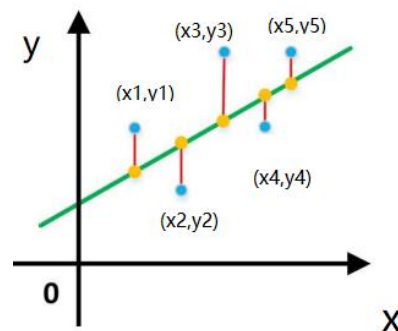


The derivation process of least square

The basic idea

The following figure is the most intuitive feeling to find out such unknown parameters to minimize the total error (distance) of sample points and fitting lines.



And this error can be directly subtracted, but the direct subtraction is going to be positive and negative, which cancel each other out, so you just square the difference

The derivation process

1. Linear equation set fitting for:

$$y = a + bx$$

2. Samples/ datasets:

$$(x_1, y_1), (x_2, y_2) \dots (x_n, y_n)$$

3. Set d_i as the distance from the sample point to the fitting line, i.e., the error.

Loss function $f(x)$.

$$f(x) = y_i - y$$

$$d_i = y_i - (a + bx_i)$$

4. Let D be the sum of the differences (why take the square to prevent the pluses and minuses from cancelling out).

Error ,

$$D = \sum_{i=1}^n d_i^2 = \sum_{i=1}^n (y_i - a - bx_i)^2$$

5. Set the first derivative is equal to 0, and the second derivative is greater than or equal to 0.

$$y = x^2 \quad y' = 2x$$

Take the first partial derivative with respect to a .

$$\begin{aligned}\frac{\partial D}{\partial a} &= \sum_{i=1}^n 2(y_i - a - bx_i)(-1) \\ &= -2 \sum_{i=1}^n (y_i - a - bx_i) \\ &= -2 \left(\sum_{i=1}^n y_i - \sum_{i=1}^n a - b \sum_{i=1}^n x_i \right) \\ &= -2(n\bar{y} - na - nb\bar{x})\end{aligned}$$

Take the first partial derivative with respect to b .

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

taking the partial derivative to be equal to 0.

$$\begin{aligned}-2(n\bar{y} - na - nb\bar{x}) &= 0 \\ \Rightarrow a &= \bar{y} - b\bar{x}\end{aligned}$$

$$-2 \left(\sum_{i=1}^n x_i y_i - na\bar{x} - b \sum_{i=1}^n x_i^2 \right) = 0 \quad \text{And simplify } a = \bar{y} - b\bar{x}$$

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

$$\begin{aligned}\therefore \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) &= \sum_{i=1}^n (x_i y_i - \bar{x} y_i - x_i \bar{y} + \bar{x} \bar{y}) = \sum_{i=1}^n x_i y_i - n\bar{x}\bar{y} - \cancel{n\bar{x}\bar{y}} + \cancel{n\bar{x}\bar{y}} \\ \sum_{i=1}^n (x_i - \bar{x})^2 &= \sum_{i=1}^n (x_i^2 - 2\bar{x}x_i + \bar{x}^2) = \sum_{i=1}^n x_i^2 - 2n\bar{x}^2 + n\bar{x}^2 = \sum_{i=1}^n x_i^2 - n\bar{x}^2\end{aligned}$$

So let's substitute that in

$$b = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$