3 Multiple Regression Model (重回帰モデル)

Up to now, only one independent variable, i.e., x_i , is taken into the regression model. We extend it to more independent variables, which is called the **multiple regression model** (重回帰モデル).

We consider the following regression model:

$$y_{i} = \beta_{1}x_{i,1} + \beta_{2}x_{i,2} + \dots + \beta_{k}x_{i,k} + u_{i} = (x_{i,1}, x_{i,2}, \dots, x_{i,k}) \begin{pmatrix} \beta_{1} \\ \beta_{2} \\ \vdots \\ \beta_{k} \end{pmatrix} + u_{i} = x_{i}\beta + u_{i},$$

for $i = 1, 2, \dots, n$, where x_i and β denote a $1 \times k$ vector of the independent variables

and a $k \times 1$ vector of the unknown parameters to be estimated, which are given by:

$$x_i = (x_{i,1}, x_{i,2}, \dots, x_{i,k}), \qquad \beta = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix}.$$

 $x_{i,j}$ denotes the *i*th observation of the *j*th independent variable.

The case of k = 2 and $x_{i,1} = 1$ for all i is exactly equivalent to (1).

Therefore, the matrix form above is a generalization of (1).

Writing all the equations for $i = 1, 2, \dots, n$, we have:

$$y_{1} = \beta_{1}x_{1,1} + \beta_{2}x_{1,2} + \dots + \beta_{k}x_{1,k} + u_{1} = x_{1}\beta + u_{1},$$

$$y_{2} = \beta_{1}x_{2,1} + \beta_{2}x_{2,2} + \dots + \beta_{k}x_{2,k} + u_{2} = x_{2}\beta + u_{2},$$

$$\vdots$$

$$y_{n} = \beta_{1}x_{n,1} + \beta_{2}x_{n,2} + \dots + \beta_{k}x_{n,k} + u_{n} = x_{n}\beta + u_{n},$$

which is rewritten as:

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,k} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1} & x_{n,2} & \cdots & x_{n,k} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix} + \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix}$$

$$= \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \beta + \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix}.$$

Again, the above equation is compactly rewritten as:

$$y = X\beta + u, (18)$$

where y, X and u are denoted by:

$$y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, \qquad X = \begin{pmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,k} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1} & x_{n,2} & \cdots & x_{n,k} \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \qquad u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix}.$$

Utilizing the matrix form (18), we derive the ordinary least squares estimator of β , denoted by $\hat{\beta}$.

In (18), replacing β by $\hat{\beta}$, we have the following equation:

$$y = X\hat{\beta} + e,$$

where e denotes a $n \times 1$ vector of the residuals.

The *i*th element of e is given by e_i .

The sum of squared residuals is written as follows:

$$S(\hat{\beta}) = \sum_{i=1}^{n} e_i^2 = e'e = (y - X\hat{\beta})'(y - X\hat{\beta}) = (y' - \hat{\beta}'X')(y - X\hat{\beta})$$

= $y'y - y'X\hat{\beta} - \hat{\beta}'X'y + \hat{\beta}'X'X\hat{\beta} = y'y - 2y'X\hat{\beta} + \hat{\beta}'X'X\hat{\beta}.$

In the last equality, note that $\hat{\beta}'X'y = y'X\hat{\beta}$ because both are scalars.

To minimize $S(\hat{\beta})$ with respect to $\hat{\beta}$, we set the first derivative of $S(\hat{\beta})$ equal to zero, i.e.,

$$\frac{\partial S(\hat{\beta})}{\partial \hat{\beta}} = -2X'y + 2X'X\hat{\beta} = 0.$$

Solving the equation above with respect to $\hat{\beta}$, the **ordinary least squares estimator** (**OLS**, 最小自乗推定量) of β is given by:

$$\hat{\beta} = (X'X)^{-1}X'y. \tag{19}$$

Thus, the ordinary least squares estimator is derived in the matrix form.

(*) Remark

The second order condition for minimization:

$$\frac{\partial^2 S(\hat{\beta})}{\partial \hat{\beta} \partial \hat{\beta}'} = 2X'X$$

is a positive definite matrix.

Set
$$c = Xd$$
.

For any $d \neq 0$, we have c'c = d'X'Xd > 0.

Now, in order to obtain the properties of $\hat{\beta}$ such as mean, variance, distribution and so on, (19) is rewritten as follows:

$$\hat{\beta} = (X'X)^{-1}X'y = (X'X)^{-1}X'(X\beta + u) = (X'X)^{-1}X'X\beta + (X'X)^{-1}X'u$$

$$= \beta + (X'X)^{-1}X'u. \tag{20}$$

Taking the expectation on both sides of (20), we have the following:

$$E(\hat{\beta}) = E(\beta + (X'X)^{-1}X'u) = \beta + (X'X)^{-1}X'E(u) = \beta,$$

because of E(u) = 0 by the assumption of the error term u_i .

Thus, unbiasedness of $\hat{\beta}$ is shown.

The variance of $\hat{\beta}$ is obtained as:

$$\begin{split} \mathbf{V}(\hat{\boldsymbol{\beta}}) &= \mathbf{E}((\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})') = \mathbf{E}\Big((X'X)^{-1}X'u((X'X)^{-1}X'u)'\Big) \\ &= \mathbf{E}((X'X)^{-1}X'uu'X(X'X)^{-1}) = (X'X)^{-1}X'\mathbf{E}(uu')X(X'X)^{-1} \\ &= \sigma^2(X'X)^{-1}X'X(X'X)^{-1} = \sigma^2(X'X)^{-1}. \end{split}$$

The first equality is the definition of variance in the case of vector.

In the fifth equality, $E(uu') = \sigma^2 I_n$ is used, which implies that $E(u_i^2) = \sigma^2$ for all i and $E(u_i u_j) = 0$ for $i \neq j$.

Remember that u_1, u_2, \dots, u_n are assumed to be mutually independently and identically distributed with mean zero and variance σ^2 .

Under normality assumption on the error term u, it is known that the distribution of $\hat{\beta}$ is given by:

$$\hat{\beta} \sim N(\beta, \sigma^2(X'X)^{-1}).$$

Proof:

First, when $X \sim N(\mu, \Sigma)$, the moment-generating function, i.e., $\phi(\theta)$, is given by:

$$\phi(\theta) \equiv E(\exp(\theta'X)) = \exp(\theta'\mu + \frac{1}{2}\theta'\Sigma\theta)$$

$$\theta_u$$
: $n \times 1$, u : $n \times 1$, θ_{β} : $k \times 1$, $\hat{\beta}$: $k \times 1$

The moment-generating function of u, i.e., $\phi_u(\theta_u)$, is:

$$\phi_u(\theta_u) \equiv \mathrm{E}(\exp(\theta'_u u)) = \exp(\frac{\sigma^2}{2}\theta'_u \theta_u),$$

which is $N(0, \sigma^2 I_n)$.

The moment-generating function of $\hat{\beta}$, i.e., $\phi_{\beta}(\theta_{\beta})$, is:

$$\begin{split} \phi_{\beta}(\theta_{\beta}) &\equiv \mathrm{E} \Big(\mathrm{exp}(\theta_{\beta}'\hat{\beta}) \Big) = \mathrm{E} \Big(\mathrm{exp}(\theta_{\beta}'\beta + \theta_{\beta}'(X'X)^{-1}X'u) \Big) \\ &= \mathrm{exp}(\theta_{\beta}'\beta) \mathrm{E} \Big(\mathrm{exp}(\theta_{\beta}'(X'X)^{-1}X'u) \Big) = \mathrm{exp}(\theta_{\beta}'\beta) \phi_u \Big(\theta_{\beta}'(X'X)^{-1}X' \Big) \\ &= \mathrm{exp}(\theta_{\beta}'\beta) \, \mathrm{exp} \Big(\frac{\sigma^2}{2} \theta_{\beta}'(X'X)^{-1}\theta_{\beta} \Big) = \mathrm{exp} \Big(\theta_{\beta}'\beta + \frac{\sigma^2}{2} \theta_{\beta}'(X'X)^{-1}\theta_{\beta} \Big), \end{split}$$

which is equivalent to the normal distribution with mean β and variance $\sigma^2(X'X)^{-1}$.

Note that
$$\theta_u = X(X'X)^{-1}\theta_{\beta}$$
. QED

Taking the *j*th element of $\hat{\beta}$, its distribution is given by:

$$\hat{\beta}_j \sim N(\beta_j, \sigma^2 a_{jj}),$$
 i.e., $\frac{\hat{\beta}_j - \beta_j}{\sigma \sqrt{a_{ij}}} \sim N(0, 1),$

where a_{ij} denotes the *j*th diagonal element of $(X'X)^{-1}$.

Replacing σ^2 by its estimator s^2 , we have the following t distribution:

$$\frac{\hat{\beta}_j - \beta_j}{s \sqrt{a_{ij}}} \sim t(n - k),$$

where t(n-k) denotes the t distribution with n-k degrees of freedom.