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

$$y = f(x) = Ax + B. \tag{1}$$

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

$$f(x_k) = y_k + e_k, \tag{2}$$

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***):

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

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	$f(x_k) = 8.6 - 1.6x_k$	$\|e_k\|$	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.

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

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

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

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.

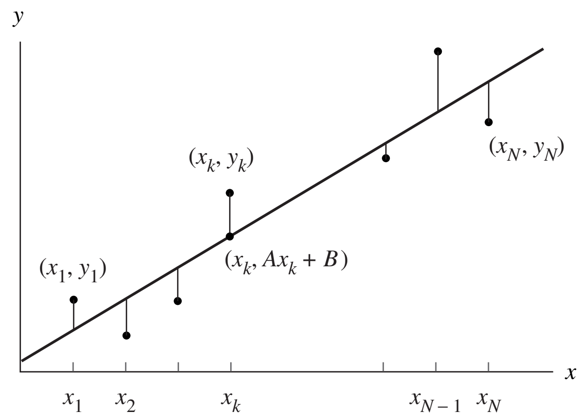

Figure 5.2 The vertical distances between the points $\{(x_k, y_k)\}$ and the least-squares line $y = Ax + B$.

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

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

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

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

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

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 the 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

$$\begin{aligned} 92A + 20B &= 25 \\ 20A + 8B &= 37. \end{aligned}$$

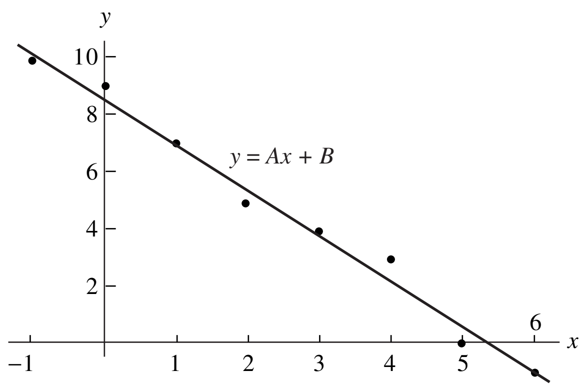

Figure 5.3 The least-squares line $y = -1.6071429x + 8.6428571$.

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)

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

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

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

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

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

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

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

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 $d = 4.9073t^2$ and $g = 2A = 9.7146$ m/sec^2. ■

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