

## NORMAL EQUATION DERIVATION

Derivation of Normal Equation.

- Squared error cost function is:

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)})^2$$

Which can be written in vectorized form:

$$J(\theta) = \frac{1}{2m} (x\theta - y)^T (x\theta - y)$$

$$= \frac{1}{2m} ((x\theta)^T - y^T) (x\theta - y)$$

Simplifying

$$= \frac{1}{2m} (x\theta)^T x\theta - (x\theta)^T y - y^T (x\theta) + y^T y$$

since  $(x\theta)^T$  and  $y$  are both vectors, so using their multiplicative property.

$$\therefore (x\theta)^T y = y^T (x\theta)$$

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$$= \frac{1}{2m} (\mathbf{x}\boldsymbol{\theta})^T \mathbf{x}\boldsymbol{\theta} - 2(\mathbf{x}\boldsymbol{\theta})^T \mathbf{y} + \mathbf{y}^T \mathbf{y}$$

$$\textcircled{O} = \frac{1}{2m} \cancel{\boldsymbol{\theta}^T \mathbf{x}} \mathbf{x}\boldsymbol{\theta} - 2(\mathbf{x}\boldsymbol{\theta})^T \mathbf{y} + \mathbf{y}^T \mathbf{y} = 0$$

So, in order to find optimal values of  $\boldsymbol{\theta}$ , we will have to derive  $J(\boldsymbol{\theta})$  w.r.t to vector  $\boldsymbol{\theta}$  and set that to 0 to find the minima.

~~Find derivatives of each term in the equation, note the  $\frac{1}{2m}$  will be removed since we have set  $J(\boldsymbol{\theta})$  to 0 on the right hand side.~~

Derivating  $2(\mathbf{x}\boldsymbol{\theta})^T \mathbf{y}$ .

For simplicity assume our input feature matrix  $\mathbf{x}$  is of dimension  $2 \times 2$ . as follow

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \quad \boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$$

$$= 2(x\theta)^T y$$

$$= 2 \left( \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \right)^T \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$= 2 \left( \begin{bmatrix} x_{11}\theta_1 + x_{12}\theta_2 \\ x_{21}\theta_1 + x_{22}\theta_2 \end{bmatrix} \right)^T \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

~~it will~~ taking transform since  $X\theta$  is a vector  
it will turn in  $1 \times 2$  matrix.

$$= 2 \left( \begin{bmatrix} x_{11}\theta_1 + x_{12}\theta_2 & x_{21}\theta_1 + x_{22}\theta_2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \right)$$

lets call the below eq as  $P_1(\theta)$

$$P_1(\theta) = 2(y_1(x_{11}\theta_1 + x_{12}\theta_2) + y_2(x_{21}\theta_1 + x_{22}\theta_2))$$

$$\frac{\partial P_1}{\partial \theta_1} = 2(x_{11}y_1 + x_{21}y_2)$$

$$\frac{\partial P_1}{\partial \theta_2} = 2(y_1x_{12} + x_{22}y_2)$$

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The results of derivatives can be written as follows:

$$= 2 \begin{bmatrix} x_{11} & x_{21} \\ x_{12} & x_{22} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

the above matrix is  $X^T$ .

$$\text{so } \frac{\partial}{\partial \theta} (\theta^T X^T) y = 2 X^T y$$

taking the derivative of other term

$\theta^T X^T \theta \neq X^T \theta$ , it doesn't matter whether we write  ~~$\theta^T$  or  $X^T \theta$~~  according to dimensions.

let's multiply  $X^T \cdot X$  first

$$X^T = \begin{bmatrix} x_{11} & x_{21} \\ x_{12} & x_{22} \end{bmatrix} \quad X = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix}$$

$X^T \cdot X \cdot \theta$ 

$$= \begin{bmatrix} x_{11}^2 + x_{21}^2 & x_{11}x_{12} + x_{21}x_{22} \\ x_{12}x_{11} + x_{22}x_{21} & x_{12}^2 + x_{22}^2 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$$

 $X^T \cdot \theta$ 

$$= \begin{bmatrix} \theta_1(x_{11}^2 + x_{21}^2) + \theta_2(x_{11}x_{12} + x_{21}x_{22}) \\ \theta_1(x_{12}x_{11} + x_{22}x_{21}) + \theta_2(x_{12}^2 + x_{22}^2) \end{bmatrix}$$

 $\theta^T \cdot X^T \cdot X \cdot \theta$ 

$$= [\theta_1 \quad \theta_2] \begin{bmatrix} \theta_1(x_{11}^2 + x_{21}^2) + \theta_2(x_{11}x_{12} + x_{21}x_{22}) \\ \theta_1(x_{12}x_{11} + x_{22}x_{21}) + \theta_2(x_{12}^2 + x_{22}^2) \end{bmatrix}$$

$$= [\theta_1^2(x_{11}^2 + x_{21}^2) + \theta_1\theta_2(x_{11}x_{12} + x_{21}x_{22}) \\ + \theta_2\theta_1(x_{12}x_{11} + x_{22}x_{21}) + \theta_2^2(x_{12}^2 + x_{22}^2)]$$

lets call the above function  $Z(\theta)$

$$Z(\theta) = [\theta_1^2(x_{11}^2 + x_{21}^2) + 2\theta_1\theta_2(x_{11}x_{12} + x_{21}x_{22}) + \theta_2^2(x_{12}^2 + x_{22}^2)]$$

$$\frac{\partial Z}{\partial \theta_1} = [2\theta_1(x_{11}^2 + x_{21}^2) + 2\theta_2(x_{11}x_{12} + x_{21}x_{22})]$$

$$\frac{\partial Z}{\partial \theta_2} = [2\theta_1(x_{11}x_{12} + x_{21}x_{22}) + 2\theta_2(x_{12}^2 + x_{22}^2)]$$

$$= \begin{bmatrix} 2(x_{11}^2 + x_{21}^2) & 2(x_{11}x_{12} + x_{21}x_{22}) \\ 2(x_{11}x_{12} + x_{21}x_{22}) & 2(x_{12}^2 + x_{22}^2) \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$$

$$= 2 X^T X \theta$$

$$\frac{\partial}{\partial \theta} \quad \theta^T X^T X \theta = 2 X^T X \theta$$

$$\frac{\partial}{\partial \theta} \quad y^T y = 0$$

Combining all :

$$\frac{\partial}{\partial \theta} \theta^T X^T X \theta - 2(X\theta)^T y + y^T y =$$

$$2X^T X \theta - 2X^T y = 0$$

$$X^T X \theta = X^T y$$

$$\boxed{\theta = (X^T X)^{-1} X^T y}$$

Normal Equation.