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:

$$y_i = \beta_1 x_{i,1} + \beta_2 x_{i,2} + \cdots + \beta_k x_{i,k} + u_i = (x_{i,1}, x_{i,2}, \cdots, x_{i,k}) \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix} + u_i = x_i \beta + u_i,$$

for $i = 1, 2, \cdots, n$, 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:

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

$x_{i,j}$ denotes the ith observation of the jth 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 $i = 1, 2, \cdots, n$, we have:

$$y_1 = \beta_1 x_{1,1} + \beta_2 x_{1,2} + \cdots + \beta_k x_{1,k} + u_1 = x_1 \beta + u_1,$$

$$y_2 = \beta_1 x_{2,1} + \beta_2 x_{2,2} + \cdots + \beta_k x_{2,k} + u_2 = x_2 \beta + u_2,$$

$$\vdots$$

$$y_n = \beta_1 x_{n,1} + \beta_2 x_{n,2} + \cdots + \beta_k x_{n,k} + u_n = x_n \beta + u_n,$$

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:

$$y = X\beta + u, \tag{18}$$

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 ith 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:

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

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

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

because of $\mathrm{E}(u) = 0$ by the assumption of the error term u_i.

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

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

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

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

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

Remember that $u_1, u_2, \cdots, u_n$ 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:

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

θ_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:

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

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

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

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

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 jth element of $\hat{\beta}$, its distribution is given by:

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

where a_{jj} denotes the jth diagonal element of $(X'X)^{-1}$.

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

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

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

[Review] Trace (トレース):

1. A: $n \times n$, $\quad \mathrm{tr}(A) = \sum_{i=1}^{n} a_{ii}$, where a_{ij} denotes an element in the ith row and the jth column of a matrix A.

2. a: scalar (1×1), $\quad \mathrm{tr}(a) = a$

3. A: $n \times k$, B: $k \times n$, $\quad \mathrm{tr}(AB) = \mathrm{tr}(BA)$

4. $\mathrm{tr}(X(X'X)^{-1}X') = \mathrm{tr}((X'X)^{-1}X'X) = \mathrm{tr}(I_k) = k$

5. When X is a square matrix of random variables, $\mathrm{E}(\mathrm{tr}(AX)) = \mathrm{tr}(A\mathrm{E}(X))$

End of Review

s^2 is taken as follows:

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

which leads to an unbiased estimator of σ^2.

Proof:

Substitute $y = X\beta + u$ and $\hat{\beta} = \beta + (X'X)^{-1}X'u$ into $e = y - X\hat{\beta}$.

$$\begin{aligned} e = y - X\hat{\beta} &= X\beta + u - X(\beta + (X'X)^{-1}X'u) \\ &= u - X(X'X)^{-1}X'u = (I_n - X(X'X)^{-1}X')u \end{aligned}$$

$I_n - X(X'X)^{-1}X'$ is idempotent and symmetric, because we have:

$$(I_n - X(X'X)^{-1}X')(I_n - X(X'X)^{-1}X') = I_n - X(X'X)^{-1}X,'$$

$$(I_n - X(X'X)^{-1}X')' = I_n - X(X'X)^{-1}X'.$$

s^2 is rewritten as follows:

$$
\begin{aligned}
s^2 &= \frac{1}{n-k} e'e = \frac{1}{n-k} \big((I_n - X(X'X)^{-1}X')u\big)'(I_n - X(X'X)^{-1}X')u \\
&= \frac{1}{n-k} u'(I_n - X(X'X)^{-1}X')'(I_n - X(X'X)^{-1}X')u \\
&= \frac{1}{n-k} u'(I_n - X(X'X)^{-1}X')u
\end{aligned}
$$

Take the expectation of $u'(I_n - X(X'X)^{-1}X')u$ and note that $\mathrm{tr}(a) = a$ for a scalar a.

$$
\begin{aligned}
\mathrm{E}(s^2) &= \frac{1}{n-k} \mathrm{E}\Big(\mathrm{tr}\Big(u'(I_n - X(X'X)^{-1}X')u\Big)\Big) = \frac{1}{n-k} \mathrm{E}\Big(\mathrm{tr}\Big((I_n - X(X'X)^{-1}X')uu'\Big)\Big) \\
&= \frac{1}{n-k} \mathrm{tr}\Big((I_n - X(X'X)^{-1}X')\mathrm{E}(uu')\Big) = \frac{1}{n-k} \sigma^2 \mathrm{tr}\Big((I_n - X(X'X)^{-1}X')I_n\Big) \\
&= \frac{1}{n-k} \sigma^2 \mathrm{tr}(I_n - X(X'X)^{-1}X') = \frac{1}{n-k} \sigma^2 (\mathrm{tr}(I_n) - \mathrm{tr}(X(X'X)^{-1}X')) \\
&= \frac{1}{n-k} \sigma^2 (\mathrm{tr}(I_n) - \mathrm{tr}((X'X)^{-1}X'X)) = \frac{1}{n-k} \sigma^2 (\mathrm{tr}(I_n) - \mathrm{tr}(I_k)) \\
&= \frac{1}{n-k} \sigma^2 (n-k) = \sigma^2
\end{aligned}
$$

$\longrightarrow$ s^2 is an unbiased estimator of σ^2.

Note that we do not need normality assumption for unbiasedness of s^2.

[Review]

- $X'X \sim \chi^2(n)$ for $X \sim N(0, I_n)$.

- $(X-\mu)'\Sigma^{-1}(X-\mu) \sim \chi^2(n)$ for $X \sim N(\mu, \Sigma)$.

- $\dfrac{X'X}{\sigma^2} \sim \chi^2(n)$ for $X \sim N(0, \sigma^2 I_n)$.

- $\dfrac{X'AX}{\sigma^2} \sim \chi^2(G)$, where $X \sim N(0, \sigma^2 I_n)$ and A is a symmetric idempotent $n \times n$ matrix of rank $G \leq n$.

Remember that $G = \mathrm{Rank}(A) = \mathrm{tr}(A)$ when A is symmetric and idempotent.

[End of Review]

Under normality assumption for u, the distribution of s^2 is:

$$\frac{(n-k)s^2}{\sigma^2} = \frac{u'(I_n - X(X'X)^{-1}X')u}{\sigma^2} \sim \chi^2(\mathrm{tr}(I_n - X(X'X)^{-1}X'))$$

Note that $\mathrm{tr}(I_n - X(X'X)^{-1}X') = n - k$, because

$$\mathrm{tr}(I_n) = n$$

$$\mathrm{tr}(X(X'X)^{-1}X') = \mathrm{tr}((X'X)^{-1}X'X) = \mathrm{tr}(I_k) = k$$

Asymptotic Normality (without normality assumption on u): Using the central limit theorem, without normality assumption we can show that as $n \longrightarrow \infty$, under the condition of $\frac{1}{n}X'X \longrightarrow M$ we have the following result:

$$\frac{\hat{\beta}_j - \beta_j}{s\sqrt{a_{jj}}} \longrightarrow N(0,1),$$

where M denotes a $k \times k$ constant matrix.

Thus, we can construct the confidence interval and the testing procedure, using the t distribution under the normality assumption or the normal distribution without the normality assumption.