

Regression analysis and resampling methods

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ABSTRACT

The ...

1. Introduction

2. Theory

* DECIDE ON z vs. y

$$\text{MSE}(\mathbf{y}, \tilde{\mathbf{y}}) = \frac{1}{n}(\mathbf{y} - \tilde{\mathbf{y}})^2 = \frac{1}{n} \sum_{i=0}^{n-1} (y_i - \tilde{y}_i)^2 \quad (1)$$

$$R^2(\mathbf{y}, \tilde{\mathbf{y}}) = 1 - \frac{(\mathbf{y} - \tilde{\mathbf{y}})^2}{(\mathbf{y}(1 - \bar{y}))^2} = 1 - \frac{\sum_{i=0}^{n-1} (y_i - \tilde{y}_i)^2}{\sum_{i=0}^{n-1} (y_i - \bar{y})^2} \quad (2)$$

$$\bar{y} = \frac{1}{n} \sum_{i=0}^{n-1} y_i$$

2.1. Regression

We assume the vector $\mathbf{y} \in \mathbb{R}^n$ consisting of observed values y_i to take the form $\mathbf{y} = f(\mathbf{x}) + \boldsymbol{\varepsilon}$ where $f(\mathbf{x}) \in \mathbb{R}^n$ is a continous function and $\boldsymbol{\varepsilon} \in \mathbb{R}^n$ is a normally distributed noise. We approximate f by $\tilde{\mathbf{y}} = X\boldsymbol{\beta}$, where $X \in \mathbb{R}^{n \times p}$ is the design matrix of n row vectors $\mathbf{x}_i \in \mathbb{R}^p$, and $\boldsymbol{\beta} \in \mathbb{R}^p$ are the unknown parameters to be determined. The integers n and p represent the number of data points and features, respectively.

For an observed value y_i we have $y_i = \mathbf{x}_i^T \boldsymbol{\beta} + \varepsilon_i = (X\boldsymbol{\beta})_i + \varepsilon_i$ ¹. The inner product $\mathbf{x}_i^T \boldsymbol{\beta}$ is non-stochastic, hence

$$\mathbb{E}[(X\boldsymbol{\beta})_i] = (X\boldsymbol{\beta})_i$$

and since

$$\mathbb{E}[\varepsilon_i] \stackrel{\text{per def.}}{=} 0,$$

we have the expectation value

$$\begin{aligned} \mathbb{E}[y_i] &= \mathbb{E}[(X\boldsymbol{\beta})_i + \varepsilon_i] \\ &= \mathbb{E}[(X\boldsymbol{\beta})_i] + \mathbb{E}[\varepsilon_i] \\ &= (X\boldsymbol{\beta})_i. \end{aligned}$$

¹ Can also write $X_{ij}\beta_j$, but we try to be consistent with our notation.

To find the variance, we need the expetation value of the outer product $\mathbf{y}\mathbf{y}^T$,

$$\begin{aligned} \mathbb{E}[\mathbf{y}\mathbf{y}^T] &= \mathbb{E}[(X\boldsymbol{\beta} + \boldsymbol{\varepsilon})(X\boldsymbol{\beta} + \boldsymbol{\varepsilon})^T] \\ &= \mathbb{E}[X\boldsymbol{\beta}\boldsymbol{\beta}^T X^T + X\boldsymbol{\beta}\boldsymbol{\varepsilon}^T + \boldsymbol{\varepsilon}\boldsymbol{\beta}^T X^T + \boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^T] \\ &= X\boldsymbol{\beta}\boldsymbol{\beta}^T X^T + \mathbb{I}\sigma^2. \end{aligned} \quad (3)$$

The variance becomes

$$\begin{aligned} \text{Var}[y_i] &= \mathbb{E}[(\mathbf{y}\mathbf{y}^T)_{ii}] - (\mathbb{E}[y_i])^2 \\ &= (X\boldsymbol{\beta})_i(X\boldsymbol{\beta})_i + \sigma^2 - (X\boldsymbol{\beta})_i(X\boldsymbol{\beta})_i \\ &= \sigma^2. \end{aligned}$$

Taking $\hat{\boldsymbol{\beta}}$ as the Ordinary Least Square (OLS) expression for the optimal parameter, i.e.

$$\hat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T \mathbf{y},$$

we get the expected value

$$\begin{aligned} \mathbb{E}[\hat{\boldsymbol{\beta}}] &= \mathbb{E}[(X^T X)^{-1} X^T \mathbf{y}] \\ &= (X^T X)^{-1} X^T \mathbb{E}[\mathbf{y}] \\ &= (X^T X)^{-1} X^T X\boldsymbol{\beta} \\ &= \boldsymbol{\beta}. \end{aligned}$$

The variance is then

$$\begin{aligned} \text{Var}[\hat{\boldsymbol{\beta}}] &= \mathbb{E}[\hat{\boldsymbol{\beta}}\hat{\boldsymbol{\beta}}^T] - \mathbb{E}[\hat{\boldsymbol{\beta}}]\mathbb{E}[\hat{\boldsymbol{\beta}}^T] \\ &= \mathbb{E}[(X^T X)^{-1} X^T \mathbf{y}\mathbf{y}^T X ((X^T X)^{-1})^T] - \boldsymbol{\beta}\boldsymbol{\beta}^T \\ &= (X^T X)^{-1} X^T \mathbb{E}[\mathbf{y}\mathbf{y}^T] X (X^T X)^{-1} - \boldsymbol{\beta}\boldsymbol{\beta}^T \\ &\stackrel{(3)}{=} (X^T X)^{-1} X^T (X\boldsymbol{\beta}\boldsymbol{\beta}^T X^T + \mathbb{I}\sigma^2) X (X^T X)^{-1} \\ &= \boldsymbol{\beta}\boldsymbol{\beta}^T + (X^T X)^{-1} X^T \sigma^2 X (X^T X)^{-1} - \boldsymbol{\beta}\boldsymbol{\beta}^T \\ &= \sigma^2 (X^T X)^{-1}. \end{aligned}$$

2.1.1. Ordinary Least Squares (OLS)

2.1.2. Ridge regression

2.1.3. Lasso regression

2.2. *Resampling*

2.2.1. Bootstrap method

2.2.2. Cross-validation

3. Analysis

4. Conclusion