Linear regression

ML Instruction Team, Fall 2022

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Formulation

- We generally formulate the linear regression model in matrix form:

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

where the target value y_i can be evaluated by

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

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

  $\epsilon = (\epsilon_1, \ldots, \epsilon_m)^T$
- X is a matrix of the features in which the column of ones incorporates the intercept.

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

Optimization Problem

- One suitable estimator of β should be the one minimizing the sum of the squared errors $\|\epsilon\|_2^2 = \sum_{i=1}^{m} \epsilon_i^2 = \epsilon^T \epsilon$.

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

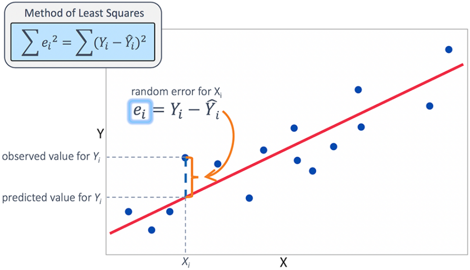

Figure: Simple Linear Regression, Source

Non-Geometric Approach

- Differentiating this term and setting it to zero, we find that the estimate for $beta$, which minimizes the squared error, satisfies the so-called Normal equation:

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

- Provided $X^T X$ 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 $H = X\left(X^T X\right)^{-1} X^T$.

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 $Y - X\hat{\beta}$.

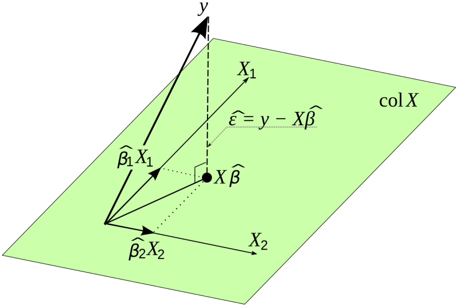

Figure: Geometric Approach of Linear Regression, Source

Extended Versions

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

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

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

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

Thank You!

Any Question?