Derivation of OLS: Simple and Multiple Linear Regression

Simple Linear Regression

The simple linear regression model is defined as:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i,$$

where:

- y_i : Dependent variable (response variable).
- x_i : Independent variable (predictor variable).
- β_0, β_1 : Regression coefficients (intercept and slope).
- ϵ_i : Error term (unobservable).

The objective of Ordinary Least Squares (OLS) is to minimize the **Sum of Squared Errors (SSE)**, which is given by:

$$SSE = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2.$$

Step 1: Partial derivatives of SSE To find the values of β_0 and β_1 that minimize SSE, we compute the partial derivatives with respect to β_0 and β_1 and set them equal to 0.

Partial derivative with respect to β_0 :

$$\frac{\partial SSE}{\partial \beta_0} = -2\sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_i)) = 0.$$

Partial derivative with respect to β_1 :

$$\frac{\partial SSE}{\partial \beta_1} = -2\sum_{i=1}^n x_i \left(y_i - (\beta_0 + \beta_1 x_i) \right) = 0.$$

Step 2: Solve for β_0 and β_1 Expanding the first equation:

$$\sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) = 0.$$

This simplifies to:

$$\sum_{i=1}^{n} y_i - n\beta_0 - \beta_1 \sum_{i=1}^{n} x_i = 0,$$

which gives:

$$\beta_0 = \bar{y} - \beta_1 \bar{x},$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$ and $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$. Expanding the second equation:

$$\sum_{i=1}^{n} x_i (y_i - \beta_0 - \beta_1 x_i) = 0.$$

Substitute $\beta_0 = \bar{y} - \beta_1 \bar{x}$:

$$\sum_{i=1}^{n} x_i y_i - \beta_0 \sum_{i=1}^{n} x_i - \beta_1 \sum_{i=1}^{n} x_i^2 = 0.$$

This simplifies to:

$$\beta_1 = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2}.$$

Thus, the OLS estimators for simple linear regression are:

$$\beta_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}, \quad \beta_0 = \bar{y} - \beta_1 \bar{x}.$$

Multiple Linear Regression

The multiple linear regression model is defined as:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where:

- $\mathbf{y} \in \mathbb{R}^n$: Dependent variable vector.
- $\mathbf{X} \in \mathbb{R}^{n \times p}$: Design matrix containing p predictors (including a column of ones for the intercept).
- $\beta \in \mathbb{R}^p$: Coefficient vector.
- $\epsilon \in \mathbb{R}^n$: Error term vector.

The objective of OLS is to minimize the **Sum of Squared Errors (SSE)**, which is given in matrix form as:

$$J(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2.$$

Expanding the norm:

$$J(\boldsymbol{\beta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^{\top} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}).$$

Step 1: Partial derivative of $J(\beta)$ Take the derivative with respect to β :

$$\frac{\partial J(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = -2\mathbf{X}^{\top}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}).$$

Set the derivative to 0:

$$\mathbf{X}^{\top}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = 0.$$

Step 2: Solve for β Rearranging:

$$\mathbf{X}^{\top}\mathbf{y} = \mathbf{X}^{\top}\mathbf{X}\boldsymbol{\beta}.$$

Assuming $\mathbf{X}^{\top}\mathbf{X}$ is invertible, multiply by its inverse:

$$\boldsymbol{\beta} = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}.$$

Thus, the OLS estimator for multiple linear regression is:

$$\boldsymbol{\beta} = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}.$$

Conclusion

In this document, we derived the OLS estimators for both simple and multiple linear regression. The simple linear regression derivation focused on solving for β_0 and β_1 analytically, while the multiple linear regression derivation utilized matrix operations to generalize the solution for multiple predictors. These derivations form the foundation for linear regression in statistics and machine learning.