in Exercise 3.
- Compute the error E for the approximations in Exercise 4.
- Use the Gram-Schmidt process to construct $\phi_0(x)$, $\phi_1(x)$, $\phi_2(x)$, and $\phi_3(x)$ for the following intervals.
 - $[0, 1]$
 - $[0, 2]$
 - $[1, 3]$
- Repeat Exercise 1 using the results of Exercise 7.
- Obtain the least squares approximation polynomial of degree 3 for the functions in Exercise 1 using the results of Exercise 7.
- Repeat Exercise 3 using the results of Exercise 7.
- Use the Gram-Schmidt procedure to calculate L_1 , L_2 , and L_3 , where $\{L_0(x), L_1(x), L_2(x), L_3(x)\}$ 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**.
- 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:
 - $f(x) = x^2$
 - $f(x) = e^{-x}$
 - $f(x) = x^3$
 - $f(x) = e^{-2x}$
- Suppose $\{\phi_0, \phi_1, \dots, \phi_n\}$ 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, \dots, c_n , such that

$$Q(x) = \sum_{k=0}^n c_k \phi_k(x).$$

- Show that if $\{\phi_0, \phi_1, \dots, \phi_n\}$ is an orthogonal set of functions on $[a, b]$ with respect to the weight function w , then $\{\phi_0, \phi_1, \dots, \phi_n\}$ is a linearly independent set.
- 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 $a_j = 0, j = 0, 1, \dots, n$. Multiply Eq. (8.6) by a_j , and sum over all j . Interchange the integral sign and the summation sign to obtain $\int_a^b [P(x)]^2 dx = 0$. Thus, $P(x) \equiv 0$, so $a_j = 0$, for $j = 0, \dots, n$. 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 $\{T_n(x)\}$ are orthogonal on $(-1, 1)$ with respect to the weight function $w(x) = (1 - x^2)^{-1/2}$. Although they can be derived by the method in the previous