Linear regression

ML Instruction Team, Fall 2022

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Formulation

It is generally much easier to formulate the linear regression model in matrix form, say we have a linear model of the form:

$$y_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_n x_{in} + \epsilon_i$$

We can write it as the matrix from:

$$Y = X\beta + \epsilon$$

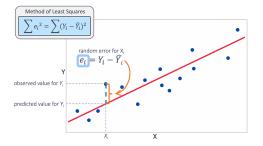


Figure: Simple Linear Regression, Source



Non-Geometric Approach

- Y represents a vector of length n containing the observed values $Y = (y_1, \dots, y_m)^T$
- β is a vector for the parameters $\beta = (\beta_0, \dots, \beta_n)^T$
- ϵ is a vector for the errors

$$\epsilon = (\epsilon_1, \dots, \epsilon_m)^T$$

X is a matrix of the features in which the column of ones incorporates the intercept.

$$X = \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1n} \\ 1 & x_{21} & x_{22} & \dots & x_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{m1} & x_{m2} & \dots & x_{mn} \end{pmatrix}$$

One suitable estimator of β should be the one minimizing the sum of the squared errors $\sum_{i=1}^{m} \epsilon_i^2 = \epsilon^T \epsilon$.

$$\sum_{i=1}^{m} \epsilon_i^2 = \epsilon^T \epsilon = (Y - X\beta)^T (Y - X\beta)$$
$$= y^T y - 2\beta X^T y + \beta^T X^T X\beta$$

Non-Geometric Approach

Differentiating this term and setting it to zero, we find that the estimate for β that minimizes the squared error satisfies the so called normal equation:

$$\boldsymbol{X}^T\boldsymbol{X}\hat{\boldsymbol{\beta}} = \boldsymbol{X}^T\boldsymbol{Y}$$

Provided X^TX is invertible,

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

We can then get the fitted values, \hat{Y} , and residuals, $\hat{\epsilon}$,

$$\hat{Y} = X\hat{\beta} = X \left(X^T X\right)^{-1} X^T Y = HY$$
$$\hat{\epsilon} = Y - X\hat{\beta} = Y - \hat{Y} = (I - H)Y$$

where the projection matrix $H = X (X^T X)^{-1} X^T$.



Geometric Approach

- Another way of looking at this problem is to say we want a solution (our fitted values) that lies in the space spanned by X become as close as possible to Y.
- In this way, the systematic component $X\hat{\beta}$ is the projection of Y onto the space spanned by X, and the residuals are $Y X\hat{\beta}$.

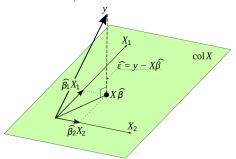


Figure: Geometric Approach of Linear Regression, Source

Geometric Approach

■ The Ridge estimate of the linear regression problem is defined as:

$$\begin{split} \hat{\beta}_{\text{Ridge}} &= \underset{\beta \in \mathbb{R}^n}{\operatorname{argmin}} \|y - X\beta\|_2^2 + \frac{1}{2}\lambda \sum_{j=1}^n |\beta_j|^2 \\ &= \underset{\beta \in \mathbb{R}^n}{\operatorname{argmin}} \|y - X\beta\|_2^2 + \frac{1}{2}\lambda \|\beta\|_2^2 \end{split}$$

The Lasso estimate of the linear regression problem is defined as:

$$\begin{split} \hat{\beta}_{\text{Lasso}} &= \underset{\beta \in \mathbb{R}^n}{\operatorname{argmin}} \|y - X\beta\|_2^2 + \lambda \sum_{j=1}^n |\beta_j| \\ &= \underset{\beta \in \mathbb{P}^n}{\operatorname{argmin}} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1 \end{split}$$



Thank You!

Any Question?