Least Squares Derivation

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Definition: Transpose of a Matrix

Given the following 3×2 matrix

$$X = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ \dots & \dots \end{pmatrix}$$

The transpose of the above matrix is of the form:

$$X^T = \begin{pmatrix} x_{11} & x_{21} & \dots \\ x_{12} & x_{22} & \dots \end{pmatrix}$$

In transpose, rows become columns and columns become rows.

You can perform transpose over numpy objects by calling or .

Definition: Inverse of a Matrix

When we multiply a number by its reciprocal, we get 1.

For a number n,

$$n \cdot \frac{1}{n} = 1$$

Similarly, when we multiply a matrix by its inverse, we get the Identity matrix.

For a matrix A,

$$A\,A^{-1} = I$$

is used to calculate the inverse of a matrix, if it exists.

Multiple Linear Regression

In Multiple Linear Regression, the model takes a simple algebraic form:

$$Y = X\,\beta$$

We will again choose the MSE as our loss function, which can be expressed in vector notation as:

$$MSE(\beta) = \frac{1}{n}||Y - X\,\beta||^2$$

$$MSE(\beta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - x_{i1}\beta_1 - x_{i2}\beta_2)^2$$

Taking the derivative of the loss i.e. MSE with respect to the model parameter β gives:

$$\frac{\partial L}{\partial \beta} = -2X^T(Y - X\beta)$$

For optimization, we set the values of the partial derivative to zero, i.e.

$$\frac{\partial L}{\partial \beta} = 0 \Rightarrow -2X^T(Y - X\beta) = 0$$

$$\Rightarrow X^T(Y - X\beta) = 0$$

Optimization of the previous equation gives:

$$X^T X\beta = X^T Y$$

Multiplying both sides with $(X^T X)^-1$, we get:

$$(X^T X)^{-1} X^T X\beta = (X^T X)^{-1} X^T Y$$

Thus, we get

$$\beta = (X^T X)^{-1} X^T Y$$

Backtracking this equation to fit the model optimization problem, we have

$$\hat{\beta} = (X^T X)^{-1} X^T Y = \underset{\beta}{\operatorname{argmin}} MSE(\beta)$$

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