MATH 302
NUMERICAL ANALYSIS

SOLVED EXERCISES

AN OVERVİEW

Chp-2
Systems of Linear Algebraic Equations

2.1 Introduction

EXAMPLE 2.1

Determine whether the following matrix is singular:

$$\mathbf{A} = \begin{bmatrix} 2.1 & -0.6 & 1.1 \\ 3.2 & 4.7 & -0.8 \\ 3.1 & -6.5 & 4.1 \end{bmatrix}$$

Solution. Laplace's development of the determinant (see Appendix A2) about the first row of **A** yields

$$\begin{aligned} |\mathbf{A}| &= 2.1 \begin{vmatrix} 4.7 & -0.8 \\ -6.5 & 4.1 \end{vmatrix} - (-0.6) \begin{vmatrix} 3.2 & -0.8 \\ 3.1 & 4.1 \end{vmatrix} + 1.1 \begin{vmatrix} 3.2 & 4.7 \\ 3.1 & -6.5 \end{vmatrix} \\ &= 2.1(14.07) + 0.6(15.60) + 1.1(35.37) = 0 \end{aligned}$$

Since the determinant is zero, the matrix is singular. It can be verified that the singularity is due to the following row dependency: $(\text{row}\,3) = (3 \times \text{row}\,1) - (\text{row}\,2)$.

EXAMPLE 2.2

Solve the equations $\mathbf{Ax} = \mathbf{b}$, where

$$\mathbf{A} = \begin{bmatrix} 8 & -6 & 2 \\ -4 & 11 & -7 \\ 4 & -7 & 6 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 28 \\ -40 \\ 33 \end{bmatrix}$$

knowing that the LU decomposition of the coefficient matrix is (you should verify this)

$$\mathbf{A} = \mathbf{LU} = \begin{bmatrix} 2 & 0 & 0 \\ -1 & 2 & 0 \\ 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 4 & -3 & 1 \\ 0 & 4 & -3 \\ 0 & 0 & 2 \end{bmatrix}$$

Solution. We first solve the equations $\mathbf{Ly} = \mathbf{b}$ by forward substitution:

$$\begin{aligned} 2y_1 &= 28 & y_1 &= 28/2 = 14 \\ -y_1 + 2y_2 &= -40 & y_2 &= (-40 + y_1)/2 = (-40 + 14)/2 = -13 \\ y_1 - y_2 + y_3 &= 33 & y_3 &= 33 - y_1 + y_2 = 33 - 14 - 13 = 6 \end{aligned}$$

The solution $\mathbf{x}$ is then obtained from $\mathbf{Ux} = \mathbf{y}$ by back substitution:

$$\begin{aligned} 2x_3 &= y_3 & x_3 &= y_3/2 = 6/2 = 3 \\ 4x_2 - 3x_3 &= y_2 & x_2 &= (y_2 + 3x_3)/4 = [-13 + 3(3)]/4 = -1 \\ 4x_1 - 3x_2 + x_3 &= y_1 & x_1 &= (y_1 + 3x_2 - x_3)/4 = [14 + 3(-1) - 3]/4 = 2 \end{aligned}$$

Hence the solution is $\mathbf{x} = \begin{bmatrix} 2 & -1 & 3 \end{bmatrix}^T$.

2.2 Gauss Elimination Method

EXAMPLE 2.3

Use Gauss elimination to solve the equations $\mathbf{AX} = \mathbf{B}$, where

$$\mathbf{A} = \begin{bmatrix} 6 & -4 & 1 \\ -4 & 6 & -4 \\ 1 & -4 & 6 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} -14 & 22 \\ 36 & -18 \\ 6 & 7 \end{bmatrix}$$

Solution. The augmented coefficient matrix is

$$\left[\begin{array}{rrr|rr} 6 & -4 & 1 & -14 & 22 \\ -4 & 6 & -4 & 36 & -18 \\ 1 & -4 & 6 & 6 & 7 \end{array}\right]$$

The elimination phase consists of the following two passes:

$$\text{row } 2 \leftarrow \text{row } 2 + (2/3) \times \text{row } 1$$

$$\text{row } 3 \leftarrow \text{row } 3 - (1/6) \times \text{row } 1$$

$$\left[\begin{array}{lrr|rr} 6 & -4 & 1 & -14 & 22 \\ 0 & 10/3 & -10/3 & 80/3 & -10/3 \\ 0 & -10/3 & 35/6 & 25/3 & 10/3 \end{array}\right]$$

and

$$\text{row } 3 \leftarrow \text{row } 3 + \text{row } 2$$

$$\left[\begin{array}{rrr|rr} 6 & -4 & 1 & -14 & 22 \\ 0 & 10/3 & -10/3 & 80/3 & -10/3 \\ 0 & 0 & 5/2 & 35 & 0 \end{array}\right]$$

In the solution phase, we first compute $\mathbf{x}_1$ by back substitution:

$$X_{31} = \frac{35}{5/2} = 14$$

$$X_{21} = \frac{80/3 + (10/3)X_{31}}{10/3} = \frac{80/3 + (10/3)14}{10/3} = 22$$

$$X_{11} = \frac{-14 + 4X_{21} - X_{31}}{6} = \frac{-14 + 4(22) - 14}{6} = 10$$

Thus the first solution vector is

$$\mathbf{x}_1 = \left[\, X_{11} \quad X_{21} \quad X_{31} \,\right]^T = \left[\, 10 \quad 22 \quad 14 \,\right]^T$$

The second solution vector is computed next, also using back substitution:

$$\begin{aligned}
X_{32} &= 0 \\
X_{22} &= \frac{-10/3 + (10/3)\,X_{32}}{10/3} = \frac{-10/3 + 0}{10/3} = -1 \\
X_{12} &= \frac{22 + 4X_{22} - X_{32}}{6} = \frac{22 + 4(-1) - 0}{6} = 3
\end{aligned}$$

Therefore,

$$\mathbf{x}_2 = \left[\, X_{12} \quad X_{22} \quad X_{32} \,\right]^T = \left[\, 3 \quad -1 \quad 0 \,\right]^T$$

EXAMPLE 2.4

An $n \times n$ Vandermode matrix **A** is defined by

$$A_{ij} = v_i^{n-j}, \quad i = 1, 2, \ldots, n, \quad j = 1, 2, \ldots, n$$

where **v** is a vector. Use the Gaussian Elimination method to compute the solution of

Ax = **b**, where **A** is the 3 × 3 Vandermode matrix generated from the vector

v =[1.0 -1.0 2.0] and **b** =[1.0 2.0 3.0]

Solution

$$\boldsymbol{A} = \begin{bmatrix} 1 & v_1 & v_1^2 \\ 1 & v_2 & v_2^2 \\ 1 & v_3 & v_3^2 \end{bmatrix} \longrightarrow \boldsymbol{A} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 2 & 4 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 2 \\ 1 & 2 & 4 & 3 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & -2 & 0 & 1 \\ 0 & 0 & 3 & 5/2 \end{bmatrix} \longrightarrow$$

$3x_3 = 5/2$

$x_3 = 5/6$

$-2x_2 = 1$

$x_2 = -1/2$

$x_1 + x_2 + x_3 = 1$

$x_1 = 2/3$

2.3 LU Decomposition Methods

EXAMPLE 2.5

Use Doolittle's decomposition method to solve the equations $\mathbf{Ax} = \mathbf{b}$, where

$$\mathbf{A} = \begin{bmatrix} 1 & 4 & 1 \\ 1 & 6 & -1 \\ 2 & -1 & 2 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 7 \\ 13 \\ 5 \end{bmatrix}$$

Solution. We first decompose $\mathbf{A}$ by Gauss elimination. The first pass consists of the elementary operations

$$\text{row 2} \leftarrow \text{row 2} - 1 \times \text{ row 1 (eliminates } A_{21})$$

$$\text{row 3} \leftarrow \text{row 3} - 2 \times \text{ row 1 (eliminates } A_{31})$$

Storing the multipliers $L_{21} = 1$ and $L_{31} = 2$ in place of the eliminated terms, we obtain

$$\mathbf{A}' = \begin{bmatrix} 1 & 4 & 1 \\ 1 & 2 & -2 \\ 2 & -9 & 0 \end{bmatrix}$$

The second pass of Gauss elimination uses the operation

$$\text{row } 3 \leftarrow \text{row } 3 - (-4.5) \times \text{ row } 2 \text{ (eliminates } A_{32}\text{)}$$

Storing the multiplier $L_{32} = -4.5$ in place of A_{32}, we get

$$\mathbf{A}'' = [\mathbf{L}\backslash\mathbf{U}] = \begin{bmatrix} 1 & 4 & 1 \\ 1 & 2 & -2 \\ 2 & -4.5 & -9 \end{bmatrix}$$

The decomposition is now complete, with

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & -4.5 & 1 \end{bmatrix} \qquad \mathbf{U} = \begin{bmatrix} 1 & 4 & 1 \\ 0 & 2 & -2 \\ 0 & 0 & -9 \end{bmatrix}$$

Solution of $\mathbf{Ly} = \mathbf{b}$ by forward substitution comes next. The augmented coefficient form of the equations is

$$\begin{bmatrix} \mathbf{L} \mid \mathbf{b} \end{bmatrix} = \left[\begin{array}{ccc|c} 1 & 0 & 0 & 7 \\ 1 & 1 & 0 & 13 \\ 2 & -4.5 & 1 & 5 \end{array}\right]$$

The solution is

$$y_1 = 7$$

$$y_2 = 13 - y_1 = 13 - 7 = 6$$

$$y_3 = 5 - 2y_1 + 4.5y_2 = 5 - 2(7) + 4.5(6) = 18$$

Finally, the equations $\mathbf{Ux} = \mathbf{y}$, or

$$\left[\mathbf{U} \;\middle|\; \mathbf{y}\right] = \left[\begin{array}{ccr|r} 1 & 4 & 1 & 7 \\ 0 & 2 & -2 & 6 \\ 0 & 0 & -9 & 18 \end{array}\right]$$

are solved by back substitution. This yields

$$x_3 = \frac{18}{-9} = -2$$

$$x_2 = \frac{6 + 2x_3}{2} = \frac{6 + 2(-2)}{2} = 1$$

$$x_1 = 7 - 4x_2 - x_3 = 7 - 4(1) - (-2) = 5$$

EXAMPLE 2.7

Solve **AX** = **B** with Doolittle's decomposition method and computes |**A**|.

$$\mathbf{A} = \begin{bmatrix} 3 & -1 & 4 \\ -2 & 0 & 5 \\ 7 & 2 & -2 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} 6 & -4 \\ 3 & 2 \\ 7 & -5 \end{bmatrix}$$

Solution

$$\boldsymbol{L} = \begin{bmatrix} 1 & 0 & 0 \\ -2/3 & 1 & 0 \\ 7/3 & -13/2 & 1 \end{bmatrix} \qquad \boldsymbol{U} = \begin{bmatrix} 3 & -1 & 4 \\ 0 & -2/3 & 23/3 \\ 0 & 0 & 231/6 \end{bmatrix}$$

|**A**|= -77

X1 =[1.0 1.0 1.0]

X2 =[1.0 1.0 0.0]

2.7 Iterative Methods
(Gauss-Seidel Method)
(Conjugate Gradient Method)

EXAMPLE 2.15

Solve the equations

$$\begin{bmatrix} 4 & -1 & 1 \\ -1 & 4 & -2 \\ 1 & -2 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 12 \\ -1 \\ 5 \end{bmatrix}$$

by the Gauss-Seidel method without relaxation.

Solution. With the given data, the iteration formulas in Eq. (2.34) become

$$x_1 = \frac{1}{4}(12 + x_2 - x_3)$$

$$x_2 = \frac{1}{4}(-1 + x_1 + 2x_3)$$

$$x_3 = \frac{1}{4}(5 - x_1 + 2x_2)$$

Choosing the starting values $x_1 = x_2 = x_3 = 0$, the first iteration gives us

$$x_1 = \frac{1}{4}(12 + 0 - 0) = 3$$

$$x_2 = \frac{1}{4}[-1 + 3 + 2(0)] = 0.5$$

$$x_3 = \frac{1}{4}[5 - 3 + 2(0.5)] = 0.75$$

The second iteration yields

$$x_1 = \frac{1}{4}(12 + 0.5 - 0.75) = 2.9375$$

$$x_2 = \frac{1}{4}[-1 + 2.9375 + 2(0.75)] = 0.859\,38$$

$$x_3 = \frac{1}{4}[5 - 2.9375 + 2(0.859\,38)] = 0\,.945\,31$$

and the third iteration results in

$$x_1 = \frac{1}{4}(12 + 0.85938 - 0\,.94531) = 2.978\,52$$

$$x_2 = \frac{1}{4}[-1 + 2.97852 + 2(0\,.94531)] = 0.967\,29$$

$$x_3 = \frac{1}{4}[5 - 2.97852 + 2(0.96729)] = 0.989\,02$$

After five more iterations the results would agree with the exact solution $x_1 = 3$, $x_2 = x_3 = 1$ within five decimal places.

EXAMPLE 2.16

Solve the equations in Example 2.15 by the conjugate gradient method.

Solution. The conjugate gradient method should converge after three iterations. Choosing again for the starting vector

$$\mathbf{x}_0 = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T,$$

the computations outlined in the text proceed as follows:

First Iteration

$$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0 = \begin{bmatrix} 12 \\ -1 \\ 5 \end{bmatrix} - \begin{bmatrix} 4 & -1 & 1 \\ -1 & 4 & -2 \\ 1 & -2 & 4 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 12 \\ -1 \\ 5 \end{bmatrix}$$

$$\mathbf{s}_0 = \mathbf{r}_0 = \begin{bmatrix} 12 \\ -1 \\ 5 \end{bmatrix}$$

$$\mathbf{A}\mathbf{s}_0 = \begin{bmatrix} 4 & -1 & 1 \\ -1 & 4 & -2 \\ 1 & -2 & 4 \end{bmatrix} \begin{bmatrix} 12 \\ -1 \\ 5 \end{bmatrix} = \begin{bmatrix} 54 \\ -26 \\ 34 \end{bmatrix}$$

$$\alpha_0 = \frac{\mathbf{s}_0^T \mathbf{r}_0}{\mathbf{s}_0^T \mathbf{A}\mathbf{s}_0} = \frac{12^2 + (-1)^2 + 5^2}{12(54) + (-1)(-26) + 5(34)} = 0.201\,42$$

$$\mathbf{x}_1 = \mathbf{x}_0 + \alpha_0 \mathbf{s}_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} + 0.201\,42 \begin{bmatrix} 12 \\ -1 \\ 5 \end{bmatrix} = \begin{bmatrix} 2.41\,704 \\ -0.201\,42 \\ 1.007\,10 \end{bmatrix}$$

Second Iteration

$$\mathbf{r}_1 = \mathbf{b} - \mathbf{A}\mathbf{x}_1 = \begin{bmatrix} 12 \\ -1 \\ 5 \end{bmatrix} - \begin{bmatrix} 4 & -1 & 1 \\ -1 & 4 & -2 \\ 1 & -2 & 4 \end{bmatrix} \begin{bmatrix} 2.41704 \\ -0.20142 \\ 1.00710 \end{bmatrix} = \begin{bmatrix} 1.12332 \\ 4.23692 \\ -1.84828 \end{bmatrix}$$

$$\beta_0 = -\frac{\mathbf{r}_1^T \mathbf{A}\mathbf{s}_0}{\mathbf{s}_0^T \mathbf{A}\mathbf{s}_0} = -\frac{1.12332(54) + 4.23692(-26) - 1.84828(34)}{12(54) + (-1)(-26) + 5(34)} = 0.133107$$

$$\mathbf{s}_1 = \mathbf{r}_1 + \beta_0 \mathbf{s}_0 = \begin{bmatrix} 1.12332 \\ 4.23692 \\ -1.84828 \end{bmatrix} + 0.133107 \begin{bmatrix} 12 \\ -1 \\ 5 \end{bmatrix} = \begin{bmatrix} 2.72076 \\ 4.10380 \\ -1.18268 \end{bmatrix}$$

$$\mathbf{A}\mathbf{s}_1 = \begin{bmatrix} 4 & -1 & 1 \\ -1 & 4 & -2 \\ 1 & -2 & 4 \end{bmatrix} \begin{bmatrix} 2.72076 \\ 4.10380 \\ -1.18268 \end{bmatrix} = \begin{bmatrix} 5.59656 \\ 16.05980 \\ -10.21760 \end{bmatrix}$$

$$\alpha_1 = \frac{\mathbf{s}_1^T \mathbf{r}_1}{\mathbf{s}_1^T \mathbf{A}\mathbf{s}_1}$$

$$= \frac{2.72076(1.12332) + 4.10380(4.23692) + (-1.18268)(-1.84828)}{2.72076(5.59656) + 4.10380(16.05980) + (-1.18268)(-10.21760)}$$

$$= 0.24276$$

$$\mathbf{x}_2 = \mathbf{x}_1 + \alpha_1 \mathbf{s}_1 = \begin{bmatrix} 2.41704 \\ -0.20142 \\ 1.00710 \end{bmatrix} + 0.24276 \begin{bmatrix} 2.72076 \\ 4.10380 \\ -1.18268 \end{bmatrix} = \begin{bmatrix} 3.07753 \\ 0.79482 \\ 0.71999 \end{bmatrix}$$

Third Iteration

$$\mathbf{r}_2 = \mathbf{b} - \mathbf{A}\mathbf{x}_2 = \begin{bmatrix} 12 \\ -1 \\ 5 \end{bmatrix} - \begin{bmatrix} 4 & -1 & 1 \\ -1 & 4 & -2 \\ 1 & -2 & 4 \end{bmatrix} \begin{bmatrix} 3.077\,53 \\ 0.794\,82 \\ 0.719\,99 \end{bmatrix} = \begin{bmatrix} -0.235\,29 \\ 0.338\,23 \\ 0.632\,15 \end{bmatrix}$$

$$\beta_1 = -\frac{\mathbf{r}_2^T \mathbf{A}\mathbf{s}_1}{\mathbf{s}_1^T \mathbf{A}\mathbf{s}_1}$$

$$= -\frac{(-0.235\,29)(5.596\,56) + 0.338\,23(16.059\,80) + 0.632\,15(-10.217\,60)}{2.720\,76(5.596\,56) + 4.103\,80(16.059\,80) + (-1.182\,68)(-10.217\,60)}$$

$$= 0.0251\,452$$

$$\mathbf{s}_2 = \mathbf{r}_2 + \beta_1 \mathbf{s}_1 = \begin{bmatrix} -0.235\,29 \\ 0.338\,23 \\ 0.632\,15 \end{bmatrix} + 0.025\,1452 \begin{bmatrix} 2.720\,76 \\ 4.103\,80 \\ -1.182\,68 \end{bmatrix} = \begin{bmatrix} -0.166\,876 \\ 0.441\,421 \\ 0.602\,411 \end{bmatrix}$$

$$\mathbf{A}\mathbf{s}_2 = \begin{bmatrix} 4 & -1 & 1 \\ -1 & 4 & -2 \\ 1 & -2 & 4 \end{bmatrix} \begin{bmatrix} -0.166\,876 \\ 0.441\,421 \\ 0.602\,411 \end{bmatrix} = \begin{bmatrix} -0.506\,514 \\ 0.727\,738 \\ 1.359\,930 \end{bmatrix}$$

$$
\begin{aligned}
\alpha_2 &= \frac{\mathbf{r}_2^T\mathbf{s}_2}{\mathbf{s}_2^T\mathbf{A}\mathbf{s}_2} \\
&= \frac{(-0.235\,29)(-0.166\,876) + 0.338\,23(0.441\,421) + 0.632\,15(0.602\,411)}{(-0.166\,876)(-0.506\,514) + 0.441\,421(0.727\,738) + 0.602\,411(1.359\,930)} \\
&= 0.464\,80
\end{aligned}
$$

$$
\mathbf{x}_3 = \mathbf{x}_2 + \alpha_2\mathbf{s}_2 = \begin{bmatrix} 3.077\,53 \\ 0.794\,82 \\ 0.719\,99 \end{bmatrix} + 0.464\,80 \begin{bmatrix} -0.166\,876 \\ 0.441\,421 \\ 0.602\,411 \end{bmatrix} = \begin{bmatrix} 2.999\,97 \\ 0.999\,99 \\ 0.999\,99 \end{bmatrix}
$$

The solution $\mathbf{x}_3$ is correct to almost five decimal places. The small discrepancy may be caused by roundoff errors in the computations.

Chp-3
Interpolation and Curve Fitting

3.2 Polynomial Interpolation
(Lagrange's Method)
(Newton's Method)

EXAMPLE 3.1

Given the data points

x	0	2	3
y	7	11	28

use Lagrange's method to determine y at $x = 1$.

Solution

$$\ell_0 = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} = \frac{(1-2)(1-3)}{(0-2)(0-3)} = \frac{1}{3}$$

$$\ell_1 = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} = \frac{(1-0)(1-3)}{(2-0)(2-3)} = 1$$

$$\ell_2 = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} = \frac{(1-0)(1-2)}{(3-0)(3-2)} = -\frac{1}{3}$$

$$y = y_0\ell_0 + y_1\ell_1 + y_2\ell_2 = \frac{7}{3} + 11 - \frac{28}{3} = 4$$

EXAMPLE 3.2

The data points

x	-2	1	4	-1	3	-4
y	-1	2	59	4	24	-53

lie on a polynomial. Determine the degree of this polynomial by constructing a divided difference table, similar to Table 3.1.

Solution

i	x_i	y_i	∇y_i	$\nabla^2 y_i$	$\nabla^3 y_i$	$\nabla^4 y_i$	$\nabla^5 y_i$
0	-2	-1					
1	1	2	1				
2	4	59	10	3			
3	-1	4	5	-2	1		
4	3	24	5	2	1	0	
5	-4	-53	26	-5	1	0	0

Here are a few sample calculations used in arriving at the figures in the table:

$$\nabla y_2 = \frac{y_2 - y_0}{x_2 - x_0} = \frac{59 - (-1)}{4 - (-2)} = 10$$

$$\nabla^2 y_2 = \frac{\nabla y_2 - \nabla y_1}{x_2 - x_1} = \frac{10 - 1}{4 - 1} = 3$$

$$\nabla^3 y_5 = \frac{\nabla^2 y_5 - \nabla^2 y_2}{x_5 - x_2} = \frac{-5 - 3}{-4 - 4} = 1$$

From the table we see that the last nonzero coefficient (last nonzero diagonal term) of Newton's polynomial is $\nabla^3 y_3$, which is the coefficient of the cubic term. Hence the polynomial is a cubic.

EXAMPLE 3.3

Given the data points

x	4.0	3.9	3.8	3.7
y	−0.06604	−0.02724	0.01282	0.05383

determine the root of $y(x) = 0$ by Neville's method.

Solution. This is an example of *inverse interpolation*, in which the roles of x and y are interchanged. Instead of computing y at a given x, we are finding x that corresponds to a given y (in this case, $y = 0$). Employing the format of Table 3.2 (with x and y interchanged, of course), we obtain

i	y_i	$P_0[\,] = x_i$	$P_1[\,,\,]$	$P_2[\,,\,,\,]$	$P_3[\,,\,,\,,\,]$
0	−0.06604	4.0	3.8298	3.8316	3.8317
1	−0.02724	3.9	3.8320	3.8318	
2	0.01282	3.8	3.8313		
3	0.05383	3.7			

The following are sample computations used in the table:

$$\begin{aligned}
P_1[y_0, y_1] &= \frac{(y - y_1)\,P_0[y_0] + (y_0 - y)\,P_0[y_1]}{y_0 - y_1} \\
&= \frac{(0 + 0.02724)(4.0) + (-0.06604 - 0)(3.9)}{-0.06604 + 0.02724} = 3.8298 \\
P_2[y_1, y_2, y_3] &= \frac{(y - y_3)\,P_1[y_1, y_2] + (y_1 - y)\,P_1[y_2, y_3]}{y_1 - y_3} \\
&= \frac{(0 - 0.05383)(3.8320) + (-0.02724 - 0)(3.8313)}{-0.02724 - 0.05383} = 3.8318
\end{aligned}$$

All the P's in the table are estimates of the root resulting from different orders of interpolation involving different data points. For example, $P_1[y_0, y_1]$ is the root obtained from linear interpolation based on the first two points, and $P_2[y_1, y_2, y_3]$ is the result from quadratic interpolation using the last three points. The root obtained from cubic interpolation over all four data points is $x = P_3[y_0, y_1, y_2, y_3] = 3.8317$.

EXAMPLE 3.4

The data points in the table lie on the plot of $f(x) = 4.8 \cos \frac{\pi x}{20}$. Interpolate this data by Newton's method at $x = 0, 0.5, 1.0, \ldots, 8.0$, and compare the results with the "exact" values $y_i = f(x_i)$.

x	0.15	2.30	3.15	4.85	6.25	7.95
y	4.79867	4.49013	4.2243	3.47313	2.66674	1.51909

Solution

$x_0 = 0.15$ $\quad y_0 = 4.79867$

$x_1 = 2.30$ $\quad y_1 = 4.49013$

$x_2 = 3.15$ $\quad y_2 = 4.2243$

$x_3 = 4.85$ $\quad y_3 = 3.47313$

$x_4 = 6.25$ $\quad y_4 = 2.66674$

$x_5 = 7.95$ $\quad y_5 = 1.51909$

$$P(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \cdots + a_5(x - x_0) \ldots (x - x_4)$$

The results are

x	yInterp	yExact
0.0	4.80003	4.80000
0.5	4.78518	4.78520
1.0	4.74088	4.74090
1.5	4.66736	4.66738
2.0	4.56507	4.56507
2.5	4.43462	4.43462
3.0	4.27683	4.27683
3.5	4.09267	4.09267
4.0	3.88327	3.88328
4.5	3.64994	3.64995
5.0	3.39411	3.39411
5.5	3.11735	3.11735
6.0	2.82137	2.82137
6.5	2.50799	2.50799
7.0	2.17915	2.17915
7.5	1.83687	1.83688
8.0	1.48329	1.48328

3.3 Interpolation with Cubic Spline

EXAMPLE 3.7

Use a natural cubic spline to determine y at $x = 1.5$. The data points are

x	1	2	3	4	5
y	0	1	0	1	0

Solution. The five knots are equally spaced at $h = 1$. Recalling that the second derivative of a natural spline is zero at the first and last knot, we have $k_0 = k_4 = 0$. The second derivatives at the other knots are obtained from Eq. (3.12). Using $i = 1, 2, 3$ results in the simultaneous equations

$$0 + 4k_1 + k_2 = 6\,[0 - 2(1) + 0] = -12$$

$$k_1 + 4k_2 + k_3 = 6\,[1 - 2(0) + 1] = 12$$

$$k_2 + 4k_3 + 0 = 6\,[0 - 2(1) + 0] = -12$$

The solution is $k_1 = k_3 = -30/7$, $k_2 = 36/7$.

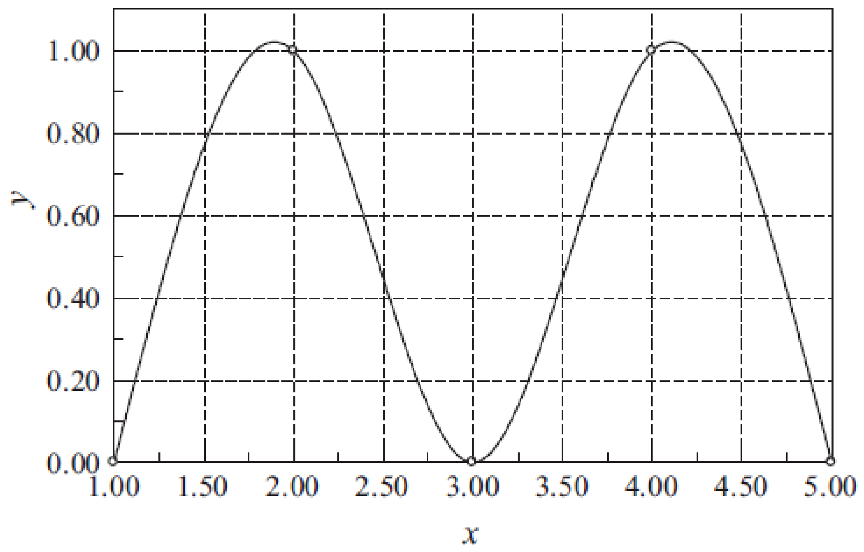
The point $x = 1.5$ lies in the segment between knots 0 and 1. The corresponding interpolant is obtained from Eq. (3.10) by setting $i = 0$. With $x_i - x_{i+1} = -h = -1$, we obtain from Eq. (3.10)

$$f_{0,1}(x) = -\frac{k_0}{6}\left[(x - x_1)^3 - (x - x_1)\right] + \frac{k_1}{6}\left[(x - x_0)^3 - (x - x_0)\right]$$
$$- [y_0(x - x_1) - y_1(x - x_0)]$$

Therefore,

$$\begin{aligned} y(1.5) &= f_{0,1}(1.5) \\ &= 0 + \frac{1}{6}\left(-\frac{30}{7}\right)\left[(1.5 - 1)^3 - (1.5 - 1)\right] - [0 - 1(1.5 - 1)] \\ &= 0.7679 \end{aligned}$$

The plot of the interpolant, which in this case is made up of four cubic segments, is shown in the figure.



EXAMPLE 3.8

Sometimes it is preferable to replace one or both of the end conditions of the cubic spline with something other than the natural conditions. Use the end condition $f'_{0,1}(0) = 0$ (zero slope), rather than $f''_{0,1}(0) = 0$ (zero curvature), to determine the cubic spline interpolant at $x = 2.6$, given the data points

x	0	1	2	3
y	1	1	0.5	0

Solution. We must first modify Eqs. (3.12) to account for the new end condition. Setting $i = 0$ in Eq. (3.10) and differentiating, we get

$$f'_{0,1}(x) = \frac{k_0}{6}\left[3\frac{(x-x_1)^2}{x_0-x_1} - (x_0-x_1)\right] - \frac{k_1}{6}\left[3\frac{(x-x_0)^2}{x_0-x_1} - (x_0-x_1)\right] + \frac{y_0-y_1}{x_0-x_1}$$

Thus the end condition $f'_{0,1}(x_0) = 0$ yields

$$\frac{k_0}{3}(x_0-x_1) + \frac{k_1}{6}(x_0-x_1) + \frac{y_0-y_1}{x_0-x_1} = 0$$

or

$$2k_0 + k_1 = -6\frac{y_0-y_1}{(x_0-x_1)^2}$$

From the given data we see that $y_0 = y_1 = 1$, so that the last equation becomes

$$2k_0 + k_1 = 0 \tag{a}$$

The other equations in Eq. (3.12) are unchanged. Knowing that $k_3 = 0$, they are

$$k_0 + 4k_1 + k_2 = 6\,[1 - 2(1) + 0.5] = -3 \tag{b}$$

$$k_1 + 4k_2 = 6\,[1 - 2(0.5) + 0] = 0 \tag{c}$$

The solution of Eqs. (a)–(c) is $k_0 = 0.4615$, $k_1 = -0.9231$, $k_2 = 0.2308$.

The interpolant can now be evaluated from Eq. (3.10). Substituting $i = 2$ and $x_i - x_{i+1} = -1$, we obtain

$$\begin{aligned} f_{2,3}(x) = \frac{k_2}{6}\left[-(x - x_3)^3 + (x - x_3)\right] - \frac{k_3}{6}\left[-(x - x_2)^3 + (x - x_2)\right] \\ - y_2(x - x_3) + y_3(x - x_2) \end{aligned}$$

Therefore,

$$\begin{aligned} y(2.6) = f_{2,3}(2.6) &= \frac{0.2308}{6}\left[-(-0.4)^3 + (-0.4)\right] - 0 - 0.5(-0.4) + 0 \\ &= 0.1871 \end{aligned}$$

3.4 Least-Squares Fit
(Fitting a Straight Line (Regression))

EXAMPLE 3.10
Fit a straight line to the data shown and compute the standard deviation.

x	0.0	1.0	2.0	2.5	3.0
y	2.9	3.7	4.1	4.4	5.0

Solution. The averages of the data are

$$\bar{x} = \frac{1}{5}\sum x_i = \frac{0.0 + 1.0 + 2.0 + 2.5 + 3.0}{5} = 1.7$$

$$\bar{y} = \frac{1}{5}\sum y_i = \frac{2.9 + 3.7 + 4.1 + 4.4 + 5.0}{5} = 4.02$$

The intercept a and slope b of the interpolant can now be determined from Eq. (3.19):

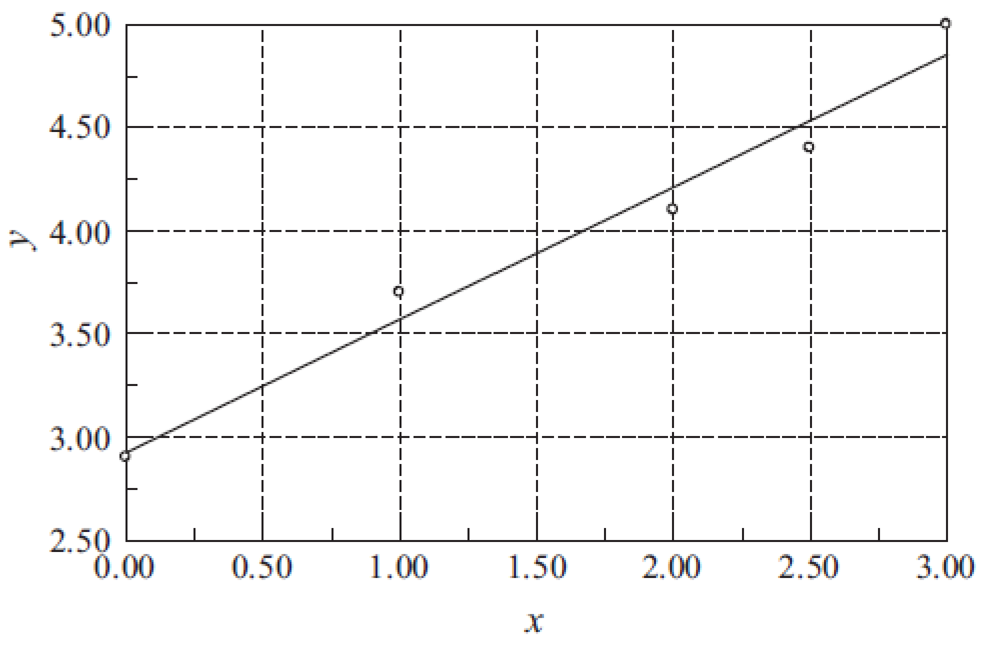
$$b = \frac{\sum y_i(x_i - \bar{x})}{\sum x_i(x_i - \bar{x})}$$

$$= \frac{2.9(-1.7) + 3.7(-0.7) + 4.1(0.3) + 4.4(0.8) + 5.0(1.3)}{0.0(-1.7) + 1.0(-0.7) + 2.0(0.3) + 2.5(0.8) + 3.0(1.3)}$$

$$= \frac{3.73}{5.8} = 0.6431$$

$$a = \bar{y} - \bar{x}b = 4.02 - 1.7(0.6431) = 2.927$$

Therefore, the regression line is $f(x) = 2.927 + 0.6431x$, which is shown in the figure together with the data points.



EXAMPLE 3.11

Determine the parameters a and b so that $f(x) = ae^{bx}$ fits the following data in the least-squares sense.

x	1.2	2.8	4.3	5.4	6.8	7.9
y	7.5	16.1	38.9	67.0	146.6	266.2

Use two different methods: (1) fit $\ln y_i$; and (2) fit $\ln y_i$ with weights $W_i = y_i$. Compute the standard deviation in each case.

Solution of Part (1). The problem is to fit the function $\ln(ae^{bx}) = \ln a + bx$ to the data

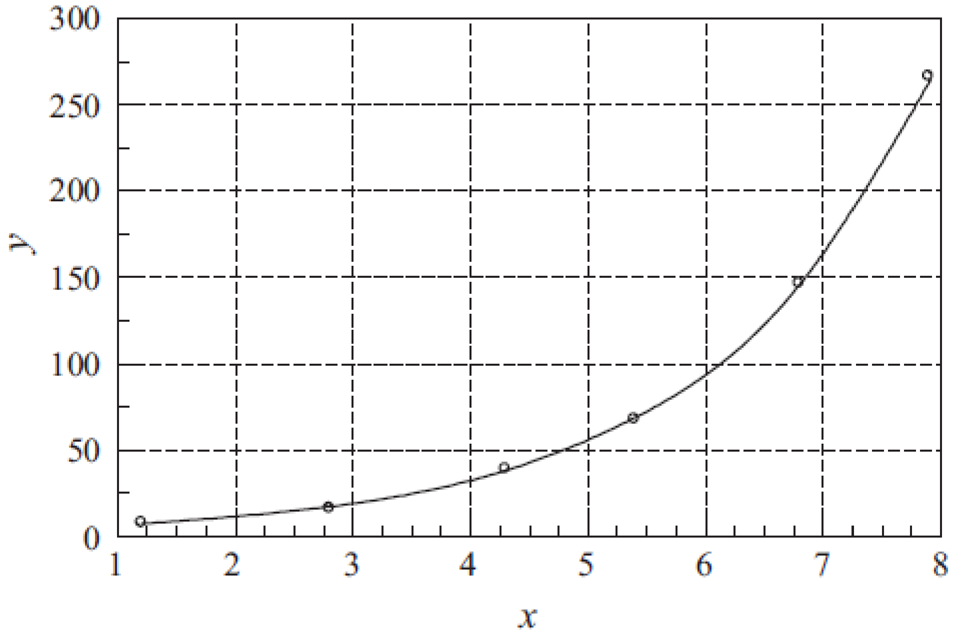
x	1.2	2.8	4.3	5.4	6.8	7.9
$z = \ln y$	2.015	2.779	3.661	4.205	4.988	5.584

We are now dealing with linear regression, where the parameters to be found are $A = \ln a$ and b. Following the steps in Example 3.8, we get (skipping some of the arithmetic details),

$$\bar{x} = \frac{1}{6}\sum x_i = 4.733 \qquad \bar{z} = \frac{1}{6}\sum z_i = 3.872$$

$$b = \frac{\sum z_i(x_i - \bar{x})}{\sum x_i(x_i - \bar{x})} = \frac{16.716}{31.153} = 0.5366 \qquad A = \bar{z} - \bar{x}b = 1.3323$$

Therefore, $a = e^{A} = 3.790$ and the fitting function becomes $f(x) = 3.790e^{0.5366}$. The plots of $f(x)$ and the data points are shown in the figure.



Solution of Part (2). We again fit $\ln(ae^{bx}) = \ln a + bx$ to $z = \ln y$, but this time using the weights $W_i = y_i$. From Eqs. (3.27) the weighted averages of the data are (recall that we fit $z = \ln y$)

$$\hat{x} = \frac{\sum y_i^2 x_i}{\sum y_i^2} = \frac{737.5 \times 10^3}{98.67 \times 10^3} = 7.474$$

$$\hat{z} = \frac{\sum y_i^2 z_i}{\sum y_i^2} = \frac{528.2 \times 10^3}{98.67 \times 10^3} = 5.353$$

and Eqs. (3.28) yield for the parameters

$$b = \frac{\sum y_i^2 z_i (x_i - \hat{x})}{\sum y_i^2 x_i (x_i - \hat{x})} = \frac{35.39 \times 10^3}{65.05 \times 10^3} = 0.5440$$

$$\ln a = \hat{z} - b\hat{x} = 5.353 - 0.5440(7.474) = 1.287$$

Therefore,

$$a = e^{\ln a} = e^{1.287} = 3.622$$

so that the fitting function is $f(x) = 3.622e^{0.5440x}$. As expected, this result is somewhat different from that obtained in Part (1).