Least Squares Algorithm Derivation

Introduction

The Least Squares Algorithm is a mathematical approach used to find the best-fitting line (or curve) for a set of data points. It minimizes the sum of squared differences (or residuals) between observed values and those predicted by a model. This technique is widely used in regression analysis, where the goal is to model the relationship between two or more variables. In linear regression, this method is used to determine the parameters (slope and intercept) of the best-fitting straight line.

The objective of this derivation is to find the parameters β_0 (intercept) and β_1 (slope) that minimize the sum of squared residuals between the observed and predicted data points.

Problem Setup

Given a set of data points $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$, where x_i represents the independent variable and y_i the dependent variable, we aim to fit a linear model to predict y_i as a function of x_i.

In linear regression, we assume a model of the form:

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

Where:

- y_i is the observed value at x_i,
- β_0 and β_1 are the parameters (intercept and slope) of the line,
- ϵ_i is the error term, the difference between the actual and predicted value of y_i.

Objective: Minimize the Error

We want to minimize the sum of squared errors (residuals), which is defined as:

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

Here, $S(\beta_0, \beta_1)$ represents the total squared error or the cost function that we want to minimize with respect to β_0 and β_1.

Derivation of Least Squares Solution

We now proceed to derive the values of β_0 and β_1 that minimize the cost function.

Expand the Error Function

First, expand the squared error term:

$$S(\beta_0, \beta_1) = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

Expanding this expression:

$$S(\beta_0, \beta_1) = \sum_{i=1}^{n} \left(y_i^2 - 2y_i(\beta_0 + \beta_1 x_i) + (\beta_0 + \beta_1 x_i)^2\right)$$

This simplifies to:

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

Take Partial Derivatives

To find the minimum, take the partial derivatives of $S(\beta_0, \beta_1)$ with respect to β_0 and β_1, and set them equal to zero.

Partial derivative with respect to β_0

$$\frac{\partial S}{\partial \beta_0} = -2 \sum_{i=1}^{n} y_i + 2n\beta_0 + 2\beta_1 \sum_{i=1}^{n} x_i$$

Set this equal to zero:

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

This simplifies to:

$$n\beta_0 + \beta_1 \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i \tag{1}$$

Partial derivative with respect to β_1

$$\frac{\partial S}{\partial \beta_1} = -2\sum_{i=1}^{n} y_i x_i + 2\beta_0 \sum_{i=1}^{n} x_i + 2\beta_1 \sum_{i=1}^{n} x_i^2$$

Set this equal to zero:

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

This simplifies to:

$$\beta_0 \sum_{i=1}^{n} x_i + \beta_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i x_i \tag{2}$$

Solve the System of Equations

We now have the system of two equations:

$$n\beta_0 + \beta_1 \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i \tag{1}$$

$$\beta_0 \sum_{i=1}^{n} x_i + \beta_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i x_i \tag{2}$$

To solve for β_0 and β_1, follow these steps:

Solve equation (1) for β_0

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

Substitute this expression for β_0 into equation (2):

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

Simplifying the equation gives:

$$\beta_1 = \frac{n\sum_{i=1}^{n} y_i x_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

Once you have β_1, substitute it back into equation (1) to get β_0:

$$\beta_0 = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

Final Results

The least squares estimates for β_0 and β_1 are:

$$\beta_1 = \frac{n\sum_{i=1}^{n} y_i x_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$\beta_0 = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

These are the coefficients of the best-fitting line in the least squares sense.