2 Some Formulas of Matrix Algebra

1. Let $A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{l1} & a_{l2} & \cdots & a_{lk} \end{pmatrix} = [a_{ij}]$,

   which is a $l \times k$ matrix, where a_{ij} denotes ith row and jth column of A.

   The **transposed matrix (転置行列)** of A, denoted by A', is defined as:

   $$A' = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{l1} \\ a_{12} & a_{22} & \cdots & a_{l2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1k} & a_{2k} & \cdots & a_{lk} \end{pmatrix} = [a_{ji}],$$

   where the ith row of A' is the ith column of A.

2. $(Ax)' = x'A'$,

   where A and x are a $l \times k$ matrix and a $k \times 1$ vector, respectively.

3. $a' = a$,

   where a denotes a scalar.

4. $\dfrac{\partial a'x}{\partial x} = a$,

   where a and x are $k \times 1$ vectors.

5. If A is symmetric, $A = A'$.

6. $\dfrac{\partial x'Ax}{\partial x} = (A + A')x$,

   where A and x are a $k \times k$ matrix and a $k \times 1$ vector, respectively.

   Especially, when A is symmetric,

$$\frac{\partial x'Ax}{\partial x} = 2Ax.$$

7. Let A and B be $k \times k$ matrices, and I_k be a $k \times k$ **identity matrix (単位行列)** (one in the diagonal elements and zero in the other elements).

   When $AB = I_k$, B is called the **inverse matrix (逆行列)** of A, denoted by $B = A^{-1}$.

   That is, $AA^{-1} = A^{-1}A = I_k$.

8. Let A be a $k \times k$ matrix and x be a $k \times 1$ vector.

   If A is a **positive definite matrix (正値定符号行列)**, for any x except for $x = 0$ we have:

$$x'Ax > 0.$$

   If A is a **positive semidefinite matrix (非負値定符号行列)**, for any x except for $x = 0$ we have:

$$x'Ax \geq 0.$$

If A is a **negative definite matrix (負値定符号行列)**, for any x except for $x = 0$ we have:

$$x'Ax < 0.$$

If A is a **negative semidefinite matrix (非正値定符号行列)**, for any x except for $x = 0$ we have:

$$x'Ax \leq 0.$$

Trace, Rank and etc.: $\quad A : k \times k, \qquad B : n \times k, \qquad C : k \times n.$

1. The **trace (トレース)** of A is: $\mathrm{tr}(A) = \sum_{i=1}^{k} a_{ii}$, where $A = [a_{ij}]$.

2. The **rank (ランク，階数)** of A is the maximum number of linearly independent column (or row) vectors of A, which is denoted by rank(A).

3. If A is an **idempotent matrix (べき等行列)**, $A = A^2$.

4. If A is an idempotent and symmetric matrix, $A = A^2 = A'A$.

5. A is idempotent if and only if the eigen values of A consist of 1 and 0.

6. If A is idempotent, rank(A) =tr(A) .

7. tr(BC) =tr(CB)

Distributions in Matrix Form:

1. Let X, μ and Σ be $k \times 1$, $k \times 1$ and $k \times k$ matrices.

When $X \sim N(\mu, \Sigma)$, the density function of X is given by:

$$f(x) = \frac{1}{(2\pi)^{k/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu)'\Sigma^{-1}(x-\mu)\Big).$$

$\mathrm{E}(X) = \mu$ and $\mathrm{V}(X) = \mathrm{E}\Big((X-\mu)(X-\mu)'\Big) = \Sigma$

The moment-generating function: $\phi(\theta) = \mathrm{E}\Big(\exp(\theta' X)\Big) = \exp(\theta'\mu + \frac{1}{2}\theta'\Sigma\theta)$

(*) In the univariate case, when $X \sim N(\mu, \sigma^2)$, the density function of X is:

$$f(x) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\Big(-\frac{1}{2\sigma^2}(x-\mu)^2\Big).$$

2. If $X \sim N(\mu, \Sigma)$, then $(X-\mu)'\Sigma^{-1}(X-\mu) \sim \chi^2(k)$.

   Note that $\quad X'X \sim \chi^2(k)$ when $X \sim N(0, I_k)$.

3. X: $n \times 1$, $\qquad Y$: $m \times 1$, $\qquad X \sim N(\mu_x, \Sigma_x)$, $\qquad Y \sim N(\mu_y, \Sigma_y)$

X is independent of Y, i.e., $\mathrm{E}\Big((X-\mu_x)(Y-\mu_y)'\Big) = 0$ in the case of normal random variables.

$$\frac{(X-\mu_x)'\Sigma_x^{-1}(X-\mu_x)/n}{(Y-\mu_y)'\Sigma_y^{-1}(Y-\mu_y)/m} \sim F(n,m)$$

4. If $X \sim N(0,\sigma^2 I_n)$ and A is a symmetric idempotent $n\times n$ matrix of rank G, then $X'AX/\sigma^2 \sim \chi^2(G)$.

   Note that $X'AX = (AX)'(AX)$ and $\mathrm{rank}(A) = \mathrm{tr}(A)$ because A is idempotent.

5. If $X \sim N(0,\sigma^2 I_n)$, A and B are symmetric idempotent $n \times n$ matrices of rank G and K, and $AB = 0$, then

$$\frac{X'AX}{G\sigma^2}\Big/\frac{X'BX}{K\sigma^2} = \frac{X'AX/G}{X'BX/K} \sim F(G,K).$$

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:

$$\begin{aligned} y_1 &= \beta_1 x_{1,1} + \beta_2 x_{1,2} + \cdots + \beta_k x_{1,k} + u_1 = x_1\beta + u_1, \\ y_2 &= \beta_1 x_{2,1} + \beta_2 x_{2,2} + \cdots + \beta_k x_{2,k} + u_2 = x_2\beta + u_2, \\ &\vdots \\ y_n &= \beta_1 x_{n,1} + \beta_2 x_{n,2} + \cdots + \beta_k x_{n,k} + u_n = x_n\beta + u_n, \end{aligned}$$

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:

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

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.