

Least Squares

Simple case: One dimension

Dataset: $(x_1, b_1) \dots (x_m, b_m)$

$$b_i = \theta' x_i + \theta'' \quad , \quad i=1, \dots, m \quad \text{--- (1)}$$

↗ linear fit ↑ offset

System of equations (1) is equivalent to

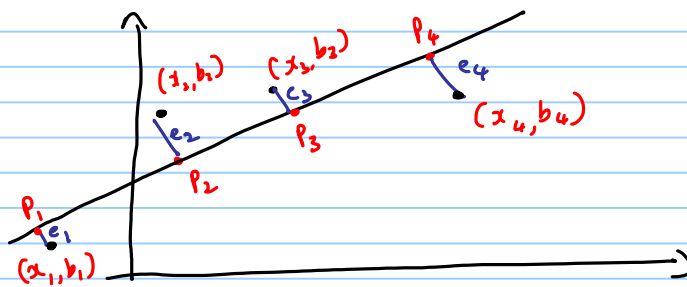
$$\begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_m & 1 \end{bmatrix} \begin{bmatrix} \theta' \\ \theta'' \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$$

$$A \theta = b, \text{ where } \theta = \begin{pmatrix} \theta' \\ \theta'' \end{pmatrix}$$

$A\theta = b$ may be inconsistent

Least squares approach: minimize $E^2 = \|b - A\theta\|^2$
 $= (b_1 - \theta'_1 x_1 - \theta''_1)^2 + \dots + (b_m - \theta'_m x_m - \theta''_m)^2$

$$(\hat{\theta}', \hat{\theta}'') = \arg \min_{\theta} \|b - A\theta\|^2$$



If the points b_1, b_2, b_3, b_4 lie on a line,
 then $P_1 = b_1, P_2 = b_2, P_3 = b_3, P_4 = b_4$

& $E^2 = 0$ & $Ax = b$ can be solved

If not, then minimize $E^2 = \|A\theta - b\|^2$

Example:

$$A\theta = b$$

$$\begin{bmatrix} -1 & 1 \\ 1 & 1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} \theta' \\ \theta'' \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 3 \end{bmatrix}$$

Is $A\theta = b$ consistent? or does $b \in C(A)$?

$$\left[\begin{array}{cc|c} -1 & 1 & 1 \\ 1 & 1 & 1 \\ 2 & 1 & 3 \end{array} \right] \rightarrow \left[\begin{array}{cc|c} 1 & -1 & -1 \\ 1 & 1 & 1 \\ 2 & 1 & 3 \end{array} \right] \rightarrow \left[\begin{array}{cc|c} 1 & -1 & -1 \\ 0 & 2 & 2 \\ 0 & 3 & 5 \end{array} \right]$$

inconsistent $A\theta = b$ or
 $b \notin C(A)$

$$\left[\begin{array}{cc|c} 1 & -1 & -1 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{array} \right] \leftarrow \left[\begin{array}{cc|c} 1 & -1 & -1 \\ 0 & 1 & 1 \\ 0 & 3 & 5 \end{array} \right]$$

Least-squares:

$$A^T A \hat{\theta} = A^T b, \text{ where } \hat{\theta} = \begin{bmatrix} \hat{\theta}' \\ \hat{\theta}'' \end{bmatrix}$$

$$A^T A = \begin{bmatrix} -1 & 1 & 2 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} -1 & 1 \\ 1 & 1 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 2 \\ 2 & 3 \end{bmatrix}, \quad A^T b = \begin{bmatrix} -1 & 1 & 2 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 6 \\ 5 \end{bmatrix}$$

$$A^T A \hat{\theta} = A^T b \quad (\Rightarrow) \quad \begin{bmatrix} 6 & 2 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} \hat{\theta}' \\ \hat{\theta}'' \end{bmatrix} = \begin{bmatrix} 6 \\ 5 \end{bmatrix}$$

$$6 \hat{\theta}' + 2 \hat{\theta}'' = 6$$

$$2 \hat{\theta}' + 3 \hat{\theta}'' = 5$$

leads to

$$\hat{\theta}'' = \frac{9}{7} \quad \text{and} \quad \hat{\theta}' = \frac{4}{7} \quad \Rightarrow \quad \hat{\theta} = \begin{bmatrix} 4/7 \\ 9/7 \end{bmatrix}$$

Best line (in the "least squares" sense) through the given data is

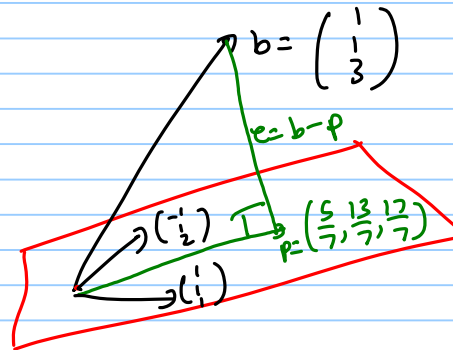
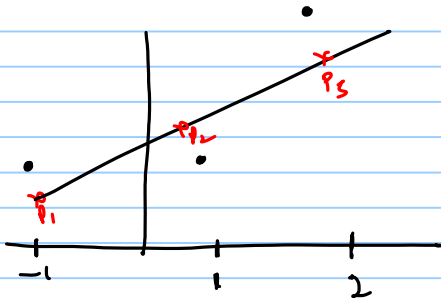
$$\boxed{\frac{4}{7}x + \frac{9}{7}}$$

Projections: $p_1 = \frac{4}{7}(-1) + \frac{9}{7} = \frac{5}{7}$, $p_2 = \frac{13}{7}$, $p_3 = \frac{17}{7}$

The original data is not on a line, so $E^2 > 0$

$$E^2 = \|b - A\hat{\theta}\|^2 = \|e\|^2$$

$$\begin{aligned} e &= \left[1 - \left(-\frac{4}{7} + \frac{9}{7}\right) \right], \left[1 - \left(\frac{4}{7} + \frac{9}{7}\right) \right], \left[3 - \left(\frac{8}{7} + \frac{9}{7}\right) \right] \\ &= \left(+\frac{2}{7}, -\frac{6}{7}, \frac{4}{7} \right) \end{aligned}$$



$$e = \left(\frac{+2}{7}, \frac{-6}{7}, \frac{4}{7} \right)$$

$$e \perp (-1, 1, 2) \quad \text{and} \quad e \perp (1, 1, 1)$$