Normal Equation

Let $x^{(i)} \in \mathbf{R}^3$ be i-th data and $y^{(i)} \in \mathbf{R}$ be i-th label for $i = 1, 2, \dots, m$. We want to find unknown weight, $w \in \mathbf{R}^3$. y, X, w are defined as

$$y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}, \tag{1}$$

$$X = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & x_3^{(1)} \\ x_1^{(2)} & x_2^{(2)} & x_3^{(2)} \\ \vdots & \vdots & \vdots \\ x_1^{(m)} & x_2^{(m)} & x_3^{(m)} \end{bmatrix},$$
 (2)

$$w = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}. \tag{3}$$

Derive a normal equation, $X^TXw = X^Ty$, to solve the following least squares problem.

$$\min_{w} \frac{1}{m} \sum_{i=1}^{m} |y^{(i)} - f(w; x^{(i)})|^2$$
(4)

where

$$f(w;x) = w_1 x_1 + w_2 x_2 + w_3 x_3 \tag{5}$$

Proof. For k = 1, 2, 3,

$$\frac{\partial J}{\partial w_k} = \frac{\partial}{\partial w_k} \left[\frac{1}{m} \sum_{i=1}^m |y^{(i)} - f(w; x^{(i)})|^2 \right]$$
 (6)

$$=$$
 (7)

$$= -\frac{2}{m} \sum_{i=1}^{m} \left(y^{(i)} - f(w; x^{(i)}) \right) \frac{\partial}{\partial w_k} (w_1 x_1^{(i)} + w_2 x_2^{(i)} + w_3 x_3^{(i)})$$
 (8)

$$= -\frac{2}{m} \sum_{i=1}^{m} \left(y^{(i)} - f(w; x^{(i)}) \right) x_k^{(i)}$$
(9)

$$= -\frac{2}{m} \sum_{i=1}^{m} x_k^{(i)} \left(y^{(i)} - \left(w_1 x_1^{(i)} + w_2 x_2^{(i)} + w_3 x_3^{(i)} \right) \right)$$
 (10)

$$\nabla J(w) = \begin{bmatrix} \frac{\partial J}{\partial w_1} & \frac{\partial J}{\partial w_2} & \frac{\partial J}{\partial w_3} \end{bmatrix}^T \tag{11}$$

$$= -\frac{2}{m}X^{T}(y - Xw) = 0 (12)$$

Therefore,

$$-\frac{2}{m}X^{T}(y - Xw) = 0 (13)$$

$$-X^{T}(y - Xw) = 0 (14)$$

$$X^T X w = X^T y \tag{15}$$

Proof. For k = 1, 2, 3,

$$\nabla J(w) = \nabla \left[\frac{1}{m} ||y - f(w; x)||^2 \right]$$
(16)

$$= \nabla \left[\frac{1}{m} ||y - Xw||^2 \right] \tag{17}$$

$$= \nabla \left[\frac{1}{m} (y - Xw)^T (y - Xw) \right] \tag{18}$$

$$= (19)$$

$$= \frac{1}{m} \nabla \left(y^T y - 2w^T X^T y + w^T X^T X w \right) \tag{20}$$

$$= \frac{1}{m} \left(\nabla(y^T y) - 2\nabla(w^T X^T y) + \nabla(w^T X^T X w) \right) \tag{21}$$

$$= (22)$$

Therefore,

$$-X^T y + X^T X w = 0 (23)$$

$$X^T X w = X^T y (24)$$