Convexity of Sum of Squared Errors for Linear Regression

เราต้องการพิสูจน์ว่า sum of squared errors สำหรับ linear regression เป็น convex function

เรามี
$$Cost = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

การตรวจสอบการเป็น convex function สามารถทำได้โดยพิจารณา second derivative ของ function นั้น ๆ ถ้า second derivative มีค่ามากกว่าหรือเท่ากับ 0 ในทุกกรณีแล้ว หมายความว่า function นั้นเป็น convex function จาก

$$\nabla^2 Cost = \begin{bmatrix} \frac{\partial^2 Cost}{\partial w_0^2} \\ \frac{\partial^2 Cost}{\partial w_1^2} \\ \vdots \\ \frac{\partial^2 Cost}{\partial w_p^2} \end{bmatrix}$$

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

$$\frac{\partial Cost}{\partial w_d} = -2\sum_{i=1}^n x_{i,d}(y_i - \hat{y}_i) \tag{1}$$

พิจารณา $\dfrac{\partial^2 Cost}{\partial w_d^2}$ เมื่อ $d \in \{0,1,...,p\}$ จะได้ว่า

$$\frac{\partial^2 Cost}{\partial w_d^2} = 2\sum_{i=1}^n x_{i,d}^2 \tag{2}$$

พิจารณา $x_{i,d}^2$

เนื่องจาก
$$x_{i,d} \in \mathbb{R}$$
 ดังนั้น $x_{i,d}^2 \geq 0$

จะได้ว่า
$$2\sum_{i=1}^n x_{i,d}^2 \geq 0$$
 นั่นคือ

$$\nabla^2 Cost = \begin{bmatrix} \frac{\partial^2 Cost}{\partial w_0^2} \\ \frac{\partial^2 Cost}{\partial w_1^2} \\ \vdots \\ \frac{\partial^2 Cost}{\partial w_n^2} \end{bmatrix} \ge \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

สรุปได้ว่า sum of squared error สำหรับ linear regression เป็น convex function

Derive Equation 1

$$\begin{split} \frac{\partial Cost}{\partial w_d} &= \frac{\partial \sum_{i=1}^n (y_i - \hat{y}_i)^2}{\partial w_d} \\ &= \sum_{i=1}^n \frac{\partial (y_i - \hat{y}_i)^2}{\partial (y_i - \hat{y}_i)} \cdot \frac{\partial (y_i - \hat{y}_i)}{\partial \hat{y}_i} \cdot \frac{\partial \hat{y}_i}{\partial w_d} \\ &= \sum_{i=1}^n 2(y_i - \hat{y}_i)(1)(-1)\frac{\partial \hat{y}_i}{\partial w_d} \\ &= \sum_{i=1}^n -2(y_i - \hat{y}_i)\frac{(w_0 + w_1x_{i,1} + \dots + w_dx_{i,d} + \dots + w_px_{i,p})}{\partial w_d} \\ &= \sum_{i=1}^n -2(y_i - \hat{y}_i)x_{i,d} \\ &= -2\sum_{i=1}^n (y_i - \hat{y}_i)x_{i,d} \\ &= -2\sum_{i=1}^n x_{i,d}(y_i - \hat{y}_i) \end{split}$$

Derive Equation 2

$$\begin{split} \frac{\partial^2 Cost}{\partial w_d^2} &= \frac{\partial}{\partial w_d} \left(\frac{\partial Cost}{\partial w_d} \right) \\ &= \frac{\partial}{\partial w_d} \left(-2 \sum_{i=1}^n x_{i,d} (y_i - \hat{y}_i) \right) \\ &= \frac{\partial \left(-2 \sum_{i=1}^n x_{i,d} (y_i - \hat{y}_i) \right)}{\partial w_d} \\ &= -2 \sum_{i=1}^n \frac{\partial x_{i,d} (y_i - \hat{y}_i)}{\partial w_d} \\ &= -2 \sum_{i=1}^n \frac{\partial \left[x_{i,d} y_i - x_{i,d} \hat{y}_i \right]}{\partial w_d} \\ &= -2 \left[\frac{\partial x_{i,d} y_i}{\partial w_d} - \frac{\partial x_{i,d} \hat{y}_i}{\partial w_d} \right] \\ &= -2 \sum_{i=1}^n \left[0 - \frac{\partial x_{i,d} \hat{y}_i}{\partial w_d} \right] \\ &= -2 \sum_{i=1}^n \left[-\frac{\partial x_{i,d} \hat{y}_i}{\partial w_d} \right] \\ &= 2 \sum_{i=1}^n \left[\frac{\partial x_{i,d} \hat{y}_i}{\partial w_d} \right] \\ &= 2 \sum_{i=1}^n \left[x_{i,d} \frac{\partial \hat{y}_i}{\partial w_d} \right] \\ &= 2 \sum_{i=1}^n \left[x_{i,d} \frac{\partial \hat{y}_i}{\partial w_d} \right] \\ &= 2 \sum_{i=1}^n \left[x_{i,d} \frac{\partial \hat{y}_i}{\partial w_d} \right] \\ &= 2 \sum_{i=1}^n \left[x_{i,d} \frac{w_0 + w_1 x_{i,1} + \dots + w_d x_{i,d} + \dots + w_p x_{i,p}}{\partial w_d} \right] \\ &= 2 \sum_{i=1}^n x_{i,d} x_{i,d} \\ &= 2 \sum_{i=1}^n x_{i,d}^2 x_{i,d} \end{split}$$