

## Regression Analysis (I)

Kutner's Applied Linear Statistical Models (5/E)

### Chapter 5: Matrix Approach to Simple Linear Regression Analysis

Thursday 09:10-12:00, 資訊 140301

**Han-Ming Wu**

Department of Statistics, National Chengchi University

<http://www.hmwu.idv.tw>

## Overview

1. The matrix approach is practically a necessity in \_\_\_\_\_ regression analysis, since it permits extensive systems of equations and large arrays of data to be denoted compactly and operated upon efficiently.
2. This chapter gives a brief introduction to a matrix algebra.
3. Then we apply matrix methods to the simple linear regression model.

## 5.1 Matrices

### Definition of Matrix

1. A matrix is a \_\_\_\_\_ array of elements arranged in rows and columns.
2. A matrix with \_\_\_\_\_ and \_\_\_\_\_ will be represented either in full:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1j} & \cdots & a_{1c} \\ a_{21} & a_{22} & \cdots & a_{2j} & \cdots & a_{2c} \\ \vdots & \vdots & & \vdots & & \vdots \\ a_{i1} & a_{i2} & \cdots & a_{ij} & \cdots & a_{ic} \\ \vdots & \vdots & & \vdots & & \vdots \\ a_{r1} & a_{r2} & \cdots & a_{rj} & \cdots & a_{rc} \end{bmatrix}$$

or in abbreviated form:

$$\mathbf{A} = \text{_____}, \quad i = 1, \dots, r; j = 1, \dots, c$$

or simply by a boldface symbol, such as  $\mathbf{A}$ .

## Square Matrix

1. A matrix is said to be square if the number of rows \_\_\_\_\_ the number of columns.

## Vector

1. A matrix containing only one column is called a \_\_\_\_\_ vector or simply a vector.

$$\mathbf{C} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix}$$

the vector  $\mathbf{C}$  is a \_\_\_\_\_.

2. A matrix containing only one row is called a \_\_\_\_\_: e.g.,  $\mathbf{B}' = [15 \ 25 \ 50]$ . We use the prime symbol ( \_\_\_\_\_ ) for row vectors. Note that the row vector  $\mathbf{B}'$  is a \_\_\_\_\_ matrix.

## Transpose

1. The transpose of a matrix  $\mathbf{A}$  is another matrix, denoted by \_\_\_\_\_', that is obtained by interchanging corresponding columns and rows of the matrix  $\mathbf{A}$ .

$$\mathbf{A} = \begin{bmatrix} 2 & 5 \\ 7 & 10 \\ 3 & 4 \end{bmatrix}$$

then the transpose  $\mathbf{A}'$  is:

$$\mathbf{A}' = \text{_____}$$



2.

if  $\mathbf{A}_{r \times c} = [a_{ij}]$ ,  $\mathbf{B}_{r \times c} = [b_{ij}]$ , then  $\mathbf{A} \pm \mathbf{B} =$  \_\_\_\_\_

3. The regression model:  $Y_i = E(Y_i) + \varepsilon_i$ ,  $i = 1, \dots, n$  can be written in matrix notation:

\_\_\_\_\_

4. The observations vector  $\mathbf{Y}$  equals the sum of two vectors, a vector containing the expected values and another containing the error terms.

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} E(Y_1) \\ E(Y_2) \\ \vdots \\ E(Y_n) \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix} = \begin{bmatrix} E(Y_1) + \varepsilon_1 \\ E(Y_2) + \varepsilon_2 \\ \vdots \\ E(Y_n) + \varepsilon_n \end{bmatrix}$$

## 5.3 Matrix Multiplication

### Multiplication of a Matrix by a Scalar

1. A scalar is an ordinary number or a symbol representing a number. In multiplication of a matrix by a scalar, every element of the matrix is multiplied by the scalar.

2. If  $\mathbf{A} = [a_{ij}]$  and  $k$  is the scalar, then

$$k\mathbf{A} = \mathbf{A}k = \underline{\hspace{2cm}}$$

### Multiplication of a Matrix by a Matrix

1. In general, the product  $\mathbf{AB}$  is defined only when the number of columns in  $\mathbf{A}$  equals the number of rows in  $\mathbf{B}$  so that there will be corresponding terms in the \_\_\_\_\_.

2. Note that the dimension of the product  $\mathbf{AB}$  is given by the number of rows in  $\mathbf{A}$  and the number of columns in  $\mathbf{B}$ . Note also that in the second case the product  $\mathbf{BA}$  would not be defined since the number of columns in  $\mathbf{B}$  is not equal to the number of rows in  $\mathbf{A}$ .

3. In general, if  $\mathbf{A} = [a_{ik}]$  has dimension  $r \times c$  and  $\mathbf{B} = [b_{kj}]$  has dimension  $c \times s$ , the product  $\mathbf{AB}$  is a matrix of dimension  $r \times s$  whose element in the  $i$ th row and  $j$ th column is:

$$\mathbf{AB} = \underline{\hspace{10em}}$$

## Regression Examples

1. A product frequently needed is  $\mathbf{Y}'\mathbf{Y}$ , where  $\mathbf{Y}$  is the vector of observations on the response variable

$$\mathbf{Y}'\mathbf{Y} = [Y_1 \ Y_2 \ \cdots \ Y_n] \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \underline{\hspace{10em}} = \underline{\hspace{10em}}$$

2.  $\mathbf{X}'\mathbf{X}$  is a  $2 \times 2$  matrix:

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ X_1 & X_2 & \cdots & X_n \end{bmatrix} \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix} = \underline{\hspace{10em}}$$

3.  $\mathbf{X}'\mathbf{Y}$  is a  $2 \times 1$  matrix:

$$\mathbf{X}'\mathbf{Y} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ X_1 & X_2 & \cdots & X_n \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \underline{\hspace{10em}}$$

## 5.4 Special Types of Matrices

Certain special types of matrices arise regularly in regression analysis. We consider the most important of these.

### Symmetric Matrix

1. If \_\_\_\_\_,  $\mathbf{A}$  is said to be symmetric.

- A symmetric matrix necessarily is \_\_\_\_\_.
- Symmetric matrices arise typically in regression analysis when we premultiply a matrix, say,  $\mathbf{X}$ , by its transpose,  $\mathbf{X}'$ . The resulting matrix, \_\_\_\_\_, is symmetric.

## Diagonal Matrix

- A diagonal matrix is a square matrix whose \_\_\_\_\_ elements are all \_\_\_\_\_.
- We will often not show all zeros for a diagonal matrix, presenting it in the form:

$$\mathbf{B} = \begin{bmatrix} 4 & & & \\ & 1 & & \\ & & 10 & \\ & & & 5 \end{bmatrix}$$

- Identity Matrix** The identity matrix or \_\_\_\_\_ matrix is denoted by \_\_\_\_\_. It is a diagonal matrix whose elements on the main diagonal are all 1s.
- Premultiplying or postmultiplying any  $r \times r$  matrix  $\mathbf{A}$  by the  $r \times r$  identity matrix  $\mathbf{I}$  leaves  $\mathbf{A}$  unchanged.

$$\mathbf{AI} = \underline{\hspace{2cm}}$$

- A **scalar matrix** is a diagonal matrix whose \_\_\_\_\_ elements are the \_\_\_\_\_. A scalar matrix can be expressed as \_\_\_\_\_, where  $k$  is the scalar.
- Multiplying an  $r \times r$  matrix  $\mathbf{A}$  by the  $r \times r$  scalar matrix  $k\mathbf{I}$  is equivalent to multiplying  $\mathbf{A}$  by the scalar  $k$ .

## Vector and Matrix with All Elements Unity

- A column vector with all elements 1 will be denoted by \_\_\_\_\_ and a square matrix with all elements 1 will be denoted by \_\_\_\_\_.

2. Note that for an  $n \times 1$  vector  $\mathbf{1}$  we obtain:

$$\mathbf{1}'\mathbf{1} = [1 \ 1 \ \dots \ 1] \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = \underline{\hspace{2cm}}$$

and

$$\mathbf{1}\mathbf{1}' = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} [1 \ 1 \ \dots \ 1] = \begin{bmatrix} 1 & \dots & 1 \\ \vdots & & \vdots \\ 1 & \dots & 1 \end{bmatrix} = \underline{\hspace{2cm}}$$

## Zero Vector

1. A zero vector is a vector containing only zeros. The zero column vector will be denoted by  $\mathbf{0}$ .

## 5.5 Linear Dependence and Rank of Matrix

### Linear Dependence

1. Consider the following matrix:

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 5 & 1 \\ 2 & 2 & 10 & 6 \\ 3 & 4 & 15 & 1 \end{bmatrix}$$

We view  $\mathbf{A}$  as being made up of four column vectors. Note that the third column vector is a multiple of the first column vector.

$$\begin{bmatrix} 5 \\ 10 \\ 15 \end{bmatrix} = 5 \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

We say that the columns of  $\mathbf{A}$  are linearly dependent. They contain redundant information, since one column can be obtained as a linear combination of the others.

2. We define the set of  $c$  column vectors  $\mathbf{C}_1, \dots, \mathbf{C}_c$  in an  $r \times c$  matrix to be linearly dependent if one vector can be expressed as a \_\_\_\_\_ of the others. If no vector in the set can be so expressed, we define the set of vectors to be \_\_\_\_\_.

3. When  $c$  scalars  $k_1, \dots, k_c$ , not all zero, can be found such that:

$$k_1\mathbf{C}_1 + k_2\mathbf{C}_2 + \dots + k_c\mathbf{C}_c = \mathbf{0}$$

where  $\mathbf{0}$  denotes the zero column vector, the  $c$  column vectors are \_\_\_\_\_. If the only set of scalars for which the equality holds is  $k_1 = 0, \dots, k_c = 0$ , the set of  $c$  column vectors is \_\_\_\_\_.

4. For our example,  $k_1 = 5, k_2 = 0, k_3 = -1, k_4 = 0$  leads to:

$$5 \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} + 0 \begin{bmatrix} 2 \\ 2 \\ 4 \end{bmatrix} - 1 \begin{bmatrix} 5 \\ 10 \\ 15 \end{bmatrix} + 0 \begin{bmatrix} 1 \\ 6 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Hence, the column vectors are linearly dependent. Note that some of the  $k_j$  equal zero here. For linear dependence, it is only required that not all  $k_j$  be zero.

## Rank of Matrix

- The rank of a matrix is defined to be the \_\_\_\_\_ of linearly independent \_\_\_\_\_ in the matrix.
- The rank of a matrix is \_\_\_\_\_ and can equivalently be defined as the maximum number of linearly independent rows.
- It follows that the rank of an  $r \times c$  matrix cannot exceed \_\_\_\_\_, the minimum of the two values  $r$  and  $c$ .
- When a matrix is the product of two matrices, its rank cannot exceed the smaller of the two ranks for the matrices being multiplied. Thus, if  $\mathbf{C} = \mathbf{AB}$ , the rank of  $\mathbf{C}$  cannot exceed \_\_\_\_\_.



## 5.6 Inverse of a Matrix

1. In matrix algebra, the inverse of a matrix  $\mathbf{A}$  is another matrix, denoted by \_\_\_\_\_, such that

$$\underline{\hspace{10em}}$$

where  $\mathbf{I}$  is the identity matrix.

### Finding the Inverse

1. An inverse of a square  $r \times r$  matrix exists if the \_\_\_\_\_ of the matrix is \_\_\_\_\_. Such a matrix is said to be nonsingular or of full rank.
2. An  $r \times r$  matrix with rank less than  $r$  is said to be \_\_\_\_\_ or \_\_\_\_\_, and does not have an inverse. The inverse of an  $r \times r$  matrix of full rank also has rank  $r$ .
3. Finding the inverse of a matrix can often require a large amount of computing. We shall take the approach that the inverse of a  $2 \times 2$  matrix and a  $3 \times 3$  matrix can be calculated by hand. For any larger matrix, one ordinarily uses a computer to find the inverse.

4. If

$$\mathbf{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

then

$$\mathbf{A}^{-1} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \underline{\hspace{10em}}$$

where \_\_\_\_\_,  $D$  is called the \_\_\_\_\_ of the matrix  $\mathbf{A}$ .

5. If  $\mathbf{A}$  were singular, its determinant would equal \_\_\_\_\_ and no inverse of  $\mathbf{A}$  would exist.

### Regression Example

1. The principal inverse matrix encountered in regression analysis is the inverse of the matrix  $\mathbf{X}'\mathbf{X}$ .

 Question ..... (p191)

Find the inverse of the matrix  $\mathbf{X}'\mathbf{X}$ :

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} n & \sum X_i \\ \sum X_i & \sum X_i^2 \end{bmatrix}$$

*sol:*

## Uses of Inverse Matrix

1. In matrix algebra, if we have an equation:

$$\mathbf{A}\mathbf{Y} = \mathbf{C}.$$

We correspondingly premultiply both sides by  $\mathbf{A}^{-1}$ , assuming  $\mathbf{A}$  has an inverse

$$\underline{\hspace{2cm}} = \underline{\hspace{2cm}}$$

we obtain the solution:

$$\mathbf{Y} = \underline{\hspace{2cm}}.$$


## 5.7 Some Basic Results for Matrices

We list here, without proof, some basic results for matrices which we will utilize in later work.

$$\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A}$$





 Question ..... (p42)

Suppose that a random vector  $\mathbf{W}$  that is obtained by premultiplying the random vector  $\mathbf{Y}$  by a constant matrix  $\mathbf{A}$ , that is  $\mathbf{W} = \mathbf{A}\mathbf{Y}$ . Find the expected value and the variance-covariance matrix of  $\mathbf{W}$ .

*sol:*

## Multivariate Normal Distribution

1. The density function of the multivariate normal distribution can now be stated as follows:

$$f(\mathbf{Y}) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{Y} - \boldsymbol{\mu})' \Sigma^{-1} (\mathbf{Y} - \boldsymbol{\mu})\right\},$$

where  $\mathbf{Y}$  containing an observation on each of the  $p$   $Y$  variables

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_p \end{bmatrix}.$$

2. The mean vector  $E(\mathbf{Y})$ , denoted by  $\boldsymbol{\mu}$ , contains the expected values for each of the  $p$   $Y$  variables:

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_p \end{bmatrix}.$$

3. The variance-covariance matrix  $\sigma^2(\mathbf{Y})$  is denoted by \_\_\_\_\_: and contains as always the variances and covariances of the  $p$   $Y$  variables:

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2p} \\ \vdots & \vdots & & \vdots \\ \sigma_{p1} & \sigma_{p2} & \cdots & \sigma_p^2 \end{bmatrix}$$

$\sigma_i^2$  denotes the variance of  $Y_i$ ,  $\sigma_{ij}$  denotes the covariance of  $Y_i$  and  $Y_j$ .

4. The multivariate normal density function has properties that correspond to the ones described for the \_\_\_\_\_ normal distribution.
5. For instance, if  $Y_1, \dots, Y_p$  are jointly normally distributed (i.e., they follow the multivariate normal distribution), the marginal probability distribution of each variable  $Y_k$  is normal, with mean  $\mu_k$  and standard deviation  $\sigma_k$ .

## 5.9 Simple Linear Regression Model in Matrix Terms

1. The normal error regression model (2.1):

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \quad i = 1, \dots, n$$

2. The normal error regression model in matrix terms:

$$\underline{\hspace{15em}},$$


where

$$\mathbf{Y} = \underline{\hspace{5em}}, \quad \mathbf{X} = \underline{\hspace{5em}}, \quad \boldsymbol{\beta} = \underline{\hspace{5em}}, \quad \boldsymbol{\varepsilon} = \underline{\hspace{5em}},$$

$\boldsymbol{\varepsilon}$  is a vector of independent normal random variables with  $E(\boldsymbol{\varepsilon}) = \mathbf{0}$  and  $\sigma^2(\boldsymbol{\varepsilon}) = \sigma^2 \mathbf{I}$

## 5.10 Least Squares Estimation of Regression Parameters

### Normal Equations

 Question ..... (p200)

Express the normal equations (1.9),

$$\begin{aligned}nb_0 + b_1 \sum X_i &= \sum Y_i \\b_0 \sum X_i + b_1 \sum X_i^2 &= \sum X_i Y_i\end{aligned}$$


in the matrix form

$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{Y}$$

where  $\mathbf{b}$  is the vector of the least squares regression coefficients:

$$\mathbf{b}_{2 \times 1} = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix}$$

*sol:*

 Question ..... (p201)

Derive the normal equations by the method of least squares in matrix notation.

*sol:*

## Estimated Regression Coefficients

1. Obtain the estimated regression coefficients from the normal equations (5.59) by matrix methods, We premultiply both sides by

\_\_\_\_\_

We then find, since  $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X} = \mathbf{I}$  and  $\mathbf{I}\mathbf{b} = \mathbf{b}$ ,

$$\mathbf{b} = \underline{\hspace{2cm}}$$



 Question ..... (p200)

Use matrix methods to obtain the estimated regression coefficients for the Toluca Company example.

*sol:*

## 5.11 Fitted Values and Residuals

### Fitted Values

1. Let the vector of the fitted values  $Y_i$  be denoted by  $\hat{\mathbf{Y}}$ , then

$$\hat{\mathbf{Y}} = \underline{\hspace{2cm}}$$

$$\begin{bmatrix} \hat{Y}_1 \\ \hat{Y}_2 \\ \vdots \\ \hat{Y}_n \end{bmatrix} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \end{bmatrix} = \begin{bmatrix} b_0 + b_1 X_1 \\ b_0 + b_1 X_2 \\ \vdots \\ b_0 + b_1 X_n \end{bmatrix}$$

2. **Hat Matrix** We can express the matrix result for  $\hat{\mathbf{Y}}$  as follows by using the expression for  $\mathbf{b}$  in (5.60):

$$\hat{\mathbf{Y}} = \underline{\hspace{2cm}}$$




3. The variance-covariance matrix of the vector of residuals  $\mathbf{e}$  involves the matrix  $\mathbf{I} - \mathbf{H}$ :

$$\sigma^2(\mathbf{e}) = \underline{\hspace{2cm}}$$

and is estimated by:

$$s^2(\mathbf{e}) = \underline{\hspace{2cm}}$$

 **Question** ..... (p204)

Show that the variance-covariance matrix of  $\mathbf{e}$  is  $\sigma^2(\mathbf{e}) = \sigma^2(\mathbf{I} - \mathbf{H})$ .

*sol:*

## 5.12 Analysis of Variance Results

### Sums of Squares

 **Question** ..... (p42)

Express the sums of squares,  $SSTO$ ,  $SSE$  and  $SSR$  in matrix notation.


*sol:*

## Sums of Squares as Quadratic Forms

1. In general, a quadratic form is defined as:

$$\mathbf{y}'\mathbf{A}\mathbf{y}, \quad \text{where } a_{ij} = a_{ji}.$$

2.  $\mathbf{A}$  is a symmetric  $n \times n$  matrix and is called the matrix of the quadratic form.
3. The ANOVA sums of squares  $SSTO$ ,  $SSE$ , and  $SSR$  are all \_\_\_\_\_, as can be seen by reexpressing  $\mathbf{b}'\mathbf{X}'$ .


 Question ..... (p42)

Show that the ANOVA sums of squares  $SSTO$ ,  $SSE$ , and  $SSR$  are all quadratic forms.

*sol:*

## 5.13 Inferences in Regression Analysis

### Regression Coefficients

 Question ..... (p42)

(a) Derive the variance-covariance matrix of the simple linear regression coefficients,  $\mathbf{b}$  by matrix methods. (b) Obtain the estimated variance-covariance matrix of  $\mathbf{b}$ .

*sol:*

Mean Response\*

Prediction of New Observation\*

 TA Class

- Problems: 5.5, 5.16, 5.22, 5.24, 5.26
- Exercises: 5.31