

Least Squares or Least Circles?

Online Supplement:

Partial derivative with respect to the parameter a equal zero is

$$\frac{\partial E_{\perp}^2}{\partial a} = \frac{-2}{(1+b^2)} \sum_{i=1}^n (y_i - (a + bx_i)) = 0$$

which implies

$$\begin{aligned} \sum_{i=1}^n (y_i - (a + bx_i)) &= 0 \\ \sum_{i=1}^n y_i &= na + b \sum_{i=1}^n x_i, \end{aligned}$$

where

$$\bar{y} = a + b\bar{x} \quad \text{and} \quad a = \bar{y} - b\bar{x}$$

Partial derivative with respect to the parameter b equal zero is

$$\begin{aligned} \frac{\partial E_{\perp}^2}{\partial b} &= \frac{(1+b^2)[-2 \sum_{i=1}^n (y_i - (a + bx_i)) - 2b \sum_{i=1}^n (y_i - (a + bx_i))]^2}{(1+b^2)^2} \\ &= \frac{-2b \sum_{i=1}^n (y_i - (a + bx_i))^2}{(1+b^2)} = 0 \end{aligned}$$

Since

$$\sum_{i=1}^n (y_i - (a + bx_i)) = 0$$

so

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

Quadratic equation of b is:

$$b^2 S_{xx} - 2b S_x S_y + S_{yy} = 0$$

where

$$b_{1,2} = \frac{-S_x S_y \pm \sqrt{(S_x S_y)^2 - 4S_x S_y}}{S_{xx}^2}$$