Derivation of Lasso Regression

Derive
$$\mathbf{w} = (X_b^T X_b + \lambda I)^{-1} X_b^T \mathbf{y}$$

เรามี
$$Cost=\sum_{i=1}^n{(y_i-\hat{y}_i)^2}+\lambda\sum_{j=0}^p{|w_j|}$$
 และเราต้องการหา $\mathbf{w}=\begin{bmatrix}w_0\\w_1\\\vdots\\w_p\end{bmatrix}$ ที่ทำให้ $Cost$ ต่ำที่สุด

จาก calculus เราทราบว่า Cost ต่ำสุดเมื่อ $\nabla Cost = 0$ ดังนั้น

$$\nabla Cost = \begin{bmatrix} \frac{\partial Cost}{\partial w_0} \\ \frac{\partial Cost}{\partial w_1} \\ \vdots \\ \frac{\partial Cost}{\partial w_d} \\ \vdots \\ \frac{\partial Cost}{\partial w_p} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

พิจารณา $\dfrac{\partial Cost}{\partial w_d}=0$ เมื่อ $d\in\{0,1,...,p\}$ จะได้ว่า

$$\sum_{i=1}^{n} x_{i,d} \hat{y}_i + \lambda \frac{\partial |w_d|}{\partial w_d} = \sum_{i=1}^{n} x_{i,d} y_i$$
 (1)

ซึ่งสามารถเขียนให้อยู่ในรูป matrix ได้ดังนี้

$$\begin{bmatrix} x_{1,d} & x_{2,d} & \cdots & x_{n,d} \end{bmatrix} \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} + \lambda \frac{\partial |w_d|}{\partial w_d} = \begin{bmatrix} x_{1,d} & x_{2,d} & \cdots & x_{n,d} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$
(2)

จากสมการ

$$\begin{bmatrix} \frac{\partial Cost}{\partial w_0} \\ \frac{\partial Cost}{\partial w_1} \\ \vdots \\ \frac{\partial Cost}{\partial w_d} \\ \vdots \\ \frac{\partial Cost}{\partial w_p} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

เราจะสามารถเขียนให้อยู่ในรูปต่อไปนี้ได้

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_{1,1} & x_{2,1} & \cdots & x_{n,1} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1,p} & x_{2,p} & \cdots & x_{n,p} \end{bmatrix} \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} + \lambda \begin{bmatrix} \frac{\partial |w_0|}{\partial |w_1|} \\ \frac{\partial |w_p|}{\partial w_n} \\ \vdots \\ \frac{\partial |w_p|}{\partial w_n} \end{bmatrix} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_{1,1} & x_{2,1} & \cdots & x_{n,1} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1,p} & x_{2,p} & \cdots & x_{n,p} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; x_{i,0} = 1; i \in \{1, 2, ..., n\}$$

กำหนดให้

$$X_b = \begin{bmatrix} 1 & x_{1,1} & \cdots & x_{1,p} \\ 1 & x_{2,1} & \cdots & x_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n,1} & \cdots & x_{n,p} \end{bmatrix}, \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix}$$

นั่นคือ $X_b^T \hat{\mathbf{y}} + \lambda \mathbf{w} = X_b^T \mathbf{y}$

$$:: \hat{\mathbf{y}} = X_b \mathbf{w} \tag{3}$$

จะได้

$$X_b^T X_b \mathbf{w} + \lambda \nabla \mathbf{w} = X_b^T \mathbf{y}$$

Derive Equation 1

เนื่องจาก

$$\begin{split} \frac{\partial \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\partial w_d} &= \sum_{i=1}^{n} \frac{\partial (y_i - \hat{y}_i)^2}{\partial (y_i - \hat{y}_i)} \cdot \frac{\partial (y_i - \hat{y}_i)}{\partial \hat{y}_i} \cdot \frac{\partial \hat{y}_i}{w_d} \\ &= \sum_{i=1}^{n} 2(y_i - \hat{y}_i)(1)(-1)\frac{\partial \hat{y}_i}{w_d} \\ &= \sum_{i=1}^{n} -2(y_i - \hat{y}_i)\frac{\partial (w_0 + w_1 x_{i,1} + \dots + w_d x_{i,d} + \dots + w_p x_{i,p})}{w_d} \\ &= \sum_{i=1}^{n} -2(y_i - \hat{y}_i)x_{i,d} \\ &= -2\sum_{i=1}^{n} (y_i - \hat{y}_i)x_{i,d} \\ &= -2\sum_{i=1}^{n} x_{i,d}y_i + 2\sum_{i=1}^{n} x_{i,d}\hat{y}_i \end{split}$$

และ

$$\begin{split} \frac{\partial \lambda \sum_{j=0}^{p} |w_{j}|}{\partial w_{d}} &= \lambda \frac{\partial \sum_{j=0}^{p} |w_{j}|}{\partial w_{d}} \\ &= \lambda \frac{\partial (|w_{0}| + |w_{1}| + \dots + |w_{d}| + \dots + |w_{p}|)}{\partial w_{d}} \\ &= \lambda \frac{\partial |w_{d}|}{\partial w_{d}} \end{split}$$

ดังนั้น

$$\begin{split} \frac{\partial Cost}{\partial w_d} &= \frac{\partial \left[\sum_{i=1}^n (y_i - \hat{y}_i)^2 + \lambda \sum_{j=0}^p |w_j|\right]}{\partial w_d} \\ 0 &= \frac{\partial \sum_{i=1}^n (y_i - \hat{y}_i)^2}{\partial w_d} + \frac{\partial \lambda \sum_{j=0}^p |w_j|}{\partial w_d} \\ 0 &= -2\sum_{i=1}^n x_{i,d}y_i + 2\sum_{i=1}^n x_{i,d}\hat{y}_i + \lambda \frac{\partial |w_d|}{\partial w_d} \\ 0 &= -\sum_{i=1}^n x_{i,d}y_i + \sum_{i=1}^n x_{i,d}\hat{y}_i + \frac{\lambda}{2} \frac{\partial |w_d|}{\partial w_d} \\ 0 &= -\sum_{i=1}^n x_{i,d}y_i + \sum_{i=1}^n x_{i,d}\hat{y}_i + \lambda \frac{\partial |w_d|}{\partial w_d} \\ \sum_{i=1}^n x_{i,d}\hat{y}_i + \lambda \frac{\partial |w_d|}{\partial w_d} &= \sum_{i=1}^n x_{i,d}y_i \end{split}$$

Derive Equation 2

พิจารณา $\sum_{i=1}^n x_{i,d} \hat{y}_i$

$$\sum_{i=1}^{n} x_{i,d} \hat{y}_{i} = x_{1,d} \hat{y}_{1} + x_{2,d} \hat{y}_{2} + \dots + x_{n,d} \hat{y}_{n}$$

$$= \begin{bmatrix} x_{1,d} & x_{2,d} & \dots & x_{n,d} \end{bmatrix}$$

$$x_{1,d} \hat{y}_{1} & \begin{bmatrix} \hat{y}_{1} \\ x_{2,d} \hat{y}_{2} & & \\ \vdots & & \\ x_{n,d} \hat{y}_{n} & \\ \hat{y}_{n} \end{bmatrix}$$

พิจารณา $\sum_{i=1}^n x_{i,d} y_i$

$$\sum_{i=1}^{n} x_{i,d}y_i = x_{1,d}y_1 + x_{2,d}y_2 + \dots + x_{n,d}y_n$$

$$= \begin{bmatrix} x_{1,d} & x_{2,d} & \dots & x_{n,d} \end{bmatrix}$$

$$x_{1,d}y_1 & \begin{bmatrix} y_1 \\ x_{2,d}y_2 & & y_2 \\ \vdots & & \vdots \\ x_{n,d}y_n & y_n \end{bmatrix}$$

ดังนั้น จะได้ว่า

$$\sum_{i=1}^{n} x_{i,d} \hat{y}_i + \lambda \frac{\partial |w_d|}{\partial w_d} = \sum_{i=1}^{n} x_{i,d} y_i$$

$$\begin{bmatrix} x_{1,d} & x_{2,d} & \cdots & x_{n,d} \end{bmatrix} \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} + \lambda \frac{\partial |w_d|}{\partial w_d} = \begin{bmatrix} x_{1,d} & x_{2,d} & \cdots & x_{n,d} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Derive Equation 3

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} w_0 + w_1 x_{1,1} + \dots + w_p x_{1,p} \\ w_0 + w_1 x_{2,1} + \dots + w_p x_{2,p} \\ \vdots \\ w_0 + w_1 x_{n,1} + \dots + w_p x_{n,p} \end{bmatrix}$$
$$= \begin{bmatrix} 1 & x_{1,1} & \dots & x_{1,p} \\ 1 & x_{2,1} & \dots & x_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n,1} & \dots & x_{n,p} \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_p \end{bmatrix}$$

กำหนดให้
$$\hat{\mathbf{y}}=\begin{bmatrix}\hat{y}_1\\\hat{y}_2\\\vdots\\\hat{y}_n\end{bmatrix}, X_b=\begin{bmatrix}1&x_{1,1}&\cdots&x_{1,p}\\1&x_{2,1}&\cdots&x_{2,p}\\\vdots&\vdots&\ddots&\vdots\\1&x_{n,1}&\cdots&x_{n,p}\end{bmatrix}, \mathbf{w}=\begin{bmatrix}w_0\\w_1\\\vdots\\w_p\end{bmatrix}$$

ดังนั้น จะได้ว่า

$$\hat{\mathbf{y}} = X_b \mathbf{w}$$