Linear Regression

Newton's three sisters

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Outline

1 Distribution of the RSS Values

2 Hypothesis Testing for $\hat{\beta}_j \neq 0$

3 Coefficient of Determination and the Detection of Collinearity

4 Confidence and Prediction Intervals

Hat matrix

• Hat matrix defined by $\hat{y} = Hy$

$$\hat{y} = X\hat{\beta} = X(X^TX)^{-1}X^Ty = Hy$$

$$H \triangleq X(X^TX)^{-1}X^T$$

• Some properties

$$\begin{split} H^2 &= X(X^TX)^{-1}X^T \cdot X(X^TX)^{-1}X^T = X(X^TX)^{-1}X^T = H \\ (I-H)^2 &= I-2H+H^2 = I-H \\ HX &= X(X^TX)^{-1}X^T \cdot X = X \end{split}$$

Residual sum of square

• RSS defined

$$RSS \triangleq ||y - \hat{y}||^2$$

• Using hat matrix

$$y-\hat{y}=y-Hy=(I-H)y=(I-H)(X\beta+\varepsilon)$$

$$=(X-HX)\beta+(I-H)\varepsilon=(I-H)\varepsilon$$

$$\mathrm{RSS} \triangleq ||y - \hat{y}||^2 = \{(I - H)\varepsilon\}^T (I - H)\varepsilon = \varepsilon^T (I - H)^2 \varepsilon = \varepsilon^T (I - H)\varepsilon$$

Eigenvalues H and I - H

- They are only zeros and ones
- Dimensions of the eigenspaces of H and I-H are both p+1

Proof using
$$rank(X) = p + 1$$

$$\label{eq:rank} \begin{split} \operatorname{rank}(H) & \leq \min\{\operatorname{rank}(X(X^TX)^{-1}), \operatorname{rank}(X)\} \leq \operatorname{rank}(X) = p+1 \\ \operatorname{rank}(H) & \geq \operatorname{rank}(HX) = \operatorname{rank}(X) = p+1 \end{split}$$

Hat matrix

• Hat matrix defined by

$$\hat{y} = X\hat{\beta} = X(X^TX)^{-1}X^Ty = Hy$$

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Residual sum of square

• RSS defined

$$\mathrm{RSS} \triangleq ||y - \hat{y}||^2$$

• Using hat matrix

$$\begin{split} y - \hat{y} &= y - Hy = (I - H)y = (I - H)(X\beta + \varepsilon) \\ &= (X - HX)\beta + (I - H)\varepsilon = (I - H)\varepsilon \end{split}$$

$$RSS \triangleq ||y - \hat{y}||^2 = \{(I - H)\varepsilon\}^T (I - H)\varepsilon = \varepsilon^T (I - H)^2 \varepsilon = \varepsilon^T (I - H)\varepsilon$$

Eigenvalues of H and Null space of (I - H)

• Proof by contrapositive

$$Hx = x \Rightarrow (I - H)x = 0$$

 $(I - H)x = 0 \Rightarrow Hx = x$

• Dimensions of the eigenspaces of H is p+1

Proof using
$$rank(X) = p + 1$$

$$\begin{aligned} & \operatorname{rank}(H) \leq \min\{\operatorname{rank}(X(X^TX)^{-1}), \operatorname{rank}(X)\} \leq \operatorname{rank}(X) = p+1 \\ & \operatorname{rank}(H) \geq \operatorname{rank}(HX) = \operatorname{rank}(X) = p+1 \end{aligned}$$

 \bullet Dimensions of the null space of I-H is N-(p+1)

$$P(I-H)P^T = \mathrm{diag}(\underbrace{1,\ldots,1}_{N-p-1},\underbrace{0,\ldots,0}_{p+1})$$

• We define $v = P\varepsilon \in \mathbb{R}^N$, then from $\varepsilon = P^T v$

$$\begin{split} \text{RSS} &= \varepsilon^T (I - H) \varepsilon = (P^T v)^T (I - H) P^T v = v^T P (I - H) P^T v \\ &= [v_1, \cdots, v_{N-p-1}, v_{N-p}, \cdots, v_n] \begin{bmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & \ddots & 0 & \cdots & \cdots & \vdots \\ \vdots & 0 & 1 & \cdots & \cdots & 0 \\ 0 & 0 & 0 & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & \cdots & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ \vdots \\ v_{N-p-1} \\ v_{N-p} \\ \vdots \\ v_N \end{bmatrix} \\ &= \sum_{i=1}^{N-p-1} v_i^2 \end{split}$$

$$\bullet \ \, \mathrm{Let} \,\, w \in \mathbb{R}^{N-p-1}$$

Average

$$E[v] = E[P\varepsilon] = 0$$

$$E[w] = 0$$

Covariance

$$\begin{split} E[vv^t] &= E[P\varepsilon(P\varepsilon)^T] = PE[\varepsilon\varepsilon^t]P = P\sigma^2IP^T = \sigma^2I\\ E[ww^T] &= \sigma^2I \end{split}$$

• We have RSS

$$\frac{RSS}{\sigma^2} \sim \chi^2_{N-p-1}$$

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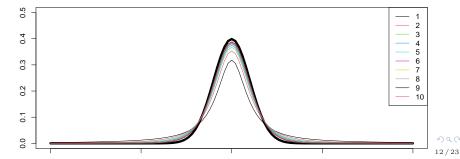
4 Confidence and Prediction Intervals

Test statistic T

- A t distribution with N-P-1 degrees of freedom
- We decide that hypothesis $\beta_i = 0$ should be rejected.
- $U \sim N(0,1), \ V \sim \chi_m^2$

$$T \triangleq U/\sqrt{V/m}$$

```
curve(dnorm(x), -10, 10, ann = FALSE, ylim = c(0, 0.5), lwd = 5)
for(i in 1:10)curve(dt(x, df= i), -10, 10, col = i, add = TRUE, ann = FALSE)
legend("topright", legend = 1:10, lty = 1, col = 1:10)
```



Significance level

•
$$\alpha = 0.01, 0.05$$

• Reject the null hypothesis

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제목 뭐라고 하지.

- 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 $\bar{y} = Wy = \sum_{i=1}^N y_i$ for $y_1, \cdots, y_N \in \mathbb{R}$
- Residual sum of squares RSS

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

- Explained sum of squres ESS

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

- Total sum of squres TSS

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

• We have relation TSS = RSS + ESS**Proof**

Sample - based correlation

• Coefficient of determination

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

• Correlation between the covariates and response

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

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

penalized

• Variance inflation factors

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

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

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

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

- 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

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

• We define

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

C 정의?

- $\bullet \ {\bf C} \sim t_{N-p-1}$
- variance in the difference between $x_*\hat{\beta}$ and $y_* \triangleq x_*\beta + \varepsilon$

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

Similarly, we can derive the following

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

• The confidence and prediction intervals

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

Q & A

Thank you:)