

Least Square

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Declaration

Independent variable

$$\mathbf{x}^T = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix}$$

Label

$$\mathbf{y}^T = \begin{bmatrix} y_1 & y_2 & \cdots & y_n \end{bmatrix}$$

Model

$$y_i = ax_i + b$$

Estimation by Model

$$\hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} \hat{a}x_1 + \hat{b} \\ \hat{a}x_2 + \hat{b} \\ \vdots \\ \hat{a}x_n + \hat{b} \end{bmatrix} = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} = \mathbf{X}\mathbf{w}$$

Error

$$\mathbf{e} = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix} = \mathbf{y} - \hat{\mathbf{y}} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} \hat{a}x_1 + \hat{b} \\ \hat{a}x_2 + \hat{b} \\ \vdots \\ \hat{a}x_n + \hat{b} \end{bmatrix} = \mathbf{y} - \mathbf{X}\mathbf{w}$$

Scalar

Cost to minimize by changing \hat{a} and \hat{b}

$$\begin{aligned} J &= \frac{1}{2} \sum_{i=1}^n e_i^2 = \frac{1}{2} \sum_{i=1}^n (y_i - \hat{a}x_i - \hat{b})^2 \\ &= \frac{1}{2} \sum_{i=1}^n (y_i^2 - y_i\hat{a}x_i - y_i\hat{b} - \hat{a}x_iy_i + \hat{a}^2x_i^2 + \hat{a}x_i\hat{b} - \hat{b}y_i + \hat{b}\hat{a}x_i + \hat{b}^2) \\ &= \frac{1}{2} \sum_{i=1}^n (y_i^2 + \hat{a}^2x_i^2 + \hat{b}^2 - 2\hat{a}x_iy_i - 2\hat{b}y_i + 2\hat{a}x_i\hat{b}) \end{aligned}$$

First Parameter \hat{a}

$$\begin{aligned} \frac{\partial J}{\partial \hat{a}} &= \frac{\partial}{\partial \hat{a}} \frac{1}{2} \sum_{i=1}^n (y_i - \hat{a}x_i - \hat{b})^2 = 0 \\ &= \frac{1}{2} \sum_{i=1}^n \frac{\partial}{\partial \hat{a}} (y_i - \hat{a}x_i - \hat{b})^2 \\ &= \sum_{i=1}^n (y_i - \hat{a}x_i - \hat{b}) \frac{\partial}{\partial \hat{a}} (y_i - \hat{a}x_i - \hat{b}) \\ &= \sum_{i=1}^n (y_i - \hat{a}x_i - \hat{b})(-x_i) = 0 \\ &= \sum_{i=1}^n (-x_iy_i + \hat{a}x_i^2 + x_i\hat{b}) = 0 \\ \hat{a} \sum_{i=1}^n x_i^2 + \hat{b} \sum_{i=1}^n x_i &= \sum_{i=1}^n x_iy_i \end{aligned}$$

Second Parameter \hat{b}

$$\begin{aligned} \frac{\partial J}{\partial \hat{b}} &= \frac{\partial}{\partial \hat{b}} \frac{1}{2} \sum_{i=1}^n (y_i - \hat{a}x_i - \hat{b})^2 = 0 \\ &= \frac{1}{2} \sum_{i=1}^n \frac{\partial}{\partial \hat{b}} (y_i - \hat{a}x_i - \hat{b})^2 \\ &= \sum_{i=1}^n (y_i - \hat{a}x_i - \hat{b}) \frac{\partial}{\partial \hat{b}} (y_i - \hat{a}x_i - \hat{b}) \\ &= \sum_{i=1}^n (y_i - \hat{a}x_i - \hat{b})(-1) = 0 \\ &= \sum_{i=1}^n (-y_i + \hat{a}x_i + \hat{b}) = 0 \\ \hat{a} \sum_{i=1}^n x_i + \hat{b} \sum_{i=1}^n 1 &= \sum_{i=1}^n y_i \end{aligned}$$

Simultaneous Equations about \hat{a} and \hat{b}

$$\begin{cases} \hat{a} \sum_{i=1}^n x_i^2 + \hat{b} \sum_{i=1}^n x_i = \sum_{i=1}^n x_i y_i \\ \hat{a} \sum_{i=1}^n x_i + \hat{b} \sum_{i=1}^n 1 = \sum_{i=1}^n y_i \end{cases}$$
$$\begin{bmatrix} \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n 1 \end{bmatrix} \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n x_i y_i \\ \sum_{i=1}^n y_i \end{bmatrix}$$

Left side

$$\begin{bmatrix} \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n 1 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \\ 1 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} = \mathbf{X}^T \mathbf{X}$$

Right side

$$\begin{bmatrix} \sum_{i=1}^n x_i y_i \\ \sum_{i=1}^n y_i \end{bmatrix} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \\ 1 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \mathbf{X}^T \mathbf{y}$$

Equation in Matrix Form

$$\mathbf{X}^T \mathbf{X} \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} = \mathbf{X}^T \mathbf{y}$$

$$(\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \mathbf{X}) \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} = \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Vector

Error in vector form

$$\mathbf{e} = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix} = \mathbf{y} - \hat{\mathbf{y}} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} \hat{a}x_1 + \hat{b} \\ \hat{a}x_2 + \hat{b} \\ \vdots \\ \hat{a}x_n + \hat{b} \end{bmatrix} = \mathbf{y} - \mathbf{X}\mathbf{w}$$

Cost to minimize

$$\begin{aligned} J &= \frac{1}{2} \sum_{i=1}^n e_i^2 = \frac{1}{2} \mathbf{e}^T \mathbf{e} = \frac{1}{2} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w}) \\ &= \frac{1}{2} (\mathbf{y}^T - \mathbf{w}^T \mathbf{X}^T) (\mathbf{y} - \mathbf{X}\mathbf{w}) \\ &= \frac{1}{2} (\mathbf{y}^T \mathbf{y} - \mathbf{w}^T \mathbf{X}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}\mathbf{w} + \mathbf{w}^T \mathbf{X}^T \mathbf{X}\mathbf{w}) \end{aligned}$$

Partial derivatives of cost about parameter \mathbf{w} (i)

$$\begin{aligned} \frac{\partial J}{\partial \mathbf{w}} &= \frac{1}{2} \frac{\partial}{\partial \mathbf{w}} [(\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})] = 0 \\ &= \frac{1}{2} \left[\left[\frac{\partial}{\partial \mathbf{w}} (\mathbf{y} - \mathbf{X}\mathbf{w})^T \right] (\mathbf{y} - \mathbf{X}\mathbf{w}) + (\mathbf{y} - \mathbf{X}\mathbf{w})^T \left[\frac{\partial}{\partial \mathbf{w}} (\mathbf{y} - \mathbf{X}\mathbf{w}) \right] \right] \\ &= \frac{1}{2} \left[-\mathbf{X}^T (\mathbf{y} - \mathbf{X}\mathbf{w}) + (\mathbf{y} - \mathbf{X}\mathbf{w})^T [-\mathbf{X}] \right] \\ &= \frac{1}{2} \left[(-\mathbf{X}^T \mathbf{y} + \mathbf{X}^T \mathbf{X}\mathbf{w}) + (\mathbf{y}^T - \mathbf{w}^T \mathbf{X}^T) [-\mathbf{X}] \right] \\ &= \frac{1}{2} \left[(-\mathbf{X}^T \mathbf{y} + \mathbf{X}^T \mathbf{X}\mathbf{w}) + (-\mathbf{y}^T \mathbf{X} + \mathbf{w}^T \mathbf{X}^T \mathbf{X}) \right] \end{aligned}$$

Partial derivatives of cost about parameter \mathbf{w} (ii)

$$\begin{aligned}\frac{\partial J}{\partial \mathbf{w}} &= \begin{bmatrix} \frac{\partial J}{\partial \hat{a}} \\ \frac{\partial J}{\partial \hat{b}} \end{bmatrix} = \frac{1}{2} \frac{\partial}{\partial \mathbf{w}} \left[(\mathbf{y}_{n \times 1} - \mathbf{X}_{n \times 2} \mathbf{w}_{n \times 2})^T_{1 \times n} (\mathbf{y}_{n \times 1} - \mathbf{X}_{n \times 2} \mathbf{w}_{n \times 2})_{n \times 1} \right] = \mathbf{0} \\ &= \frac{1}{2} \left[\left[\frac{\partial}{\partial \mathbf{w}} (\mathbf{y}_{n \times 1} - \mathbf{X}_{n \times 2} \mathbf{w}_{n \times 2})^T \right] (\mathbf{y}_{n \times 1} - \mathbf{X}_{n \times 2} \mathbf{w}_{n \times 2})_{n \times 1} + (\mathbf{y}_{n \times 1} - \mathbf{X}_{n \times 2} \mathbf{w}_{n \times 2})^T_{1 \times n} \left[\frac{\partial}{\partial \mathbf{w}} (\mathbf{y} - \mathbf{X} \mathbf{w}) \right] \right] \\ &= \frac{1}{2} \left[-\mathbf{X}^T (\mathbf{y} - \mathbf{X} \mathbf{w}) + (\mathbf{y} - \mathbf{X} \mathbf{w})^T [-\mathbf{X}] \right] \\ &= \frac{1}{2} \left[(-\mathbf{X}^T \mathbf{y} + \mathbf{X}^T \mathbf{X} \mathbf{w}) + (\mathbf{y}^T - \mathbf{w}^T \mathbf{X}^T) [-\mathbf{X}] \right] \\ &= \frac{1}{2} \left[(-\mathbf{X}^T \mathbf{y} + \mathbf{X}^T \mathbf{X} \mathbf{w}) + (-\mathbf{y}^T \mathbf{X} + \mathbf{w}^T \mathbf{X}^T \mathbf{X}) \right]\end{aligned}$$

Size

$$\begin{aligned}J &= \frac{1}{2} (\mathbf{y}^T_{1 \times n} \mathbf{y}_{n \times 1} - \mathbf{w}^T_{1 \times 2} \mathbf{X}^T_{2 \times n} \mathbf{y}_{n \times 1} - \mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} + \mathbf{w}^T_{1 \times 2} \mathbf{X}^T_{2 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1}) \\ \frac{\partial J}{\partial \mathbf{w}} &= \begin{bmatrix} \frac{\partial J}{\partial w_1} \\ \frac{\partial J}{\partial w_2} \end{bmatrix} = \frac{\partial}{\partial \mathbf{w}} \frac{1}{2} (\mathbf{y}^T_{1 \times n} \mathbf{y}_{n \times 1} - \mathbf{w}^T_{1 \times 2} \mathbf{X}^T_{2 \times n} \mathbf{y}_{n \times 1} - \mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} + \mathbf{w}^T_{1 \times 2} \mathbf{X}^T_{2 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1}) \\ &= \frac{1}{2} \left(\frac{\partial}{\partial \mathbf{w}} \mathbf{y}^T_{1 \times n} \mathbf{y}_{n \times 1} - \frac{\partial}{\partial \mathbf{w}} \mathbf{w}^T_{1 \times 2} \mathbf{X}^T_{2 \times n} \mathbf{y}_{n \times 1} - \frac{\partial}{\partial \mathbf{w}} \mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} + \frac{\partial}{\partial \mathbf{w}} \mathbf{w}^T_{1 \times 2} \mathbf{X}^T_{2 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} \right) \\ &= \frac{1}{2} \left(-\mathbf{X}^T_{2 \times n} \mathbf{y}_{n \times 1} - \frac{\partial}{\partial \mathbf{w}} \mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} + \frac{\partial}{\partial \mathbf{w}} \mathbf{w}^T_{1 \times 2} \mathbf{X}^T_{2 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} \right)\end{aligned}$$

Simplifying partial derivatives of cost function

$$\begin{aligned}\frac{\partial}{\partial \mathbf{w}} \mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} &= \begin{bmatrix} \frac{\partial}{\partial w_1} (\mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1}) \\ \frac{\partial}{\partial w_2} (\mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1}) \end{bmatrix} \\ \frac{\partial}{\partial w_1} (\mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1}) &= \mathbf{y}^T_{1 \times n} \mathbf{x}_{n \times 1} \\ \frac{\partial}{\partial w_2} (\mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1}) &= \mathbf{y}^T_{1 \times n} \mathbf{1}_{n \times 1} \\ \frac{\partial}{\partial \mathbf{w}} \mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} &= \begin{bmatrix} \frac{\partial}{\partial w_1} (\mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1}) \\ \frac{\partial}{\partial w_2} (\mathbf{y}^T_{1 \times n} \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1}) \end{bmatrix} = \begin{bmatrix} \mathbf{y}^T_{1 \times n} \mathbf{x}_{n \times 1} \\ \mathbf{y}^T_{1 \times n} \mathbf{1}_{n \times 1} \end{bmatrix} = \mathbf{X}^T_{2 \times n} \mathbf{y}_{n \times 1}\end{aligned}$$

$$\frac{\partial J}{\partial \mathbf{w}} = \begin{bmatrix} \frac{\partial J}{\partial w_1} \\ \frac{\partial J}{\partial w_2} \end{bmatrix} = \frac{1}{2} \left(-\mathbf{X}_{2 \times n}^T \mathbf{y}_{n \times 1} - \mathbf{X}_{2 \times n}^T \mathbf{y}_{n \times 1} + \frac{\partial}{\partial \mathbf{w}} \mathbf{w}_{1 \times 2}^T \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} \right)$$

$$= \frac{1}{2} \left(\frac{\partial}{\partial \mathbf{w}} \mathbf{w}_{1 \times 2}^T \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} \right) - \mathbf{X}_{2 \times n}^T \mathbf{y}_{n \times 1}$$

$$\frac{\partial}{\partial \mathbf{w}} \mathbf{w}_{1 \times 2}^T \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} = \begin{bmatrix} \frac{\partial}{\partial w_1} \mathbf{w}_{1 \times 2}^T \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} \\ \frac{\partial}{\partial w_2} \mathbf{w}_{1 \times 2}^T \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} \end{bmatrix}$$

$$\mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} = \begin{bmatrix} \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n 1 \end{bmatrix}$$

$$\mathbf{w}_{1 \times 2}^T \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} = \begin{bmatrix} w_1 & w_2 \end{bmatrix} \begin{bmatrix} \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$

$$= \begin{bmatrix} w_1 \sum_{i=1}^n x_i^2 + w_2 \sum_{i=1}^n x_i & w_1 \sum_{i=1}^n x_i + w_2 \sum_{i=1}^n 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$

$$= w_1^2 \sum_{i=1}^n x_i^2 + 2w_1 w_2 \sum_{i=1}^n x_i + w_2^2 \sum_{i=1}^n 1$$

$$\frac{\partial}{\partial w_1} \mathbf{w}_{1 \times 2}^T \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} = \frac{\partial}{\partial w_1} \left(w_1^2 \sum_{i=1}^n x_i^2 + 2w_1 w_2 \sum_{i=1}^n x_i + w_2^2 \sum_{i=1}^n 1 \right)$$

$$= 2w_1 \sum_{i=1}^n x_i^2 + 2w_2 \sum_{i=1}^n x_i$$

$$= 2 \begin{bmatrix} \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$

$$= 2 \begin{bmatrix} \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i \end{bmatrix} \mathbf{w}$$

$$\begin{aligned}
\frac{\partial}{\partial w_2} \mathbf{w}_{1 \times 2}^T \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} &= \frac{\partial}{\partial w_2} \left(w_1^2 \sum_{i=1}^n x_i^2 + 2w_1 w_2 \sum_{i=1}^n x_i + w_2^2 \sum_{i=1}^n 1 \right) \\
&= 2w_1 \sum_{i=1}^n x_i + 2w_2 \sum_{i=1}^n 1 \\
&= 2 \begin{bmatrix} \sum_{i=1}^n x_i & \sum_{i=1}^n 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \\
&= 2 \begin{bmatrix} \sum_{i=1}^n x_i & \sum_{i=1}^n 1 \end{bmatrix} \mathbf{w}
\end{aligned}$$

$$\frac{\partial}{\partial \mathbf{w}} \mathbf{w}_{1 \times 2}^T \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} = 2 \mathbf{X}^T \mathbf{X} \mathbf{w}$$

Finally

$$\begin{aligned}
\frac{\partial J}{\partial \mathbf{w}} &= \frac{1}{2} \left(\frac{\partial}{\partial \mathbf{w}} \mathbf{w}_{1 \times 2}^T \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} \right) - \mathbf{X}_{2 \times n}^T \mathbf{y}_{n \times 1} \\
&= \frac{1}{2} (2 \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1}) - \mathbf{X}_{2 \times n}^T \mathbf{y}_{n \times 1} \\
&= \mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} - \mathbf{X}_{2 \times n}^T \mathbf{y}_{n \times 1} = 0 \\
\mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2} \mathbf{w}_{2 \times 1} &= \mathbf{X}_{2 \times n}^T \mathbf{y}_{n \times 1} \\
\mathbf{w}_{2 \times 1} &= (\mathbf{X}_{2 \times n}^T \mathbf{X}_{n \times 2})^{-1} \mathbf{X}_{2 \times n}^T \mathbf{y}_{n \times 1}
\end{aligned}$$