

Fitting a line. — Minh Quoc Nguyen
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Call N data points

$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(N)}, y^{(N)})$$

Finding a and b for fitting the line

$$y = ax + b$$

to the data points, that means minimizing predefined error.

Mean squared error:

$$l(a, b) = \frac{1}{N} \sum_{i=1}^N (y^{(i)} - y(x^{(i)}))^2$$

Taking partial derivatives:

$$\begin{aligned} \frac{\partial l}{\partial a} &= \frac{1}{N} \sum_{i=1}^N 2(y^{(i)} - (ax^{(i)} + b))(-x^{(i)}) \\ &= \frac{2}{N} \sum_{i=1}^N (ax^{(i)} + b - y^{(i)})x^{(i)} \end{aligned}$$

$$\frac{\partial l}{\partial b} = \frac{1}{N} \sum_{i=1}^N 2(y^{(i)} - (ax^{(i)} + b)) \cdot 1$$

Simplifying the

Then

$$0 = \frac{\partial l}{\partial a} \Rightarrow 0 = \frac{2}{N} \left[a \sum_{i=1}^N (x^{(i)})^2 + b \sum_{i=1}^N x^{(i)} - \sum_{i=1}^N y^{(i)} x^{(i)} \right]$$

$$\Leftrightarrow 0 = a \bar{x}^2 + b \bar{x} - \bar{xy} \quad (1)$$

where $\bar{x}^2 = \frac{1}{N} \sum_{i=1}^N (x^{(i)})^2$, $\bar{x} = \frac{1}{N} \sum_{i=1}^N x^{(i)}$, $\bar{xy} = \frac{1}{N} \sum_{i=1}^N y^{(i)} x^{(i)}$

$$0 = \frac{\partial l}{\partial b} \Rightarrow 0 = \frac{2}{N} \left[\sum_{i=1}^N y^{(i)} - a \sum_{i=1}^N x^{(i)} + b \sum_{i=1}^N 1 \right]$$

$$\Leftrightarrow 0 = \bar{y} - a \bar{x} + b \quad (2)$$

From (1), (2):

$$\begin{cases} a \bar{x}^2 + b \bar{x} = \bar{xy} \\ a \bar{x} + b = \bar{y} \end{cases}$$

(Suppose the system have unique solution $\begin{vmatrix} \bar{x}^2 & \bar{x} \\ \bar{x} & 1 \end{vmatrix} \neq 0$)

$$\Rightarrow \begin{cases} a = \frac{\bar{xy} - \bar{x} \bar{y}}{\bar{x}^2 - (\bar{x})^2} \\ b = \frac{\bar{x}^2 \bar{y} - \bar{x} \bar{xy}}{\bar{x}^2 - (\bar{x})^2} \end{cases}$$

If now each data points have m attributes:
 $(x^{(i)}, y^{(i)}) \rightarrow (x_1^{(i)}, x_2^{(i)}, \dots, x_m^{(i)}, y^{(i)})$

The predicted value becomes:

$$y = w_0 + [w_1, \dots, w_m] \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}$$

$$= w_0 + w^T x$$

Also taking the derivative: for $1 \leq j \leq m$.

$$\begin{aligned} \frac{\partial l}{\partial w_j} &= \frac{1}{N} \sum_{i=1}^N 2(y^{(i)} - y^{(i)}) x_j^{(i)} \\ &= \frac{2}{N} \sum_{i=1}^N [w_0 + w^T x^{(i)} - y^{(i)}] x_j^{(i)} \\ &= \frac{2}{N} \sum_{i=1}^N [w_1^T x^{(i)} - y^{(i)}] x_j^{(i)} \end{aligned}$$

where $w^T = [w_1, w_2, \dots, w_m]$, $x^{(i)} = \begin{bmatrix} x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_m^{(i)} \end{bmatrix}$

$$\begin{aligned} \frac{\partial l}{\partial w_0} &= \frac{1}{N} \sum_{i=1}^N 2(y^{(i)} - y^{(i)}) \cdot 1 \\ &= \frac{2}{N} \sum_{i=1}^N [w^T x^{(i)} - y^{(i)}] \end{aligned}$$

Denote

$$X = \begin{bmatrix} 1 & \dots & x^{(1)} & \dots \\ 1 & \dots & x^{(2)} & \dots \\ \vdots & & \vdots & \\ 1 & \dots & x^{(N)} & \dots \end{bmatrix} \quad \begin{matrix} X \text{ size} \\ N \times (m+1) \end{matrix}$$

$$y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{bmatrix} \quad y \in \mathbb{R}^N$$

Then

$$\begin{bmatrix} \frac{\partial \ell}{\partial w_0} \\ \frac{\partial \ell}{\partial w_1} \\ \vdots \\ \frac{\partial \ell}{\partial w_m} \end{bmatrix} = X^T (Xw' - Y)$$

$$\Rightarrow \nabla \ell(w) = 0 \Leftrightarrow X^T (Xw' - Y) = 0$$

$$\Leftrightarrow X^T X w' - X^T Y = 0$$

$$\Leftrightarrow w' = (X^T X)^{-1} (X^T Y)$$

(Suppose $(X^T X)^{-1}$ is invertible)