

Example 3: If the curve $y = a + bx + \frac{c}{x}$ is to be used to represent the points (1,4.5), (2,4.75), and (4,7.125), find the values of a , b , and c by using linear least squares regression.

Solution:

Since the given curve is not a polynomial, we cannot use the general least squares matrix, and we must use the general least squares derivation.

Let the approximating equation (model) $g(x) = a + bx + \frac{c}{x}$.

The local error is $e_i = g_i - y_i$ and the total error is $E = \sum_{i=1}^n e_i^2$ which must be

minimized by letting $\frac{\partial E}{\partial a} = 0$, $\frac{\partial E}{\partial b} = 0$, and $\frac{\partial E}{\partial c} = 0$.

$$E = \sum_{i=1}^n (g_i - y_i)^2 \Rightarrow E = \sum_{i=1}^n (a + bx_i + \frac{c}{x_i} - y_i)^2,$$

$$\frac{\partial E}{\partial a} = 2 \sum_{i=1}^n (a + bx_i + \frac{c}{x_i} - y_i), \quad \frac{\partial E}{\partial a} = 0 \Rightarrow 2 \sum_{i=1}^n (a + bx_i + \frac{c}{x_i} - y_i) = 0,$$

$$\sum_{i=1}^n a + \sum_{i=1}^n bx_i + \sum_{i=1}^n \frac{c}{x_i} - \sum_{i=1}^n y_i = 0, \quad \text{but } \sum_{i=1}^n a = n.a,$$

$$\therefore n.a + \sum_{i=1}^n bx_i + \sum_{i=1}^n \frac{c}{x_i} = \sum_{i=1}^n y_i. \quad \dots\dots\dots (1)$$

$$\frac{\partial E}{\partial b} = 2 \sum_{i=1}^n (a + bx_i + \frac{c}{x_i} - y_i)x_i, \quad \frac{\partial E}{\partial b} = 0 \Rightarrow 2 \sum_{i=1}^n (ax_i + bx_i^2 + c - x_i y_i) = 0,$$

$$\sum_{i=1}^n x_i a + \sum_{i=1}^n x_i^2 b + \sum_{i=1}^n c - \sum_{i=1}^n x_i y_i = 0, \quad \text{but } \sum_{i=1}^n c = n.c,$$

$$\therefore \sum_{i=1}^n x_i a + \sum_{i=1}^n x_i^2 b + n.c = \sum_{i=1}^n x_i y_i \quad \dots\dots\dots (2)$$

$$\frac{\partial E}{\partial c} = 2 \sum_{i=1}^n (a + bx_i + \frac{c}{x_i} - y_i) \frac{1}{x_i}, \quad \frac{\partial E}{\partial c} = 0 \Rightarrow 2 \sum_{i=1}^n (\frac{1}{x_i} a + b + \frac{1}{x_i^2} c - \frac{1}{x_i} y_i) = 0,$$

$$\sum_{i=1}^n \frac{1}{x_i} a + \sum_{i=1}^n b + \sum_{i=1}^n \frac{1}{x_i^2} c - \sum_{i=1}^n \frac{y_i}{x_i} = 0, \quad \text{but } \sum_{i=1}^n b = n.b,$$

$$\therefore \sum_{i=1}^n \frac{1}{x_i} a + n.b + \sum_{i=1}^n \frac{1}{x_i^2} c = \sum_{i=1}^n \frac{y_i}{x_i}. \quad \dots\dots\dots (3)$$

In matrix form:

$$\begin{bmatrix} n & \sum_{i=1}^n x_i & \sum_{i=1}^n \frac{1}{x_i} \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 & n \\ \sum_{i=1}^n \frac{1}{x_i} & n & \sum_{i=1}^n \frac{1}{x_i^2} \end{bmatrix} \begin{Bmatrix} a \\ b \\ c \end{Bmatrix} = \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \\ \sum_{i=1}^n \frac{y_i}{x_i} \end{bmatrix},$$

$$n = 3, \quad \sum_{i=1}^n x_i = 1 + 2 + 4 = 7, \quad \sum_{i=1}^n x_i^2 = 1^2 + 2^2 + 4^2 = 21,$$

$$\sum_{i=1}^n \frac{1}{x_i} = \frac{1}{1} + \frac{1}{2} + \frac{1}{4} = 1.75, \quad \sum_{i=1}^n \frac{1}{x_i^2} = \frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{4^2} = 1.3125,$$

$$\sum_{i=1}^n y_i = 4.5 + 4.75 + 7.125 = 16.375, \quad \sum_{i=1}^n x_i y_i = 1(4.5) + 2(4.75) + 4(7.125) = 42.5,$$

$$\sum_{i=1}^n \frac{y_i}{x_i} = \frac{4.5}{1} + \frac{4.75}{2} + \frac{7.125}{4} = 8.65625.$$

$$\therefore \begin{bmatrix} 3 & 7 & 1.75 \\ 7 & 21 & 3 \\ 1.75 & 3 & 1.3125 \end{bmatrix} \begin{Bmatrix} a \\ b \\ c \end{Bmatrix} = \begin{bmatrix} 16.375 \\ 42.5 \\ 8.65625 \end{bmatrix}.$$

Solving the above matrix, we get: $a = 0.5$, $b = 1.5$, and $c = 2.5$.

Non-polynomial models

Linear least-squares regression may be used to fit a non-polynomial model by transforming it to a polynomial model, such as

$$* \quad y = \alpha e^{\beta x} \Rightarrow \ln y = \ln \alpha + \beta x \Rightarrow y^* = a + \beta x \quad (\text{polynomial}),$$

where $y^* = \ln y$ and $a = \ln \alpha$.

$$* \quad y = \alpha x^\beta \Rightarrow \log y = \log \alpha + \beta \log x \Rightarrow y^* = a + \beta x^* \quad (\text{polynomial}),$$

where $x^* = \log x$, $y^* = \log y$, and $a = \log \alpha$.

$$* \quad y = \frac{\alpha x}{\beta + x} \Rightarrow \frac{1}{y} = \frac{\beta + x}{\alpha x} \Rightarrow \frac{1}{y} = \frac{1}{\alpha} + \frac{\beta}{\alpha} \cdot \frac{1}{x} \Rightarrow y^* = a + bx^* \quad (\text{polynomial}),$$

where $x^* = \frac{1}{x}$, $y^* = \frac{1}{y}$, $a = \frac{1}{\alpha}$, and $b = \frac{\beta}{\alpha}$.

Example: The stress-strain data obtained from a compression test of a concrete cylinder is listed below. Perform a least-squares fit using the equation $\sigma = Ae^{B\varepsilon}$, where A and B are constants.

Strain ε ($\times 10^{-6}$)	500	1000	1500	2000	2375
Stress σ (MPa)	15.5	24.6	29.3	30.3	30.6

Solution:

Since the given model $\sigma = Ae^{B\varepsilon}$ is a non-polynomial, thus we must first transform it to a polynomial form.

$$\sigma = Ae^{B\varepsilon} \Rightarrow \ln \sigma = \ln A + B\varepsilon \Rightarrow y = a + Bx \quad (\text{polynomial}),$$

where $x = \varepsilon$, $y = \ln \sigma$ and $a = \ln A$.

$x, (= \varepsilon), (\times 10^{-6})$	500	1000	1500	2000	2375
$y, (= \ln \sigma)$	2.74084	3.202746	3.377588	3.411148	3.421

Now, use the least squares criterion,

$$\begin{bmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{bmatrix} \begin{Bmatrix} a \\ B \end{Bmatrix} = \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \end{bmatrix},$$

$$n = 5, \quad \sum_{i=1}^n x_i = (500 + 1000 + 1500 + 2000 + 2375) \times 10^{-6} = 7375 \times 10^{-6},$$

$$\sum_{i=1}^n x_i^2 = 1.314 \times 10^{-5}, \quad \sum_{i=1}^n y_i = 16.153322, \quad \text{and} \quad \sum_{i=1}^n x_i y_i = 0.024587.$$

$$\therefore \begin{bmatrix} 5 & 7375 \times 10^{-6} \\ 7375 \times 10^{-6} & 1.314 \times 10^{-5} \end{bmatrix} \begin{Bmatrix} a \\ B \end{Bmatrix} = \begin{bmatrix} 16.153322 \\ 0.024587 \end{bmatrix}.$$

Solving the above matrix, we get: $a = 2.734504$ and $B = 336.380242$.

But $a = \ln A \Rightarrow A = e^a \Rightarrow A = e^{2.734504} = 15.402102$.

\therefore The required equation is $\sigma \approx 15.4e^{336.38\varepsilon}$.