

## Ch6. Multiple Regression

### 6.1 The model

Multiple Linear Regression Model with  $p$  independent variables is defined as

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip} + \epsilon_i \quad (6.1)$$

where  $i = 1, \dots, n$  ( $n$  is the sample size), or in matrix form

$$\mathbf{y}_{n \times 1} = \mathbf{X}_{n \times r} \boldsymbol{\beta}_{r \times 1} + \boldsymbol{\epsilon}_{n \times 1}$$

where  $r = p + 1$ .

■ What are  $\mathbf{y}$ ,  $\mathbf{X}$ ,  $\boldsymbol{\beta}$  and  $\boldsymbol{\epsilon}$ ?

■ Main assumptions of the model are

- 1  $E(\boldsymbol{\epsilon}) = \mathbf{0}$ ;
- 2  $\text{Cov}(\boldsymbol{\epsilon}) = \sigma^2 \mathbf{I}$ , thus  $\epsilon_i$  or  $y_i$  are uncorrelated for  $i = 1, \dots, n$ ;
- 3  $\mathbf{X}$  is full column rank (for now).

## 6.2 Least Squares Estimation (LSE)

### 6.2.1 LSE

Minimize the sum of squares of deviations of observed and predicted values  $(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})'(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})$ , we have

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

**Proof.**

## 6.2.1 LSE – residuals and estimator of $\sigma^2$

- Vector of residuals  $\hat{\mathbf{e}} = \mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}$ :

$$\begin{aligned}\hat{\mathbf{e}} &= \mathbf{y} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \\ &= [\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}']\mathbf{y} \\ &= [\mathbf{I} - \mathbf{H}]\mathbf{y}\end{aligned}$$

where  $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ .

- Fitted value:  $\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \mathbf{H}\mathbf{y}$ .
- The unbiased estimator of  $\sigma^2$  is

$$\hat{\sigma}^2 = \frac{\hat{\mathbf{e}}'\hat{\mathbf{e}}}{n - r}.$$

## 6.2.1 LSE – residuals and estimator of $\sigma^2$

- $\mathbf{X}'\hat{\boldsymbol{\epsilon}} = \mathbf{0}$  ( $\mathbf{X}'\mathbf{H} = \mathbf{X}'$ ,  $\mathbf{H}\mathbf{X} = \mathbf{X}$  and  $\mathbf{X}'(\mathbf{I} - \mathbf{H}) = \mathbf{0}$ ,  $(\mathbf{I} - \mathbf{H})\mathbf{X} = \mathbf{0}$ );
- $\mathbf{H}$  is symmetric idempotent;
- $\hat{\mathbf{y}}'\hat{\boldsymbol{\epsilon}} = 0$ ;
- $\mathbf{I} - \mathbf{H}$  is symmetric idempotent;
- $E(\hat{\boldsymbol{\beta}}) = \boldsymbol{\beta}$  (unbiased estimator);
- $\text{Cov}(\hat{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{X})^{-1}\sigma^2$ ;
- $\text{tr}(\mathbf{I} - \mathbf{H}) = n - r$ ;
- $\hat{\boldsymbol{\epsilon}}'\hat{\boldsymbol{\epsilon}} = \text{tr}(\mathbf{y}\mathbf{y}'(\mathbf{I} - \mathbf{H}))$ ;
- $E(\mathbf{y}\mathbf{y}') = \sigma^2\mathbf{I} + \mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}'$ ;
- $E\left(\frac{\hat{\boldsymbol{\epsilon}}'\hat{\boldsymbol{\epsilon}}}{n-r}\right) = \sigma^2$ .

## 6.2.2 Generalized Least Squares Estimation

Assume that  $\text{Cov}(\epsilon) = \sigma^2 \mathbf{V}$ ,  $\mathbf{V}$  known

### ■ Estimation of $\beta$

- Ordinary Least Squares Estimator:

$$\text{minimize } (\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta) \Rightarrow \hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

- Generalized Least Squares Estimator: minimize

$$(\mathbf{y} - \mathbf{X}\mathbf{a})'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\mathbf{a})$$

Let

$$\begin{aligned} S &= (\mathbf{y} - \mathbf{X}\mathbf{a})'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\mathbf{a}) \\ &= \mathbf{y}'\mathbf{V}^{-1}\mathbf{y} - 2\mathbf{y}'\mathbf{V}^{-1}\mathbf{X}\mathbf{a} + \mathbf{a}'\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\mathbf{a} \end{aligned}$$

$$\frac{\partial S}{\partial \mathbf{a}} = -2\mathbf{X}'\mathbf{V}^{-1}\mathbf{y} + 2\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\mathbf{a} = 0$$

$$\Rightarrow \mathbf{X}'\mathbf{V}^{-1}\mathbf{y} = \mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\mathbf{a}$$

$$\Rightarrow \tilde{\mathbf{a}} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$$

Note: If  $\mathbf{V} = \sigma^2 \mathbf{I}$ , OLS = GLS

- Weighted Least Squares Estimator.

## 6.2.3 Properties of LSE

**Gauss-Markov Theorem: The best linear unbiased estimator (b.l.u.e.):** Let  $\mathbf{t}$  be a vector and we need to construct the b.l.u.e. of  $\mathbf{t}'\beta$ .

- Let  $\lambda'\mathbf{y}$  be a linear function of the observations and an estimator of  $\mathbf{t}'\beta$ .
- If  $\lambda'\mathbf{y}$  is an unbiased estimator of  $\mathbf{t}'\beta$ ,  $E(\lambda'\mathbf{y}) = \mathbf{t}'\beta$ .

$$\text{But } E(\lambda'\mathbf{y}) = \lambda'E(\mathbf{y}) = \lambda'\mathbf{X}\beta$$

Hence,  $\lambda'\mathbf{X}\beta = \mathbf{t}'\beta$  which is true for all  $\beta$

$$\Rightarrow \lambda'\mathbf{X} = \mathbf{t}'$$

- Find the linear unbiased estimator of  $\mathbf{t}'\beta$  which has minimum variance.

$$\text{Var}(\lambda'\mathbf{y}) = \sigma^2 \lambda' \mathbf{V} \lambda$$

## 6.2.3 Properties of LSE

**Gauss-Markov Theorem:**  $W = \lambda' V \lambda$  is minimum if

$$\lambda' = t'(X' V^{-1} X)^{-1} X' V^{-1}$$

subject to the constraint that  $X' \lambda = t$ ; i.e. GLS is the b.l.u.e.

## 6.3 Maximum likelihood estimation

A normal model is defined by (6.1) with an additional assumption

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon}_{n \times 1} \sim N(\mathbf{0}, \sigma^2 \mathbf{I}),$$

where  $\sigma^2$  is unknown.

- The likelihood function is

$$L(\boldsymbol{\beta}, \sigma^2) = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{n}{2}} e^{-\frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})}$$

Take log, we have

$$\begin{aligned} & \log L(\boldsymbol{\beta}, \sigma^2) \\ &= -\frac{n}{2} \log 2\pi - \frac{n}{2} \log \sigma^2 - \frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \\ &= -\frac{n}{2} \log 2\pi - \frac{n}{2} \log \sigma^2 - \frac{1}{2\sigma^2} (\mathbf{y}'\mathbf{y} - 2\mathbf{y}'\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta}) \end{aligned}$$



## 6.3 Maximum likelihood estimation

- MLE for  $\beta$  and  $\sigma^2$

$$\frac{\partial \log L}{\partial \beta} = \frac{1}{\sigma^2} (\mathbf{X}'\mathbf{y} - \mathbf{X}'\mathbf{X}\beta)$$

$$\frac{\partial \log L}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} (\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta)$$

- Put the above 2 equations to zero and we obtain the MLEs:

$$\text{MLE}(\beta) = \hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

$$\begin{aligned}\text{MLE}(\sigma^2) &= \hat{\sigma}^2 = \frac{1}{n} (\mathbf{y} - \mathbf{X}\hat{\beta})'(\mathbf{y} - \mathbf{X}\hat{\beta}) \\ &= \frac{1}{n} (\mathbf{y} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y})'(\mathbf{y} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}) \\ &= \frac{1}{n} \mathbf{y}'(\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}')\mathbf{y} \\ &= \frac{1}{n} \mathbf{y}'(\mathbf{I} - \mathbf{H})\mathbf{y} = \frac{1}{n} [\mathbf{y}'\mathbf{y} - \hat{\beta}'\mathbf{X}'\mathbf{y}]\end{aligned}$$

## 6.3 Maximum likelihood estimation: properties

- Distribution of  $\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \sim N(\beta, (\mathbf{X}'\mathbf{X})^{-1}\sigma^2)$  Since

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

$$\text{Cov}(\hat{\beta}) = \text{Cov}((\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}) = (\mathbf{X}'\mathbf{X})^{-1}\sigma^2.$$

- Let  $SSE = \mathbf{y}'(\mathbf{I} - \mathbf{H})\mathbf{y}$ :

- $\hat{\sigma}^2 = \frac{SSE}{n}$  is the MLE

- $\tilde{\sigma}^2 = \frac{SSE}{n-r(\mathbf{X})}$  is an unbiased estimator of  $\sigma^2$  with  
 $r(\mathbf{X}) = \text{rank of } \mathbf{X}$ .

- $\hat{\beta}$  and SSE are independent.

- Distribution of  $\hat{\sigma}^2$

$$\frac{[n - r(\mathbf{X})]\tilde{\sigma}^2}{\sigma^2} \sim \chi^2_{(n-r(\mathbf{X}))}.$$

## 6.3 Maximum likelihood estimation: Example 6.1

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i \quad i = 1, 2, \dots, n; \quad \varepsilon_i \stackrel{\text{ind}}{\sim} N(0, \sigma^2).$$

In matrix notation,  $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}, \quad \mathbf{X}'\mathbf{y} = \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \end{bmatrix}$$

$$\begin{aligned} (\mathbf{X}'\mathbf{X})^{-1} &= \frac{1}{n \sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2} \begin{bmatrix} \sum_{i=1}^n x_i^2 & -\sum_{i=1}^n x_i \\ -\sum_{i=1}^n x_i & n \end{bmatrix} \\ &= \frac{1}{n \sum_{i=1}^n (x_i - \bar{x})^2} \begin{bmatrix} \sum_{i=1}^n x_i^2 & -\sum_{i=1}^n x_i \\ -\sum_{i=1}^n x_i & n \end{bmatrix} \end{aligned}$$

## 6.3 Maximum likelihood estimation: Example 6.1

$$\begin{aligned}\hat{\beta} &= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \\&= \frac{1}{n \sum_{i=1}^n (x_i - \bar{x})^2} \begin{bmatrix} \sum_{i=1}^n y_i \sum_{i=1}^n x_i^2 - \sum_{i=1}^n x_i \sum_{i=1}^n x_i y_i \\ n \sum_{i=1}^n x_i y_i - \sum_{i=1}^n x_i \sum_{i=1}^n y_i \end{bmatrix} \\&= \begin{bmatrix} \frac{\bar{y} - \hat{\beta}_1 \bar{x}}{\frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}} \end{bmatrix} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix}\end{aligned}$$

## 6.3 Maximum likelihood estimation: Example 6.1

$$\begin{aligned}\hat{\sigma}^2 &= \frac{1}{n-2}(\mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y}) \\&= \frac{1}{n-2}\left[\sum_{i=1}^n y_i^2 - \hat{\beta}_0 \sum_{i=1}^n y_i - \hat{\beta}_1 \sum_{i=1}^n x_i y_i\right] \\&= \frac{1}{n-2}\left[\sum_{i=1}^n y_i^2 - \bar{y} \sum_{i=1}^n y_i + \hat{\beta}_1 \bar{x} \sum_{i=1}^n y_i - \hat{\beta}_1 \sum_{i=1}^n x_i y_i\right] \\&= \frac{1}{n-2}\left[\sum_{i=1}^n (y_i - \bar{y})^2 - \hat{\beta}_1 \left(\sum_{i=1}^n x_i y_i - n \sum_{i=1}^n x_i \sum_{i=1}^n y_i\right)\right] \\&= \frac{1}{n-2}\left[\sum_{i=1}^n (y_i - \bar{y})^2 - \frac{[\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})]^2}{\sum_{i=1}^n (x_i - \bar{x})^2}\right]\end{aligned}$$

## 6.4. The model in centered form

- The centered form of the multiple linear regression model is

$$\begin{aligned} y_i &= \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip} + \epsilon_i \\ &= \alpha + b_1(x_{i1} - \bar{x}_1) + b_2(x_{i2} - \bar{x}_2) + \cdots + b_p(x_{ip} - \bar{x}_p) + \epsilon_i \end{aligned}$$

where  $\alpha = \beta_0 + \beta_1 \bar{x}_1 + \beta_2 \bar{x}_2 + \cdots + \beta_p \bar{x}_p$ , and  $\bar{x}_j$  is the average of  $\{x_{ij}, i = 1, \dots, n\}$  for  $j = 1, 2, \dots, p$ .

- The matrix form can be expressed as

$$\mathbf{y}_{n \times 1} = \begin{pmatrix} \mathbf{1} & \mathbf{Z} \end{pmatrix} \begin{pmatrix} \alpha \\ \mathbf{b} \end{pmatrix} + \boldsymbol{\epsilon}_{n \times 1},$$

where  $(\mathbf{Z} = \mathbf{X}_1 - \mathbf{1}\bar{\mathbf{X}}')$ ,  $\bar{\mathbf{X}}' = (\bar{x}_1, \bar{x}_2, \dots, \bar{x}_p)$  and  $\mathbf{b}' = (b_1, \dots, b_p)$ .

- We can prove that

$$\hat{\alpha} = \hat{\beta}_0 + \hat{\beta}_1 \bar{x}_1 + \hat{\beta}_2 \bar{x}_2 + \cdots + \hat{\beta}_p \bar{x}_p$$

and  $\hat{\mathbf{b}} = \hat{\boldsymbol{\beta}}_1$ .

## 6.4. The model in centered form

$$\begin{aligned}\text{Var}(\hat{\beta}) &= \text{Var} \begin{pmatrix} \hat{\beta}_0 \\ \hat{\mathbf{b}} \end{pmatrix} = (\mathbf{X}'\mathbf{X})^{-1}\sigma^2 \\ &= \begin{bmatrix} \frac{1}{n} + \bar{\mathbf{X}}'(\mathbf{Z}'\mathbf{Z})^{-1}\bar{\mathbf{X}} & -\bar{\mathbf{X}}'(\mathbf{Z}'\mathbf{Z})^{-1} \\ -(\mathbf{Z}'\mathbf{Z})^{-1}\bar{\mathbf{X}} & (\mathbf{Z}'\mathbf{Z})^{-1} \end{bmatrix} \sigma^2\end{aligned}$$

Then

$$\begin{aligned}\text{Var}(\hat{\mathbf{b}}) &= (\mathbf{Z}'\mathbf{Z})^{-1}\sigma^2 \\ \text{Var}(\hat{\beta}_0) &= \frac{\sigma^2}{n} + \bar{\mathbf{X}}'(\mathbf{Z}'\mathbf{Z})^{-1}\bar{\mathbf{X}}\sigma^2 \\ &= \frac{\sigma^2}{n} + \bar{\mathbf{X}}' \text{Var}(\hat{\mathbf{b}}) \bar{\mathbf{X}} \\ \text{Cov}(\hat{\beta}_0, \hat{\mathbf{b}}') &= -\bar{\mathbf{X}}'(\mathbf{Z}'\mathbf{Z})^{-1}\sigma^2 = -\bar{\mathbf{X}}' \text{Var}(\hat{\mathbf{b}})\end{aligned}$$

## 6.5. Partitioning Total Sum of Squares

- SST (Total sum of squares corrected for the mean),

$$SST = \mathbf{y}'\mathbf{y} - \frac{1}{n}\mathbf{y}'\mathbf{1}\mathbf{1}'\mathbf{y} = \mathbf{y}'(\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}')\mathbf{y}$$

$$\frac{SST}{\sigma^2} \sim \chi^2_{(n-1, \frac{\beta'\mathbf{X}'\mathbf{X}\beta - \frac{1}{n}(\mathbf{1}'\mathbf{X}\beta)^2}{2\sigma^2})}$$

- SSR (Sum of squares of regression ) = SST - SSE,

$$SSR = \mathbf{y}'(\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}')\mathbf{y} - \mathbf{y}'(\mathbf{I} - \mathbf{H})\mathbf{y}$$

$$= \mathbf{y}'(\mathbf{H} - \frac{1}{n}\mathbf{1}\mathbf{1}')\mathbf{y}$$

$$\frac{SSR}{\sigma^2} \sim \chi^2_{(k, \frac{\mathbf{b}'(\mathbf{Z}'\mathbf{Z})\mathbf{b}}{2\sigma^2})}$$

$$- R^2 = \frac{SSR}{SST}.$$



## 6.5. Partitioning Total Sum of Squares: Anova Table

Source	df	SS	MS	F-statistics
Regression	$r(\mathbf{X}) - 1$	$\hat{\mathbf{b}}' \mathbf{Z}' \mathbf{y}$	$\frac{SSR}{r(\mathbf{X}) - 1}$	$F = \frac{MSR}{MSE}$
Error	$n - r(\mathbf{X})$	$\mathbf{y}' \mathbf{y} - \hat{\beta}' \mathbf{X}' \mathbf{y}$	$\frac{SSE}{n - r(\mathbf{X})}$	
Total	$n - 1$	$\mathbf{y}' (\mathbf{I} - \frac{1}{n} \mathbf{1} \mathbf{1}') \mathbf{y}$		

- SSR is independent of SSE
- $F \sim F_{(r(\mathbf{X})-1, n-r(\mathbf{X}), \frac{\mathbf{b}'(\mathbf{Z}'\mathbf{Z})\mathbf{b}}{2\sigma^2})}$
- Under  $H_0 : \mathbf{b} = \mathbf{0}$ ,

$$F \sim F_{(r(\mathbf{X})-1, n-r(\mathbf{X}), 0)}.$$

## 6.6. Model Misspecification – Misspecification of the error structure

- Suppose the true model is

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad \text{Cov}(\mathbf{y}) = \sigma^2 \mathbf{V},$$

- but the working model is

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad \text{Cov}(\mathbf{y}) = \sigma^2 \mathbf{I}.$$

- This will still have an unbiased estimate of  $\boldsymbol{\beta}$ , but it is not the BLUE.

## 6.6. Model Misspecification – Misspecification of the mean

We consider the following two models

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\epsilon}, \quad \text{Cov}(\mathbf{y}) = \sigma^2 \mathbf{I}, \quad (6.2)$$

and

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\epsilon}, \quad \text{Cov}(\mathbf{y}) = \sigma^2 \mathbf{I}. \quad (6.3)$$

- Under-fitting: if the true model is (6.2), but use the model (6.3);
- Over-fitting: if the true model is (6.3), but use the model (6.2).