Least Square Fit of a Line

Problem: Given a set of N pairs of numbers, $\{(x_i, y_i) \mid i = 1, ..., N\}$, what is the best linear fit, $y = ax + b$, in the sense that it minimizes the square error, $S = \sum_{i=1}^{N}\left(ax_i + b - y_i\right)^2$.

Answer: S is a quadratic function of both a and b, and it becomes $+\infty$ for $a \to \pm\infty$ or $b \to \pm\infty$. There is a unique combination of a and b, at which S takes the minimum value and its derivatives with respect to a and b are zero, i.e.,

$$\begin{cases} \dfrac{\partial S}{\partial a} = 2\sum_{i=1}^{N}\left(ax_i + b - y_i\right)x_i = 0 \\ \dfrac{\partial S}{\partial b} = 2\sum_{i=1}^{N}\left(ax_i + b - y_i\right) = 0 \end{cases}$$

This is a set of linear equations,

$$\begin{cases} \left(\sum_{i=1}^{N} x_i^2\right)a + \left(\sum_{i=1}^{N} x_i\right)b = \sum_{i=1}^{N} x_i y_i \\ \left(\sum_{i=1}^{N} x_i\right)a + Nb = \sum_{i=1}^{N} y_i \end{cases}$$

which, in the matrix notation, becomes

$$\begin{bmatrix} \sum_{i=1}^{N} x_i^2 & \sum_{i=1}^{N} x_i \\ \sum_{i=1}^{N} x_i & N \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} x_i y_i \\ \sum_{i=1}^{N} y_i \end{bmatrix}$$

The solution is

$$\begin{aligned}\begin{bmatrix} a \\ b \end{bmatrix} &= \begin{bmatrix} \sum_{i=1}^{N} x_i^2 & \sum_{i=1}^{N} x_i \\ \sum_{i=1}^{N} x_i & N \end{bmatrix}^{-1}\begin{bmatrix} \sum_{i=1}^{N} x_i y_i \\ \sum_{i=1}^{N} y_i \end{bmatrix} \\ &= \frac{1}{\sum_{i=1}^{N} x_i^2 N - \left(\sum_{i=1}^{N} x_i\right)^2}\begin{bmatrix} N & -\sum_{i=1}^{N} x_i \\ -\sum_{i=1}^{N} x_i & \sum_{i=1}^{N} x_i^2 \end{bmatrix}\begin{bmatrix} \sum_{i=1}^{N} x_i y_i \\ \sum_{i=1}^{N} y_i \end{bmatrix} \\ &= \frac{1}{\sum_{i=1}^{N} x_i^2 N - \left(\sum_{i=1}^{N} x_i\right)^2}\begin{bmatrix} N\sum_{i=1}^{N} x_i y_i - \sum_{i=1}^{N} x_i \sum_{i=1}^{N} y_i \\ -\sum_{i=1}^{N} x_i \sum_{i=1}^{N} x_i y_i + \sum_{i=1}^{N} x_i^2 \sum_{i=1}^{N} y_i \end{bmatrix}\end{aligned}$$

Or

$$\begin{cases} a = \dfrac{N\sum\limits_{i=1}^{N} x_i y_i - \sum\limits_{i=1}^{N} x_i \sum\limits_{i=1}^{N} y_i}{\sum\limits_{i=1}^{N} x_i^2 N - \left(\sum\limits_{i=1}^{N} x_i\right)^2} \\ b = \dfrac{-\sum\limits_{i=1}^{N} x_i \sum\limits_{i=1}^{N} x_i y_i + \sum\limits_{i=1}^{N} x_i^2 \sum\limits_{i=1}^{N} y_i}{\sum\limits_{i=1}^{N} x_i^2 N - \left(\sum\limits_{i=1}^{N} x_i\right)^2} \end{cases}$$