3.43. An investment of \$300,000 yields an annual profit of \$86,000 that is spread uniformly over the year and is reinvested immediately (thus continuously compounded). The life is 6 years, and there is no salvage value. What is the rate of return on the investment?

Ans.: 20%.

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CHAPTER 4

EQUATION FITTING

4.1 MATHEMATICAL MODELING

This chapter and the next present procedures for developing equations that represent the performance characteristics of equipment, the behavior of processes, and thermodynamic properties of substances. Engineers may have a variety of reasons for wanting to develop equations, but the crucial ones in the design of thermal systems are (1) to facilitate the process of system simulation and (2) to develop a mathematical statement for optimization. Most large, realistic simulation and optimization problems must be executed on the computer, and it is usually more expedient to operate with equations than with tabular data. An emerging need for expressing equations is in *equipment selection;* some designers are automating equipment selection, storing performance data in the computer, and then automatically retrieving them when a component is being selected.

Equation development will be divided into two different categories; this chapter treats equation fitting and Chapter 5 concentrates on modeling thermal equipment. The distinction between the two is that this chapter approaches the development of equations as purely a number-processing operation, while Chapter 5 uses some physical laws to help equation development. Both approaches are appropriate. In modeling a reciprocating compressor, for example, obviously there are physical explanations for the performance, but by the time the complicated flow processes, compression, reexpansion, and valve mechanics are incorporated, the model is so complex that it is simpler to use experimental or catalog data and treat the problem as a number-processing exercise. On the other hand, heat exchangers follow certain laws that suggest a form for the equation, and this insight can be used to advantage, as shown in Chapter 5.

Where do the data come from on which equations are based? Usually the data used by a designer come from tables or graphs. Experimental data from the laboratory might provide the basis, and the techniques in this and the next chapter are applicable to processing laboratory data. But system designers are usually one step removed from the laboratory and are selecting commercially available components for which the manufacturer has provided performance data. In a few rare instances manufacturers may reserve several lines on a page of tabular data to provide the equation that represents the table. If and when that practice becomes widespread, the system designer's task will be made easier. That stage, however, has not yet been reached.

Much of this chapter presents systematic techniques for determining the constants and coefficients in equations, a process of following rules. The other facet of equation fitting is that of proposing the form of the equation, and this operation is an art. Some suggestions will be offered for the execution of this art. Methods will be presented for determining equations that fit a limited number of data points perfectly. Also explained is the method of least squares, which provides an equation of best fit to a large number of points.

4.2 MATRICES

All the operations in this chapter can be performed without using matrix terminology, but the use of matrices provides several conveniences and insights. In particular, the application of matrix terminology is applicable to the solution of sets of simultaneous equations.

A matrix is a rectangular array of numbers, for example,

$$\begin{bmatrix} 5 & -2 & 0 \\ 3 & 1 & -1 \\ 0 & 1 & 1 \end{bmatrix} \quad \begin{bmatrix} 2 & 3 \\ -1 & 0 \\ 2 & 2 \end{bmatrix} \quad \begin{bmatrix} 7 & 3 \\ 1 & 2 \end{bmatrix} \quad \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & 1_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

The numbers that make up the array are called *elements*. The orders of these matrices, from left to right, are $3 \times 3, 3 \times 2, 2 \times 2$, and $m \times n$.

A transpose of a matrix $[A]$, designated $[A]^T$, is formed by interchanging rows and columns. Thus, if

$$[A] = \begin{bmatrix} 3 & -1 \\ 2 & 0 \\ 4 & -2 \end{bmatrix} \quad \text{then} \quad [A]^T = \begin{bmatrix} 3 & 2 & 4 \\ -1 & 0 & -2 \end{bmatrix}$$

To multiply two matrices, multiply elements of the first row of the left matrix by the corresponding elements of the first column of the right matrix; then sum the products to give the element of the first row and first column of the product matrix. For example, the multiplication of the two matrices

$$\begin{bmatrix} 1 & -1 & 0 \\ 2 & 0 & 1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} -2 & 1 \\ 3 & 0 \\ 1 & 4 \end{bmatrix}$$

gives

$$\begin{bmatrix} (1)(-2) + (-1)(3) + (0)(1) & (1)(1) + (-1)(0) + (0)(4) \\ (2)(-2) + (0)(3) + (1)(1) & (2)(1) + (0)(0) + (1)(4) \end{bmatrix} = \begin{bmatrix} -5 & 1 \\ -3 & 6 \end{bmatrix}$$

The convention for the multiplication of two matrices offers a slightly shorter form for writing a system of simultaneous linear equations. The three equations

$$2x_1 - x_2 + 3x_3 = 6$$

$$x_1 + 3x_2 = 1$$

$$4x_1 - 2x_2 + x_3 = 0$$

can be written in matrix form as

$$\begin{bmatrix} 2 & -1 & 3 \\ 1 & 3 & 0 \\ 4 & -2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 6 \\ 1 \\ 0 \end{bmatrix}$$

The determinant is a scalar (which is simply a number) and is written between vertical lines. For a 1×1 matrix it is the element itself; thus

$$|a_{11}| = a_{11}$$

A technique for evaluating the determinant of a 2×2 matrix is to sum the products of diagonal elements, assigning a positive sign to the diagonal moving downward to the right and a negative sign to the product moving upward to the right:

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = + \searrow - \nearrow = a_{11}a_{22} - a_{21}a_{12}$$

An extension of this method applies to computing the determinant of a 3×3 matrix:

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = + \searrow + \searrow + \searrow - \nearrow - \nearrow - \nearrow$$

$$= a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32}$$
$$- a_{31}a_{22}a_{13} - a_{32}a_{23}a_{11} - a_{33}a_{21}a_{12}$$

Evaluation of determinants 4 × 4 and larger requires a more general procedure, which applies also to 2 × 2 and 3 × 3 matrices. This procedure is *row expansion* or *column expansion*. The determinant of a 3 × 3 matrix found by expanding about the first column is

$$\det = a_{11}A_{11} + a_{21}A_{21} + a_{31}A_{31}$$

where A_{ij} is the *cofactor* of the element a_{ij}. The cofactor is found as follows:

$$A_{ij} = [(-1)^{i+j}] \begin{vmatrix} \text{submatrix formed} \\ \text{by striking out} \\ i\text{th row and } j\text{th} \\ \text{column of } [A] \end{vmatrix}$$

For example, the cofactor of a_{21}, which is A_{21}, is

$$A_{21} = [(-1)^{2+1}] \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = (-1)^3 \begin{vmatrix} a_{12} & a_{13} \\ a_{32} & a_{33} \end{vmatrix}$$

$$A_{21} = -(a_{12}a_{33} - a_{32}a_{13})$$

Example 4.1. Evaluate

$$\begin{vmatrix} 1 & 2 & -1 & 0 \\ 0 & 1 & 2 & 0 \\ 3 & -1 & 1 & 2 \\ 4 & 2 & 1 & 5 \end{vmatrix}$$

Solution. Two elements of the second row are zero, so that row would be a convenient one about which to expand.

$$\det = a_{21}A_{21} + a_{22}A_{22} + a_{23}A_{23} + a_{24}A_{24}$$

$$= (0)A_{21} + (1)(-1)^{2+2} \begin{vmatrix} 1 & -1 & 0 \\ 3 & 1 & 2 \\ 4 & 1 & 5 \end{vmatrix}$$

$$+ (2)(-1)^{2+3} \begin{vmatrix} 1 & 2 & 0 \\ 3 & -1 & 2 \\ 4 & 2 & 5 \end{vmatrix} + (0)A_{24}$$

$$= 0 + 10 + 46 + 0 = 56$$

4.3 SOLUTION OF SIMULTANEOUS EQUATIONS

There are many ways of solving sets of simultaneous equations, two of which will be described in this section, Cramer's rule and gaussian elimination. For a set of linear simultaneous equations

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 &= b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 &= b_3 \end{aligned} \tag{4.1}$$

which can be written in matrix form

$$[A][X] = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = [B] \tag{4.2}$$

Cramer's rule states that

$$x_i = \frac{|[A] \text{ matrix with } [B] \text{ matrix substituted in } i\text{th column}|}{|A|} \tag{4.3}$$

Example 4.2. Using Cramer's rule, solve for x_2 in this set of simultaneous linear equations:

$$\begin{bmatrix} 2 & 1 & -1 \\ 1 & -2 & 2 \\ -1 & 0 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 9 \\ 0 \end{bmatrix}$$

Solution

$$x_2 = \frac{\begin{vmatrix} 2 & 3 & -1 \\ 1 & 9 & 2 \\ -1 & 0 & 3 \end{vmatrix}}{\begin{vmatrix} 2 & 1 & -1 \\ 1 & -2 & 2 \\ -1 & 0 & 3 \end{vmatrix}} = \frac{30}{-15} = -2$$

Equation (4.3) suggests that none of the x's can be determined if $|A|$ is zero. The equations are dependent in this case, and there is no unique solution to the set.

Another method of solving simultaneous linear equations is gaussian elimination, which will be illustrated by solving

$$x_1 - 4x_2 + 3x_3 = -7 \tag{4.4}$$

$$3x_1 + x_2 - 2x_3 = 14 \tag{4.5}$$

$$2x_1 + x_2 + x_3 = 5 \tag{4.6}$$

The two major steps in gaussian elimination are conversion of the coefficient matrix into a triangular matrix and solution for x_n to x_1 by back substitution.

In the example set of equations, the first part of step 1 is to eliminate the coefficients of x_1 in Eq. (4.5) by multiplying Eq. (4.4) by a suitable constant and adding the product to Eq. (4.5). Specifically, multiply Eq. (4.4) by −3 and add to Eq. (4.5). Similarly, multiply Eq. (4.4) by −2 and add to Eq. (4.6):

$$x_1 - 4x_2 + 3x_3 = -7 \qquad (4.7)$$

$$13x_2 - 11x_3 = 35 \qquad (4.8)$$

$$9x_2 - 5x_3 = 19 \qquad (4.9)$$

The last part of step 1 is to multiply Eq. (4.8) by $-\frac{9}{13}$ and add to Eq. (4.9), which completes the triangularization

$$x_1 - 4x_2 + 3x_3 = -7 \qquad (4.10)$$

$$13x_2 - 11x_3 = 35 \qquad (4.11)$$

$$\frac{34}{13}x_3 = -\frac{68}{13} \qquad (4.12)$$

In step 2 the value of x_3 can be determined directly from Eq. (4.12) as $x_3 = -2$. Substituting the value of x_3 into Eq. (4.11) and solving gives $x_2 = 1$. Finally, substitute the values of x_2 and x_3 into Eq. (4.10) to find that $x_1 = 3$.

If a different set of equations were being solved, and in the equation corresponding to Eq. (4.8) if the coefficient of x_2 had been zero instead of 13, it would have been necessary to exchange the positions of Eqs. (4.8) and (4.9). If both the x_2 coefficients in Eqs. (4.8) and (4.9) had been zero, this would indicate that the set of equations is dependent.

Most computer departments have in their library a routine for solving a set of simultaneous linear equations which can be called as needed. It may be convenient to write one's own subprogram using a method like gaussian elimination.[1] It will be useful for future work in this text to have access to an equation-solving routine on a digital computer.

4.4 POLYNOMIAL REPRESENTATIONS

Probably the most obvious and most useful form of equation representation is a polynomial. If y is to be represented as a function of x, the polynomial form is

$$y = a_o + a_1x + a_2x^2 + \cdots + a_nx^n \qquad (4.13)$$

where a_o to a_n are constants. The degree of the equation is the highest exponent of x, which in Eq. (4.13) is n.

Equation (4.13) is an expression giving the function of one variable in terms of another. In other common situations one variable is a function of two or more variables, e.g., in an axial-flow compressor

Flow rate $= f$ (inlet pressure, inlet temperature, compressor speed, outlet pressure)

This form of equation will be presented in Sec. 4.8.

When the number of data points available is precisely the same as the degree of the equation plus 1, $n + 1$, a polynomial can be devised that exactly expresses those data points. When the number of available data points exceeds $n + 1$, it may be advisable to seek a polynomial that gives the "best fit" to the data points (see Sec. 4.10).

The first and simplest case to be considered is where one variable is a function of another variable and the number of data points equals $n + 1$.

4.5 POLYNOMIAL, ONE VARIABLE A FUNCTION OF ANOTHER VARIABLE AND $n + 1$ DATA POINTS

Two available data points are adequate to describe a first-degree, or linear, equation (Fig. 4-1). The form of this first-degree equation is

$$y = a_o + a_1x \qquad (4.14)$$

The xy pairs for the two known points (x_o, y_o) and (x_1, y_1) can be substituted into Eq. (4.14), providing two linear equations with two unknowns, a_o and a_1

$$y_o = a_o + a_1x_o$$

$$y_1 = a_o + a_1x_1$$

For a second-degree, or quadratic, equation, three data points are needed; for example, points 0, 1, and 2 in Fig. 4-2. The xy pairs for the three known points can be substituted into the general form for the quadratic equation

$$y = a_o + a_1x + a_2x^2 \qquad (4.15)$$

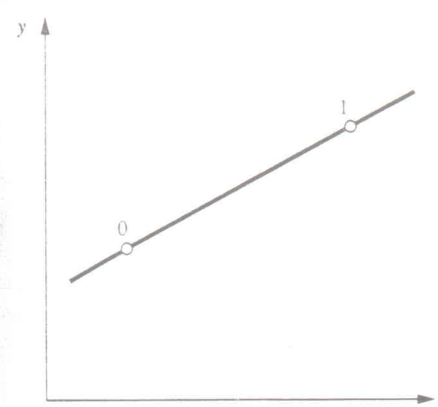

FIGURE 4-1
Two points describing a linear equation.

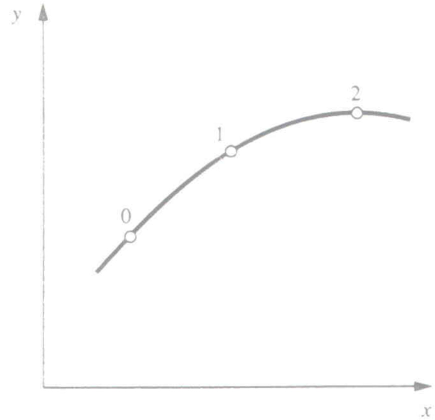

FIGURE 4-2
Three points describing a quadratic equation.

which gives three equations

$$\begin{bmatrix} 1 & x_0 & x_0^2 \\ 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \end{bmatrix}$$

The solution of these three linear simultaneous equations provides the values of a_o, a_1, and a_2.

The coefficients of the high-degree terms in a polynomial may be quite small, particularly if the independent variable is large. For example, if the enthalpy of saturated water vapor h is a function of temperature t in the equation

$$h = a_o + a_1 t + \cdots + a_5 t^5 + a_6 t^6$$

where the range of t extends into hundreds of degrees, the value of a_5 and a_6 may be so small that precision problems result. Sometimes this difficulty can be surmounted by defining a new independent variable, for example, $t/100$.

$$h = a_o + a_1 \frac{t}{100} + \cdots + a_5 \left(\frac{t}{100}\right)^5 + a_6 \left(\frac{t}{100}\right)^6$$

4.6 SIMPLIFICATIONS WHEN THE INDEPENDENT VARIABLE IS UNIFORMLY SPACED

Sometimes a polynomial is used to represent a function, say $y = f(x)$, where the values of y are known at equally spaced values of x. This situation exists, for instance, when the data points are read off a graph and the points can be chosen at equal intervals of x. The solution of simultaneous equations to determine the coefficients in the polynomial can be performed symbolically in advance,[2] and the execution of the calculations requires a relatively small effort thereafter.

Suppose that the curve in Fig. 4-3 is to be reproduced by a fourth-degree polynomial. The $n + 1$ data points (five in this case) establish a polynomial of degree n (four in this case). The spacing of the points is $x_1 - x_0 = x_2 - x_1 = x_3 - x_2 = x_4 - x_3$. The range of $x, x_4 - x_o$, is designated R, and the symbols are $\Delta y_1 = y_1 - y_0, \Delta y_2 = y_2 - y_0$, etc.

Instead of the polynomial form of Eq. (4.13), an alternate form is used

$$y - y_0 = a_1 \left[\frac{n}{R}(x - x_0)\right] + a_2 \left[\frac{n}{R}(x - x_0)\right]^2 + a_3 \left[\frac{n}{R}(x - x_0)\right]^3 + a_4 \left[\frac{n}{R}(x - x_0)\right]^4 \qquad (4.16)$$

To find a_1 to a_4, first substitute the (x_1, y_1) pair into Eq. (4.16)

$$\Delta y_1 = a_1 \frac{4(x_1 - x_0)}{R} + a_2 \left[\frac{4(x_1 - x_0)}{R}\right]^2 + a_3 \left[\frac{4(x_1 - x_0)}{R}\right]^3 + a_4 \left[\frac{4(x_1 - x_0)}{R}\right]^4 \qquad (4.17)$$

Because of the uniform spacing of the points along the x axis, $n(x_1 - x_0)/R = 1$, and so Eq. (4.17) can be rewritten as

$$\Delta y_1 = a_1 + a_2 + a_3 + a_4 \qquad (4.18)$$

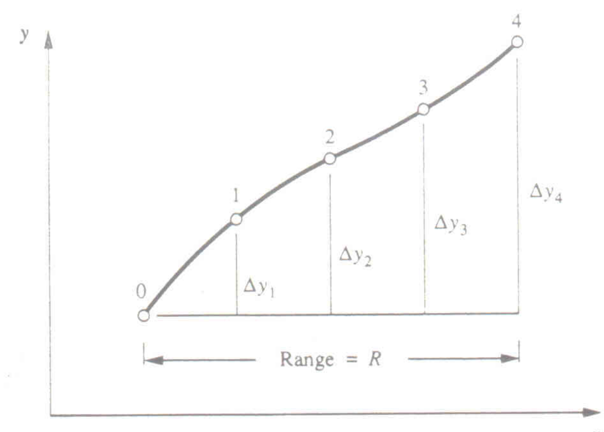

FIGURE 4-3
Polynomial representation when points are equally spaced along the x axis.

TABLE 4.1
Constants in Eq. (4.16)

Equation	a_4	a_3	a_2	a_1
Fourth degree	$\frac{1}{24}(\Delta y_4 - 4\Delta y_3 + 6\Delta y_2 - 4\Delta y_1)$	$\frac{\Delta y_3}{6} - \frac{\Delta y_2}{2} + \frac{\Delta y_1}{2} - 6a_4$	$\frac{\Delta y_2}{2} - \Delta y_1 - 3a_3 - 7a_4$	$\Delta y_1 - a_2 - a_3 - a_4$
Cubic		$\frac{1}{6}(3\Delta y_1 + \Delta y_3 - 3\Delta y_2)$	$\frac{1}{2}(\Delta y_2 - 2\Delta y_1) - 3a_3$	$\Delta y_1 - a_2 - a_3$
Quadratic			$\frac{1}{2}(\Delta y_2 - 2\Delta y_1)$	$\Delta y_1 - a_2$
Linear				Δy_1

Using the (x_2, x_2) pair and the fact that $n(x_2 - x_0)/R = 2$ gives

$$\Delta y_2 = 2a_1 + 4a_2 + 8a_3 + 16a_4 \tag{4.19}$$

Similarly, for (x_3, y_3) and (x_4, y_4)

$$\Delta y_3 = 3a_1 + 9a_2 + 27a_3 + 81a_4 \tag{4.20}$$

$$\Delta y_4 = 4a_1 + 16a_2 + 64a_3 + 256a_4 \tag{4.21}$$

The expressions for a_1 to a_4 found by solving Eqs. (4.18) to (4.21) simultaneously are shown in Table 4.1, along with the constants for the cubic, quadratic, and linear equations.

4.7 LAGRANGE INTERPOLATION

Another form of polynomial results when using Lagrange interpolation. This method is applicable, unlike the method described in Sec. 4.6, to arbitrary spacing along the x axis. It has the advantage of not requiring the simultaneous solution of equations but is cumbersome to write out. This disadvantage is not applicable if the calculation is performed on a digital computer, in which case the programming is quite compact.

With a quadratic equation as an example, the usual form for a function of one variable is

$$y = a_o + a_1 x + a_2 x^2 \tag{4.22}$$

For Lagrange interpolation, a revised form is used

$$y = c_1(x - x_2)(x - x_3) + c_2(x - x_1)(x - x_3) + c_3(x - x_1)(x - x_2) \tag{4.23}$$

The three available data points are (x_1, y_1), (x_2, y_2), and (x_3, y_3). Equation (4.23) could be multiplied out and terms collected to show the correspondence to the form in Eq. (4.22).

By setting $x = x_1, x_2$, and x_3 in turn in Eq. (4.23) the constants can be found quite simply:

$$c_1 = \frac{y_1}{(x_1 - x_2)(x_1 - x_3)}$$

$$c_2 = \frac{y_2}{(x_2 - x_1)(x_2 - x_3)}$$

$$c_3 = \frac{y_3}{(x_3 - x_1)(x_3 - x_2)}$$

The general form of the equation for finding the value of y for a given x when n data points are known is

$$y = \sum_{i=1}^{n} y_i \prod_{j=1}^{n} \frac{(x - x_j) \text{ omitting } (x - x_i)}{(x_i - x_j) \text{ omitting } (x_i - x_i)} \tag{4.24}$$

where the pi, or product sign, indicates multiplication.

The equation represented by Eq. (4.24) is a polynomial of degree $n - 1$.

4.8 FUNCTION OF TWO VARIABLES

A performance variable of a component is often a function of two other variables,[3] not just one. For example, the pressure rise developed by the centrifugal pump shown in Fig. 4-4 is a function of both the speed S and the flow rate Q.

If a polynomial expression for the pressure rise Δp is sought in terms of a second-degree equation in S and Q, separate equations can be written for each of the three curves in Fig. 4-4. Three points on the 30 r/s curve would provide the constants in the equation

$$\Delta p_1 = a_1 + b_1 Q + c_1 Q^2 \tag{4.25}$$

Similar equations for the curves for the 24 and 16 r/s speeds are

$$\Delta p_2 = a_2 + b_2 Q + c_2 Q^2 \tag{4.26}$$

$$\Delta p_3 = a_3 + b_3 Q + c_3 Q^2 \tag{4.27}$$

Next the a constants can be expressed as a second-degree equation in terms of S, using the three data points $(a_1, 30)$, $(a_2, 24)$, and $(a_3, 16)$. Such an equation would have the form

$$a = A_0 + A_1 S + A_2 S^2 \tag{4.28}$$

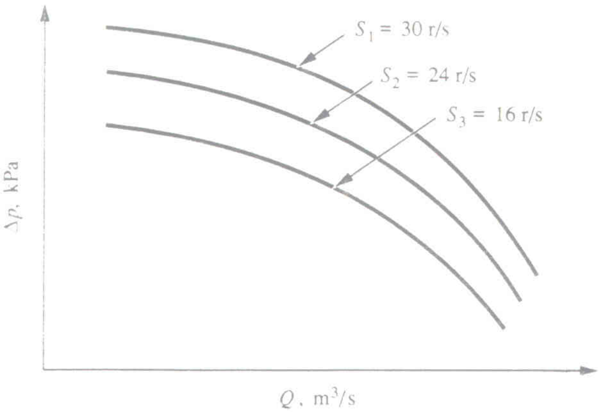

FIGURE 4-4
Performance of a centrifugal pump.

Similarly for b and c

$$b = B_0 + B_1 S + B_2 S^2 \tag{4.29}$$

$$c = C_0 + C_1 S + C_2 S^2 \tag{4.30}$$

Finally, the constants of Eqs. (4.28) to (4.30) are put into the general equation

$$\Delta p = A_0 + A_1 S + A_2 S^2 + (B_0 + B_1 S + B_2 S^2)Q + (C_0 + C_1 S + C_2 S^2)Q^2 \tag{4.31}$$

The A, B, and C constants can be computed if nine data points from Fig. 4-4 are available.

Example 4.3. Manufacturers of cooling towers often present catalog data showing the outlet-water temperature as a function of the wet-bulb temperature of the ambient air and the range. The range is the difference between the inlet and outlet temperatures of the water. In Table 4.2, for example, when the wet-bulb temperature is 20°C and the range is 10°C, the temperature of leaving water is 25.9°C, and so the temperature of the entering water is 25.9 + 10 = 35.9°C. Express the outlet-water temperature t in Table 4.2 as a function of the wet-bulb temperature (WBT) and the range R.

Solution. A second-degree polynomial equation in both independent variables will be chosen as the form of the equation, and three different methods for developing the equation will be illustrated.

Method 1. The three pairs of points for WBT = 20°C, (10, 25.9), (16, 27.0), and (22, 28.4), can be represented by a parabola

$$t = 24.733 + 0.075006R + 0.004146R^2$$

TABLE 4.2
Outlet-water temperature, °C, of cooling tower in Example 4.2

	Wet-bulb temperature, °C		
Range, °C	**20**	**23**	**26**
10	25.9	27.5	29.4
16	27.0	28.4	30.2
22	28.4	29.6	31.3

For WBT = 23°C

$$t = 26.667 + 0.041659R + 0.0041469R^2$$

and for WBT = 26°C

$$t = 28.733 + 0.024999R + 0.0041467R^2$$

Next, the constant terms 24.733, 26.667, and 28.733 can be expressed by a second-degree equation of WBT,

$$15.247 + 0.32637\text{WBT} + 0.007380\text{WBT}^2$$

The coefficients of R and R^2 can also be expressed by equations in terms of the WBT, which then provide the complete equation

$$t = (15.247 + 0.32637\text{WBT} + 0.007380\text{WBT}^2) + (0.72375 - 0.050978\text{WBT} + 0.000927\text{WBT}^2)R + (0.004147 + 0\text{WBT} + 0\text{WBT}^2)R^2 \tag{4.32}$$

Method 2. An alternate polynomial form using second-degree expressions for R and WBT is

$$t = c_1 + c_2\text{WBT} + c_3\text{WBT}^2 + c_4 R + c_5 R^2 + c_6(R)(\text{WBT}) + c_7(\text{WBT})^2(R) + c_8(\text{WBT})(R)^2 + c_9(\text{WBT})^2(R)^2 \tag{4.33}$$

The nine sets of t-R-WBT combinations expressed in Table 4.2 can be substituted into Eq. (4.33) to develop nine simultaneous equations, which can be solved for the unknowns c_1 to c_9. The c values thus obtained are

$c_1 = 15.247$ $c_2 = 0.32631$ $c_3 = 0.0073991$
$c_4 = 0.723753$ $c_5 = 0.0041474$ $c_6 = -0.0509782$
$c_7 = 0.00092704$ $c_8 = 0.0$ $c_9 = 0.0$

It is possible to multiply and collect the terms in Eq. (4.32) to develop the equation of the form of Eq. (4.33).

Method 3. Section 4.7 described a polynomial representation of a dependent variable as a function of one independent variable by use of Lagrange interpolation. Lagrange interpolation can be extended to a function of two independent variables. For example, if $z = f(x, y)$, the form can be chosen

$$\begin{aligned} z = {} & c_{11}(x - x_2)(x - x_3)(y - y_2)(y - y_3) \\ & + c_{12}(x - x_2)(x - x_3)(y - y_1)(y - y_3) \\ & + c_{13}(x - x_2)(x - x_3)(y - y_1)(y - y_2) \\ & + \cdots + c_{33}(x - x_1)(x - x_2)(y - y_1)(y - y_2) \end{aligned} \tag{4.34}$$

To represent the data in Table 4.2, z could refer to the outlet-water temperature, x the WBT, and y the range. In Eq. (4.34) $x_1 = 20$, $x_2 = 23$, and $x_3 = 26$, while $y_1 = 10$, $y_2 = 16$, and $y_3 = 22$.

To determine the magnitude of c_{12}, for example, values applicable when $x = x_1$ and $y = y_2$ can be substituted into Eq. (4.34).

$$c_{12} = \frac{27.0}{(20 - 23)(20 - 26)(16 - 10)(16 - 22)} = -0.04167$$

4.9 EXPONENTIAL FORMS

The dependence of one variable on a second variable raised to an exponent is a physical relation occurring frequently in engineering practice. The graphical method of determining the constants b and m in the equation

$$y = bx^m \tag{4.35}$$

is a simple example of mathematical modeling of an exponential form. On a graph of the known values of x and y on a log-log plot (Fig. 4-5) the slope of the straight line through the points equals m, and the intercept at $x = 1$ defines b.

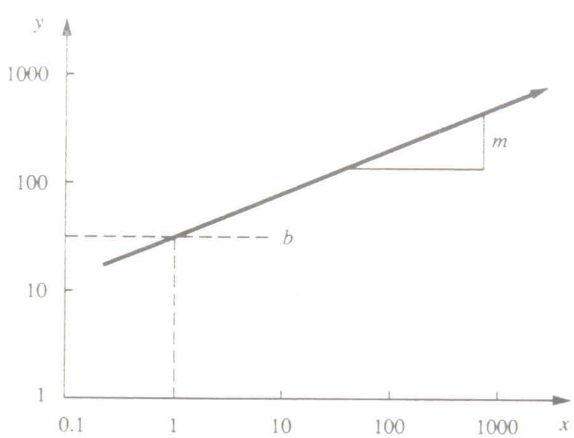

FIGURE 4-5
Graphical determination of the constant b and exponent m.

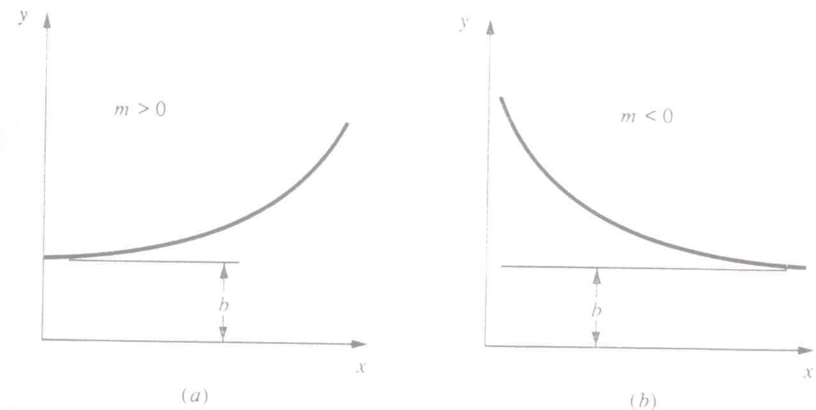

FIGURE 4-6
Curve of the equation $y = b + ax^m$.

The simple exponential form of Eq. (4.35) can be extended to include a constant

$$y = b + ax^m \tag{4.36}$$

The equation permits representations of curves similar to those shown in Fig. 4-6. The curve shown in Fig. 4-6*b* is especially common in engineering practice. The function y approaches some value b asymptotically as x increases.

One possible graphical method of determining a, b, and m in Eq. (4.36) when pairs of xy values are known is as follows:

1. Estimate the value of b.
2. Use the steep portion of the curve to evaluate m by a log-log plot of $y - b$ vs. x in a manner similar to that shown in Fig. 4-5.
3. With the value of m from step 2, plot a graph of y vs. x^m. The resulting curve should be a straight line with a slope of a and an intercept that indicates a more correct value of b. Iterate starting at step 2 if desired.

4.10 BEST FIT: METHOD OF LEAST SQUARES

This chapter has concentrated so far on finding equations that give a perfect fit to a limited number of points. If m coefficients are to be determined in an equation, m data points are required. If more than m points are available, it is possible to determine the m coefficients that result in the best fit of the equation to the data. One definition of a best fit is the one where the sum of the absolute values of the deviations from the data points is a minimum. In another type of best fit slightly different from the one just mentioned the sum of the squares of the deviation is a minimum. The procedure in establishing the coefficients in such an equation is called the *method of least squares*.

Some people proudly announce their use of the method of least squares in order to emphasize the care they have lavished on their data analysis. Misuses of the method, as illustrated in Fig. 4-7*a* and *b*, are not uncommon. In Fig. 4-7*a*, while a straight line can be found that results in the least-squares deviation, the correlation between the x and y variables seems questionable and perhaps no such device can improve the correlation. The scatter may be due to the omission of some significant variable(s). In Fig. 4-7*b* it would have been preferable to eyeball in the curve, rather than to fit a straight line to the data by the least-squares method. The error was not in using least squares but in applying a curve of too low a degree.

The procedure for using the least-squares method for first- and second-degree polynomials will be explained here. Consider first the linear equation of the form

$$y = a + bx \tag{4.37}$$

where m pairs of data points are available: (x_1, y_1), (x_2, y_2), . . . , (x_m, y_m). The deviation of the data point from that calculated from the equation is $a + bx_i - y_i$. We wish to choose an a and a b such that the summation

$$\sum_{i=1}^{m}(a + bx_i - y_i)^2 \rightarrow \text{minimum} \tag{4.38}$$

The minimum occurs when the partial derivatives of Eq. (4.38) with respect to a and b equal zero.

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

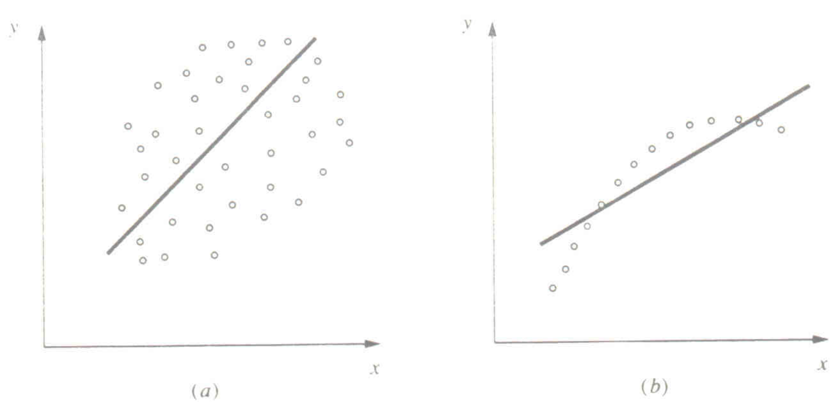

FIGURE 4-7
Misuses of the method of least squares.

and

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

Dividing by 2 and separating the above two equations into individual terms gives

$$ma + b\Sigma x_i = \Sigma y_i \tag{4.39}$$

$$a\Sigma x_i + b\Sigma x_i^2 = \Sigma x_i y_i \tag{4.40}$$

Example 4.4. Determine a_0 and a_1 in the equation $y = a_0 + a_1 x$ to provide a best fit in the sense of least-squares deviation to the data points (1, 4.9), (3, 11.2), (4, 13.7), and (6, 20.1).

Solution. The summations to substitute into Eqs. (4.39) and (4.40) are

	x_i	y_i	x_i^2	$x_i y_i$
	1	4.9	1	4.9
	3	11.2	9	33.6
	4	13.7	16	54.8
	6	20.1	36	120.6
Σ	14	49.9	62	213.9

and $m = 4$

The simultaneous equations to be solved are

$$4a_0 + 14a_1 = 49.9$$

$$14a_0 + 62a_1 = 213.9$$

yielding $a_0 = 1.908$ and $a_1 = 3.019$. Thus

$$y = 1.908 + 3.019x$$

A similar procedure can be followed when fitting a parabola of the form

$$y = a + bx + cx^2 \tag{4.41}$$

to m data points. The summation to be minimized is

$$\sum_{i=1}^{m}(a + bx_i + cx_i^2 - y_i)^2 \rightarrow \text{minimum}$$

Differentiating partially with respect to a, b, and c, in turn, results in three linear simultaneous equations expressed in matrix form

$$\begin{bmatrix} m & \Sigma x_i & \Sigma x_i^2 \\ \Sigma x_i & \Sigma x_i^2 & \Sigma x_i^3 \\ \Sigma x_i^2 & \Sigma x_i^3 & \Sigma x_i^4 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} \Sigma y_i \\ \Sigma x_i y_i \\ \Sigma x_i^2 y_i \end{bmatrix} \tag{4.42}$$

A comparison of the matrix equation (4.42) with Eqs. (4.39) and (4.40) shows a pattern evolving which by analogy permits developing the equations for higher degree polynomials without even differentiating the summation of the squared deviation.

4.11 METHOD OF LEAST SQUARES APPLIED TO NONPOLYNOMIAL FORMS

The explanation of the method of least squares was applied to polynomial forms in Sec. 4.10, but it should not be suggested that the method is limited to those forms. The method is applicable to any form which contains constant coefficients. For example, if the form of the equation is

$$y = a \sin 2x + b \ln x^2$$

the summation comparable to Eq. (4.38) is

$$\sum_{i=1}^{m} (y_i - a \sin 2x_i - b \ln x_i^2)^2 \tag{4.43}$$

Partial differentiation with respect to a and b yields

$$a \Sigma(\sin 2x_i)^2 + b \Sigma(\sin 2x_i)(\ln x_1^2) = \Sigma\, y_i \sin 2x_i$$

$$a \Sigma(\sin 2x_i)(\ln x_i^2) + b \Sigma(\ln x_i^2)^2 = \Sigma\, y_i \ln x_i^2$$

which can be solved for a and b.

A crucial characteristic of the equation form that makes it tractable to the method of least squares is that the equation have constant coefficients. In an equation of the form

$$y = \sin 2ax + bx^c$$

the terms a and c do not appear as coefficients, and this equation cannot be handled in a straightforward manner by least squares.

4.12 THE ART OF EQUATION FITTING

While there are methodical procedures for fitting equations to data, the process is also an art. The art of intuition is particularly needed in deciding upon the form of the equation, namely, the choice of independent variables to be included and the form in which these variables should appear. There are no fixed rules for knowing what variables to include or what their form should be in the equation, but making at least a rough plot of the data will often provide some insight. If the dependent variable is a function of two independent variables, as in $z = f(x, y)$, two plots might be made, as illustrated in Fig. 4-8.

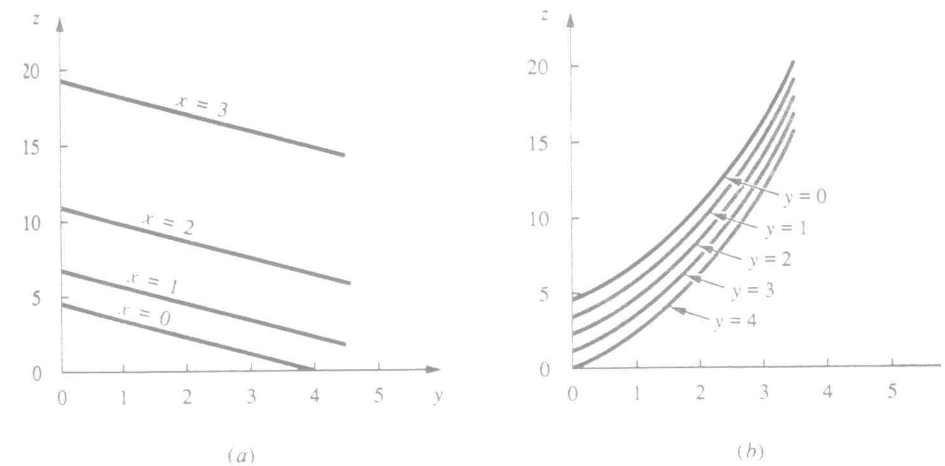

FIGURE 4-8
Cross plots to aid in developing the form of the equation.

The insight provided by Fig. 4-8*a* is that z bears a linear relation to y, and the fact that the straight lines are parallel shows no influence of x on the slope. Figure 4-8*b* suggests at least a second-degree representation of z as a function of x. A reasonable form to propose, then, is

$$z = a_0 + a_1x + a_2y + a_3x^2$$

Several frequently used forms merit further discussion.

Polynomials

If there is a lack of special indicators that other forms are more applicable, a polynomial would probably be explored. When the curve has a reverse curvature (inflection point), as shown in Fig. 4-9, at least a third-degree polynomial must be chosen. Extrapolation of a polynomial beyond the

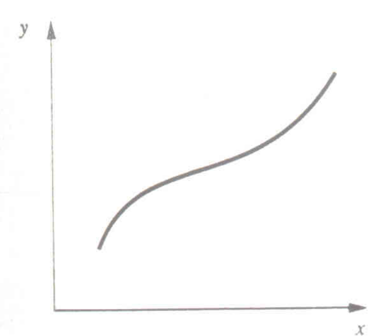

FIGURE 4-9
At least a third-degree polynomial needed.

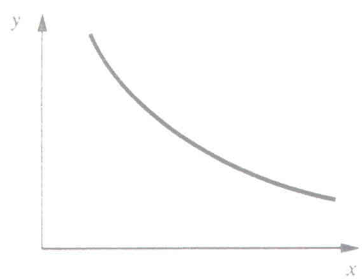

FIGURE 4-10
Negative exponents of polynomials for a curve that flattens out.

borders of the data used to develop the equation often results in serious error.

Polynomials with Negative Exponents

When curves approach a constant value at large magnitudes of the independent variable, polynomials with negative exponents

$$y = a_0 + a_1 x^{-1} + a_2 x^{-2}$$

may provide a good representation; see Fig. 4-10.

Exponential Equations

Section 4.9 has described several examples of exponential forms. The shape of the curve in Fig. 4-10 might also include a c^{-x} term. Plots on log-log paper would be a routine procedure, although a simple plot of log y vs. log x yields a straight line only with equations in the form of Eq. (4.35).

Gompertz Equation

The Gompertz equation,[4] or S curve (Fig. 4-11), appears frequently in engineering practice. The Gompertz curve, for example, represents the

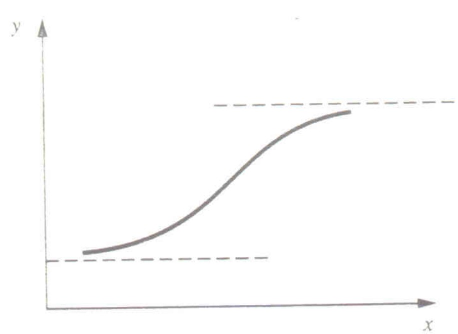

FIGURE 4-11
Gompertz, or S curve.

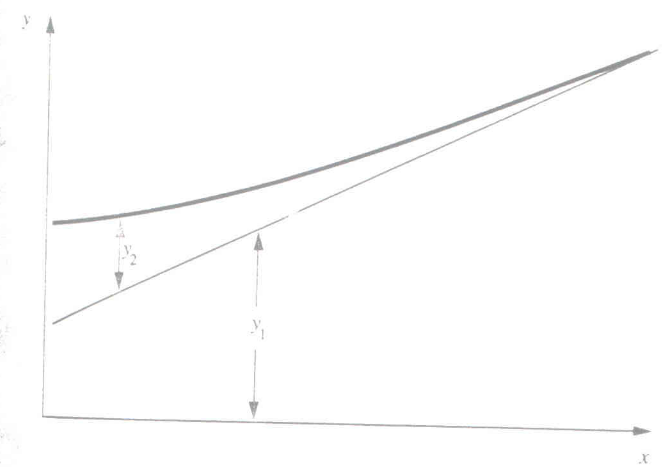

FIGURE 4-12
Combination of two forms.

sales volume vs. years for many products which have low sales when first introduced, experience a period of rapid increase, then reach saturation. The personnel required in many projects also often follows the curve. The form that represents Fig. 4-11 is

$$y = ab^{c^x} \tag{4.44}$$

where a, b, and c are constants and b and c have magnitudes less than unity.

Combination of Forms

It may be possible to fit a curve by combining two or more forms. For example, in Fig. 4-12, suppose that the value of y approaches asymptotically a straight line as x increases. A reasonable way to attack this modeling task would be to propose that

$$y = y_1 + y_2 = (a + bx) + (c + dx^m)$$

where m is a negative exponent.

4.13 AN OVERVIEW OF EQUATION FITTING

The task of finding suitable equations to represent the performance of components or thermodynamic properties is a common preliminary step to simulating and optimizing complex systems. Data may be available in tabular or graphic form, and we seek to represent the data with an equation that is both simple and faithful. A requirement for keeping the equation simple is to choose the proper terms (exponential, polynomial, etc.) to include in the equation. It is possible, of course, to include all the terms that could possibly be imagined, evaluate the coefficients by the method of least squares, and then eliminate terms that provide little contribution. This process is essentially one of *regression analysis*,[5] which also is used to assess which variables are important in representing the dependent variable.

The field of statistical analysis of data is an extensive one, and this chapter has only scratched the surface. On the other hand, much of the effort in the statistical analysis of data is directed toward fitting experimental data to equations where random experimental error occurs. In equation fitting for the design of thermal systems, since catalog tables and charts are the most frequent source of data, there usually has already been a process of smoothing of the experimental data coming from the laboratory. Because of the growing need for fitting catalog data to equations, many designers hope that manufacturers will present the equation that represents the table or graph to save each engineer the effort of developing the equation again when needed.

This chapter presented one approach to mathematical modeling where the relationship of dependent and independent variables was developed without the help of physical laws. Chapter 5 explores some special important cases where physical insight into some thermal equipment can be used to advantage in fitting equations to performance data. Chapter 13 extends the experience on mathematical modeling and also concentrates on the important topic of thermodynamic properties.

PROBLEMS

4.1. Compute

$$\begin{vmatrix} 2 & -1 & 0 & 3 \\ 1 & -2 & 2 & 4 \\ -3 & 1 & 0 & -1 \\ 4 & 2 & 0 & 3 \end{vmatrix}$$

Ans.: 50.

4.2. Test the coefficient matrix in the set of linear equations

$$\begin{bmatrix} 1 & 2 & -2 & 3 \\ 2 & -1 & 3 & -2 \\ -1 & 3 & 1 & -4 \\ 1 & -3 & 5 & -5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 5 \\ 18 \\ -6 \\ 13 \end{bmatrix}$$

and determine whether the set of equations is dependent or independent.

4.3. Using a computer program (gaussian elimination or any other that is available for solving a set of linear simultaneous equations), solve for the x's:

$$\begin{aligned} 2x_1 + x_2 - 4x_3 + 6x_4 + 3x_5 - 2x_6 &= 16 \\ -x_1 + 2x_2 + 3x_3 + 5x_4 - 2x_5 &= -7 \\ x_1 - 2x_2 - 5x_3 + 3x_4 + 2x_5 + x_6 &= 1 \\ 4x_1 + 3x_2 - 2x_3 + 2x_4 + x_6 &= -1 \\ 3x_1 + x_2 - x_3 + 4x_4 + 3x_5 + 6x_6 &= -11 \\ 5x_1 + 2x_2 - 2x_3 + 3x_4 + x_5 + x_6 &= 5 \end{aligned}$$

Ans.: 2, −1, 1, 0, 3, −4.

4.4. A second-degree equation of the form

$$y = a + bx + cx^2$$

has been proposed to pass through the three (x, y) points (1,3), (2,4), and (2, 6). Proceed with the solution for a, b, and c.

(*a*) Describe any unusual problems encountered.

(*b*) Propose an alternate second-degree relation between x and y that will successfully represent these three points.

4.5. Use data from Table 4.3 at t = 0, 50, and 100°C to establish a second-degree polynomial that fits h_g to t. Using the equation, compute h_g at 80°C.

Ans.: 2643.3 kJ/kg.

4.6. Using the data from Table 4.3 for v_g at t = 40, 60, 80 and 100°C, develop a third-degree equation similar in form to Eq. (4.16). Compute v_g at 70°C using this equation.

Ans.: 4.91 m³/kg.

4.7. Lagrange interpolation is to be used to represent the enthalpy of saturated air, h_s kJ/kg, as a function of the temperature t°C. The pairs of (h_s, t) values to be used as the basis are (9.470, 0), (29.34, 10), (57.53, 20), and (99.96, 30).

(*a*) Determine the values of the coefficients c_1 to c_4 in the equation for h_s.

(*b*) Calculate h_s at 15°C.

Ans.: (b) From tables 42.09 kJ/kg.

TABLE 4.3
Properties of saturated water

Temperature		Pressure	Specific volume	Enthalpy	
t, °C	T, K	p, kPa	v_g, m³/kg	h_f, kJ/kg	h_g, kJ/kg
0	273.15	0.6108	206.3	−0.04	2501.6
10	283.15	1.227	106.4	41.99	2519.9
20	293.15	2.337	57.84	83.86	2538.2
30	303.15	4.241	32.93	125.66	2556.4
40	313.15	7.375	19.55	167.45	2574.4
50	323.15	12.335	12.05	209.26	2592.2
60	333.15	19.92	7.679	251.09	2609.7
70	343.15	31.16	5.046	292.97	2626.9
80	353.15	47.36	3.409	334.92	2643.8
90	363.15	70.11	2.361	376.94	2660.1
100	373.15	101.33	1.673	419.06	2676.0

4.8. An equation of the form

$$y - y_0 = a_1(x-1) + a_2(x-1)^2$$

is to fit the following three (x, y) points: (1, 4), (2, 8), and (3, 10). What are the values of y_0, a_1, and a_2?

Ans.: $a_1 = 5$.

4.9. The pumping capacity of a refrigerating compressor (and thus the capability for developing refrigerating capacity) is a function of the evaporating and condensing pressures. The refrigerating capacities in kilowatts of a certain reciprocating compressor at combinations of three different evaporating and condensing temperatures are shown in Table 4.4. Develop an equation similar to the form of Eq. (4.33), namely,

$$q_e = c_1 + c_2 t_e + c_3 t_e^2 + c_4 t_c + \cdots + c_9 t_e^2 t_c^2$$

Ans.: c_1 to c_9 are 239.51, 10.073, −0.10901, −3.4100, −0.0025000, −0.20300, 0.0082004, 0.0013000, −0.000080005.

4.10. The data in Table 4.4 are to be fit to an equation using Lagrange interpolation with a form similar to Eq. (4.34). The variable x corresponds to t_e, y corresponds to t_c, and z to q_e. Compute the coefficient c_{23}.

Ans.: −0.02026.

4.11. The values of c_1 and c_2 are to be determined so that the curve represented by the equation $y = c_1/(c_2 + x)^2$ passes through the (x, y) points (2, 4) and (3, 1). Find the *two* $c_1 - c_2$ combinations.

Ans.: One value of c_1 is $\frac{4}{9}$.

4.12. Using the graphical method for the form $y = b + ax^m$ described in Sec. 4.9, determine the equation that represents the following pairs of (x, y) points: (0.2, 26), (0.5, 7), (1, 2.8), (2, 1.3), (4, 0.79), (6, 0.65), (10, 0.58), (15, 0.54).

Ans.: $y = 0.5 + 2.3x^{-1.5}$.

4.13. A function y is expected to be of the form $y = cx^m$ and the xy data develop a straight line on log-log paper. The line passes through the (x, y) points (100, 50) and (1000, 10). What are the values of c and m?

Ans.: $c = 1250$.

4.14. Compute the constants in the equation $y = a_0 + a_1 x + a_2 x^2$ to provide a best fit in the sense of least squares for the following (x, y) points: (1, 9.8), (3, 13.0), (6, 9.1), and (8, 0.6).

Ans.: 6.424, 3.953, −0.585.

TABLE 4.4
Refrigerating capacity q, kW

Evaporating temperature t_e, °C	Condensing temperature, t_c, °C 25	35	45
0	152.7	117.1	81.0
5	182.9	141.9	101.3
10	215.4	170.7	126.5

4.15. An equation of the form $y = ax + b/x$ has been chosen to fit the following (x, y) pairs of points: (1, 10.5), (3, 8), and (8,18). Choose a and b to give the best fit to the points in the sense of least sum of the deviations squared.

Ans.: $b = 8.14$.

4.16. The proposed form of the equation to represent z as a function of x and y is $z = ax + b[\ln(xy)]$, where a and b are constants. Some data relating these variables are

z	x	y
2	1	2
5	2	1
4	2	2

Determine the values of a and b that give the best fit of the equation to the data in the sense of least square deviation.

Ans.: $b = -0.35$.

4.17. With the method of least squares, fit the enthalpy of saturated liquid h_f by means of a cubic equation to the temperature t in degrees Celsius using the 11 points on Table 4.3. Then compute the values of h_f at the 11 points with the equation just developed.

Ans.: $h_f = -0.0037 + 4.2000t - 0.000505t^2 + 0.000003935t^3$.

4.18. A frequently used form of equation to relate saturation pressures to temperatures is

$$\ln p = A + \frac{B}{T}$$

where p = saturation pressure, kPa
T = absolute temperature, K

With the method of least squares and the 11 points for Table 4.3, determine the values of A and B that give the best fit. Then compute the values of p at the 11 points using the equation just developed.

Ans.: $\ln p = 18.60 - 5206.9/T$.

4.19. The variable z is to be expressed in an equation of the form

$$z = ax + by + cxy$$

The following data points are available, and a least-squares fit is desired:

z	x	y
0.1	1	1
−0.9	1	2
2.0	2	2
−1.8	3	1

Determine the values of a, b, and c.

Ans.: −2.0467, −0.9167, and 1.8833.

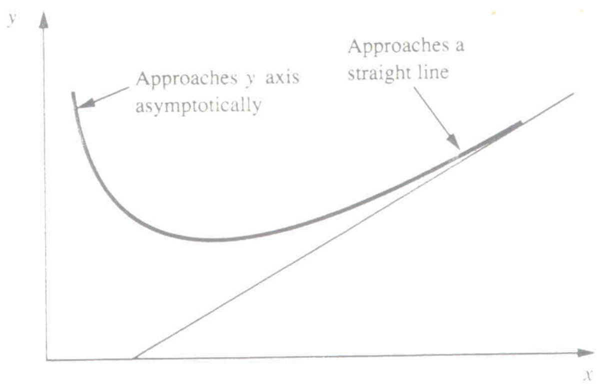

FIGURE 4-13
Function in Prob. 4.19.

4.20. Three points, (x_1, y_1), (x_2, y_2), and (x_3, y_3), lie precisely on the straight line $y = a + bx$. If a least-squares best fit were applied to these three points to determine the values of A and B in the equation $y = A + Bx$, show that the process would indeed give $A = a$, and $B = b$.

4.21. An equation is to be found that represents the function shown in Fig. 4-13. Since one single simple expression seems inadequate, propose that $y = f_1(x) + f_2(x)$. Suggest appropriate forms for f_1 and f_2 and sketch these functions.

4.22. The enthalpy of a solution is a function of the temperature t and the concentration x and consists of straight lines at a constant temperature, as shown in Fig. 4-14. Develop an equation that accurately represents h as a function of x and t.

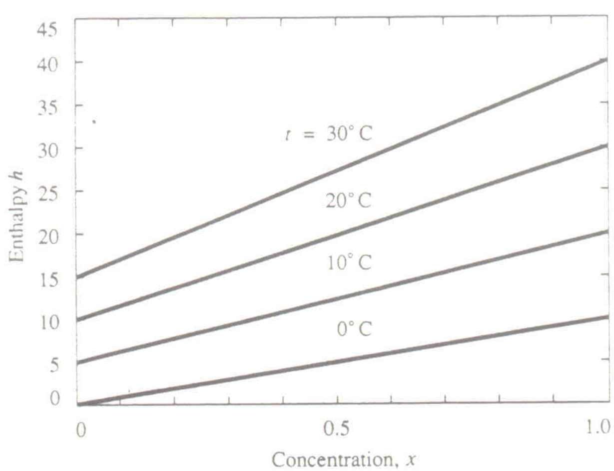

FIGURE 4-14
Enthalpy as a function of temperature and concentration in Prob. 4.20.

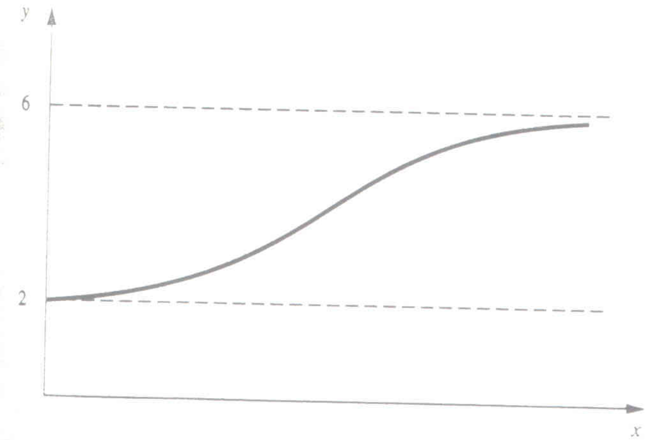

FIGURE 4-15
Gompertz equation in Prob. 4.23.

4.23. In a certain Gompertz equation which is $y = ab^{c^x}$ and represented by Fig. 4-15, $c = 0.5$, $y_0 = 2$ and the asymptote has a value of 6. Determine the values of a and b.

Ans.: $a = 6$.

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