Method of Least Squares

C&K 12.1 (pp. 495-501)

Motivation

Surface tension S in a liquid is known to be a linear function of temperature T. For a particular liquid, measurements have been made of the surface tension at certain temperatures. The results were as follows:

T	0	10	20	30	40	80	90	95
S	68.0	67.1	66.4	65.6	64.6	61.8	61.0	60.0

How can the most probable values of the constants in the equation

$$S = aT + b$$

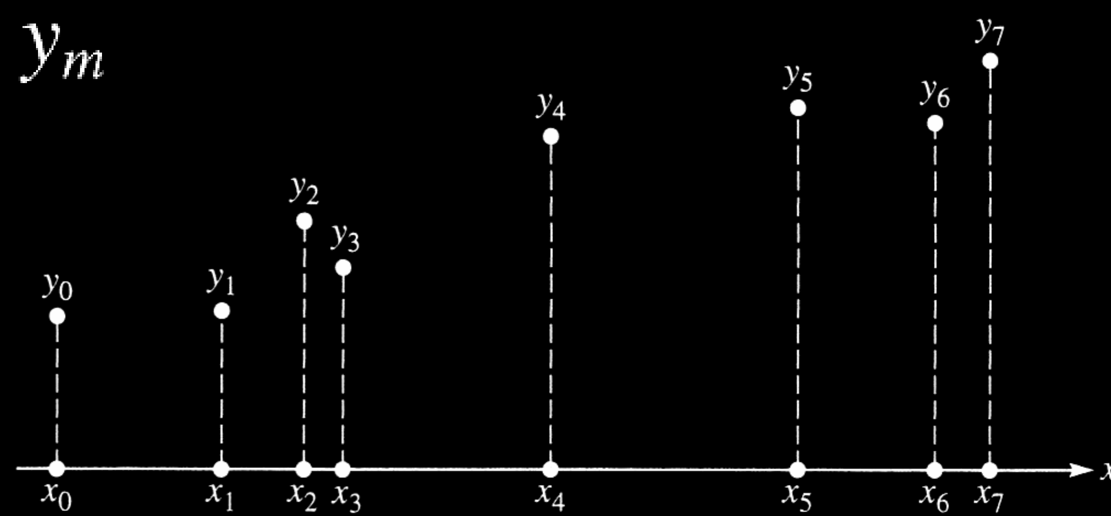
be determined? Methods for solving such problems are developed in this chapter.

(C&K p. 495)

Linear Least Squares

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

FIGURE 12.1 Experimental data



What straight line best fits the data?

$$y = ax + b$$

Minimizing sum of squared errors

Sum of squared errors:

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

Necessary conditions for minimum (from multivariate calculus):

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

Which leads to the normal equations…

… leads to the Normal Equations

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

Or…

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

Solution (ugly)

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

Simply notation:

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

Yields:

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

Solve simple 2x2 system using Cramer's rule:

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

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

$$d = \text{Det} \begin{bmatrix} s & p \\ p & m+1 \end{bmatrix}$$

Linear Least Squares

Another form of this result is

$$a = \frac{1}{d}\left[(m+1)\left(\sum_{k=0}^{m} x_k y_k\right) - \left(\sum_{k=0}^{m} x_k\right)\left(\sum_{k=0}^{m} y_k\right)\right]$$

$$b = \frac{1}{d}\left[\left(\sum_{k=0}^{m} x_k^2\right)\left(\sum_{k=0}^{m} y_k\right) - \left(\sum_{k=0}^{m} x_k\right)\left(\sum_{k=0}^{m} x_k y_k\right)\right]$$

where

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

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.

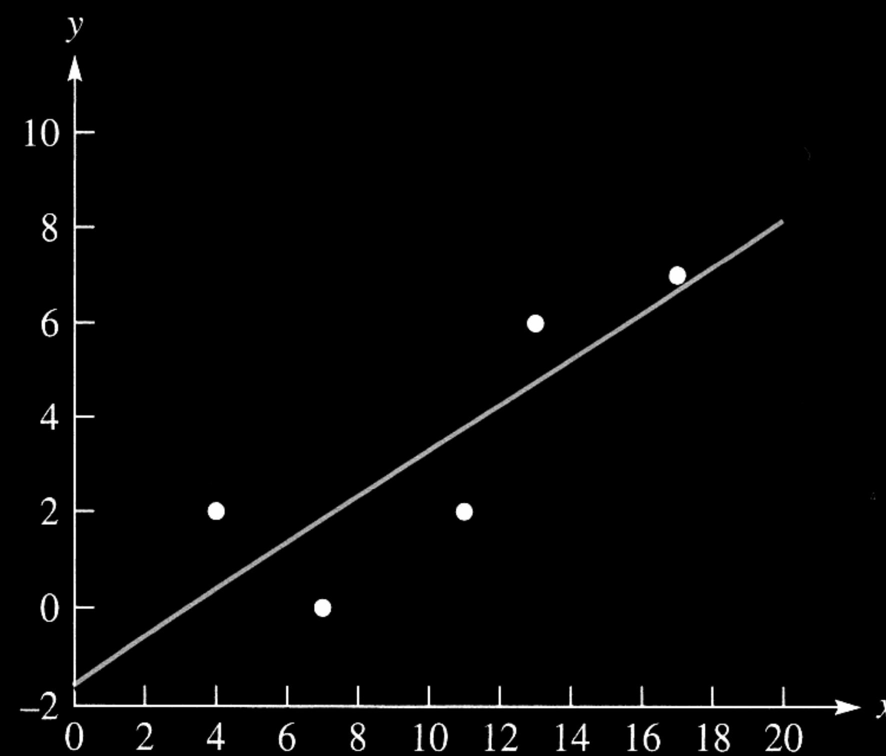


FIGURE 12.2 Linear least squares

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Matrix View of Normal Eqns

Line constraints yield linear system:

$$\boldsymbol{Ax} = \boldsymbol{y}$$

where

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

Minimizing sum of squared error (residual's two-norm squared):

$$||\boldsymbol{Ax} - \boldsymbol{b}||_2^2$$

Yields normal equations:

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

Basis Function View (p. 500)

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

Sum of squared errors:

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

Matrix view… (usually much easier & more convenient)

Example

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

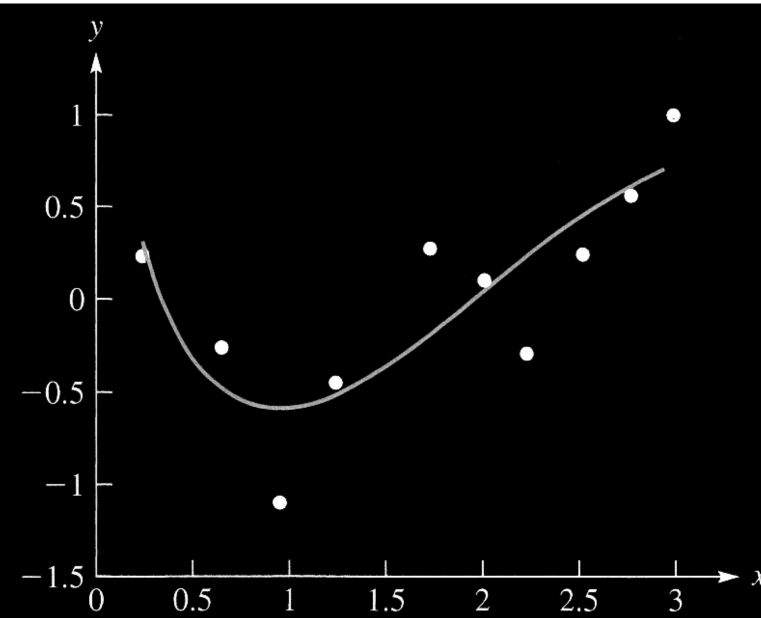
$$\varphi(a, b, c) = \sum_{k=0}^{m} (a \ln x_k + b \cos x_k + ce^{x_k} - y_k)^2$$

Example (cont'd)

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:

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

Example (with data)



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

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

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