

Prompt:

Consider a set of bivariate data $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$. Show that the line that minimizes the total squared error is given by $y = \hat{a}x + \hat{b}$ where

$$\hat{a} = \frac{n \sum(x_i y_i) - (\sum(x_i))(\sum(y_i))}{n \sum(x_i)^2 - (\sum(x_i))^2}$$

and

$$\hat{b} = \bar{y} - \hat{a}\bar{x}$$

Derivation:

We will consider the equation $E = \sum_{i=1}^n (y_i - ax_i - b)^2$. In order to minimize the equation we will take the derivative and then set it equal to zero for each of the variables, a and b. We will begin by taking the partial derivative with respect to b:

$$\begin{aligned} \frac{\partial E}{\partial b} &= \sum_{i=1}^n [2(y_i - ax_i - b)(-1)] = -2 \sum_{i=1}^n (y_i - ax_i - b) = -2 \left(\sum_{i=1}^n y_i - \sum_{i=1}^n ax_i - \sum_{i=1}^n b \right) \\ &= -2(n\bar{y} - an\bar{x} - b) = -2n(\bar{y} - a\bar{x} - b) \end{aligned}$$

Setting $\frac{\partial E}{\partial b} = 0$ to minimize the error E yields:

$$0 = \frac{\partial E}{\partial b} = -2n(\bar{y} - a\bar{x} - \hat{b}) \Rightarrow 0 = \bar{y} - a\bar{x} - \hat{b} \Rightarrow \hat{b} = \bar{y} - a\bar{x}$$

We have now shown that $\hat{b} = \bar{y} - a\bar{x}$ when the total squared error E is minimized. Now we will take the partial derivative with respect to a:

$$\begin{aligned} \frac{\partial E}{\partial a} &= \sum_{i=1}^n [2(y_i - ax_i - b)(-x_i)] = -2 \left(\sum_{i=1}^n x_i y_i - \sum_{i=1}^n ax_i^2 - \sum_{i=1}^n bx_i \right) \\ &= -2 \left(\sum_{i=1}^n x_i y_i - a \sum_{i=1}^n x_i^2 - bn\bar{x} \right) \end{aligned}$$

Setting $\frac{\partial E}{\partial a} = 0$ to minimize the error E yields:

$$0 = \frac{\partial E}{\partial a} = -2 \left(\sum_{i=1}^n x_i y_i - \hat{a} \sum_{i=1}^n x_i^2 - \hat{b}n\bar{x} \right)$$

Since $\hat{b} = \bar{y} - \hat{a}\bar{x}$, substitution yields:

$$\begin{aligned}
0 &= -2 \left(\sum_{i=1}^n x_i y_i - \hat{a} \sum_{i=1}^n x_i^2 - (\bar{y} - \hat{a}\bar{x}) n\bar{x} \right) \\
\Rightarrow 0 &= -2 \left(\sum_{i=1}^n x_i y_i - \hat{a} \sum_{i=1}^n x_i^2 - n\bar{x}\bar{y} + \hat{a}n\bar{x}^2 \right) \\
\Rightarrow 0 &= \sum_{i=1}^n x_i y_i - \hat{a} \sum_{i=1}^n x_i^2 - n \left(\frac{\sum_{i=1}^n x_i}{n} \right) \left(\frac{\sum_{i=1}^n y_i}{n} \right) + \hat{a}n \left(\frac{\sum_{i=1}^n x_i}{n} \right)^2 \\
\Rightarrow 0 &= n \sum_{i=1}^n x_i y_i - \hat{a}n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right) + \hat{a} \left(\sum_{i=1}^n x_i \right)^2 \\
\Rightarrow \hat{a}n \sum_{i=1}^n x_i^2 - \hat{a} \left(\sum_{i=1}^n x_i \right)^2 &= n \sum_{i=1}^n x_i y_i - \left(\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right) \\
\Rightarrow \hat{a} \left[n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i \right)^2 \right] &= n \sum_{i=1}^n x_i y_i - \left(\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right) \\
\Rightarrow \hat{a} &= \frac{n \sum_{i=1}^n x_i y_i - \left(\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right)}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i \right)^2}
\end{aligned}$$

Thus we have shown that $\hat{a} = \frac{n \sum_{i=1}^n x_i y_i - \left(\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right)}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i \right)^2}$ when the total squared error E is minimized. Therefore, the line that minimizes the total squared error E is given by $y = \hat{a}x + \hat{b}$ where $\hat{a} = \frac{n \sum_{i=1}^n x_i y_i - \left(\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right)}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i \right)^2}$ and $\hat{b} = \bar{y} - \hat{a}\bar{x}$.