Algebra for Least Squares

1. Function to minimize w.r.t. β_0, β_1

$$Q = \sum_{i=1}^{n} (Y_i - (\beta_0 + \beta_1 X_i))^2$$

2. Minimize this by maximizing $-Q$
3. Find partials and set both equal to zero

$$\begin{aligned} \frac{dQ}{d\beta_0} &= 0 \\ \frac{dQ}{d\beta_1} &= 0 \end{aligned}$$

Normal Equations

1. The result of this maximization step are called the normal equations. b_0 and b_1 are called point estimators of β_0 and β_1 respectively.

$$\begin{aligned} \sum Y_i &= nb_0 + b_1 \sum X_i \\ \sum X_i Y_i &= b_0 \sum X_i + b_1 \sum X_i^2 \end{aligned}$$

Goal: select values of β_0, β_1 that minimize Q and label them as b_0, b_1

$$(i): \frac{\partial Q}{\partial \beta_0} = 2\sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_i)(-1) \overset{\text{set}}{=} 0 \Rightarrow \sum_{i=1}^{n} Y_i = nb_0 + b_1 \sum_{i=1}^{n} X_i$$

$$(ii): \frac{\partial Q}{\partial \beta_1} = 2\sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_i)(-X_i) \overset{\text{set}}{=} 0 \Rightarrow \sum_{i=1}^{n} X_i Y_i = b_0 \sum_{i=1}^{n} X_i + b_1 \sum_{i=1}^{n} X_i^2$$

This is a system of two equations and two unknowns. The solution is given by . . .

Solving (by multiplying (i) by $\sum_{i=1}^{n} X_i$ and (ii) by n and taking $(ii)-(i)$):

$$n\sum_{i=1}^{n} X_iY_i - \sum_{i=1}^{n} X_i \sum_{i=1}^{n} Y_i = b_1\left(n\sum_{i=1}^{n} X_i^2 - \left(\sum_{i=1}^{n} X_i\right)^2\right) \Rightarrow$$

$$\sum_{i=1}^{n} X_iY_i - \frac{\sum_{i=1}^{n} X_i \sum_{i=1}^{n} Y_i}{n} = b_1\left(\sum_{i=1}^{n} X_i^2 - \frac{\left(\sum_{i=1}^{n} X_i\right)^2}{n}\right) \Rightarrow$$

$$b_1 = \frac{\sum_{i=1}^{n} X_iY_i - \frac{\sum_{i=1}^{n} X_i \sum_{i=1}^{n} Y_i}{n}}{\sum_{i=1}^{n} X_i^2 - \frac{\left(\sum_{i=1}^{n} X_i\right)^2}{n}} = \frac{\sum_{i=1}^{n}\left(X_i - \overline{X}\right)\left(Y_i - \overline{Y}\right)}{\sum_{i=1}^{n}\left(X_i - \overline{X}\right)^2} = \frac{SS_{XY}}{SS_{XX}} = \sum_{i=1}^{n} \frac{\left(X_i - \overline{X}\right)}{SS_{XX}} Y_i = \sum_{i=1}^{n} k_i Y_i$$

From (i): $$b_0 = \overline{Y} - b_1\overline{X} = \sum_{i=1}^{n}\left(\frac{1}{n} + \frac{\overline{X}\left(X_i - \overline{X}\right)}{SS_{XX}}\right)Y_i = \sum_{i=1}^{n} l_i Y_i$$

Fitted Values and Residuals

True Regression Function: $E\{Y\} = \beta_0 + \beta_1 X$ (Unknown, since $\beta_0, \beta_1 \equiv$ parameters)

Estimated Regression Function (Fitted): $\hat{Y} = b_0 + b_1 X$

For the i^{th} observation: $\hat{Y}_i = b_0 + b_1 X_i \quad i = 1, \ldots, n$

Residuals: Differences between observed and fitted (predicted) values:

$$e_i = Y_i - \hat{Y}_i = Y_i - \left(b_0 + b_1 X_i\right) \quad i = 1, \ldots, n$$

Properties of Residuals:

$$\sum_{i=1}^{n} e_i = 0 \quad \text{(From LS eq } (i))$$

$$\sum_{i=1}^{n} X_i e_i = 0 \quad \text{(From LS eq } (ii))$$

$$\Rightarrow \sum_{i=1}^{n} \hat{Y}_i e_i = \sum_{i=1}^{n}\left(b_0 + b_1 X_i\right)e_i = b_0\sum_{i=1}^{n} e_i + b_1 \sum_{i=1}^{n} X_i e_i = 0$$