

Chapter 2 : Linear Regression

Newton's three sisters

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1 Coefficient of Determination and the Detection of Collinearity

2 Confidence and Prediction Intervals

- We define a matrix $W \in \mathbb{R}^{N \times N}$ such that all the elements are $1/N$
 $Wy \in \mathbb{R}^N$ are $\bar{y} = Wy = \frac{1}{N} \sum_{i=1}^N y_i$ for $y_1, \dots, y_N \in \mathbb{R}$

$$Wy = \begin{bmatrix} 1/N & \cdots & 1/N \\ \vdots & \cdots & \vdots \\ 1/N & \cdots & 1/N \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} (y_1 + \cdots y_N)/N \\ \vdots \\ (y_1 + \cdots y_N)/N \end{bmatrix} = \bar{y}$$

- We can express that $\hat{y} = Hy$

- Residual Sum of Squares RSS

$$\text{RSS} = \|\hat{y} - y\|^2 = \|Hy - y\|^2 = \|(H - I)y\|^2 = \|(I - H)y\|^2$$

- Explained Sum of Squares ESS

$$\text{ESS} \triangleq \|\hat{y} - \bar{y}\|^2 = \|Hy - Wy\|^2 = \|(H - W)y\|^2$$

- Total Sum of Squares TSS

$$\text{TSS} \triangleq \|y - \bar{y}\|^2 = \|y - Wy\|^2 = \|(I - W)y\|^2$$

- **Proof** by $TSS - RSS - ESS = 0$

$$\|y - \bar{y}\|^2 - \|y - \hat{y}\|^2 - \|\hat{y} - \bar{y}\|^2 = 0$$

$$\Rightarrow (y - \bar{y})^T (y - \bar{y}) - (y - \hat{y})^T (y - \hat{y}) - (\hat{y} - \bar{y})^T (\hat{y} - \bar{y}) = 0$$

$$\Rightarrow y^T y - y^T \bar{y} - \bar{y}^T y + \bar{y}^T y - y^T y + y^T \hat{y} + \hat{y}^T y - \hat{y}^T \hat{y} - \hat{y}^T \hat{y} + \hat{y}^T \bar{y} + \bar{y}^T \hat{y} - \bar{y}^T \bar{y} = 0$$

$$\Rightarrow -2\bar{y}^T y + 2\hat{y}^T y + 2\bar{y}^T \hat{y} - 2\hat{y}^T \hat{y} = 0$$

$$\Rightarrow -\bar{y}^T (y - \hat{y}) + \hat{y}^T (y - \hat{y}) = 0$$

$$\Rightarrow (\hat{y} - \bar{y})^T (y - \hat{y}) = 0$$

- Coefficient of determination

$$R^2 = \frac{\text{ESS}}{\text{TSS}} = 1 - \frac{\text{RSS}}{\text{TSS}}$$

- Correlation between the covariates and response

$$\hat{\rho} \triangleq \frac{\sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^N (x_i - \bar{x})^2 \sum_{i=1}^N (y_i - \bar{y})^2}}$$

Relationship Between R^2 and the Correlation Coefficient

- If $p = 1$, R^2 coincides with the square of the sample-based correlation coefficient

$$\begin{aligned}\frac{\text{ESS}}{\text{TSS}} &= \frac{\hat{\beta}_1^2 ||x - \bar{x}||^2}{||y - \bar{y}||^2} = \left\{ \frac{\sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^N (x_i - \bar{x})^2} \right\}^2 \frac{\sum_{i=1}^N (x_i - \bar{x})^2}{\sum_{i=1}^N (y_i - \bar{y})^2} \\ &= \frac{\left\{ \sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y}) \right\}^2}{\sum_{i=1}^N (x_i - \bar{x})^2 \sum_{i=1}^N (y_i - \bar{y})^2} = \hat{\rho}^2\end{aligned}$$

- We sometimes use a variant of the coefficient of determination which is the adjusted coefficient of determination

$$1 - \frac{\text{RSS}/(N - p - 1)}{\text{TSS}/(N - 1)}$$

- VIF measures the redundancy of each covariate when the other covariates are present

$$\text{VIF} \triangleq \frac{1}{1 - R_{X_j|X_{-j}}^2}$$

- The minimum value of VIF is one, and we say that the collinearity of covariate is strong when its VIF value is large

1 Coefficient of Determination and the Detection of Collinearity

2 Confidence and Prediction Intervals

- We have showed how to obtain the estimate $\hat{\beta}$ of $\beta \in \mathbb{R}^{p+1}$, confidence interval of $\hat{\beta}$ as follows

$$\beta_i = \hat{\beta}_i \pm t_{N-p-1}(\alpha/2)\text{SE}(\hat{\beta}_i), \quad \text{for } i = 0, 1, \dots, p$$

- Confidence interval of $x_*\hat{\beta}$ for another point $x_* \in \mathbb{R}^{p+1}$

- The average

$$E[x_*\hat{\beta}] = x_*E[\hat{\beta}]$$

- The variance

$$V[x_*\hat{\beta}] = x_*V(\hat{\beta})x_*^T = \sigma^2 x_*(X^T X)^{-1}x_*^T$$

- We define

$$\hat{\sigma} \triangleq \sqrt{\text{RSS}/(N-p-1)}, \quad \text{SE}(x_*\hat{\beta}) \triangleq \hat{\sigma}\sqrt{x_*(X^T X)^{-1}x_*^T}$$

Confidence and Prediction Intervals in Regression

- $C \sim t_{N-p-1}$

- variance in the difference between $x_*\hat{\beta}$ and $y_* \triangleq x_*\beta + \varepsilon$

$$V[x_*\hat{\beta} - (x_*\beta + \varepsilon)] = V[x_*(\hat{\beta} - \beta)] + V[\varepsilon] = \sigma^2 x_*(X^T X)^{-1} x_*^T + \sigma^2$$

- Similarly, we can derive the following

$$P \triangleq \frac{x_*\hat{\beta} - y_*}{\text{SE}(x_*\hat{\beta} - y_*)} = \frac{x_*\hat{\beta} - y_*}{\sigma(1 + \sqrt{x_*(X^T X)^{-1} x_*^T})} / \sqrt{\frac{\text{RSS}}{\sigma^2} / (N - p - 1)} \sim t_{N-p-1}$$

- The confidence and prediction intervals

$$\begin{aligned} x_*\beta &= x_*\hat{\beta} \pm t_{N-p-1}(\alpha/2)\hat{\sigma}\sqrt{x_*(X^T X)^{-1} x_*^T} \\ y_* &= x_*\hat{\beta} \pm t_{N-p-1}(\alpha/2)\hat{\sigma}\sqrt{1 + x_*(X^T X)^{-1} x_*^T} \end{aligned}$$

Q & A

Thank you :)