Numerical Methods

Using MATLAB

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Curve Fitting

Applications of numerical techniques in science and engineering often involve curve fitting of experimental data. For example, in 1601 the German astronomer Johannes Kepler formulated the third law of planetary motion, $T = Cx^{3/2}$, where x is the distance to the sun measured in millions of kilometers, T is the orbital period measured in days, and C is a constant. The observed data pairs (x, T) for the first four planets, Mercury, Venus, Earth, and Mars, are (58, 88), (108, 225), (150, 365), and (228, 687), and the coefficient C obtained from the method of least squares is $C = 0.199769$. The curve $T = 0.199769x^{3/2}$ and the data points are shown in Figure 5.1.

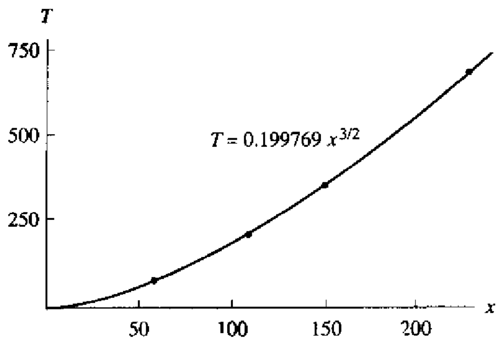

Figure 5.1 The least-squares fit $T = 0.199769x^{3/2}$ for the first four planets using Kepler's third law of planetary motion.

5.1 Least-squares Line

In science and engineering it is often the case that an experiment produces a set of data points $(x_1, y_1), \ldots, (x_N, y_N)$, where the abscissas $\{x_k\}$ are distinct. One goal of numerical methods is to determine a formula $y = f(x)$ that relates these variables. Usually, a class of allowable formulas is chosen and then coefficients must be determined. There are many different possibilities for the type of function that can be used. Often there is an underlying mathematical model, based on the physical situation, that will determine the form of the function. In this section we emphasize the class of linear functions of the form

(1) $$y = f(x) = Ax + B.$$

In Chapter 4 we saw how to construct a polynomial that passes through a set of points. If all the numerical values $\{x_k\}$, $\{y_k\}$ are known to several significant digits of accuracy, then polynomial interpolation can be used successfully; otherwise it cannot. Some experiments are devised using specialized equipment so that the data points will have at least five digits of accuracy. However, many experiments are done with equipment that is reliable only to three or fewer digits of accuracy. Often there is an experimental error in the measurements, and although three digits are recorded for the values $\{x_k\}$ and $\{y_k\}$, it is realized that the true value $f(x_k)$ satisfies

(2) $$f(x_k) = y_k + e_k,$$

where e_k is the measurement error.

How do we find the best linear approximation of the form (1) that goes near (not always through) the points? To answer this question, we need to discuss the ***errors*** (also called ***deviations*** or ***residuals***):

(3) $$e_k = f(x_k) - y_k \quad \text{for} \quad 1 \le k \le N.$$

There are several norms that can be used with the residuals in (3) to measure how far the curve $y = f(x)$ lies from the data.

(4) Maximum error: $$E_\infty(f) = \max_{1 \le k \le N} \{|f(x_k) - y_k|\},$$

(5) Average error: $$E_1(f) = \frac{1}{N} \sum_{k=1}^{N} |f(x_k) - y_k|,$$

(6) Root-mean-square error: $$E_2(f) = \left(\frac{1}{N} \sum_{k=1}^{N} |f(x_k) - y_k|^2 \right)^{1/2}.$$

The next example shows how to apply these norms when a function and a set of points are given.

Table 5.1 Calculations for Finding $E_1(f)$ and $E_2(f)$ for Example 5.1

x_k	y_k	$f(x_k) = 8.6 - 1.6x_k$	$\lvert e_k \rvert$	e_k^2
−1	10.0	10.2	0.2	0.04
0	9.0	8.6	0.4	0.16
1	7.0	7.0	0.0	0.00
2	5.0	5.4	0.4	0.16
3	4.0	3.8	0.2	0.04
4	3.0	2.2	0.8	0.64
5	0.0	0.6	0.6	0.36
6	−1.0	−1.0	0.0	0.00
			2.6	1.40

Example 5.1. Compare the maximum error, average error, and rms error for the linear approximation $y = f(x) = 8.6 - 1.6x$ to the data points $(-1, 10)$, $(0, 9)$, $(1, 7)$, $(2, 5)$, $(3, 4)$, $(4, 3)$, $(5, 0)$, and $(6, -1)$.

The errors are found using the values for $f(x_k)$ and e_k given in Table 5.1.

$$E_\infty(f) = \max\{0.2, 0.4, 0.0, 0.4, 0.2, 0.8, 0.6, 0.0\} = 0.8, \tag{7}$$

$$E_1(f) = \frac{1}{8}(2.6) = 0.325, \tag{8}$$

$$E_2(f) = \left(\frac{1.4}{8}\right)^{1/2} \approx 0.41833 \tag{9}$$

We can see that the maximum error is largest, and if one point is badly in error, its value determines $E_\infty(f)$. The average error $E_1(f)$ simply averages the absolute value of the error at the various points. It is often used because it is easy to compute. The error $E_2(f)$ is often used when the statistical nature of the errors is considered.

A best-fitting line is found by minimizing one of the quantities in equations (4) through (6). Hence there are three best-fitting lines that we could find. The third norm $E_2(f)$ is the traditional choice because it is much easier to minimize computationally. ■

Finding the Least-squares Line

Let $\{(x_k, y_k)\}_{k=1}^N$ be a set of N points, where the abscissas $\{x_k\}$ are distinct. The ***least-squares line*** $y = f(x) = Ax + B$ is the line that minimizes the root-mean-square error $E_2(f)$.

The quantity $E_2(f)$ will be a minimum if and only if the quantity $N(E_2(f))^2 = \sum_{k=1}^N (Ax_k + B - y_k)^2$ is a minimum. The latter is visualized geometrically by minimizing the sum of the squares of the vertical distances from the points to the line. The next result explains this process.

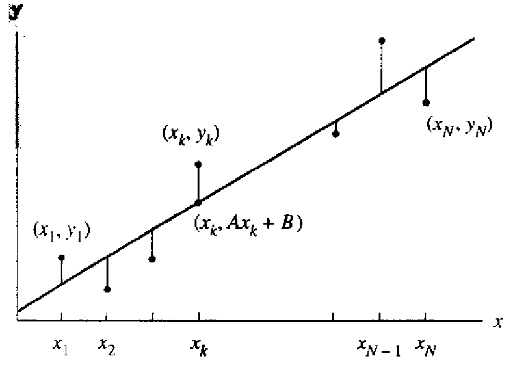

Figure 5.2 The vertical distances between the points $\{(x_k, y_k)\}$ and the least-squares line $y = Ax + B$.

Theorem 5.1 (Least-squares Line). Suppose that $\{(x_k, y_k)\}_{k=1}^N$ are N points, where the abscissas $\{x_k\}_{k=1}^N$ are distinct. The coefficients of the least-squares line

$$y = Ax + B$$

are the solution to the following linear system, known as the ***normal equations***:

$$\begin{aligned}\left(\sum_{k=1}^N x_k^2\right) A + \left(\sum_{k=1}^N x_k\right) B &= \sum_{k=1}^N x_k y_k,\\ \left(\sum_{k=1}^N x_k\right) A + NB &= \sum_{k=1}^N y_k.\end{aligned} \tag{10}$$

Proof. Geometrically, we start with the line $y = Ax + B$. The vertical distance d_k from the point (x_k, y_k) to the point $(x_k, Ax_k + B)$ on the line is $d_k = |Ax_k + B - y_k|$ (see Figure 5.2). We must minimize the sum of the squares of the vertical distances d_k:

$$E(A, B) = \sum_{k=1}^N (Ax_k + B - y_k)^2 = \sum_{k=1}^N d_k^2. \tag{11}$$

The minimum value of $E(A, B)$ is determined by setting the partial derivatives $\partial E/\partial A$ and $\partial E/\partial B$ equal to zero and solving these equations for A and B. Notice that $\{x_k\}$ and $\{y_k\}$ are constants in equation (11) and that A and B are the variables! Hold B fixed, differentiate $E(A, B)$ with respect to A, and get

$$\frac{\partial E(A, B)}{\partial A} = \sum_{k=1}^N 2(Ax_k + B - y_k)(x_k) = 2\sum_{k=1}^N (Ax_k^2 + Bx_k - x_k y_k) \tag{12}$$

Table 5.2 Obtaining the Coefficients for Normal Equations

x_k	y_k	x_k^2	$x_k y_k$
−1	10	1	−10
0	9	0	0
1	7	1	7
2	5	4	10
3	4	9	12
4	3	16	12
5	0	25	0
6	−1	36	−6
20	37	92	25

Now hold A fixed and differentiate $E(A, B)$ with respect to B and get

$$(13)\qquad \frac{\partial E(A,B)}{\partial B} = \sum_{k=1}^{N} 2(Ax_k + B - y_k) = 2\sum_{k=1}^{N}(Ax_k + B - y_k).$$

Setting the partial derivatives equal to zero in (12) and (13), use the distributive properties of summation to obtain

$$(14)\qquad 0 = \sum_{k=1}^{N}(Ax_k^2 + Bx_k - x_k y_k) = A\sum_{k=1}^{N} x_k^2 + B\sum_{k=1}^{N} x_k - \sum_{k=1}^{N} x_k y_k,$$

$$(15)\qquad 0 = \sum_{k=1}^{N}(Ax_k + B - y_k) = A\sum_{k=1}^{N} x_k + NB - \sum_{k=1}^{N} y_k. \qquad \bullet$$

Equations (14) and (15) can be rearranged in the standard form for a system and result in the normal equations (10). The solution to this system can be obtained by one of the techniques for solving a linear system from Chapter 3. However, the method employed in Program 5.1 translates the data points so that a well-conditioned matrix is employed (see exercises).

Example 5.2. Find the least-squares line for the data points given in Example 5.1.

The sums required for the normal equations (10) are easily obtained using the values in Table 5.2. The linear system involving A and B is

$$92A + 20B = 25$$
$$20A + \ 8B = 37.$$

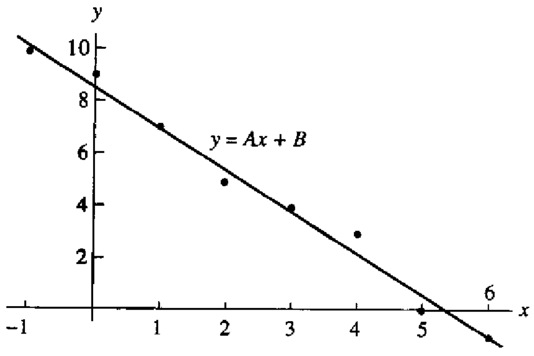

Figure 5.3 The least-squares line $y = -1.6071429x + 8.6428571$.

The solution of the linear system is $A \approx -1.6071429$ and $B \approx 8.6428571$. Therefore, the least-squares line is (see Figure 5.3)

$$y = -1.6071429x + 8.6428571 \qquad \blacksquare$$

The Power Fit $y = Ax^M$

Some situations involve $f(x) = Ax^M$, where M is a known constant. The example of planetary motion given in Figure 5.1 is an example. In these cases there is only one parameter A to be determined.

Theorem 5.2 (Power Fit). Suppose that $\{(x_k, y_k)\}_{k=1}^{N}$ are N points, where the abscissas are distinct. The coefficient A of the least-squares power curve $y = Ax^M$ is given by

$$(16)\qquad A = \left(\sum_{k=1}^{N} x_k^M y_k\right) \Big/ \left(\sum_{k=1}^{N} x_k^{2M}\right).$$

Using the least-squares technique, we seek a minimum of the function $E(A)$:

$$(17)\qquad E(A) = \sum_{k=1}^{N}(Ax_k^M - y_k)^2.$$

In this case it will suffice to solve $E'(A) = 0$. The derivative is

$$(18)\qquad E'(A) = 2\sum_{k=1}^{N}(Ax_k^M - y_k)(x_k^M) = 2\sum_{k=1}^{N}(Ax_k^{2M} - x_k^M y_k).$$

Table 5.3 Obtaining the Coefficient for a Power Fit

Time, t_k	Distance, d_k	$d_k t_k^2$	t_k^4
0.200	0.1960	0.00784	0.0016
0.400	0.7850	0.12560	0.0256
0.600	1.7665	0.63594	0.1296
0.800	3.1405	2.00992	0.4096
1.000	4.9075	4.90750	1.0000
		7.68680	1.5664

Hence the coefficient A is the solution of the equation

$$0 = A \sum_{k=1}^{N} x_k^{2M} - \sum_{k=1}^{N} x_k^M y_k, \tag{19}$$

which reduces to the formula in equation (16).

Example 5.3. Students collected the experimental data in Table 5.3. The relation is $d = \frac{1}{2}gt^2$, where d is distance in meters and t is time in seconds. Find the gravitational constant g.

The values in Table 5.3 are used to find the summations required in formula (16), where the power used is $M = 2$.

The coefficient is $A = 7.68680/1.5664 = 4.9073$, and we get $d = 4.9073t^3$ and $g = 2A = 9.7146$ m/sec^2. ■

The following program for constructing a least-squares line is computationally stable: it gives reliable results in cases when the normal equations (10) are ill conditioned. The reader is asked to develop the algorithm for this program in Exercises 4 through 7.

Program 5.1 (Least-squares Line). To construct the least-squares line $y = Ax + B$ that fits the N data points $(x_1, y_1), \ldots, (x_N, y_N)$.

```
function [A,B]=lsline(X,Y)
%Input  - X is the 1xn abscissa vector
%       - Y is the 1xn ordinate vector
%Output - A is the coefficient of x in Ax + B
%       - B is the constant coefficient in Ax + B
xmean=mean(X);
ymean=mean(Y);
sumx2=(X-xmean)*(X-xmean)';
sumxy=(Y-ymean)*(X-xmean)';
```



```
A=sumxy/sumx2;
B=ymean-A*xmean;
```

Exercises for Least-squares Line

In Exercises 1 and 2, find the least-squares line $y = f(x) = Ax + B$ for the data and calculate $E_2(f)$

1. (a)

x_k	y_k	$f(x_k)$
−2	1	1.2
−1	2	1.9
0	3	2.6
1	3	3.3
2	4	4.0

(b)

x_k	y_k	$f(x_k)$
−6	7	7.0
−2	5	4.6
0	3	3.4
2	2	2.2
6	0	−0.2

(c)

x_k	y_k	$f(x_k)$
−4	−3	−3.0
−1	−1	−0.9
0	0	−0.2
2	1	1.2
3	2	1.9

2. (a)

x_k	y_k	$f(x_k)$
−4	1.2	0.44
−2	2.8	3.34
0	6.2	6.24
2	7.8	9.14
4	13.2	12.04

(b)

x_k	y_k	$f(x_k)$
−6	−5.3	−6.00
−2	−3.5	−2.84
0	−1.7	−1.26
2	0.2	0.32
6	4.0	3.48

(c)

x_k	y_k	$f(x_k)$
−8	6.8	7.32
−2	5.0	3.81
0	2.2	2.64
4	0.5	0.30
6	−1.3	−0.87

3. Find the power fit $y = Ax$, where $M = 1$, which is a line through the origin, for the data and calculate $E_2(f)$.

(a)

x_k	y_k	$f(x_k)$
−4	−3	−2.8
−1	−1	−0.7
0	0	0.0
2	1	1.4
3	2	2.1

(b)

x_k	y_k	$f(x_k)$
3	1.6	1.722
4	2.4	2.296
5	2.9	2.870
6	3.4	3.444
8	4.6	4.592

(c)

x_k	y_k	$f(x_k)$
1	1.6	1.58
2	2.8	3.16
3	4.7	4.74
4	6.4	6.32
5	8.0	7.90

4. Define the means $\overline{x}$ and $\overline{y}$ for the points $\{(x_k, y_k)\}_{k=1}^{N}$ by

$$\overline{x} = \frac{1}{N}\sum_{k=1}^{N} x_k \quad \text{and} \quad \overline{y} = \frac{1}{N}\sum_{k=1}^{N} y_k.$$

Show that the point $(\overline{x}, \overline{y})$ lies on the least-squares line determined by the given set of points.

5. Show that the solution of the system in (10) is given by

$$A = \frac{1}{D}\left(N\sum_{k=1}^{N} x_k y_k - \sum_{k=1}^{N} x_k \sum_{k=1}^{N} y_k\right),$$

$$B = \frac{1}{D}\left(\sum_{k=1}^{N} x_k^2 \sum_{k=1}^{N} y_k - \sum_{k=1}^{N} x_k \sum_{k=1}^{N} x_k y_k\right),$$

where

$$D = N\sum_{k=1}^{N} x_k^2 - \left(\sum_{k=1}^{N} x_k\right)^2.$$

Hint. Use Gaussian elimination on the system in (10).

6. Show that the value of D in Exercise 5 is nonzero.
Hint. Show that $D = N\sum_{k=1}^{N}(x_k - \overline{x})^2$.

7. Show that the coefficients A and B for the least-squares line can be computed as follows. First compute the means $\overline{x}$ and $\overline{y}$ in Exercise 4, and then perform the calculations:

$$C = \sum_{k=1}^{N}(x_k - \overline{x})^2, \quad A = \frac{1}{C}\sum_{k=1}^{N}(x_k - \overline{x})(y_k - \overline{y}), \quad B = \overline{y} - A\overline{x}.$$

Hint. Use $X_k = x_k - \overline{x}$, $Y_k = y_k - \overline{y}$ and first find the line $Y = AX$.

8. Find the power fits $y = Ax^2$ and $y = Bx^3$ for the following data and use $E_2(f)$ to determine which curve fits best.

(a)

x_k	y_k
2.0	5.1
2.3	7.5
2.6	10.6
2.9	14.4
3.2	19.0

(b)

x_k	y_k
2.0	5.9
2.3	8.3
2.6	10.7
2.9	13.7
3.2	17.0

9. Find the power fits $y = A/x$ and $y = B/x^2$ for the following data and use $E_2(f)$ to determine which curve fits best.

(a)

x_k	y_k
0.5	7.1
0.8	4.4
1.1	3.2
1.8	1.9
4.0	0.9

(b)

x_k	y_k
0.7	8.1
0.9	4.9
1.1	3.3
1.6	1.6
3.0	0.5

10. (a) Derive the normal equation for finding the least-squares linear fit through the origin $y = Ax$.
(b) Derive the normal equation for finding the least-squares power fit $y = Ax^2$.
(c) Derive the normal equations for finding the least-squares parabola $y = Ax^2 + B$.

11. Consider the construction of a least-squares line for each of the sets of data points determined by $S_N = \{(\frac{k}{N}, (\frac{k}{N})^2)\}_{k=1}^{N}$, where $N = 2, 3, 4, \ldots$. Note that, for each value of N the points in S_N all lie on the graph of $f(x) = x^2$ over the closed interval $[0, 1]$. Let $\overline{x}_N$ and $\overline{y}_N$ be the means for the given data points (see Exercise 4). Let $\widehat{x}$ be the mean of the values of x in the interval $[0, 1]$, and let $\widehat{y}$ be the mean (average) value of $f(x) = x^2$ over the interval $[0, 1]$.
(a) Show $\lim_{N\to\infty} \overline{x}_N = \widehat{x}$.
(b) Show $\lim_{N\to\infty} \overline{y}_N = \widehat{y}$.

12. Consider the construction of a least-squares line for each of the sets of data points:

$$S_N = \left\{((b-a)\frac{k}{N} + a, f((b-a)\frac{k}{N} + a))\right\}_{k=1}^{N}$$

for $N = 2, 3, 4, \ldots$. Assume that $y = f(x)$ is an integrable function over the closed interval $[a, b]$. Repeat parts (a) and (b) from Exercise 11.

Algorithms and Programs

1. Hooke's law states that $F = kx$, where F is the force (in ounces) used to stretch a spring and x is the increase in its length (in inches). Use Program 5.1 to find an approximation to the spring constant k for the following data.

(a)

x_k	F_k
0.2	3.6
0.4	7.3
0.6	10.9
0.8	14.5
1.0	18.2

(b)

x_k	F_k
0.2	5.3
0.4	10.6
0.6	15.9
0.8	21.2
1.0	26.4

2. Write a program to find the gravitational constant g for the following sets of data. Use the power fit that was shown in Example 5.3.

(a)

Time, t_k	Distance, d_k
0.200	0.1960
0.400	0.7835
0.600	1.7630
0.800	3.1345
1.000	4.8975

(b)

Time, t_k	Distance, d_k
0.200	0.1965
0.400	0.7855
0.600	1.7675
0.800	3.1420
1.000	4.9095

3. The following data give the distances of the nine planets from the sun and their sidereal period in days.

Planet	Distance from sun (km $\times 10^6$)	Sidereal period (days)
Mercury	57.59	87.99
Venus	108.11	224.70
Earth	149.57	365.26
Mars	227.84	686.98
Jupiter	778.14	4,332.4
Saturn	1427.0	10,759
Uranus	2870.3	30,684
Neptune	4499.9	60,188
Pluto	5909.0	90,710

Modify your program from Problem 2 to also calculate $E_2(f)$. Use it to find the power fit of the form $y = Cx^{3/2}$ for **(a)** the first four planets and **(b)** all nine planets.

4. (a) Find the least-squares line for the data points $\{(x_k, y_k)\}_{k=1}^{50}$, where $x_k = (0.1)k$ and $y_k = x_k + \cos(k^{1/2})$.
   (b) Calculate $E_2(f)$.
   (c) Plot the set of data points and the least-squares line on the same coordinate system.

5.2 Curve Fitting

Data Linearization Method for $y = Ce^{Ax}$

Suppose that we are given the points $(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$ and want to fit an exponential curve of the form

$$y = Ce^{Ax}. \tag{1}$$

The first step is to take the logarithm of both sides:

$$\ln(y) = Ax + \ln(C). \tag{2}$$

Then introduce the change of variables:

$$Y = \ln(y), \qquad X = x, \qquad \text{and} \qquad B = \ln(C). \tag{3}$$

This results in a linear relation between the new variables X and Y:

$$Y = AX + B. \tag{4}$$

The original points (x_k, y_k) in the xy-plane are transformed into the points $(X_k, Y_k) = (x_k, \ln(y_k))$ in the XY-plane. This process is called ***data linearization***. Then the least-squares line (4) is fit to the points $\{(X_k, Y_k)\}$. The normal equations for finding A and B are

$$\begin{aligned} \left(\sum_{k=1}^{N} X_k^2\right) A + \left(\sum_{k=1}^{N} X_k\right) B &= \sum_{k=1}^{N} X_k Y_k, \\ \left(\sum_{k=1}^{N} X_k\right) A + \quad NB \quad &= \sum_{k=1}^{N} Y_k. \end{aligned} \tag{5}$$

After A and B have been found, the parameter C in equation (1) is computed:

$$C = e^B. \tag{6}$$

Example 5.4. Use the data linearization method and find the exponential fit $y = Ce^{Ax}$ for the five data points $(0, 1.5)$, $(1, 2.5)$, $(2, 3.5)$, $(3, 5.0)$, and $(4, 7.5)$.

Apply the transformation (3) to the original points and obtain

$$\begin{aligned} \{(X_k, Y_k)\} &= \{(0, \ln(1.5)), (1, \ln(2.5)), (2, \ln(3.5)), (3, \ln(5.0)), (4, \ln(7.5))\} \\ &= \{(0, 0.40547), (1, 0.91629), (2, 1.25276), (3, 1.60944), (4, 2.01490)\}. \end{aligned} \tag{7}$$

These transformed points are shown in Figure 5.4 and exhibit a linearized form. The equation of the least-squares line $Y = AX + B$ for the points (7) in Figure 5.4 is

$$Y = 0.391202X + 0.457367. \tag{8}$$

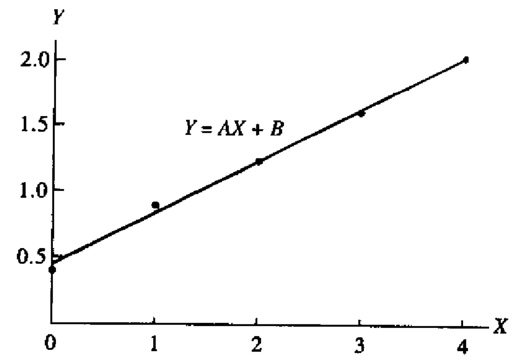

Figure 5.4 The transformed data points $\{(X_k, Y_k)\}$.

Table 5.4 Obtaining Coefficients of the Normal Equations for the Transformed Data Points $\{(X_k, Y_k)\}$

x_k	y_k	X_k	$Y_k = \ln(y_k)$	X_k^2	$X_k Y_k$
0.0	1.5	0.0	0.405465	0.0	0.000000
1.0	2.5	1.0	0.916291	1.0	0.916291
2.0	3.5	2.0	1.252763	4.0	2.505526
3.0	5.0	3.0	1.609438	9.0	4.828314
4.0	7.5	4.0	2.014903	16.0	8.059612
		10.0 $= \sum X_k$	6.198860 $= \sum Y_k$	30.0 $= \sum X_k^2$	16.309743 $= \sum X_k Y_k$

Calculation of the coefficients for the normal equations in (5) is shown in Table 5.4.
The resulting linear system (5) for determining A and B is

(9)
$$\begin{aligned} 30A + 10B &= 16.309742 \\ 10A + \ \ 5B &= \ \ 6.198860. \end{aligned}$$

The solution is $A = 0.3912023$ and $B = 0.457367$. Then C is obtained with the calculation $C = e^{0.457367} = 1.579910$, and these values for A and C are substituted into equation (1) to obtain the exponential fit (see Figure 5.5):

(10) $$y = 1.579910e^{0.3912023x} \quad \text{(fit by data linearization).}$$ ∎

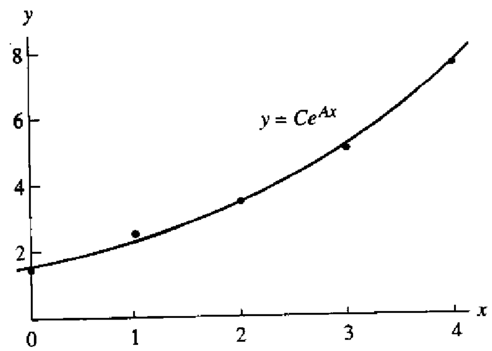

Figure 5.5 The exponential fit $y = 1.579910e^{0.3912023x}$ obtained by using the data linearization method.

Nonlinear Least-squares Method for $y = Ce^{Ax}$

Suppose that we are given the points $(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$ and want to fit an exponential curve:

(11) $$y = Ce^{Ax}.$$

The nonlinear least-squares procedure requires that we find a minimum of

(12) $$E(A, C) = \sum_{k=1}^{N} (Ce^{Ax_k} - y_k)^2.$$

The partial derivatives of $E(A, C)$ with respect to A and C are

(13) $$\frac{\partial E}{\partial A} = 2\sum_{k=1}^{N} (Ce^{Ax_k} - y_k)(Cx_k e^{Ax_k})$$

and

(14) $$\frac{\partial E}{\partial C} = 2\sum_{k=1}^{N} (Ce^{Ax_k} - y_k)(e^{Ax_k}).$$

When the partial derivatives in (13) and (14) are set equal to zero and then simplified, the resulting normal equations are

(15)
$$\begin{aligned} C\sum_{k=1}^{N} x_k e^{2Ax_k} - \sum_{k=1}^{N} x_k y_k e^{Ax_k} &= 0, \\ C\sum_{k=1}^{N} e^{Ax_k} - \sum_{k=1}^{N} y_k e^{Ax_k} &= 0. \end{aligned}$$

The equations in (15) are nonlinear in the unknowns A and C and can be solved using Newton's method. This is a time-consuming computation and the iteration involved requires good starting values for A and C. Many software packages have a built-in minimization subroutine for functions of several variables that can be used to minimize $E(A, C)$ directly, For example, the Nedler-Mead simplex algorithm can be used to minimize (12) directly and bypass the need for equations (13) through (15).

Example 5.5. Use the least-squares method and determine the exponential fit $y = Ce^{Ax}$ for the five data points (0, 1.5), (1, 2.5), (2, 3.5), (3, 5.0), and (4, 7.5).

For this solution we must minimize the quantity $E(A, C)$, which is

$$E(A,C) = (C - 1.5)^2 + (Ce^A - 2.5)^2 + (Ce^{2A} - 3.5)^2 + (Ce^{3A} - 5.0)^2 + (Ce^{4A} - 7.5)^2. \tag{16}$$

We use the `fmins` command in MATLAB to approximate the values of A and C that minimize $E(A, C)$. First we define $E(A, C)$ as an M-file in MATLAB.

```
function z=E(u)
A=u(1);
C=u(2);
z=(C-1.5).^2+(C.*exp(A)-2.5).^2+(C.*exp(2*A)-3.5).^2+...
   (C.*exp(3*A)-5.0).^2+(C.*exp(4*A)-7.5).^2;
```

Using the `fmins` command in the MATLAB Command Window and the initial values $A = 1.0$ and $C = 1.0$, we find

```
>>fmins('E',[1 1])
ans =
   0.38357046980073 1.61089952247928
```

Thus the exponential fit to the five data points is

$$y = 1.6108995e^{0.3835705} \quad \text{(fit by nonlinear least squares).} \tag{17}$$

A comparison of the solutions using data linearization and nonlinear least squares is given in Table 5.5. There is a slight difference in the coefficients. For the purpose of interpolation it can be seen that the approximations differ by no more than 2% over the interval [0, 4] (see Table 5.5 and Figure 5.6). If there is a normal distribution of the errors in the data, (17) is usually the preferred choice. When extrapolation beyond the range of the data is made, the two solutions will diverge and the discrepancy increases to about 6% when $x = 10$.

Transformations for Data Linearization

The technique of data linearization has been used by scientists to fit curves such as $y = Ce^{(Ax)}$, $y = A\ln(x) + B$, and $y = A/x + B$. Once the curve has been chosen, a suitable transformation of the variables must be found so that a linear relation is

Table 5.5 Comparison of the Two Exponential Fits

x_k	y_k	$1.5799e^{0.39120x}$	$1.6109e^{0.38357x}$
0.0	1.5	1.5799	1.6109
1.0	2.5	2.3363	2.3640
2.0	3.5	3.4548	3.4692
3.0	5.0	5.1088	5.0911
4.0	7.5	7.5548	7.4713
5.0		11.1716	10.9644
6.0		16.5202	16.0904
7.0		24.4293	23.6130
8.0		36.1250	34.6527
9.0		53.4202	50.8535
10.0		78.9955	74.6287

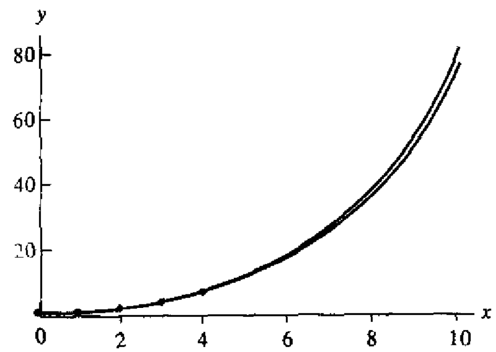

Figure 5.6 A graphical comparison of the two exponential curves.

obtained. For example, the reader can verify that $y = D/(x + C)$ is transformed into a linear problem $Y = AX + B$ by using the change of variables (and constants) $X = xy$, $Y = y$, $C = -1/A$, and $D = -B/A$. Graphs of several cases of the possibilities for the curves are shown in Figure 5.7, and other useful transformations are given in Table 5.6.

Linear Least Squares

The linear least-squares problem is stated as follows. Suppose that N data points $\{(x_k, y_k)\}$ and a set of M linear independent functions $\{f_j(x)\}$ are given. We want

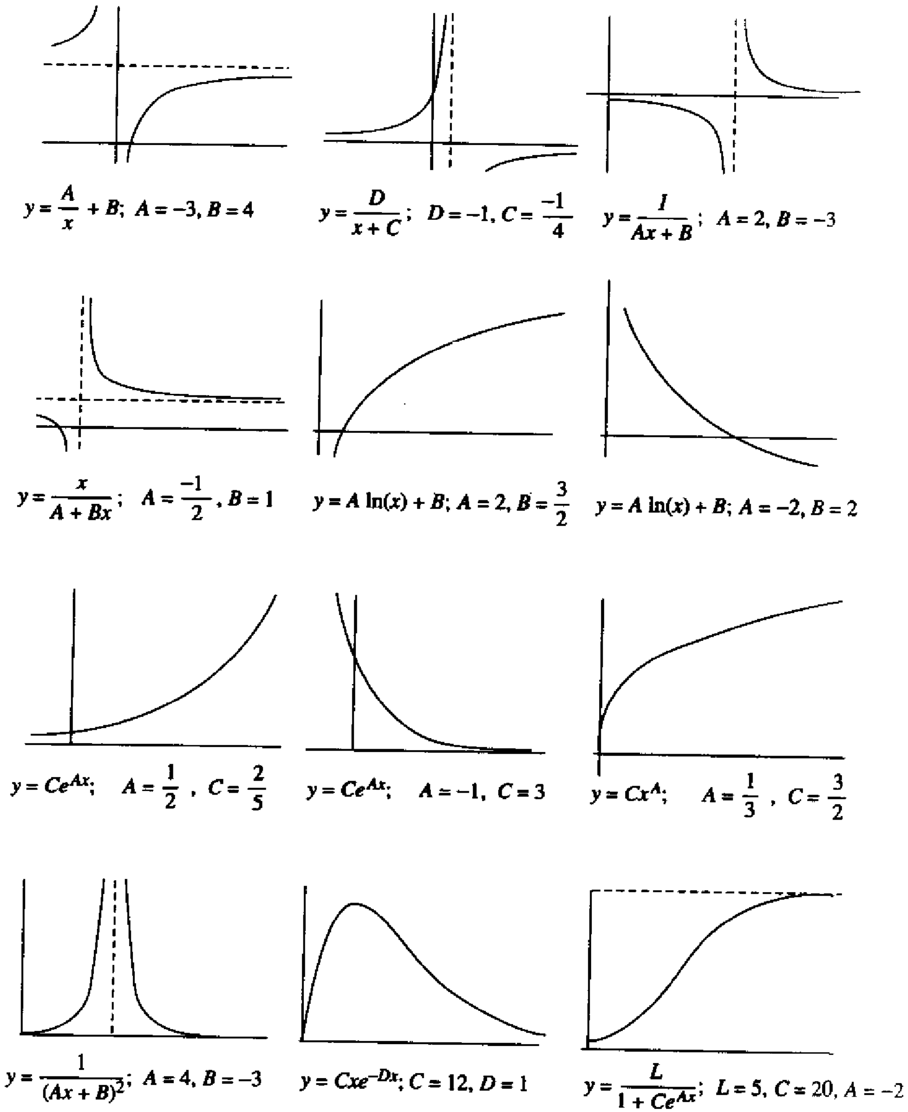

Figure 5.7 Possibilities for the curves used in "data linearization".

Table 5.6 Change of Variable(s) for Data Linearization

Function, $y = f(x)$	Linearized form, $Y = Ax + B$	Change of variable(s) and constants
$y = \frac{A}{x} + B$	$y = A\frac{1}{x} + B$	$X = \frac{1}{x}, Y = y$
$y = \frac{D}{x + C}$	$y + \frac{-1}{C}(xy) + \frac{D}{C}$	$X = xy, Y = y$ $C = \frac{-1}{A}, D = \frac{-B}{A}$
$y = \frac{1}{Ax + B}$	$\frac{1}{y} = Ax + B$	$X = x, Y = \frac{1}{y}$
$y = \frac{x}{Ax + B}$	$\frac{1}{y} = A\frac{1}{x} + B$	$X = \frac{1}{x}, Y = \frac{1}{y}$
$y = A\ln(x) + B$	$y = A\ln(x) + B$	$X = \ln(x), Y = y$
$y = Ce^{Ax}$	$\ln(y) = Ax + \ln(C)$	$X = x, Y = \ln(y)$ $C = e^{B}$
$y = Cx^{A}$	$\ln(y) = A\ln(x) + \ln(C)$	$X = \ln(x), Y = \ln(y)$ $C = e^{B}$
$y = (Ax + B)^{-2}$	$y^{-1/2} = Ax + B$	$X = x, Y = y^{-1/2}$
$y = Cxe^{-Dx}$	$\ln\left(\frac{y}{x}\right) = -Dx + \ln(C)$	$X = x, Y = \ln\left(\frac{y}{x}\right)$ $C = e^{B}, D = -A$
$y = \frac{L}{1 + Ce^{Ax}}$	$\ln\left(\frac{L}{y} - 1\right) = Ax + \ln(C)$	$X = x, Y = \ln\left(\frac{L}{y} - 1\right)$ $C = e^{B}$ and L is a constant that must be given

to find M coefficients $\{c_j\}$ so that the function $f(x)$ given by the linear combination

$$f(x) = \sum_{j=1}^{M} c_j f_j(x) \tag{18}$$

will minimize the sum of the squares of the errors

$$E(c_1, c_2, \ldots, c_M) = \sum_{k=1}^{N} (f(x_k) - y_k)^2 = \sum_{k=1}^{N} \left(\left(\sum_{j=1}^{M} c_j f_j(x_k) \right) - y_k \right)^2. \tag{19}$$

For E to be minimized it is necessary that each partial derivative be zero (i.e., $\partial E/\partial c_i = 0$ for $i = 1, 2, \ldots, M$), and this results in the system of equations

$$\sum_{k=1}^{N}\left(\left(\sum_{j=1}^{M} c_j f_j(x_k)\right) - y_k\right)(f_i(x_k)) = 0 \quad \text{for } i = 1,\ 2,\ \ldots,\ M. \tag{20}$$

Interchanging the order of the summations in (20) will produce an $M \times M$ system of linear equations where the unknowns are the coefficients $\{c_j\}$. They are called the normal equations:

$$\sum_{j=1}^{M}\left(\sum_{k=1}^{N} f_i(x_k) f_j(x_k)\right) c_j = \sum_{k=1}^{N} f_i(x_k) y_k \quad \text{for } i = 1,\ 2,\ \ldots,\ M. \tag{21}$$

The Matrix Formulation

Although (21) is easily recognized as a system of M linear equations in M unknowns, one must be clever so that wasted computations are not performed when writing the system in matrix notation. The key is to write down the matrices $\boldsymbol{F}$ and $\boldsymbol{F}'$ as follows:

$$\boldsymbol{F} = \begin{bmatrix} f_1(x_1) & f_2(x_1) & \cdots & f_M(x_1) \\ f_1(x_2) & f_2(x_2) & \cdots & f_M(x_2) \\ f_1(x_3) & f_2(x_3) & \cdots & f_M(x_3) \\ \vdots & \vdots & & \vdots \\ f_1(x_N) & f_2(x_N) & \cdots & f_M(x_N) \end{bmatrix},$$

$$\boldsymbol{F}' = \begin{bmatrix} f_1(x_1) & f_1(x_2) & f_1(x_3) & \cdots & f_1(x_N) \\ f_2(x_1) & f_2(x_2) & f_2(x_3) & \cdots & f_2(x_N) \\ \vdots & \vdots & \vdots & & \vdots \\ f_M(x_1) & f_M(x_2) & f_M(x_3) & \cdots & f_M(x_N) \end{bmatrix}.$$

Consider the product of $\boldsymbol{F}'$ and the column matrix $\boldsymbol{Y}$:

$$\boldsymbol{F}'\boldsymbol{Y} = \begin{bmatrix} f_1(x_1) & f_1(x_2) & f_1(x_3) & \cdots & f_1(x_N) \\ f_2(x_1) & f_2(x_2) & f_2(x_3) & \cdots & f_2(x_N) \\ \vdots & \vdots & \vdots & & \vdots \\ f_M(x_1) & f_M(x_2) & f_M(x_3) & \cdots & f_M(x_N) \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}. \tag{22}$$

The element in the ith row of the product $\boldsymbol{F}'\boldsymbol{Y}$ in (22) is the same as the ith element in the column matrix in equation (21); that is,

$$\sum_{k=1}^{N} f_i(x_k) y_k = \text{row}_i\, \boldsymbol{F}' \cdot [y_1 \quad y_2 \quad \ldots \quad y_N]'. \tag{23}$$

Now consider the product $\boldsymbol{F}'\boldsymbol{F}$, which is an $M \times M$ matrix:

$$\boldsymbol{F}'\boldsymbol{F} = \begin{bmatrix} f_1(x_1) & f_1(x_2) & f_1(x_3) & \cdots & f_1(x_N) \\ f_2(x_1) & f_2(x_2) & f_2(x_3) & \cdots & f_2(x_N) \\ \vdots & \vdots & \vdots & & \vdots \\ f_M(x_1) & f_M(x_2) & f_M(x_3) & \cdots & f_M(x_N) \end{bmatrix}\begin{bmatrix} f_1(x_1) & f_2(x_1) & \cdots & f_M(x_1) \\ f_1(x_2) & f_2(x_2) & \cdots & f_M(x_2) \\ f_1(x_3) & f_2(x_3) & \cdots & f_M(x_3) \\ \vdots & \vdots & & \vdots \\ f_1(x_N) & f_2(x_N) & \cdots & f_M(x_N) \end{bmatrix}.$$

The element in the ith row and jth column of $\boldsymbol{F}'\boldsymbol{F}$ is the coefficient of c_j in the ith row in equation (21); that is,

$$\sum_{k=1}^{N} f_i(x_k) f_j(x_k) = f_i(x_1) f_j(x_1) + f_i(x_2) f_j(x_2) + \cdots + f_i(x_N) f_j(x_N). \tag{24}$$

When M is small, a computationally efficient way to calculate the linear least-squares coefficients for (18) is to store the matrix $\boldsymbol{F}$, compute $\boldsymbol{F}'\boldsymbol{F}$, and $\boldsymbol{F}'\boldsymbol{Y}$ and then solve the linear system

$$\boldsymbol{F}'\boldsymbol{F}\boldsymbol{C} = \boldsymbol{F}'\boldsymbol{Y} \quad \text{for the coefficient matrix} \quad \boldsymbol{C}. \tag{25}$$

Polynomial Fitting

When the foregoing method is adapted to using the functions $\{f_j(x) = x^{j-1}\}$ and the index of summation ranges from $j = 1$ to $j = M + 1$, the function $f(x)$ will be a polynomial of degree M:

$$f(x) = c_1 + c_2 x + c_3 x^2 + \cdots + c_{M+1} x^M. \tag{26}$$

We now show how to find the ***least-squares parabola***, and the extension to a polynomial of higher degree is easily made and is left for the reader.

Theorem 5.3 (Least-squares Parabola). Suppose that $\{(x_k, y_k)\}_{k=1}^{N}$ are N points, where the abscissas are distinct. The coefficients of the least-squares parabola

$$y = f(x) = Ax^2 + Bx + C \tag{27}$$

are the solution values A, B, and C of the linear system

$$\begin{aligned} \left(\sum_{k=1}^{N} x_k^4\right) A + \left(\sum_{k=1}^{N} x_k^3\right) B + \left(\sum_{k=1}^{N} x_k^2\right) C &= \sum_{k=1}^{N} y_k x_k^2, \\ \left(\sum_{k=1}^{N} x_k^3\right) A + \left(\sum_{k=1}^{N} x_k^2\right) B + \left(\sum_{k=1}^{N} x_k\right) C &= \sum_{k=1}^{N} y_k x_k, \\ \left(\sum_{k=1}^{N} x_k^2\right) A + \left(\sum_{k=1}^{N} x_k\right) B + NC &= \sum_{k=1}^{N} y_k. \end{aligned} \tag{28}$$

Table 5.7 Obtaining the Coefficients for the Least-Squares Parabola of Example 5.6

x_k	y_k	x_k^2	x_k^3	x_k^4	$x_k y_k$	$x_k^2 y_k$
−3	3	9	−27	81	−9	27
0	1	0	0	0	0	0
2	1	4	8	16	2	4
4	3	16	64	256	12	48
3	8	29	45	353	5	79

Proof. The coefficients A, B, and C will minimize the quantity:

$$E(A, B, C) = \sum_{k=1}^{N} (Ax_k^2 + Bx_k + C - y_k)^2 \tag{29}$$

The partial derivatives $\partial E/\partial A$, $\partial E/\partial B$, and $\partial E/\partial C$ must all be zero. This results in

$$\begin{aligned} 0 &= \frac{\partial E(A, B, C)}{\partial A} = 2\sum_{k=1}^{N} (Ax_k^2 + Bx_k + C - y_k)^1 (x_k^2), \\ 0 &= \frac{\partial E(A, B, C)}{\partial B} = 2\sum_{k=1}^{N} (Ax_k^2 + Bx_k + C - y_k)^1 (x_k), \\ 0 &= \frac{\partial E(A, B, C)}{\partial C} = 2\sum_{k=1}^{N} (Ax_k^2 + Bx_k + C - y_k)^1 (1). \end{aligned} \tag{30}$$

Using the distributive property of addition, we can move the values A, B, and C outside the summations in (30) to obtain the normal equations that are given in (28). •

Example 5.6. Find the least-squares parabola for the four points $(-3, 3)$, $(0, 1)$, $(2, 1)$, and $(4, 3)$.

The entries in Table 5.7 are used to compute the summations required in the linear system (28).

The linear system (28) for finding A, B, and C becomes

$$\begin{aligned} 353A + 45B + 29C &= 79 \\ 45A + 29B + 3C &= 5 \\ 29A + 3B + 4C &= 8. \end{aligned}$$

The solution to the linear system is $A = 585/3278$, $B = -631/3278$, and $C = 1394/1639$, and the desired parabola is (see Figure 5.8)

$$y = \frac{585}{3278}x^2 - \frac{631}{3278}x + \frac{1394}{1639} = 0.178462x^2 - 0.192495x + 0.850519. \qquad \blacksquare$$

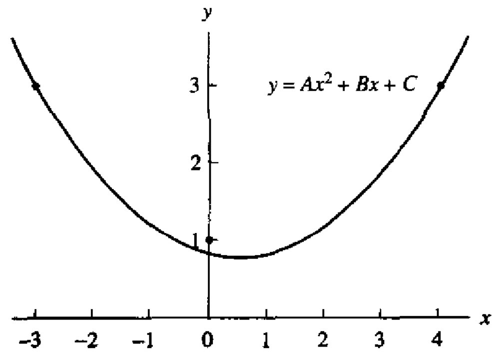

Figure 5.8 The least-squares parabola for Example 5.6.

Polynomial Wiggle

It is tempting to use a least-squares polynomial to fit data that is nonlinear. But if the data do not exhibit a polynomial nature, the resulting curve may exhibit large oscillations. This phenomenon, called ***polynomial wiggle***, becomes more pronounced with higher-degree polynomials. For this reason we seldom use a polynomial of degree 6 or above unless it is known that the true function we are working with is a polynomial.

For example, let $f(x) = 1.44/x^2 + 0.24x$ be used to generate the six data points $(0.25, 23.1)$, $(1.0, 1.68)$, $(1.5, 1.0)$, $(2.0, 0.84)$, $(2.4, 0.826)$, and $(5.0, 1.2576)$. The result of curve fitting with the least-squares polynomials

$$\begin{aligned} P_2(x) &= 22.93 - 16.96x + 2.553x^2, \\ P_3(x) &= 33.04 - 46.51x + 19.51x^2 - 2.296x^3, \\ P_4(x) &= 39.92 - 80.93x + 58.39x^2 - 17.15x^3 + 1.680x^4, \end{aligned}$$

and

$$P_5(x) = 46.02 - 118.1x + 119.4x^2 - 57.51x^3 + 13.03x^4 - 1.085x^5$$

is shown in Figure 5.9(a) through (d). Notice that $P_3(x)$, $P_4(x)$, and $P_5(x)$ exhibit a large wiggle in the interval $[2, 5]$. Even though $P_5(x)$ goes through the six points, it produces the worst fit. If we must fit a polynomial to these data, $P_2(x)$ should be the choice.

The following program uses the matrix F with entries $f_j(x) = x^{j-1}$ from equation (18).

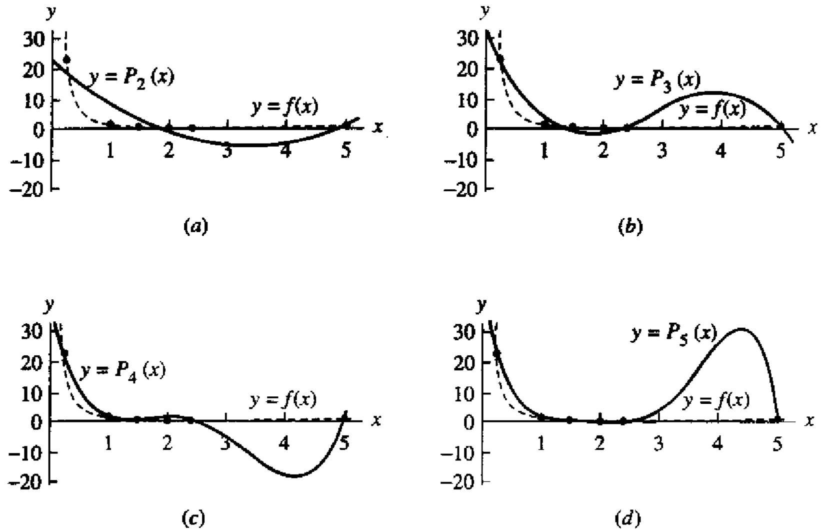

Figure 5.9 (a) Using $P_2(x)$ to fit data. (b) Using $P_3(x)$ to fit data. (c) Using $P_4(x)$ to fit data. (d) Using $P_5(x)$ to fit data.

Program 5.2 (Least-squares Polynomial). To construct the least-squares polynomial of degree M of the form

$$P_M(x) = c_1 + c_2x + c_3x^2 + \cdots + c_Mx^{M-1} + c_{M+1}x^M$$

that fits the N data points $\{(x_k, y_k)\}_{k=1}^N$.

```
function C = lspoly(X,Y,M)
%Input   - X is the 1xn abscissa vector
%        - Y is the 1xn ordinate vector
%        - M is the degree of the least-squares polynomial
% Output - C is the coefficient list for the polynomial
n=length(X);
B=zeros(1:M+1);
F=zeros(n,M+1);
%Fill the columns of F with the powers of X
for k=1:M+1
   F(:,k)=X'.^(k-1);
end
%Solve the linear system from (25)
```



```
A=F'*F;
B=F'*Y';
C=A\B;
C=flipud(C);
```

Exercises for Curve Fitting

1. Find the least-squares parabola $f(x) = Ax^2 + Bx + C$ for each set of data.

(a)

x_k	y_k
−3	15
−1	5
1	1
3	5

(b)

x_k	y_k
−3	−1
−1	25
1	25
3	1

2. Find the least-squares parabola $f(x) = Ax^2 + Bx + C$ for each set of data.

(a)

x_k	y_k
−2	−5.8
−1	1.1
0	3.8
1	3.3
2	−1.5

(b)

x_k	y_k
−2	2.8
−1	2.1
0	3.25
1	6.0
2	11.5

(c)

x_k	y_k
−2	10
−1	1
0	0
1	2
2	9

3. For the given set of data, find the least-squares curve:

   (a) $f(x) = Ce^{Ax}$, by using the change of variables $X = x$, $Y = \ln(y)$, and $C = e^B$, from Table 5.6, to linearize the data points.

   (b) $f(x) = Cx^A$, by using the change of variables $X = \ln(x)$, $Y = \ln(y)$, and $C = e^B$, from Table 5.6, to linearize the data points.

   (c) Use $E_2(f)$ to determine which curve gives the best fit.

x_k	y_k
1	0.6
2	1.9
3	4.3
4	7.6
5	12.6

4. For the given set of data, find the least-squares curve:

(a) $f(x) = Ce^{Ax}$, by using the change of variables $X = x$, $Y = \ln(y)$, and $C = e^B$, from Table 5.6, to linearize the data points.

(b) $f(x) = 1/(Ax + B)$, by using the change of variables $X = x$ and $Y = 1/y$, from Table 5.6, to linearize the data points.

(c) Use $E_2(f)$ to determine which curve gives the best fit.

x_k	y_k
−1	6.62
0	3.94
1	2.17
2	1.35
3	0.89

5. For each set of data, find the least-squares curve:

(a) $f(x) = Ce^{Ax}$, by using the change of variables $X = x$, $Y = \ln(y)$, and $C = e^B$ from Table 5.6, to linearize the data points.

(b) $f(x) = (Ax + B)^{-2}$, by using the change of variables $X = x$ and $Y = y^{-1/2}$, from Table 5.6, to linearize the data points.

(c) Use $E_2(f)$ to determine which curve gives the best fit.

(i)

x_k	y_k
−1	13.45
0	3.01
1	0.67
2	0.15

(ii)

x_k	y_k
−1	13.65
0	1.38
1	0.49
3	0.15

6. *Logistic population growth.* When the population $P(t)$ is bounded by the limiting value L, it follows a logistic curve and has the form $P(t) = L/(1 + Ce^{At})$. Find A and C for the following data, where L is a known value.

(a) (0, 200), (1, 400), (2, 650), (3, 850), (4, 950), and $L = 1000$.

(b) (0, 500), (1, 1000), (2, 1800), (3, 2800), (4, 3700), and $L = 5000$.

7. Use the data for the U.S. population and find the logistic curve $P(t)$. Estimate the population in the year 2000.

(a) Assume that $L = 8 \times 10^8$

Year	t_k	P_k
1800	−10	5.3
1850	−5	23.2
1900	0	76.1
1950	5	152.3

(b) Assume that $L = 8 \times 10^8$

Year	t_k	P_k
1900	0	76.1
1920	2	106.5
1940	4	132.6
1960	6	180.7
1980	8	226.5

In Exercises 8 through 15, carry out the indicated change of variables in Table 5.6, and derive the linearized form for each of the following functions.

8. $y = \dfrac{A}{x} + B$

9. $y = \dfrac{D}{x + C}$

10. $y = \dfrac{1}{Ax + B}$

11. $y = \dfrac{x}{A + Bx}$

12. $y = A\ln(x) + B$

13. $y = Cx^A$

14. $y = (Ax + B)^{-2}$

15. $y = Cxe^{-Dx}$

16. (a) Follow the procedure outlined in the proof of Theorem 5.3 and derive the normal equations for the least-squares curve $f(x) = A\cos(x) + B\sin(x)$.

(b) Use the results from part (a) to find the least-squares curve $f(x) = A\cos(x) + B\sin(x)$ for the following data:

x_k	y_k
−3.0	−0.1385
−1.5	−2.1587
0.0	0.8330
1.5	2.2774
3.0	−0.5110

17. The least-squares plane $z = Ax + By + C$ for the N points $(x_1, y_1, z_1), \ldots, (x_N, y_N, z_N)$ is obtained by minimizing

$$E(A, B, C) = \sum_{k=1}^{N} (Ax_k + By_k + C - z_k)^2.$$

Derive the normal equations:

$$\left(\sum_{k=1}^{N} x_k^2\right) A + \left(\sum_{k=1}^{N} x_k y_k\right) B + \left(\sum_{k=1}^{N} x_k\right) C = \sum_{k=1}^{N} z_k x_k,$$

$$\left(\sum_{k=1}^{N} x_k y_k\right) A + \left(\sum_{k=1}^{N} y_k^2\right) B + \left(\sum_{k=1}^{N} y_k\right) C = \sum_{k=1}^{N} z_k y_k,$$

$$\left(\sum_{k=1}^{N} x_k\right) A + \left(\sum_{k=1}^{N} y_k\right) B + NC = \sum_{k=1}^{N} z_k.$$

18. Find the least-squares planes for the following data.

(a) (1, 1, 7), (1, 2, 9), (2, 1, 10), (2, 2, 11), (2, 3, 12)

(b) (1, 2, 6), (2, 3, 7), (1, 1, 8), (2, 2, 8), (2, 1, 9)

(c) (3, 1, −3), (2, 1, −1), (2, 2, 0), (1, 1, 1), (1, 2, 3)

19. Consider the following table of data

x_k	y_k
1.0	2.0
2.0	5.0
3.0	10.0
4.0	17.0
5.0	26.0

When the change of variables $X = xy$ and $Y = 1/y$ are used with the func $y = D/(x + C)$, the transformed least-squares fit is

$$y = \frac{-17.719403}{x - 5.476617}.$$

When the change of variables $X = x$ and $Y = 1/y$ are used with the function $1/(Ax + B)$, the transformed least-squares fit is

$$y = \frac{1}{-0.1064253x + 0.4987330}.$$

Determine which fit is best and why one of the solutions is completely absurd.

Algorithms and Programs

1. The temperature cycle in a suburb of Los Angeles on November 8 is given in accompanying table below. There are 24 data points.

(a) Follow the procedure outlined in Example 5.5 (use the `fmins` command) to the least-squares curve of the form $f(x) = A\cos(Bx) + C\sin(Dx)$ for the g set of data.

(b) Determine $E_2(f)$.

(c) Plot the data and the least-squares curve from part (a) on the same coordinate system.

Time, p.m.	Degrees	Time, a.m.	Degrees
1	66	1	58
2	66	2	58
3	65	3	58
4	64	4	58
5	63	5	57
6	63	6	57
7	62	7	57
8	61	8	58
9	60	9	60
10	60	10	64
11	59	11	67
Midnight	58	Noon	68

5.3 Interpolation by Spline Functions

Polynomial interpolation for a set of $N + 1$ points $\{(x_k, y_k)\}_{k=0}^{N}$ is frequently unsatisfactory. As discussed in Section 5.2, a polynomial of degree N can have $N - 1$ relative maxima and minima, and the graph can wiggle in order to pass through the points. Another method is to piece together the graphs of lower-degree polynomials $S_k(x)$ and interpolate between the successive nodes (x_k, y_k) and (x_{k+1}, y_{k+1}) (see Figure 5.10).

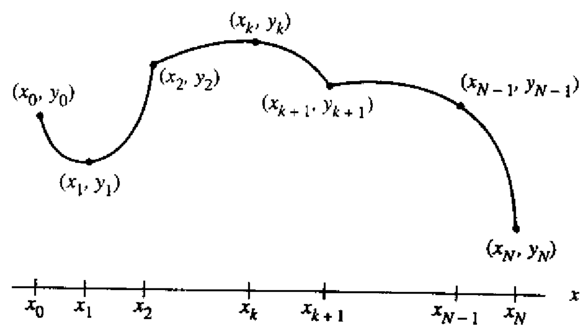

Figure 5.10 Piecewise polynomial interpolation.

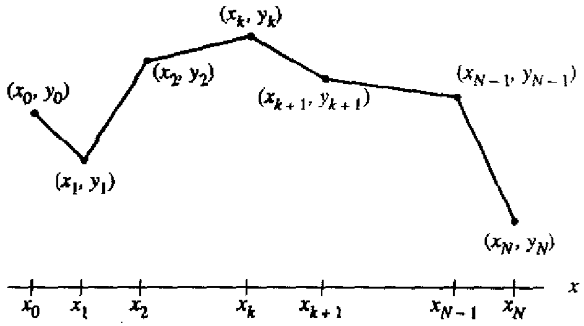

Figure 5.11 Piecewise linear interpolation (a linear spline).

The two adjacent portions of the curve $y = S_k(x)$ and $y = S_{k+1}(x)$, which lie above $[x_k, x_{k+1}]$ and $[x_{k+1}, x_{k+2}]$, respectively, pass through the common ***knot*** (x_{k+1}, y_{k+1}). The two portions of the graph are tied together at the knot (x_{k+1}, y_{k+1}), and the set of functions $\{S_k(x)\}$ forms a piecewise polynomial curve, which is denoted by $S(x)$.

Piecewise Linear Interpolation

The simplest polynomial to use, a polynomial of degree 1, produces a polygonal path that consists of line segments that pass through the points. The Lagrange polynomial from Section 4.3 is used to represent this piecewise linear curve:

$$(1) \qquad S_k(x) = y_k \frac{x - x_{k+1}}{x_k - x_{k+1}} + y_{k+1} \frac{x - x_k}{x_{k+1} - x_k} \quad \text{for} \quad x_k \le x \le x_{k+1}.$$

The resulting curve looks like a broken line (see Figure 5.11).

An equivalent expression can be obtained if we use the point-slope formula for a line segment:

$$S_k(x) = y_k + d_k(x - x_k),$$

where $d_k = (y_{k+1} - y_k)/(x_{k+1} - x_k)$. The resulting ***linear spline*** function can be written in the form

$$(2) \qquad S(x) = \begin{cases} y_0 + d_0(x - x_0) & \text{for } x \text{ in } [x_0, x_1], \\ y_1 + d_1(x - x_1) & \text{for } x \text{ in } [x_1, x_2], \\ \vdots & \vdots \\ y_k + d_k(x - x_k) & \text{for } x \text{ in } [x_k, x_{k+1}], \\ \vdots & \vdots \\ y_{N-1} + d_{N-1}(x - x_{N-1}) & \text{for } x \text{ in } [x_{N-1}, x_N]. \end{cases}$$

The form of equation (2) is better than equation (1) for the explicit calculation of $S(x)$. It is assumed that the abscissas are ordered $x_0 < x_1 < \cdots < x_{N-1} < x_N$. For a fixed value of x, the interval $[x_k, x_{k+1}]$ containing x can be found by successively computing the differences $x - x_1, \ldots, x - x_k, x - x_{k+1}$ until $k + 1$ is the smallest integer such that $x - x_{k+1} < 0$. Hence we have found k so that $x_k \le x \le x_{k+1}$, and the value of the spline function $S(x)$ is

$$(3) \qquad S(x) = S_k(x) = y_k + d_k(x - x_k) \quad \text{for} \quad x_k \le x \le x_{k+1}.$$

These techniques can be extended to higher-order polynomials. For example, if an odd number of nodes $x_0, x_1, \ldots, x_{2M}$ is given, then a piecewise quadratic polynomial can be constructed on each subinterval $[x_{2k}, x_{2k+2}]$, for $k = 0, 1, \ldots, M - 1$. A shortcoming of the resulting quadratic spline is that the curvature at the even nodes x_{2k} changes abruptly, and this can cause an undesired bend or distortion in the graph. The second derivative of a quadratic spline is discontinuous at the even nodes. If we use piecewise cubic polynomials, then both the first and second derivatives can be made continuous.

Piecewise Cubic Splines

The fitting of a polynomial curve to a set of data points has applications in CAD (computer-assisted design), CAM (computer-assisted manufacturing), and computer graphics systems. An operator wants to draw a smooth curve through data points that are not subject to error. Traditionally, it was common to use a french curve or an architect's spline and subjectively draw a curve that looks smooth when viewed by the eye. Mathematically, it is possible to construct cubic functions $S_k(x)$ on each interval $[x_k, x_{k+1}]$ so that the resulting piecewise curve $y = S(x)$ and its first and second derivatives are all continuous on the larger interval $[x_0, x_N]$. The continuity of $S'(x)$ means that the graph $y = S(x)$ will not have sharp corners. The continuity of $S''(x)$ means that the *radius of curvature* is defined at each point.

Definition 5.1 (Cubic Spline Interpolant). Suppose that $\{(x_k, y_k)\}_{k=0}^{N}$ are $N + 1$ points, where $a = x_0 < x_1 < \cdots < x_N = b$. The function $S(x)$ is called a ***cubic spline*** if there exist N cubic polynomials $S_k(x)$ with coefficients $s_{k,0}$, $s_{k,1}$, $s_{k,2}$, and $s_{k,3}$ that satisfy the properties:

I. $S(x) = S_k(x) = s_{k,0} + s_{k,1}(x - x_k) + s_{k,2}(x - x_k)^2 + s_{k,3}(x - x_k)^3$
for $x \in [x_k, x_{k+1}]$ and $k = 0, 1, \ldots, N - 1$.

II. $S(x_k) = y_k$ for $k = 0, 1, \ldots, N$.

III. $S_k(x_{k+1}) = S_{k+1}(x_{k+1})$ for $k = 0, 1, \ldots, N - 2$.

IV. $S'_k(x_{k+1}) = S'_{k+1}(x_{k+1})$ for $k = 0, 1, \ldots, N - 2$.

V. $S''_k(x_{k+1}) = S''_{k+1}(x_{k+1})$ for $k = 0, 1, \ldots, N - 2$. ▲

Property I states that $S(x)$ consists of piecewise cubics. Property II states that the piecewise cubics interpolate the given set of data points. Properties III and IV require that the piecewise cubics represent a smooth continuous function. Property V states that the second derivative of the resulting function is also continuous.

Existence of Cubic Splines

Let us try to determine if it is possible to construct a cubic spline that satisfies properties I through V. Each cubic polynomial $S_k(x)$ has four unknown constants ($s_{k,0}$, $s_{k,1}$, $s_{k,2}$, and $s_{k,3}$); hence there are $4N$ coefficients to be determined. Loosely speaking, we have $4N$ degrees of freedom or conditions that must be specified. The data points supply $N+1$ conditions, and properties III, IV, and V each supply $N-1$ conditions. Hence, $N+1+3(N-1) = 4N-2$ conditions are specified. This leaves us two additional degrees of freedom. We will call them ***end-point constraints***: they will involve either $S'(x)$ or $S''(x)$ at x_0 and x_N and will be discussed later. We now proceed with the construction.

Since $S(x)$ is piecewise cubic, its second derivative $S''(x)$ is piecewise linear on $[x_0, x_N]$. The linear Lagrange interpolation formula gives the following representation for $S''(x) = S_k''(x)$:

(4) $$S_k''(x) = S''(x_k)\frac{x - x_{k+1}}{x_k - x_{k+1}} + S''(x_{k+1})\frac{x - x_k}{x_{k+1} - x_k}$$

Use $m_k = S''(x_k)$, $m_{k+1} = S''(x_{k+1})$, and $h_k = x_{k+1} - x_k$ in (4) to get

(5) $$S_k''(x) = \frac{m_k}{h_k}(x_{k+1} - x) + \frac{m_{k+1}}{h_k}(x - x_k)$$

for $x_k \le x \le x_{k+1}$ and $k = 0, 1, \ldots, N-1$. Integrating (5) twice will introduce two constants of integration, and the result can be manipulated so that it has the form

(6) $$S_k(x) = \frac{m_k}{6h_k}(x_{k+1} - x)^3 + \frac{m_{k+1}}{6h_k}(x - x_k)^3 + p_k(x_{k+1} - x) + q_k(x - x_k).$$

Substituting x_k and x_{k+1} into equation (6) and using the values $y_k = S_k(x_k)$ and $y_{k+1} = S_k(x_{k+1})$ yields the following equations that involve p_k and q_k, respectively:

(7) $$y_k = \frac{m_k}{6}h_k^2 + p_k h_k \quad \text{and} \quad y_{k+1} = \frac{m_{k+1}}{6}h_k^2 + q_k h_k.$$

These two equations are easily solved for p_k and q_k, and when these values are substituted into equation (6), the result is the following expression for the cubic function $S_k(x)$:

(8) $$\begin{aligned} S_k(x) = &-\frac{m_k}{6h_k}(x_{k+1} - x)^3 + \frac{m_{k+1}}{6h_k}(x - x_k)^3 \\ &+ \left(\frac{y_k}{h_k} - \frac{m_k h_k}{6}\right)(x_{k+1} - x) + \left(\frac{y_{k+1}}{h_k} - \frac{m_{k+1}h_k}{6}\right)(x - x_k). \end{aligned}$$

Notice that the representation (8) has been reduced to a form that involves only the unknown coefficients $\{m_k\}$. To find these values, we must use the derivative of (8), which is

(9) $$\begin{aligned} S_k'(x) = &-\frac{m_k}{2h_k}(x_{k+1} - x)^2 + \frac{m_{k+1}}{2h_k}(x - x_k)^2 \\ &- \left(\frac{y_k}{h_k} - \frac{m_k h_k}{6}\right) + \frac{y_{k+1}}{h_k} - \frac{m_{k+1}h_k}{h_k}. \end{aligned}$$

Evaluating (9) at x_k and simplifying the result yield

(10) $$S_k'(x_k) = -\frac{m_k}{3}h_k - \frac{m_{k+1}}{6}h_k + d_k, \quad \text{where} \quad d_k = \frac{y_{k+1} - y_k}{h_k}.$$

Similarly, we can replace k by $k-1$ in (9) to get the expression for $S_{k-1}'(x)$ and evaluate it at x_k to obtain

(11) $$S_{k-1}'(x_k) = \frac{m_k}{3}h_{k-1} + \frac{m_{k-1}}{6}h_{k-1} + d_{k-1}.$$

Now use property IV and equations (10) and (11) to obtain an important relation involving m_{k-1}, m_k, and m_{k+1}:

(12) $$h_{k-1}m_{k-1} + 2(h_{k-1} + h_k)m_k + h_k m_{k+1} = u_k$$

where $u_k = 6(d_k - d_{k-1})$ for $k = 1, 2, \ldots, N-1$.

Construction of Cubic Splines

Observe that the unknowns in (12) are the desired values $\{m_k\}$, and the other terms are constants obtained by performing simple arithmetic with the data points $\{(x_k, y_k)\}$. Therefore, in reality system (12) is an underdetermined system of $N-1$ linear equations involving $N+1$ unknowns. Hence two additional equations must be supplied. They are used to eliminate m_0 from the first equation and m_N from the $(N-1)$st equation in system (12). The standard strategies for the end-point constraints are summarized in Table 5.8.

Consider strategy (v) in Table 5.8. If m_0 is given, then $h_0 m_0$ can be computed, and the first equation (when $k = 1$) of (12) is

(13) $$2(h_0 + h_1)m_1 + h_1 m_2 = u_1 - h_0 m_0.$$

Similarly, if m_N is given, then $h_{N-1}m_N$ can be computed, and the last equation (when $k = N-1$) of (12) is

(14) $$h_{N-2}m_{N-2} + 2(h_{N-2} + h_{N-1})m_{N-1} = u_{N-1} - h_{N-1}m_N.$$

Table 5.8 End-point Constraints for a Cubic Spline

Description of the strategy	Equations involving m_0 and m_N
(i) *Clamped cubic spline:* specify $S'(x_0)$, $S'(x_n)$ (the "best choice" if the derivatives are known)	$m_0 = \frac{3}{h_0}(d_0 - S'(x_0)) - \frac{m_1}{2}$ $m_N = \frac{3}{h_{N-1}}(S'(x_N) - d_{N-1}) - \frac{m_{N-1}}{2}$
(ii) *Natural cubic spline* (a "relaxed curve")	$m_0 = 0, m_N = 0$
(iii) Extrapolate $S''(x)$ to the endpoints	$m_0 = m_1 - \frac{h_0(m_2 - m_1)}{h_1}$, $m_N = m_{N-1} + \frac{h_{N-1}(m_{N-1} - m_{N-2})}{h_{N-2}}$
(iv) $S''(x)$ is constant near the endpoints	$m_0 = m_1, m_N = m_{N-1}$
(v) Specify $S''(X)$ at each endpoint	$m_0 = S''(x_0), m_N = S''(x_N)$

Equations (13) and (14) with (12) used for $k = 2, 3, \ldots, N-2$ form $N-1$ lines equations involving the coefficients $m_1, m_2, \ldots, m_{N-1}$.

Regardless of the particular strategy chosen in Table 5.8, we can rewrite equations 1 and $N-1$ in (12) and obtain a tridiagonal linear system of the form $HM = V$, which involves $m_1, m_2, \ldots, m_{N-1}$:

$$
(15) \quad \begin{bmatrix} b_1 & c_1 & & & & \\ a_1 & b_2 & c_2 & & & \\ & & \ddots & & & \\ & & & a_{N-3} & b_{N-2} & c_{N-2} \\ & & & & a_{N-2} & b_{N-1} \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_{N-2} \\ m_{N-1} \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_{N-2} \\ v_{N-1} \end{bmatrix}.
$$

The linear system in (15) is strictly diagonally dominant and has a unique solution (see Chapter 3 for details). After the coefficients $\{m_k\}$ are determined, the spline coefficients $\{s_{k,j}\}$ for $S_k(x)$ are computed using the formulas

$$
(16) \quad s_{k,0} = y_k, \qquad s_{k,1} = d_k - \frac{h_k(2m_k + m_{k+1})}{6},
$$
$$
s_{k,2} = \frac{m_k}{2}, \qquad s_{k,3} = \frac{m_{k+1} - m_k}{6h_k}.
$$

Each cubic polynomial $S_k(x)$ can be written in nested multiplication form for efficient computation:

$$
(17) \quad S_k(x) = ((s_{k,3}w + s_{k,2})w + s_{k,1})w + y_k, \qquad \text{where} \qquad w = x - x_k
$$

and $S_k(x)$ is used on the interval $x_k \le x \le x_{k+1}$.

Equations (12) together with a strategy from Table 5.8 can be used to construct a cubic spline with distinctive properties at the end points. Specifically, the values for m_0 and m_N in Table 5.8 are used to customize the first and last equations in (12) and form the system of $N-1$ equations given in (15). Then the tridiagonal system is solved for the remaining coefficients $m_1, m_2, \ldots, m_{N-1}$. Finally, the formulas in (16) are used to determine the spline coefficients. For reference, we now state how the equations must be prepared for each different type of spline.

End-point Constraints

The following five lemmas show the form of the tridiagonal linear system that must be solved for each of the different endpoint constraints in Table 5.8.

Lemma 5.1 (Clamped Spline). There exists a unique cubic spline with the first derivative boundary conditions $S'(a) = d_0$ and $S'(b) = d_N$.

Proof. Solve the linear system

$$
\left(\frac{3}{2}h_0 + 2h_1\right)m_1 + h_1 m_2 = u_1 - 3(d_0 - S'(x_0))
$$
$$
h_{k-1}m_{k-1} + 2(h_{k-1} + h_k)m_k + h_k m_{k+1} = u_k \qquad \text{for } k = 2, 3, \ldots, N-2
$$
$$
h_{N-2}m_{N-2} + (2h_{N-2} + \frac{3}{2}h_{N-1})m_{N-1} = u_{N-1} - 3(S'(x_N) - d_{N-1}). \qquad \bullet
$$

Remark. The clamped spline involves slope at the ends. This spline can be visualized as the curve obtained when a flexible elastic rod is forced to pass through the data points, and the rod is clamped at each end with a fixed slope. This spline would be useful to a draftsman for drawing a smooth curve through several points.

Lemma 5.2 (Natural Spline). There exists a unique cubic spline with the free boundary conditions $S''(a) = 0$ and $S''(b) = 0$.

Proof. Solve the linear system

$$
\begin{aligned}
2(h_0 + h_1)m_1 + h_1 m_2 &= u_1 \\
h_{k-1}m_{k-1} + 2(h_{k-1} + h_k)m_k + h_k m_{k+1} &= u_k \qquad \text{for } k = 2, 3, \ldots, N-2. \\
h_{N-2}m_{N-2} + 2(h_{N-2} + h_{N-1})m_{N-1} &= u_{N-1}.
\end{aligned}
$$
•

Remark. The natural spline is the curve obtained by forcing a flexible elastic rod through the data points, but letting the slope at the ends be free to equilibrate to the position that minimizes the oscillatory behavior of the curve. It is useful for fitting a curve to experimental data that are significant to several significant digits.

Lemma 5.3 (Extrapolated Spline). There exists a unique cubic spline that uses extrapolation from the interior nodes at x_1 and x_2 to determine $S''(a)$ and extrapolation from the nodes at x_{N-1} and x_{N-2} to determine $S''(b)$.

Proof. Solve the linear system

$$
\begin{aligned}
&\left(3h_0 + 2h_1 + \frac{h_0^2}{h_1}\right) m_1 + \left(h_1 - \frac{h_0^2}{h_1}\right) m_2 = u_1 \\
&h_{k-1}m_{k-1} + 2(h_{k-1} + h_k)m_k + h_k m_{k+1} = u_k \qquad \text{for } k = 2, 3, \ldots, N-2 \\
&\left(h_{N-2} - \frac{h_{N-1}^2}{h_{N-2}}\right) m_{N-2} + \left(2h_{N-2} + 3h_{N-1} + \frac{h_{N-1}^2}{h_{N-2}}\right) m_{N-1} = u_{N-1}.
\end{aligned}
$$
•

Remark. The extrapolated spline is equivalent to assuming that the end cubic is an extension of the adjacent cubic; that is, the spline forms a single cubic curve over the interval $[x_0, x_2]$ and another single cubic over the interval $[x_{N-2}, x_N]$.

Lemma 5.4 (Parabolically Terminated Spline). There exists a unique cubic spline that uses $S'''(x) \equiv 0$ on the interval $[x_0, x_1]$ and $S'''(x) \equiv 0$ on $[x_{N-1}, x_N]$.

Proof. Solve the linear system

$$
\begin{aligned}
(3h_0 + 2h_1)m_1 + h_1 m_2 &= u_1 \\
h_{k-1}m_{k-1} + 2(h_{k-1} + h_k)m_k + h_k m_{k+1} &= u_k \qquad \text{for } k = 2, 3, \ldots, N-2 \\
h_{N-2}m_{N-2} + (2h_{N-2} + 3h_{N-1})m_{N-1} &= u_{N-1}.
\end{aligned}
$$

Remark. The assumption that $S'''(x) \equiv 0$ on the interval $[x_0, x_1]$ forces the cubic to degenerate to a quadratic over $[x_0, x_1]$, and a similar situation occurs over $[x_{N-1}, x_N]$.

Lemma 5.5 (End-point Curvature-adjusted Spline). There exists a unique cubic spline with the second derivative boundary conditions $S''(a)$ and $S''(b)$ specified.

Proof. Solve the linear system

$$
\begin{aligned}
2(h_0 + h_1)m_1 + h_1 m_2 &= u_1 - h_0 S''(x_0) \\
h_{k-1}m_{k-1} + 2(h_{k-1} + h_k)m_k + h_k m_{k+1} &= u_k \qquad \text{for } k = 2, 3, \ldots, N-2 \\
h_{N-2}m_{N-2} + 2(h_{N-2} + h_{N-1})m_{N-1} &= u_{N-1} - h_{N-1}S''(x_N).
\end{aligned}
$$
•

Remark. Imposing values for $S''(a)$ and $S''(b)$ permits the practitioner to adjust the curvature at each endpoint.

The next five examples illustrate the behavior of the various splines. It is possible to mix the end conditions to obtain an even wider variety of possibilities, but we leave these variations to the reader to investigate.

Example 5.7. Find the clamped cubic spline that passes through (0, 0), (1, 0.5), (2, 2.0), and (3, 1.5) with the first derivative boundary conditions $S'(0) = 0.2$ and $S'(3) = -1$.

First, compute the quantities

$$
\begin{aligned}
h_0 &= h_1 = h_2 = 1 \\
d_0 &= (y_1 - y_0)/h_0 = (0.5 - 0.0)/1 = 0.5 \\
d_1 &= (y_2 - y_1)/h_1 = (2.0 - 0.5)/1 = 1.5 \\
d_2 &= (y_3 - y_2)/h_2 = (1.5 - 2.0)/1 = -0.5 \\
u_1 &= 6(d_1 - d_0) = 6(1.5 - 0.5) = 6.0 \\
u_2 &= 6(d_2 - d_1) = 6(-0.5 - 1.5) = -12.0.
\end{aligned}
$$

Then use Lemma 5.1 and obtain the equations

$$
\begin{aligned}
\left(\frac{3}{2} + 2\right) m_1 + m_2 &= 6.0 - 3(0.5 - 0.2) = 5.1, \\
m_1 + \left(2 + \frac{3}{2}\right) m_2 &= -12.0 - 3(-1.0 - (-0.5)) = -10.5.
\end{aligned}
$$

When these equations are simplified and put in matrix notation, we have

$$
\begin{bmatrix} 3.5 & 1.0 \\ 1.0 & 3.5 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} 5.1 \\ -10.5 \end{bmatrix}.
$$

It is a straightforward task to compute the solution $m_1 = 2.25$ and $m_2 = -3.72$. Now apply the equations in (i) of Table 5.8 to determine the coefficients m_0 and m_3:

$$
\begin{aligned}
m_0 &= 3(0.5 - 0.2) - \frac{2.52}{2} = -0.36, \\
m_3 &= 3(-1.0 + 0.5) - \frac{-3.72}{2} = 0.36.
\end{aligned}
$$

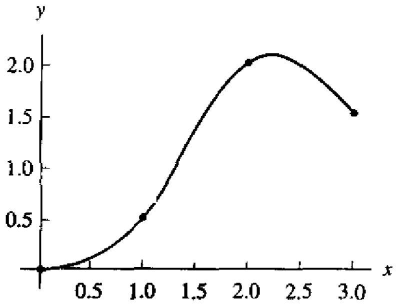

Figure 5.12 The clamped cubic spline with derivative boundary conditions: $S'(0) = 0.2$ and $S'(3) = -1$

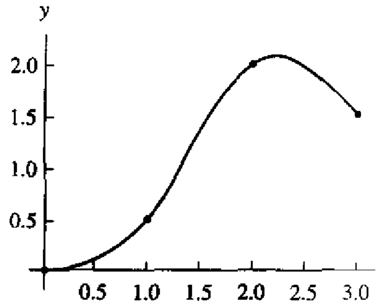

Figure 5.13 The natural cubic spline with $S''(0) = 0$ and $S''(3) = 0$.

Next, the values $m_0 = -0.36$, $m_1 = 2.25$, $m_2 = -3.72$, and $m_3 = 0.36$ are substituted into the equations (16) to find the spline coefficients. The solution is

$$
\begin{aligned}
S_0(x) &= 0.48x^3 - 0.18x^2 + 0.2x && \text{for } 0 \le x \le 1,\\
S_1(x) &= -1.04(x-1)^3 + 1.26(x-1)^2 &&\\
&\quad + 1.28(x-1) + 0.5 && \text{for } 1 \le x \le 2,\\
S_2(x) &= 0.68(x-2)^3 - 1.86(x-2)^2 &&\\
&\quad + 0.68(x-2) + 2.0 && \text{for } 2 \le x \le 3.
\end{aligned} \tag{18}
$$

This clamped cubic spline is shown in Figure 5.12. ■

Example 5.8. Find the natural cubic spline that passes through (0, 0.0), (1, 0.5), (2, 2.0), and (3, 1.5) with the free boundary conditions $S''(x) = 0$ and $S''(3) = 0$.

Use the same values $\{h_k\}$, $\{d_k\}$, and $\{u_k\}$ that were computed in Example 5.7. Then use Lemma 5.2 and obtain the equations

$$
\begin{aligned}
2(1+1)m_1 + m_2 &= 6.0,\\
m_1 + 2(1+1)m_2 &= -12.0.
\end{aligned}
$$

The matrix form of this linear system is

$$
\begin{bmatrix} 4.0 & 1.0 \\ 1.0 & 4.0 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} 6.0 \\ -12.0 \end{bmatrix}.
$$

It is easy to find the solution $m_1 = 2.4$ and $m_2 = -3.6$. Since $m_0 = S''(0) = 0$ and

$m_3 = S''(3) = 0$, when equations (16) are used to find the spline coefficients, the result is

$$
\begin{aligned}
S_0(x) &= 0.4x^3 + 0.1x && \text{for } 0 \le x \le 1,\\
S_1(x) &= -(x-1)^3 + 1.2(x-1)^2 &&\\
&\quad + 1.3(x-1) + 0.5 && \text{for } 1 \le x \le 2,\\
S_2(x) &= 0.6(x-2)^3 - 1.8(x-2)^2 &&\\
&\quad + 0.7(x-2) + 2.0 && \text{for } 2 \le x \le 3.
\end{aligned} \tag{19}
$$

This natural cubic spline is shown in Figure 5.13. ■

Example 5.9. Find the extrapolated cubic spline through (0, 0.0), (1, 0.5), (2, 2.0), and (3, 1.5).

Use the values $\{h_k\}$, $\{d_k\}$, and $\{u_k\}$ from Example 5.7 with Lemma 5.3 and obtain the linear system

$$
\begin{aligned}
(3+2+1)m_1 + (1-1)m_2 &= 6.0,\\
(1-1)m_1 + (2+3+1)m_2 &= -12.0.
\end{aligned}
$$

The matrix form is

$$
\begin{bmatrix} 6.0 & 0.0 \\ 0.0 & 6.0 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} 6.0 \\ -12.0 \end{bmatrix},
$$

and it is trivial to obtain $m_1 = 1.0$ and $m_2 = -2.0$. Now apply the equations in (iii) of Table 5.8 to compute m_0 and m_3:

$$
\begin{aligned}
m_0 &= 1.0 - (-2.0 - 1.0) = 4.0,\\
m_3 &= -2.0 + (-2.0 - 1.0) = -5.0.
\end{aligned}
$$

Finally, the values for $\{m_k\}$ are substituted in equations (16) to find the spline coefficients. The solution is

$$
\begin{aligned}
S_0(x) &= -0.5x^3 + 2.0x^2 - x && \text{for } 0 \le x \le 1,\\
S_1(x) &= -0.5(x-1)^3 + 0.5(x-1)^2 &&\\
&\quad + 1.5(x-1) + 0.5 && \text{for } 1 \le x \le 2,\\
S_2(x) &= -0.5(x-2)^3 - (x-2)^2 &&\\
&\quad + (x-2) + 2.0 && \text{for } 2 \le x \le 3.
\end{aligned} \tag{20}
$$

The extrapolated cubic spline is shown in Figure 5.14. ■

Example 5.10. Find the parabolically terminated cubic spline through (0, 0.0), (1, 0.5), (2, 2.0), and (3, 1.5).

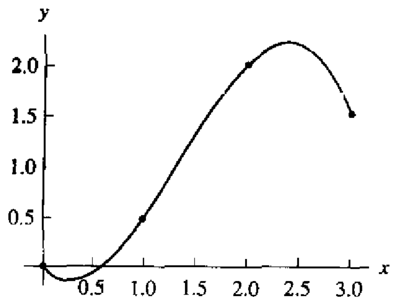

Figure 5.14 The extrapolated cubic spline.

Use $\{h_k\}$, $\{d_k\}$, and $\{u_k\}$ from Example 5.7 and then apply Lemma 5.4 to obtain

$$(3+2)m_1 + m_2 = 6.0,$$
$$m_1 + (2+3)m_2 = -12.0.$$

The matrix form is

$$\begin{bmatrix} 5.0 & 1.0 \\ 1.0 & 5.0 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} 6.0 \\ -12.0 \end{bmatrix},$$

and the solution is $m_1 = 1.75$ and $m_2 = -2.75$. Since $S''(x) \equiv 0$ on the subinterval at each end, formulas (iv) in Table 5.8 imply that we have $m_0 = m_1 = 1.75$, and $m_3 = m_2 = -2.75$. Then the values for $\{m_k\}$ are substituted in equations (16) to get the solution

(21)
$$\begin{aligned} S_0(x) &= 0.875x^2 - 0.375x && \text{for } 0 \le x \le 1, \\ S_1(x) &= -0.75(x-1)^3 + 0.875(x-1)^2 \\ &\quad + 1.375(x-1) + 0.5 && \text{for } 1 \le x \le 2, \\ S_2(x) &= -1.375(x-2)^2 + 0.875(x-2) + 2.0 && \text{for } 2 \le x \le 3. \end{aligned}$$

This parabolically terminated cubic spline is shown in Figure 5.15. ∎

Example 5.11. Find the curvature-adjusted cubic spline through (0, 0.0), (1, 0.5), (2, 2.0), and (3, 1.5) with the second derivative boundary conditions $S''(0) = -0.3$ and $S''(3) = 3.3$.

Use $\{h_k\}$, $\{d_k\}$, and $\{u_k\}$ from Example 5.7 and then apply Lemma 5.5 to obtain

$$2(1+1)m_1 + m_2 = 6.0 - (-0.3) = 6.3,$$
$$m_1 + 2(1+1)m_2 = -12.0 - (3.3) = -15.3.$$

The matrix form is

$$\begin{bmatrix} 4.0 & 1.0 \\ 1.0 & 4.0 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} 6.3 \\ -15.3 \end{bmatrix},$$

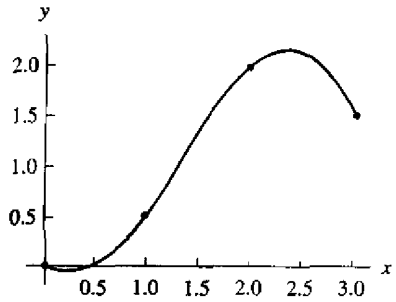

Figure 5.15 The parabolically terminated cubic spline.

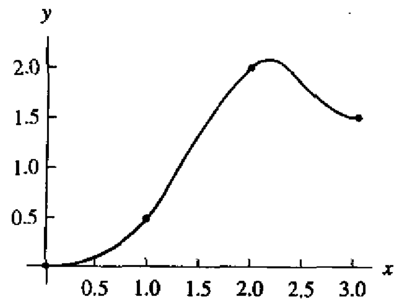

Figure 5.16 The curvature adjusted cubic spline with $S''(0) = -0.3$ and $S''(3) = 3.3$.

and the solution is $m_1 = 2.7$ and $m_2 = -4.5$. The given boundary conditions are used to determine $m_0 = S''(0) = -0.3$ and $m_3 = S''(3) = 3.3$. Substitution of $\{m_k\}$ in equations (16) produces the solution

(22)
$$\begin{aligned} S_0(x) &= 0.5x^3 - 0.15x^2 + 0.15x && \text{for } 0 \le x \le 1, \\ S_1(x) &= -1.2(x-1)^3 + 1.35(x-1)^2 \\ &\quad + 1.35(x-1) + 0.5 && \text{for } 1 \le x \le 2, \\ S_2(x) &= 1.3(x-2)^3 - 2.25(x-2)^2 \\ &\quad + 0.45(x-2) + 2.0 && \text{for } 2 \le x \le 3. \end{aligned}$$

This curvature-adjusted cubic spline is shown in Figure 5.16. ∎

Suitability of Cubic Splines

A practical feature of splines is the minimum of the oscillatory behavior that they possess. Consequently, among all functions $f(x)$ that are twice continuously differentiable on $[a, b]$ and interpolate a given set of data points $\{(x_k, y_k)\}_{k=0}^{N}$, the cubic spline has less wiggle. The next result explains this phenomenon.

Theorem 5.4 (Minimum Property of Cubic Splines). Assume that $f \in C^2[a,b]$ and $S(x)$ is the unique cubic spline interpolant for $f(x)$ that passes through the points $\{(x_k, f(x_k))\}_{k=0}^N$ and satisfies the clamped end conditions $S'(a) = f'(a)$ and $S'(b) = f'(b)$. Then

$$\int_a^b (S''(x))^2\,dx \le \int_a^b (f''(x))^2\,dx. \tag{23}$$

Proof. Use integration by parts and the end conditions to obtain

$$\begin{aligned}
&\int_a^b S''(x)(f''(x) - S''(x))\,dx \\
&= S''(x)(f'(x) - S'(x))\Big|_{x=a}^{x=b} - \int_a^b S'''(x)(f'(x) - S'(x))\,dx \\
&= 0 - 0 - \int_a^b S'''(x)(f'(x) - S'(x))\,dx.
\end{aligned}$$

Since $S'''(x) = 6s_{k,3}$ on the subinterval $[x_k, x_{k+1}]$, it follows that

$$\int_{x_k}^{x_{k+1}} S'''(x)(f'(x) - S'(x))\,dx = 6s_{k,3}(f(x) - S(x))\Big|_{x=x_k}^{x=x_{k+1}} = 0$$

for $k = 0, 1, \ldots, N-1$. Hence $\int_a^b S''(x)(f''(x) - S''(x))\,dx = 0$, and it follows that

$$\int_a^b S''(x) f''(x)\,dx = \int_a^b (S''(x))^2\,dx. \tag{24}$$

Since $0 \le (f''(x) - S''(x))^2$, we get the integral relationship

$$\begin{aligned}
0 &\le \int_a^b (f''(x) - S''(x))^2\,dx \\
&= \int_a^b (f''(x))^2\,dx - 2\int_a^b f''(x)S''(x)\,dx + \int_a^b (S''(x))^2\,dx.
\end{aligned} \tag{25}$$

Now the result in (24) is substituted into (25) and the result is

$$0 \le \int_a^b (f''(x))^2\,dx - \int_a^b (S''(x))^2\,dx.$$

This is easily rewritten to obtain the relation (23) and the result is proved. •

The following program constructs a clamped cubic spline interpolant for the data points $\{(x_k, y_k)\}_{k=0}^N$. The coefficients, in descending order, of $S_k(x)$, for $k = 0, 1, \ldots, N-1$, are found in the $(k-1)$st row of the output matrix S. In the exercises the reader will be asked to modify the program for the other end-point constraints listed in Table 5.8 and described in Lemmas 5.2 through 5.5.

Program 5.3 (Clamped Cubic Spline). To construct and evaluate a clamped cubic spline interpolant $S(x)$ for the $N+1$ data points $\{(x_k, y_k)\}_{k=0}^N$.

```
function S=csfit(X,Y,dx0,dxn)

%Input  - X is the 1xn abscissa vector
%       - Y is the 1xn ordinate vector
%       - dx0 = S'(x0) first derivative boundary condition
%       - dxn = S'(xn) first derivative boundary condition
%Output - S: rows of S are the coefficients, in descending
%         order, for the cubic interpolants

N=length(X)-1;
H=diff(X);
D=diff(Y)./H;
A=H(2:N-1);
B=2*(H(1:N-1)+H(2:N));
C=H(2:N);
U=6*diff(D);

%Clamped spline endpoint constraints
B(1)=B(1)-H(1)/2;
U(1)=U(1)-3*(D(1)-dx0);
B(N-1)=B(N-1)-H(N)/2;
U(N-1)=U(N-1)-3*(dxn-D(N));

for k=2:N-1
   temp=A(k-1)/B(k-1);
   B(k)=B(k)-temp*C(k-1);
   U(k)=U(k)-temp*U(k-1);
end

M(N)=U(N-1)/B(N-1);

for k=N-2:-1:1
   M(k+1)=(U(k)-C(k)*M(k+2))/B(k);
end

M(1)=3*(D(1)-dx0)/H(1)-M(2)/2;
M(N+1)=3*(dxn-D(N))/H(N)-M(N)/2;

for k=0:N-1
   S(k+1,1)=(M(k+2)-M(k+1))/(6*H(k+1));
   S(k+1,2)=M(k+1)/2;
   S(k+1,3)=D(k+1)-H(k+1)*(2*M(k+1)+M(k+2))/6;
   S(k+1,4)=Y(k+1);
end
```

Example 5.12. Find the clamped cubic spline that passes through (0, 0.0), (1, 0.5), (2, 2.0), and (3, 1.5) with the first derivative boundary conditions $S'(0) = 0.2$ and $S'(3) = -1$.

In MATLAB:

```
>>X=[0 1 2 3]; Y=[0 0.5 2.0 1.5];dx0=0.2; dxn=-1;
>>S=csfit(X,Y,dx0,dxn)
S =
  0.4800 -0.1800 0.2000 0
 -1.0400  1.2600 1.2800 0.5000
  0.6800 -1.8600 0.6800 2.0000
```

Notice that the rows of S are precisely the coefficients of the cubic spline interpolants in equation (18) in Example 5.7. The following commands show how to plot the cubic spline interpolant using the `polyval` command. The resulting graph is the same as Figure 5.12.

```
>>x1=0:.01:1; y1=polyval(S(1,:),x1-X(1));
>>x2=1:.01:2; y2=polyval(S(2,:),x2-X(2));
>>x3=2:.01:3; y3=polyval(S(3,:),x3-X(3));
>>plot(x1,y1,x2,y2,x3,y3,X,Y,'.')
```

Exercises for Interpolation by Spline Functions

1. Consider the polynomial $S(x) = a_0 + a_1x + a_2x^2 + a_3x^3$.
   (a) Show that the conditions $S(1) = 1$, $S'(1) = 0$, $S(2) = 2$, and $S'(2) = 0$ produce the system of equations

$$\begin{aligned} a_0 + a_1 + a_2 + a_3 &= 1 \\ a_1 + 2a_2 + 3a_3 &= 0 \\ a_0 + 2a_1 + 4a_2 + 8a_3 &= 2 \\ a_1 + 4a_2 + 12a_3 &= 0 \end{aligned}$$

   (b) Solve the system in part (a) and graph the resulting cubic polynomial.

2. Consider the polynomial $S(x) = a_0 + a_1x + a_2x^2 + a_3x^3$.
   (a) Show that the conditions $S(1) = 3$, $S'(1) = -4$, $S(2) = 1$, and $S'(2) = 2$ produce the system of equations

$$\begin{aligned} a_0 + a_1 + a_2 + a_3 &= 3 \\ a_1 + 2a_2 + 3a_3 &= -4 \\ a_0 + 2a_1 + 4a_2 + 8a_3 &= 1 \\ a_1 + 4a_2 + 12a_3 &= 2 \end{aligned}$$

   (b) Solve the system in part (a) and graph the resulting cubic polynomial.

3. Determine which of the following functions are cubic splines. *Hint.* Which, if any, of the five parts of Definition 5.1 does a given function $f(x)$ not satisfy?

   (a) $f(x) = \begin{cases} \frac{19}{2} - \frac{81}{4}x + 15x^2 - \frac{13}{4}x^3 & \text{for } 1 \le x \le 2 \\ \frac{-77}{2} + \frac{207}{4}x - 21x^2 + \frac{11}{4}x^3 & \text{for } 2 \le x \le 3 \end{cases}$

   (b) $f(x) = \begin{cases} 11 - 24x + 18x^2 - 4x^3 & \text{for } 1 \le x \le 2 \\ -54 + 72x - 30x^2 + 4x^3 & \text{for } 2 \le x \le 3 \end{cases}$

   (c) $f(x) = \begin{cases} 18 - \frac{75}{2}x + 26x^2 - \frac{11}{2}x^3 & \text{for } 1 \le x \le 2 \\ -70 + \frac{189}{2}x - 40x^2 + \frac{11}{2}x^3 & \text{for } 2 \le x \le 3 \end{cases}$

   (d) $f(x) = \begin{cases} 13 - 31x + 23x^2 - 5x^3 & \text{for } 1 \le x \le 2 \\ -35 + 51x - 22x^2 + 3x^3 & \text{for } 2 \le x \le 3 \end{cases}$

4. Find the clamped cubic spline that passes through the points $(-3, 2)$, $(-2, 0)$, $(1, 3)$, and $(4, 1)$ with the first derivative boundary conditions $S'(-3) = -1$ and $S'(4) = 1$.

5. Find the natural cubic spline that passes through the points $(-3, 2)$, $(-2, 0)$, $(1, 3)$, and $(4, 1)$ with the free boundary conditions $S''(-3) = 0$ and $S''(4) = 0$.

6. Find the extrapolated cubic spline that passes through the points $(-3, 2)$, $(-2, 0)$, $(1, 3)$, and $(4, 1)$.

7. Find the parabolically terminated cubic spline that passes through the points $(-3, 2)$, $(-2, 0)$, $(1, 3)$, and $(4, 1)$.

8. Find the curvature-adjusted cubic spline that passes through the points $(-3, 2)$, $(-2, 0)$, $(1, 3)$, and $(4, 1)$ with the second derivative boundary conditions $S''(-3) = -1$ and $S''(4) = 2$.

9. (a) Find the clamped cubic spline that passes through the points $\{(x_k, f(x_k))\}_{k=0}^{3}$, on the graph of $f(x) = x + \frac{2}{x}$, using the nodes $x_0 = 1/2$, $x_1 = 1$, $x_2 = 3/2$, and $x_3 = 2$. Use the first derivative boundary conditions $S'(x_0) = f'(x_0)$ and $S'(x_3) = f'(x_3)$. Graph f and the clamped cubic spline interpolant on the same coordinate system.
   (b) Find the natural cubic spline that passes through the points $\{(x_k, f(x_k))\}_{k=0}^{3}$, on the graph of $f(x) = x + \frac{2}{x}$, using the nodes $x_0 = 1/2$, $x_1 = 1$, $x_2 = 3/2$, and $x_3 = 2$. Use the free boundary conditions $S''(x_0) = 0$ and $S''(x_3) = 0$. Graph f and the natural cubic spline interpolant on the same coordinate system.

10. (a) Find the clamped cubic spline that passes through the points $\{(x_k, f(x_k))\}_{k=0}^{3}$, on the graph of $f(x) = \cos(x^2)$, using the nodes $x_0 = 0$, $x_1 = \sqrt{\pi/2}$, $x_2 = \sqrt{3\pi/2}$, and $x_3 = \sqrt{5\pi/2}$. Use the first derivative boundary conditions $S'(x_0) = f'(x_0)$ and $S'(x_3) = f'(x_3)$. Graph f and the clamped cubic spline interpolant on the same coordinate system.
    (b) Find the natural cubic spline that passes through the points $\{(x_k, f(x_k))\}_{k=0}^{3}$, on the graph of $f(x) = \cos(x^2)$, using the nodes $x_0 = 0$, $x_1 = \sqrt{\pi/2}$, $x_2 = \sqrt{3\pi/2}$, and $x_3 = \sqrt{5\pi/2}$. Use the free boundary conditions $S''(x_0) = 0$ and

$S''(x_3) = 0$. Graph f and the natural cubic spline interpolant on the same coordinate system.

11. Use the substitutions

$$x_{k+1} - x = h_k + (x_k - x)$$

and

$$(x_{k+1} - x)^3 = h_k^3 + 3h_k^2(x_k - x) + 3h_k(x_k - x)^2 + (x_k - x)^3$$

to show that when equation (8) is expanded into powers of $(x_k - x)$, the coefficients are those given in equations (16).

12. Consider each cubic function $S_k(x)$ over the interval $[x_k, x_{k+1}]$.
(a) Give a formula for $\int_{x_k}^{x_{k+1}} S_k(x)\,dx$.
Then evaluate $\int_{x_0}^{x_3} S(x)\,dx$ in part (a) of
(b) Exercise 10 **(c)** Exercise 11

13. Show how strategy (i) in Table 5.8 and system (12) are combined to obtain the equations in Lemma 5.1.

14. Show how strategy (iii) in Table 5.8 and system (12) are combined to obtain the equation in Lemma 5.3.

15. **(a)** Using the nodes $x_0 = -2$ and $x_1 = 0$, show that $f(x) = x^3 - x$ is its own clamped cubic spline on the interval $[-2, 0]$.
(b) Using the nodes $x_0 = -2$, $x_1 = 0$, and $x_2 = 2$, show that $f(x) = x^3 - x$ is its own clamped cubic spline on the interval $[-2, 2]$. *Note.* f has an inflection point at x_1.
(c) Use the results from parts (a) and (b) to show that any third-degree polynomial, $f(x) = a_0 + a_1x + a_2x^2 + a_3x^3$, is its own clamped cubic spline on any closed interval $[a, b]$.
(d) What, if anything, can be said about the other four types of cubic splines described in Lemmas 5.2 through 5.5?

Algorithms and Programs

1. The distance d_k that a car traveled at time t_k is given in the follwoing table. Use Program 5.3 with the first derivative boundary conditions $S'(0) = 0$ and $S'(8) = 98$ and find the clamped cubic spline for the points.

Time, t_k	0	2	4	6	8
Distance, d_k	0	40	160	300	480

2. Modify Program 5.3 to find the **(a)** natural, **(b)** extrapolated, **(c)** parabolically terminated, or **(d)** end-point curvature-adjusted cubic splines for a given set of points.

3. Use your programs from Problem 2 to find the five different cubic splines for the points (0, 1), (1, 0), (2, 0), (3, 1), (4, 2), (5, 2), and (6, 1), where $S'(0) = -0.6$, $S'(6) = -1.8$, $S''(0) = 1$, and $S''(6) = -1$. Plot the five cubic splines and the points on the same coordinate system.

4. Use your programs from Problem 2 to find the five different cubic splines for the points (0, 0), (1, 4), (2, 8), (3, 9), (4, 9), (5, 8) and (6, 6), where $S'(0) = 1$, $S'(6) = -2$, $S''(0) = 1$, and $S''(6) = -1$. Plot the five cubic splines and the points on the same coordinate system.

5. The accompanying table gives the hourly temperature readings (Fahrenheit) during a 12-hour period in a suburb of Los Angeles. Find the natural cubic spline for the data. Graph the natural cubic spline and the data on the same coordinate system. Use the natural cubic spline and the results of part (a) of Exercise 12 to approximate the average temperature during the 12-hour period.

Time, a.m.	Degrees	Time, a.m.	Degrees
1	58	7	57
2	58	8	58
3	58	9	60
4	58	10	64
5	57	11	67
6	57	Noon	68

6. Approximate the graph of $f(x) = x - \cos(x^3)$ over the interval $[-3, 3]$ using a clamped cubic spline.

5.4 Fourier Series and Trigonometric Polynomials

Scientists and engineers often study physical phenomena, such as light and sound, that have a periodic character. They are described by functions $f(x)$ that are periodic,

$$g(x + P) = g(x) \quad \text{for all } x. \tag{1}$$

The number P is called a ***period*** of the function.

It will suffice to consider functions that have period 2π. If $g(x)$ has period P, then $f(x) = g(Px/2\pi)$ will be periodic with period 2π. This is verified by the observation

$$f(x + 2\pi) = g\left(\frac{Px}{2\pi} + P\right) = g\left(\frac{Px}{2\pi}\right) = f(x). \tag{2}$$

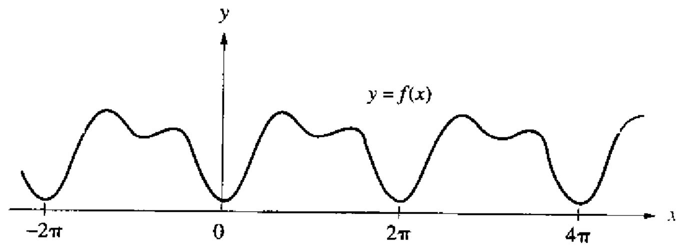

Figure 5.17 A continuous function $f(x)$ with period 2π.

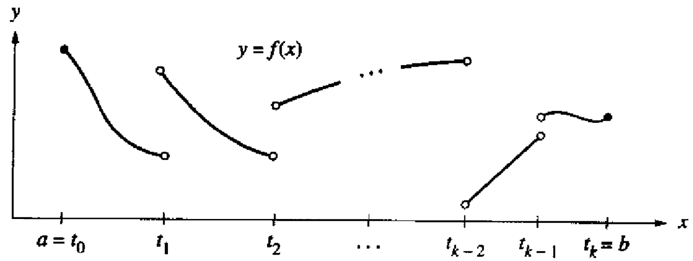

Figure 5.18 A piecewise continuous function over $[a, b]$.

Henceforth in this section we shall assume that $f(x)$ is a function that is periodic with period 2π, that is,

$$f(x + 2\pi) = f(x) \quad \text{for all } x. \tag{3}$$

The graph $y = f(x)$ is obtained by repeating the portion of the graph in any interval of length 2π, as shown in Figure 5.17.

Examples of functions with period 2π are $\sin(jx)$ and $\cos(jx)$, where j is an integer. This raises the following question: Can a periodic function be represented by the sum of terms involving $a_j \cos(jx)$ and $b_j \sin(jx)$? We will soon see that the answer is yes.

Definition 5.2 (Piecewise Continuous). The function $f(x)$ is said to be ***piecewise continuous*** on $[a, b]$ if there exist values $t_0, t_1, \ldots, t_K$ with $a = t_0 < t_1 < \cdots t_K = b$ such that $f(x)$ is continuous on each open interval $t_{i-1} < x < t_i$ for $i = 1, \ldots, K$, and $f(x)$ has left- and right-hand limits at each of the points t_i. The situation is illustrated in Figure 5.18. ▲

Definition 5.3 (Fourier Series). Assume that $f(x)$ is periodic with period 2π and that $f(x)$ is piecewise continuous on $[-\pi, \pi]$. The ***Fourier series*** $S(x)$ for $f(x)$ is

$$S(x) = \frac{a_0}{2} + \sum_{j=1}^{\infty}(a_j \cos(jx) + b_j \sin(jx)), \tag{4}$$

where the coefficients a_j and b_j are computed with Euler's formulas:

$$a_j = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos(jx)\,dx \quad \text{for } j = 0, 1, \ldots \tag{5}$$

and

$$b_j = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin(jx)\,dx \quad \text{for } j = 1, 2, \ldots. \tag{6}$$ ▲

The factor $\frac{1}{2}$ in the constant term $a_0/2$ in the Fourier series (4) has been introduced for convenience so that a_0 could be obtained from the general formula (5) by setting $j = 0$. Convergence of the Fourier series is discussed in the next result.

Theorem 5.5 (Fourier Expansion). Assume that $S(x)$ is the Fourier series for $f(x)$ over $[-\pi, \pi]$. If $f'(x)$ is piecewise continuous on $[-\pi, \pi]$ and has both a left- and right-hand derivative at each point in this interval, then $S(x)$ is convergent for all $x \in [-\pi, \pi]$. The relation

$$S(x) = f(x)$$

holds at all points $x \in [-\pi, \pi]$, where $f(x)$ is continuous. If $x = a$ is a point of discontinuity of f, then

$$S(a) = \frac{f(a^-) + f(a^+)}{2},$$

where $f(a^-)$ and $f(a^+)$ denote the left- and right-hand limits, respectively. With this understanding, we obtain the Fourier expansion:

$$f(x) = \frac{a_0}{2} + \sum_{j=1}^{\infty}(a_j \cos(jx) + b_j \sin(jx)). \tag{7}$$

A brief outline of the derivation of formulas (5) and (6) is given at the end of the section.

Example 5.13. Show that the function $f(x) = x/2$ for $-\pi < x < \pi$, extended periodically by the equation $f(x + 2\pi) = f(x)$, has the Fourier series representation

$$f(x) = \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{2} \sin(jx) = \sin(x) - \frac{\sin(2x)}{2} + \frac{\sin(3x)}{3} - \cdots.$$

Using Euler's formulas and integration by parts, we get

$$a_j = \frac{1}{\pi}\int_{-\pi}^{\pi} \frac{x}{2}\cos(jx)\,dx = \frac{x\sin(jx)}{2\pi j} + \frac{\cos(jx)}{2\pi j^2}\Big|_{-\pi}^{\pi} = 0$$

for $j = 1, 2, 3, \ldots$, and

$$b_j = \frac{1}{\pi}\int_{-\pi}^{\pi} \frac{x}{2}\sin(jx)\,dx = \frac{-x\cos(jx)}{2\pi j} + \frac{\sin(jx)}{2\pi j^2}\Big|_{-\pi}^{\pi} = \frac{(-1)^{j+1}}{j}$$

for $j = 1, 2, 3, \ldots$. The coefficient a_0 is obtained by a separate calculation:

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} \frac{x}{2}\,dx = \frac{x^2}{4\pi}\Big|_{-\pi}^{\pi} = 0.$$

These calculations show that all the coefficients of the cosine functions are zero. The graph of $f(x)$ and the partial sums

$$S_2(x) = \sin(x) - \frac{\sin(2x)}{2},$$
$$S_3(x) = \sin(x) - \frac{\sin(2x)}{2} + \frac{\sin(3x)}{3},$$

and

$$S_4(x) = \sin(x) - \frac{\sin(2x)}{2} + \frac{\sin(3x)}{3} - \frac{\sin(4x)}{4}$$

are shown in Figure 5.19. ■

We now state some general properties of Fourier series. The proofs are left as exercises.

Theorem 5.6 (Cosine Series). Suppose that $f(x)$ is an even function; that is, suppose $f(-x) = f(x)$ holds for all x. If $f(x)$ has period 2π and if $f(x)$ and $f'(x)$ are piecewise continuous, then the Fourier series for $f(x)$ involves only cosine terms:

(8) $$f(x) = \frac{a_0}{2} + \sum_{j=1}^{\infty} a_j \cos(jx),$$

where

(9) $$a_j = \frac{2}{\pi}\int_0^{\pi} f(x)\cos(jx)\,dx \quad \text{for } j = 0, 1, \ldots.$$

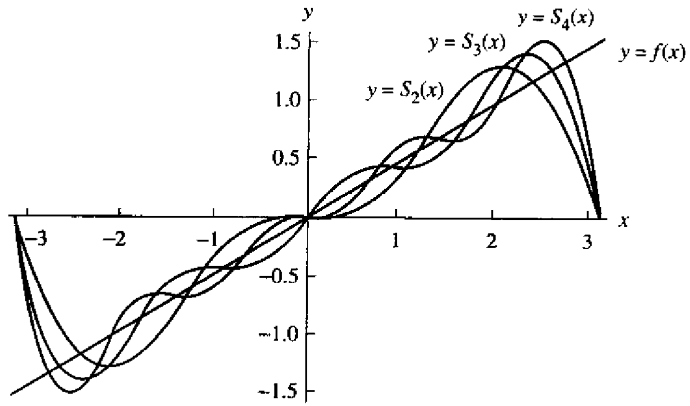

Figure 5.19 The function $f(x) = x/2$ over $[-\pi, \pi]$ and its trigonometric approximation $S_2(x)$, $S_3(x)$ and $S_4(x)$.

Theorem 5.7 (Sine Series). Suppose that $f(x)$ is an odd function; that is, $f(-x) = -f(x)$ holds for all x. If $f(x)$ has period 2π and if $f(x)$ and $f'(x)$ are piecewise continuous, then the Fourier series for $f(x)$ involves only the sine terms:

(10) $$f(x) = \sum_{j=1}^{\infty} b_j \sin(jx),$$

where

(11) $$b_j = \frac{2}{\pi}\int_0^{\pi} f(x)\sin(jx)\,dx \quad \text{for } j = 1, 2, \ldots.$$

Example 5.14. Show that the function $f(x) = |x|$ for $-\pi < x < \pi$, extended periodically by the equation $f(x + 2\pi) = f(x)$, has the Fourier cosine representation

(12) $$f(x) = \frac{\pi}{2} - \frac{4}{\pi}\sum_{j=1}^{\infty} \frac{\cos((2j-1)x)}{(2j-1)^2} = \frac{\pi}{2} - \frac{4}{\pi}\left(\cos(x) + \frac{\cos(3x)}{3^2} + \frac{\cos(5x)}{5^2} + \cdots\right).$$

The function $f(x)$ is an even function, so we can use Theorem 5.6 and need only to compute the coefficients $\{a_j\}$:

$$a_j = \frac{2}{\pi}\int_0^{\pi} x\cos(jx)\,dx = \frac{2x\sin(jx)}{\pi j} + \frac{2\cos(jx)}{\pi j^2}\Big|_0^{\pi}$$
$$= \frac{2\cos(j\pi) - 2}{\pi j^2} = \frac{2((-1)^j - 1)}{\pi j^2} \quad \text{for } j = 1, 2, 3, \ldots.$$

Since $((-1)^j - 1) = 0$ when j is even, the cosine series will involve only the odd terms. The odd coefficients have the pattern

$$a_1 = \frac{-4}{\pi}, \quad a_3 = \frac{-4}{\pi 3^2}, \quad a_5 = \frac{-4}{\pi 5^2}, \quad \ldots.$$

The coefficient a_0 is obtained by the separate calculation

$$a_0 = \frac{2}{\pi}\int_0^{\pi} x\,dx = \frac{x^2}{\pi}\Big|_0^{\pi} = \pi.$$

Therefore, we have found the desired coefficients in (12). ■

Proof of Euler's Formulas for Theorem 5.5. The following heuristic argument assumes the existence and convergence of the Fourier series representation. To determine a_0, we can integrate both sides of (7) and get

(13)
$$\begin{aligned}\int_{-\pi}^{\pi} f(x)\,dx &= \int_{-\pi}^{\pi}\left(\frac{a_0}{2} + \sum_{j=1}^{\infty}(a_j\cos(jx) + b_j\sin(jx))\right)dx \\ &= \int_{-\pi}^{\pi}\frac{a_0}{2}\,dx + \sum_{j=1}^{\infty} a_j\int_{-\pi}^{\pi}\cos(jx)\,dx + \sum_{j=1}^{\infty} b_j\int_{-\pi}^{\pi}\sin(jx)\,dx \\ &= \pi a_0 + 0 + 0.\end{aligned}$$

Justification for switching the order of integration and summation requires a detailed treatment of uniform convergence and can be found in advanced texts. Hence we have shown that

(14)
$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\,dx.$$

To determine a_m, we let $m > 0$ be a fixed integer, multiply both sides of (7) by $\cos(mx)$, and integrate both sides to obtain

(15)
$$\begin{aligned}\int_{-\pi}^{\pi} f(x)\cos(mx)\,dx &= \frac{a_0}{2}\int_{-\pi}^{\pi}\cos(mx)\,dx + \sum_{j=1}^{\infty} a_j\int_{-\pi}^{\pi}\cos(jx)\cos(mx)\,d \\ &\quad + \sum_{j=1}^{\infty} b_j\int_{-\pi}^{\pi}\sin(jx)\cos(mx)\,dx.\end{aligned}$$

Equation (15) can be simplified by using the orthogonal properties of the trigonometric functions, which are now stated. The value of the first term on the right-hand side of (15) is

(16)
$$\frac{a_0}{2}\int_{-\pi}^{\pi}\cos(mx)\,dx = \frac{a_0\sin(mx)}{2m}\Big|_{-\pi}^{\pi} = 0.$$

The value of the term involving $\cos(jx)\cos(mx)$ is found by using the trigonometric identity

(17)
$$\cos(jx)\cos(mx) = \frac{1}{2}\cos((j+m)x) + \frac{1}{2}\cos((j-m)x).$$

When $j \neq m$, then (17) is used to get

(18)
$$\begin{aligned}a_j\int_{-\pi}^{\pi}\cos(jx)\cos(mx)\,dx &= \frac{1}{2}a_j\int_{-\pi}^{\pi}\cos((j+m)x)\,dx \\ &\quad + \frac{1}{2}a_j\int_{-\pi}^{\pi}\cos((j-m)x)\,dx = 0 + 0 = 0.\end{aligned}$$

When $j = m$, the value of the integral is

(19)
$$a_m\int_{-\pi}^{\pi}\cos(jx)\cos(mx)\,dx = a_m\pi.$$

The value of the term on the right side of (15) involving $\sin(jx)\cos(mx)$ is found by using the trigonometric identity

(20)
$$\sin(jx)\cos(mx) = \frac{1}{2}\sin((j+m)x) + \frac{1}{2}\sin((j-m)x).$$

For all values of j and m in (20), we obtain

(21)
$$\begin{aligned}b_j\int_{-\pi}^{\pi}\sin(jx)\cos(mx)\,dx &= \frac{1}{2}b_j\int_{-\pi}^{\pi}\sin((j+m)x)\,dx \\ &\quad + \frac{1}{2}b_j\int_{-\pi}^{\pi}\sin((j-m)x)\,dx = 0 + 0 = 0.\end{aligned}$$

Therefore, using the results of (16), (18), (19), and (21) in equation (15), we conclude that

(22)
$$\pi a_m = \int_{-\pi}^{\pi} f(x)\cos(mx)\,dx, \qquad \text{for } m = 1, 2, \ldots.$$

Therefore, Euler's formula (5) is established. Euler's formula (6) is proved similarly. •

Trigonometric Polynomial Approximation

Definition 5.4 (Trigonometric Polynomial). A series of the form

(23)
$$T_M(x) = \frac{a_0}{2} + \sum_{j=1}^{M}(a_j\cos(jx) + b_j\sin(jx))$$

is called a ***trigonometric polynomial*** of order M. ▲

Theorem 5.8 (Discrete Fourier Series). Suppose that $\{(x_j, y_j)\}_{j=0}^{N}$ are $N+1$ points where $y_j = f(x_j)$, and the abscissas are equally spaced:

$$x_j = -\pi + \frac{2j\pi}{N} \quad \text{for } j = 0, 1, \ldots, N. \tag{24}$$

If $f(x)$ is periodic with period 2π and $2M < N$, then there exists a trigonometric polynomial $T_M(x)$ of the form (23) that minimizes the quantity

$$\sum_{k=1}^{N} (f(x_k) - T_M(x_k))^2. \tag{25}$$

The coefficients a_j and b_j of this polynomial are computed with the formulas

$$a_j = \frac{2}{N} \sum_{k=1}^{N} f(x_k)\cos(jx_k) \quad \text{for } j = 0, 1, \ldots, M, \tag{26}$$

and

$$b_j = \frac{2}{N} \sum_{k=1}^{N} f(x_k)\sin(jx_k) \quad \text{for } j = 1, 2, \ldots, M. \tag{27}$$

Although formulas (26) and (27) are defined with the least-squares procedure, they can also be viewed as numerical approximations to the integrals in Euler's formulas (5) and (6). Euler's formulas give the coefficients for the Fourier series of a continuous function, whereas formulas (26) and (27) give the trigonometric polynomial coefficients for curve fitting to data points. The next example uses data points generated by the function $f(x) = x/2$ at discrete points. When more points are used, the trigonometric polynomial coefficients get closer to the Fourier series coefficients.

Example 5.15. Use the 12 equally spaced points $x_k = -\pi + k\pi/6$, for $k = 1, 2, \ldots, 12$, and find the trigonometric polynomial approximation for $M = 5$ to the 12 data points $\{(x_k, f(x_k))\}_{k=1}^{12}$, where $f(x) = x/2$. Also compare the results when 60 and 360 points are used and with the first five terms of the Fourier series expansion for $f(x)$ that is given in Example 5.13.

Since the periodic extension is assumed, at a point of discontinuity, the function value $f(\pi)$ must be computed using the formula

$$f(\pi) = \frac{f(\pi^-) + f(\pi^+)}{2} = \frac{\pi/2 - \pi/2}{2} = 0. \tag{28}$$

The function $f(x)$ is an odd function; hence the coefficients for the cosine terms are all zero (i.e., $a_j = 0$ for all j). The trigonometric polynomial of degree $M = 5$ involves only the sine terms, and when formula (27) is used with (28), we get

$$\begin{aligned} T_5(x) = {} & 0.9770486\sin(x) - 0.4534498\sin(2x) + 0.26179938\sin(3x) \\ & - 0.1511499\sin(4x) + 0.0701489\sin(5x). \end{aligned} \tag{29}$$

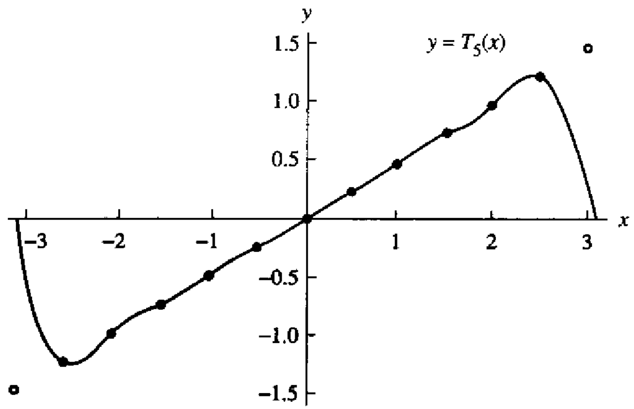

Figure 5.20 The trigonometric polynomial $T_5(x)$ of degree $M = 5$, based on 12 data points that lie on the line $y = x/2$.

Table 5.9 Comparison of Trigonometric Polynomial Coefficients for Approximations to $f(x) = x/2$ over $[-\pi, \pi]$

	Trigonometric polynomial coefficients			Fourier series coefficients
	12 points	60 points	360 points	
b_1	0.97704862	0.99908598	0.99997462	1.0
b_2	−0.45344984	−0.49817096	−0.49994923	−0.5
b_3	0.26179939	0.33058726	0.33325718	0.33333333
b_4	−0.15114995	−0.24633386	−0.24989845	−0.25
b_5	0.07014893	0.19540972	0.19987306	0.2

The graph of $T_5(x)$ is shown in Figure 5.20.

The coefficients of the fifth-degree trigonometric polynomial change slightly when the number of interpolation points increases to 60 and 360. As the number of points increases, they get closer to the coefficients of the Fourier series expansion of $f(x)$. The results are compared in Table 5.9. ∎

The following program constructs matrices A and B that contain the coefficients a_j and b_j, respectively, of the trigonometric polynomial (23) of order M.

Program 5.4 (Trigonometric Polynomials). To construct the trigonometric polynomial of order M of the form

$$P(x) = \frac{a_0}{2} + \sum_{j=1}^{M}(a_j \cos(jx) + b_j \sin(jx))$$

based on the N equally spaced values $x_k = -\pi + 2\pi k/N$, for $k = 1, 2, \ldots, N$. The construction is possible provided that $2M + 1 \le N$.

```
function [A,B]=tpcoeff(X,Y,M)
%Input  - X is a vector of equally spaced abscissas in [-pi,pi]
%       - Y is a vector of ordinates
%       - M is the degree of the trigonometric polynomial
%Output - A is a vector containing the coefficients of cos(jx)
%       - B is a vector containing the coefficients of sin(jx)
N=length(X)-1;
max1=fix((N-1)/2);
if M>max1
   M=max1;
end
A=zeros(1,M+1);
B=zeros(1,M+1);
Yends=(Y(1)+Y(N+1))/2;
Y(1)=Yends;
Y(N+1)=Yends;
A(1)=sum(Y);
for j=1:M
   A(j+1)=cos(j*X)*Y';
   B(j+1)=sin(j*X)*Y';
end
A=2*A/N;
B=2*B/N;
A(1)=A(1)/2;
```

The following short program will evaluate the trigonometric polynomial $P(x)$ of order M from Program 5.4 at a particular value of x.

```
function z=tp(A,B,x,M)
z=A(1);
for j= 1:M
   z=z+A(j+1)*cos(j*x)+B(j+1)*sin(j*x);
end
```


For example, the following sequence of commands in the MATLAB command window will produce a graph analogous to Figure 5.20.

```
>>x=-pi:.01:pi;
>>y=tp(A,B,x,M);
>>plot(x,y,X,Y,'o')
```

Exercises for Fourier Series and Trigonometric Polynomials

In Exercises 1 through 5, find the Fourier series representation of the given function. *Hint.* Follow the procedures outlined in Examples 5.13 and 5.14. Graph each function and the partial sums $S_2(x)$, $S_3(x)$, and $S_4(x)$ of its Fourier series representation on the same coordinate system (see Figure 5.19).

1. $f(x) = \begin{cases} -1 & \text{for } -\pi < x < 0 \\ 1 & \text{for } 0 < x < \pi \end{cases}$

2. $f(x) = \begin{cases} \frac{\pi}{2} + x & \text{for } -\pi \le x < 0 \\ \frac{\pi}{2} - x & \text{for } 0 \le x < \pi \end{cases}$

3. $f(x) = \begin{cases} 0 & \text{for } -\pi \le x < 0 \\ x & \text{for } 0 \le x < \pi \end{cases}$

4. $f(x) = \begin{cases} -1 & \text{for } \frac{\pi}{2} < x < \pi \\ 1 & \text{for } \frac{-\pi}{2} < x < \frac{\pi}{2} \\ -1 & \text{for } -\pi < x < \frac{-\pi}{2} \end{cases}$

5. $f(x) = \begin{cases} -\pi - x & \text{for } -\pi \le x < \frac{-\pi}{2} \\ x & \text{for } \frac{-\pi}{2} \le x < \frac{\pi}{2} \\ \pi - x & \text{for } \frac{\pi}{2} \le x < \pi \end{cases}$

6. In Exercise 1, set $x = \pi/2$ and show that

$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \cdots.$$

7. In Exercise 2, set $x = 0$ and show that

$$\frac{\pi^2}{8} = 1 + \frac{1}{3^2} + \frac{1}{5^2} + \frac{1}{7^2} + \cdots.$$

8. Find the Fourier cosine series representation for the periodic function whose definition on one period is $f(x) = x^2/4$ where $-\pi \le x < \pi$.

9. Suppose that $f(x)$ is a periodic function with period $2P$; that is, $f(x + 2P) = f(x)$ for all x. By making an appropriate substitution, show that Euler's formulas (5) and (6) for f are

$$a_0 = \frac{1}{P}\int_{-P}^{P} f(x)\,dx$$

$$a_j = \frac{1}{P}\int_{-P}^{P} f(x)\cos\left(\frac{j\pi x}{P}\right)dx \quad \text{for } j = 1,\ 2,\ \ldots$$

$$b_j = \frac{1}{P}\int_{-P}^{P} f(x)\sin\left(\frac{j\pi x}{P}\right)dx \quad \text{for } j = 1,\ 2,\ \ldots.$$

In Exercises 10 through 12, use the results of Exercise 9 to find the Fourier series rep resentation of the given function. Graph $f(x)$, $S_4(x)$, and $S_6(x)$ on the same coordinat system.

10. $f(x) = \begin{cases} 0 & \text{for } -2 \le x < 0 \\ 1 & \text{for } 0 \le x < 2 \end{cases}$

11. $f(x) = \begin{cases} -1 & \text{for } -3 \le x < -1 \\ |x| & \text{for } -1 \le x < 1 \\ 1 & \text{for } 1 \le x < 3 \end{cases}$

12. $f(x) = -x^2 + 9 \quad \text{for } -3 \le x < 3.$

13. Prove Theorem 5.6.

14. Prove Theorem 5.7.

Algorithms and Programs

1. Use Program 5.4 with $N = 12$ points and follow Example 5.15 to find the trigono metric polynomial of degree $M = 5$ for the equally spaced points $\{(x_k, f(x_k))\}_{k=1}^{12}$, where $f(x)$ is the function in (a) Exercise 1, (b) Exercise 2, (c) Exercise 3, and (d) Exercise 4. In each case, produce a graph of $f(x)$, $T_5(x)$, and $\{(x_k, f(x_k))\}_{k=1}^{12}$ on the same coordinate system.
2. Use Program 5.4 to find the coefficients of $T_5(x)$ in Example 5.15 when first 60 and then 360 equally spaced points are used.
3. Modify Program 5.4 so that it will find the trigonometric polynomial of period $2P = b - a$ when the data points are equally spaced over the interval $[a, b]$.
4. Use Program 5.4 to find $T_5(x)$ for (a) $f(x)$ in Exercise 10, using 12 equally spaced data points, and (b) $f(x)$ in Exercise 12, using 60 equally spaced data points. In eacl case, graph $T_5(x)$ and the data points on the same coordinate system.
5. The temperature cycle (Fahrenheit) in a suburb of Los Angeles on November 8 i given in Table 5.10. There are 24 data points.
   (a) Find the trigonometric polynomial $T_7(x)$.
   (b) Graph $T_7(x)$ and the 24 data points on the same coordinate system.
   (c) Repeat parts (a) and (b) using temperatures from your locale.
6. The yearly temperature cycle (Fahrenheit) for Fairbanks, Alaska, is given in Ta ble 5.11. There are 13 equally spaced data points, which correspond to a measuremen every 28 days.
   (a) Find the trigonometric polynomial $T_6(x)$.
   (b) Graph $T_6(x)$ and the 13 data points on the same coordinate system.

Table 5.10 Data for Problem 5

Time, p.m.	Degrees	Time, a.m.	Degrees
1	66	1	58
2	66	2	58
3	65	3	58
4	64	4	58
5	63	5	57
6	63	6	57
7	62	7	57
8	61	8	58
9	60	9	60
10	60	10	64
11	59	11	67
Midnight	58	Noon	68

Table 5.11 Data for Problem 6

Calendar date	Average degrees
Jan. 1	−14
Jan. 29	−9
Feb. 26	2
Mar. 26	15
Apr. 23	35
May 21	52
June 18	62
July 16	63
Aug. 13	58
Sept. 10	50
Oct. 8	34
Nov. 5	12
Dec. 3	−5