12.1 Method of Least Squares

Linear Least Squares

In experimental, social, and behavioral sciences, an experiment or survey often produces a mass of data. To interpret the data, the investigator may resort to graphical methods. For instance, an experiment in physics might produce a numerical table of the form

x	x_0	x_1	$\cdots$	x_m
y	y_0	y_1	$\cdots$	y_m

(1)

and from it, $m+1$ points on a graph could be plotted. Suppose that the resulting graph looks like Figure 12.1. A reasonable tentative conclusion is that the underlying function is *linear* and that the failure of the points to fall *precisely* on a straight line is due to experimental error. If one proceeds on this assumption—or if theoretical reasons exist for believing that the function is indeed linear—the next step is to determine the correct function. Assuming that

$$y = ax + b$$

what are the coefficients a and b? Thinking geometrically, we ask: *What line most nearly passes through the eight points plotted*?

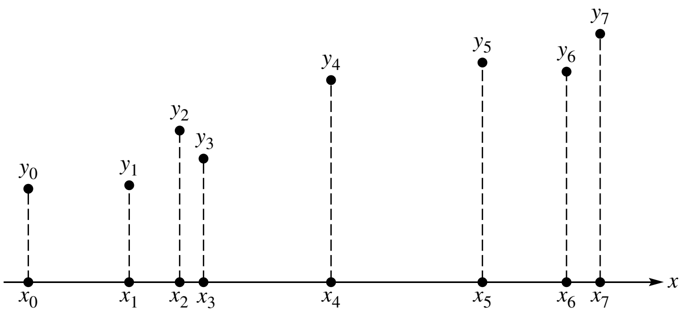

FIGURE 12.1 Experimental data

To answer this question, suppose that a guess is made about the correct values of a and b. This is equivalent to deciding on a specific line to represent the data. In general, the data points will not fall on the line $y = ax + b$. If by chance the kth datum falls on the line, then

$$ax_k + b - y_k = 0$$

If it does not, then there is a discrepancy or *error* of magnitude

$$|\, ax_k + b - y_k \,|$$

The total absolute error for all $m + 1$ points is therefore

$$\sum_{k=0}^{m} |\, ax_k + b - y_k \,|$$

This is a function of a and b, and it would be reasonable to choose a and b so that the function assumes its minimum value. This problem is an example of $\boldsymbol{\ell}_1$ **approximation** and can be solved by the techniques of linear programming, a subject dealt with in Chapter 17. (The methods of calculus do not work on this function because it is not generally differentiable.)

In practice, it is common to minimize a different error function of a and b:

$$\varphi(a, b) = \sum_{k=0}^{m} (ax_k + b - y_k)^2 \qquad (2)$$

This function is suitable because of statistical considerations. Explicitly, if the errors follow a *normal probability distribution,* then the minimization of φ produces a best estimate of a and b. This is called an $\boldsymbol{\ell}_2$ **approximation**. Another advantage is that the methods of calculus can be used on Equation (2).

The ℓ_1 and ℓ_2 approximations are related to specific cases of the $\boldsymbol{\ell}_p$ **norm** defined by

$$\|x\|_p = \left\{ \sum_{i=1}^{n} |x_i|^p \right\}^{1/p} \qquad (1 \leqq p < \infty)$$

for the vector $x = [x_1, x_2, \dots, x_n]^T$.

Let us try to make $\varphi(a, b)$ a minimum. By calculus, the conditions

$$\frac{\partial \varphi}{\partial a} = 0 \qquad \frac{\partial \varphi}{\partial b} = 0$$

(partial derivatives of φ with respect to a and b, respectively) are *necessary* at the minimum. Taking derivatives in Equation (2), we obtain

$$\begin{cases} \displaystyle\sum_{k=0}^{m} 2(ax_k + b - y_k)x_k = 0 \\ \displaystyle\sum_{k=0}^{m} 2(ax_k + b - y_k) = 0 \end{cases}$$

This is a pair of simultaneous linear equations in the unknowns a and b. They are called the **normal equations** and can be written as

$$\begin{cases} \left(\displaystyle\sum_{k=0}^{m} x_k^2\right) a + \left(\displaystyle\sum_{k=0}^{m} x_k\right) b = \displaystyle\sum_{k=0}^{m} y_k x_k \\ \left(\displaystyle\sum_{k=0}^{m} x_k\right) a + \quad (m+1) b = \displaystyle\sum_{k=0}^{m} y_k \end{cases} \tag{3}$$

Here, of course, $\sum_{k=0}^{m} 1 = m + 1$, which is the number of data points. To simplify the notation, we set

$$p = \sum_{k=0}^{n} x_k \qquad q = \sum_{k=0}^{n} y_k \qquad r = \sum_{k=0}^{n} x_k y_k \qquad s = \sum_{k=0}^{n} x_k^2$$

The system of Equations (3) is now

$$\begin{bmatrix} s & p \\ p & m+1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ q \end{bmatrix}$$

We solve this pair of equations by Gaussian elimination and obtain the following algorithm. Alternatively, since this is a 2×2 linear system, we can use Cramer's Rule* to solve it. The determinant of the coefficient matrix is

$$d = \text{Det} \begin{bmatrix} s & p \\ p & m+1 \end{bmatrix} = (m+1)s - p^2$$

Moreover, we obtain

$$a = \frac{1}{d} \text{Det} \begin{bmatrix} r & p \\ q & m+1 \end{bmatrix} = \frac{1}{d}[(m+1)r - pq]$$

$$b = \frac{1}{d} \text{Det} \begin{bmatrix} s & r \\ p & q \end{bmatrix} = \frac{1}{d}[sq - pr]$$

We can write this as an algorithm:

■ ALGORITHM 1 *Linear Least Squares*

The coefficients in the least-squares line $y = ax + b$ through the set of $m + 1$ data points (x_k, y_k) for $k = 0, 1, 2, \ldots, m$ are computed (in order) as follows:

1. $p = \sum_{k=0}^{m} x_k$

2. $q = \sum_{k=0}^{m} y_k$

*Cramer's Rule is given in Appendix D.

3. $r = \sum_{k=0}^{m} x_k y_k$
4. $s = \sum_{k=0}^{m} x_k^2$
5. $d = (m+1)s - p^2$
6. $a = [(m+1)r - pq]/d$
7. $b = [sq - pr]/d$

Another form of this result is

$$\begin{aligned} a &= \frac{1}{d}\left[(m+1)\left(\sum_{k=0}^{m} x_k y_k\right) - \left(\sum_{k=0}^{m} x_k\right)\left(\sum_{k=0}^{m} y_k\right)\right] \\ b &= \frac{1}{d}\left[\left(\sum_{k=0}^{m} x_k^2\right)\left(\sum_{k=0}^{m} y_k\right) - \left(\sum_{k=0}^{m} x_k\right)\left(\sum_{k=0}^{m} x_k y_k\right)\right] \end{aligned} \quad (4)$$

where

$$d = (m+1)\left(\sum_{k=0}^{m} x_k^2\right) - \left(\sum_{k=0}^{m} x_k\right)^2$$

Linear Example

The preceding analysis illustrates the **least-squares** procedure in the simple linear case.

EXAMPLE 1 As a concrete example, find the linear least-squares solution for the following table of values:

x	4	7	11	13	17
y	2	0	2	6	7

Plot the original data points and the line using a finer set of grid points.

Solution The equations in Algorithm 1 leads to this system of two equations:

$$\begin{cases} 644a + 52b = 227 \\ 52a + 5b = 17 \end{cases}$$

whose solution is $a = 0.4864$ and $b = -1.6589$. By Equation (3), we obtain the value $\varphi(a, b) = 10.7810$. Figure 12.2 is a plot of the given data and the linear least squares straight line.

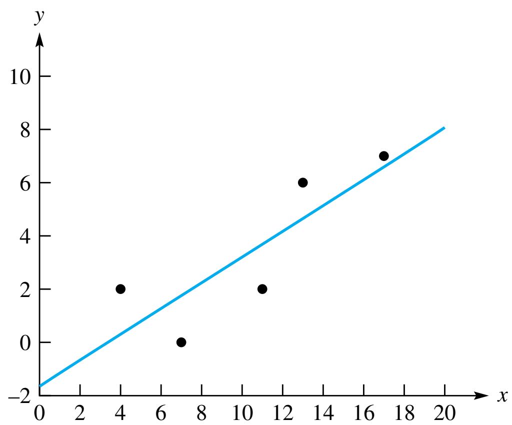

FIGURE 12.2 Linear least squares ■

We can use mathematical software such as Matlab, Maple, or Mathematica to fit a linear least-squares polynomial to the data and verify the value of φ. (See Computer Problem 12.1.5.)

To understand what is going on here, we want to determine the equation of a line of the form $y = ax + b$ that fits the data best in the least-squares sense. With four data points (x_i, y_i), we have four equations $y_i = ax_i + b$ for $i = 1, 2, 3, 4$ that can be written as

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{y}$$

where

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \\ x_4 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

In general, we want to solve a linear system

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$$

where $\boldsymbol{A}$ is an $m \times n$ matrix and $m > n$. The solution coincides with the solution of the **normal equations**

$$\boldsymbol{A}^T\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}^T\boldsymbol{b}$$

This corresponds to minimizing $||\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}||_2^2$.

Nonpolynomial Example

The method of least squares is not restricted to linear (first-degree) polynomials or to any specific functional form. Suppose, for instance, that we want to fit a table of values (x_k, y_k), where $k = 0, 1, \ldots, m$, by a function of the form

$$y = a \ln x + b \cos x + ce^x$$

in the least-squares sense. The unknowns in this problem are the three coefficients a, b, and c. We consider the function

$$\varphi(a, b, c) = \sum_{k=0}^{m} (a \ln x_k + b \cos x_k + ce^{x_k} - y_k)^2$$

and set $\partial\varphi/\partial a = 0$, $\partial\varphi/\partial b = 0$, and $\partial\varphi/\partial c = 0$. This results in the following three normal equations:

$$\begin{cases} a \displaystyle\sum_{k=0}^{m} (\ln x_k)^2 + b \sum_{k=0}^{m} (\ln x_k)(\cos x_k) + c \sum_{k=0}^{m} (\ln x_k)e^{x_k} = \sum_{k=0}^{m} y_k \ln x_k \\ a \displaystyle\sum_{k=0}^{m} (\ln x_k)(\cos x_k) + b \sum_{k=0}^{m} (\cos x_k)^2 + c \sum_{k=0}^{m} (\cos x_k)e^{x_k} = \sum_{k=0}^{m} y_k \cos x_k \\ a \displaystyle\sum_{k=0}^{m} (\ln x_k)e^{x_k} + b \sum_{k=0}^{m} (\cos x_k)e^{x_k} + c \sum_{k=0}^{m} (e^{x_k})^2 = \sum_{k=0}^{m} y_k e^{x_k} \end{cases}$$

EXAMPLE 2 Fit a function of the form $y = a \ln x + b \cos x + ce^x$ to the following table values:

x	0.24	0.65	0.95	1.24	1.73	2.01	2.23	2.52	2.77	2.99
y	0.23	−0.26	−1.10	−0.45	0.27	0.10	−0.29	0.24	0.56	1.00

Solution Using the table and the equations above, we obtain the 3×3 system

$$\begin{cases} 6.79410a - 5.34749b + 63.25889c = 1.61627 \\ -5.34749a + 5.10842b - 49.00859c = -2.38271 \\ 63.25889a - 49.00859b + 1002.50650c = 26.77277 \end{cases}$$

It has the solution $a = -1.04103$, $b = -1.26132$, and $c = 0.03073$. So the curve

$$y = -1.04103 \ln x - 1.26132 \cos x + 0.03073e^x$$

has the required form and fits the table in the least-squares sense. The value of $\varphi(a, b, c)$ is 0.92557. Figure 12.3 is a plot of the given data and the nonpolynomial least squares curve.

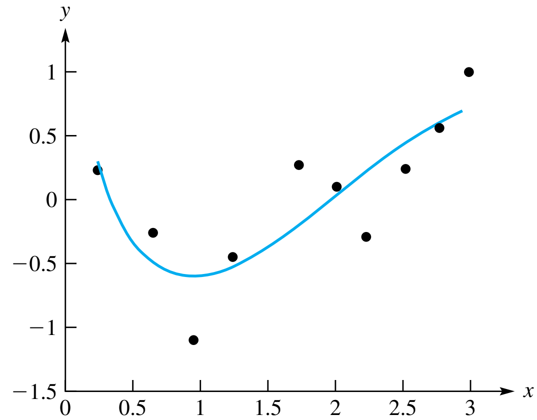

FIGURE 12.3 Nonpolynomial least squares

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We can use mathematical software such as Matlab, Maple, or Mathematica to verify these results and to plot the solution curve. (See Computer Problem 12.1.6.)

Basis Functions $\{g_0, g_1, \ldots, g_n\}$

The principle of least squares, illustrated in these two simple cases, can be extended to general linear families of functions without involving any new ideas. Suppose that the data in Equation (1) are thought to conform to a relationship such as

$$y = \sum_{j=0}^{n} c_j g_j(x) \tag{5}$$

in which the functions $g_0, g_1, \ldots, g_n$ (called **basis functions**) are known and held fixed. The coefficients $c_0, c_1, \ldots, c_n$ are to be determined according to the principle of least squares.

In other words, we define the expression

$$\varphi(c_0, c_1, \ldots, c_n) = \sum_{k=0}^{m} \left[\sum_{j=0}^{n} c_j g_j(x_k) - y_k \right]^2 \tag{6}$$

and select the coefficients to make it as small as possible. Of course, the expression $\varphi(c_0, c_1, \ldots, c_n)$ is the sum of the squares of the errors associated with each entry (x_k, y_k) in the given table.

Proceeding as before, we write down as necessary conditions for the minimum the n equations

$$\frac{\partial \varphi}{\partial c_i} = 0 \qquad (0 \leqq i \leqq n)$$

These partial derivatives are obtained from Equation (7). Indeed,

$$\frac{\partial \varphi}{\partial c_i} = \sum_{k=0}^{m} 2 \left[\sum_{j=0}^{n} c_j g_j(x_k) - y_k \right] g_i(x_k) \qquad (0 \leqq i \leqq n)$$

When set equal to zero, the resulting equations can be rearranged as

$$\sum_{j=0}^{n} \left[\sum_{k=0}^{m} g_i(x_k) g_j(x_k) \right] c_j = \sum_{k=0}^{m} y_k g_i(x_k) \qquad (0 \leqq i \leqq n) \tag{7}$$

These are the **normal equations** in this situation and serve to determine the best values of the parameters $c_0, c_1, \ldots, c_n$. The normal equations are linear in c_i; thus, in principle, they can be solved by the method of Gaussian elimination (see Chapter 7).

In practice, the normal equations may be difficult to solve if care is not taken in choosing the basis functions $g_0, g_1, \ldots, g_n$. First, the set $\{g_0, g_1, \ldots, g_n\}$ should be **linearly independent**. This means that no linear combination $\sum_{i=0}^{n} c_i g_i$ can be the zero function (except in the trivial case when $c_0 = c_1 = \cdots = c_n = 0$). Second, the functions $g_0, g_1, \ldots, g_n$ should be *appropriate* to the problem at hand. Finally, one should choose a set of basis functions that is *well conditioned* for numerical work. We elaborate on this aspect of the problem in the next section.

Summary

(1) We wish to find a line $y = ax + b$ that most nearly passes through the $m + 1$ pairs of points (x_i, y_i) for $0 \leqq i \leqq m$. An example of **ℓ_1 approximation** is to choose a and b so that the total absolute error for all these points is minimized:

$$\sum_{k=0}^{m} | a x_k + b - y_k |$$

This can be solved by the techniques of linear programming.

(2) An **ℓ_2 approximation** will minimize a different error function of a and b:

$$\varphi(a, b) = \sum_{k=0}^{m} (a x_k + b - y_k)^2$$

The minimization of φ produces a best estimate of a and b in the least-squares sense. One solves the **normal equations**

$$\begin{cases} \left(\sum_{k=0}^{m} x_k^2\right) a + \left(\sum_{k=0}^{m} x_k\right) b = \sum_{k=0}^{m} y_k x_k \\ \left(\sum_{k=0}^{m} x_k\right) a + \quad (m+1) b = \sum_{k=0}^{m} y_k \end{cases}$$

(3) In a more general case, the data points conform to a relationship such as

$$y = \sum_{j=0}^{n} c_j g_j(x)$$

in which the **basis functions** $g_0, g_1, \dots, g_n$ are known and held fixed. The coefficients $c_0, c_1, \dots, c_n$ are to be determined according to the principle of least squares. The **normal equations** in this situation are

$$\sum_{j=0}^{n} \left[\sum_{k=0}^{m} g_i(x_k) g_j(x_k) \right] c_j = \sum_{k=0}^{m} y_k g_i(x_k) \qquad (0 \leqq i \leqq n)$$

and can be solved, in principle, by the method of Gaussian elimination to determine the best values of the parameters $c_0, c_1, \dots, c_n$.