

MULTIVARIATE ANALYSIS AND PRELIMINARIES

1 Aspects of Multivariate Analysis

Reference: Johnson & Wichern (2002) *Applied Multivariate Statistical Analysis* Chapter 1.

- (a) Multivariate analysis is concerned with two or more random variables.
- (b) Many multivariate methods are based on an underlying probability model known as the multivariate normal distribution.
- (c) The objectives of the investigation for multivariate analysis include:
 - Data reduction
 - Sorting and grouping
 - Investigation of the dependence among variables
 - Prediction
 - Hypothesis construction and testing
- (d) The multivariate statistical methods are:
 - Principal component analysis (PCA)
 - Factor analysis (FA)
 - Discrimination and classification analysis (DCA)
 - Cluster analysis (CA)
 - Multivariate linear regression model (LRM)
- (e) Applications: Multivariate methods have been widely applied to many practical problems arising in
 - Medicine science : (discrimination)
 - Physics : (linear regression model)
 - Sociology
 - Business and Economics

- Environmental study
- Meteorology
- Geology
- Psychology

1.1 Multivariate Graphical Techniques

Reference: Johnson & Wichern (2002) *Applied Multivariate Statistical Analysis* Fifth Edition, Chapter 1, pages 11-49.

- Multiple Scatter Plots
- Multiple Scatter and/or boxplots.
- Three-dimensional scatter plot for trivariate data.
- Three-dimensional scatter plots with rotation.
- Three-dimensional perspectives.
- Growth curves
- Chernoff faces
- Distances between the data points.

2 Matrix Algebra

Reference: Johnson & Wichern (2002) *Applied Multivariate Statistical Analysis*, Chapter 2.

2.1 Vectors

An array of \mathbf{x} of n real numbers x_1, x_2, \dots, x_n is called a vector of dimension n and it is written as

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}_{n \times 1} \quad \text{or} \quad \mathbf{x}^T = (x_1 \ x_2 \ \dots \ x_n)_{1 \times n}$$

- (a) A vector can be multiply by a constant. Multiplying vector \mathbf{x} by constant a is given by

$$a\mathbf{x} = \begin{pmatrix} ax_1 \\ ax_2 \\ \vdots \\ ax_n \end{pmatrix}_{n \times 1}$$

- (b) Two vectors may be added. Addition of \mathbf{x} and \mathbf{y} :

$$\mathbf{x} + \mathbf{y} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}_{n \times 1} + \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}_{n \times 1} = \begin{pmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_n + y_n \end{pmatrix}_{n \times 1}$$

- (c) The length of a vector \mathbf{x} is defined by $L_x = |\mathbf{x}| = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}$.

- (d) Multiplication of Two Vectors:

- (1) Multiplication of \mathbf{x}^T by \mathbf{y} gives a single number. Note $L_x = \sqrt{\mathbf{x}^T \mathbf{x}} = |\mathbf{x}|$

$$\mathbf{x}^T \mathbf{y} = (x_1 \ x_2 \ \dots \ x_n)_{1 \times n} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}_{n \times 1} = x_1 y_1 + x_2 y_2 + \dots + x_n y_n$$

- (2) Multiplication of \mathbf{x} by \mathbf{y}^T gives a $n \times n$ matrix.

$$\mathbf{x} \mathbf{y}^T = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}_{n \times 1} (y_1 \ y_2 \ \dots \ y_n)_{1 \times n} = \begin{pmatrix} x_1 y_1 & x_1 y_2 & \dots & x_1 y_n \\ x_2 y_1 & x_2 y_2 & \dots & x_2 y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_n y_1 & x_n y_2 & \dots & x_n y_n \end{pmatrix}_{n \times n}$$

2.2 Matrices

- (a) A matrix is a rectangular array of real numbers. A matrix with m rows and n columns is denoted by

$$\mathcal{A} = \mathcal{A}_{m \times n} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{pmatrix}_{m \times n} = (a_{ij})_{m \times n}$$

- (b) Transpose of \mathcal{A} is matrix of $n \times m$ and denoted by \mathcal{A}^T . That is, $\mathcal{A}^T = (a_{ji})_{n \times m}$.
- (c) Multiplication of Two Matrices: $\mathcal{A}_{m \times n} = (a_{ij})_{m \times n}$ and $\mathcal{B}_{n \times p} = (b_{ij})_{n \times p}$ give matrix $\mathcal{C}_{m \times p} = (c_{ij})_{m \times p}$ where $c_{ij} = \sum_{k=1}^n a_{ik}b_{kj}$.
- (d) Square Matrix: If the number of rows and number of columns of a matrix are equal, then it is called a square matrix (e.g. $m = n$).

$$\mathcal{A} = \mathcal{A}_{n \times n} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix}_{n \times n}$$

- (e) Symmetric Matrix: If \mathcal{A} is a square matrix of order n and the elements $a_{ij} = a_{ji}$ for all i and j , then \mathcal{A} is called a symmetric matrix.

Note : \mathcal{A} is a symmetric matrix iff $\mathcal{A}^T = \mathcal{A}$.

- (f) Identity matrix: A square matrix with ones on the diagonal and zeros elsewhere is called an identity matrix. The identity matrix of order n is given by

$$\mathcal{I}_n = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix}_{n \times n} = \text{diag}(1 \ 1 \ \dots \ 1)$$

- (g) Inverse of a Matrix: If there exists a matrix \mathcal{B} for a given square matrix \mathcal{A} such that $\mathcal{AB} = \mathcal{BA} = \mathcal{I}$ then \mathcal{B} is called the inverse of \mathcal{A} and is denoted by \mathcal{A}^{-1} .

- (h) Orthogonal Matrix: A square matrix \mathcal{Q} is said to be orthogonal if

$$\mathcal{Q}^T \mathcal{Q} = \mathcal{Q} \mathcal{Q}^T = \mathcal{I}.$$

Note : $\mathcal{Q}^{-1} = \mathcal{Q}^T$.

- (i) The Trace of a Matrix: Let $\mathcal{A} = (a_{ij})_{n \times n}$, a square matrix of order n . The trace of the matrix \mathcal{A} is the sum of the diagonal elements of \mathcal{A} and it is denoted by $\text{tr}(\mathcal{A})$. That is,

$$\text{tr}(\mathcal{A}) = \sum_{i=1}^n a_{ii}.$$

- (j) If \mathcal{B} and \mathcal{C} are square matrices, then

$$\text{tr}(\mathcal{B}\mathcal{C}) = \text{tr}(\mathcal{C}\mathcal{B}).$$

- (k) For a quadratic form $\mathbf{x}^T \mathcal{A} \mathbf{x}$, we have

$$\mathbf{x}^T \mathcal{A} \mathbf{x} = \text{tr}(\mathbf{x}^T \mathcal{A} \mathbf{x}) = \text{tr}(\mathbf{x} \mathbf{x}^T \mathcal{A}) = \text{tr}(\mathcal{A} \mathbf{x} \mathbf{x}^T)$$

- (l) Determinant: The determinant of a square matrix \mathcal{A} is denoted by $|\mathcal{A}|$ or $\det(\mathcal{A})$ and it is a numerical value computed from

$$|\mathcal{A}| = \det(\mathcal{A}) = \sum_{i=1}^n (-1)^{i+1} a_{1i} |\mathcal{A}_{1i}|$$

where \mathcal{A}_{1i} is the square matrix of order $(n-1)$ obtained by deleting the first row and i^{th} column of \mathcal{A} .

- (m) Eigenvalues and Eigenvectors: Let \mathcal{A} be a square matrix of order n and \mathbf{e} be a n dimensional vector. The values of λ and \mathbf{e} which satisfy the equation

$$\mathcal{A} \mathbf{e} = \lambda \mathbf{e}$$

are respectively called the eigenvalues and eigenvectors of \mathcal{A} .

Note:

- (1) The eigenvalues of \mathcal{A} can be obtained by solving $|\mathcal{A} - \lambda \mathcal{I}| = 0$.
- (2) There are n eigenvalues for a matrix of order n .

- (n) Let $(\lambda_i, \mathbf{e}_i)$, $i = 1, 2, \dots, n$, be the eigenvalue-eigenvector pairs of \mathcal{A} . Then

$$\mathcal{A}\mathbf{e}_i = \lambda_i\mathbf{e}_i$$

for $i = 1, 2, \dots, n$. If we chose \mathbf{e}_i such that $\mathbf{e}_i^T \mathbf{e}_i = 1$, then \mathbf{e}_i is called the **normalized eigenvector** corresponding to λ_i .

- (o) Spectral Decomposition: If $(\lambda_i, \mathbf{e}_i)$, $i = 1, 2, \dots, n$, be the eigenvalue, normalized eigenvector pairs of the square matrix \mathcal{A} , then

$$\mathcal{A} = \lambda_1 \mathbf{e}_1 \mathbf{e}_1^T + \lambda_2 \mathbf{e}_2 \mathbf{e}_2^T + \dots + \lambda_n \mathbf{e}_n \mathbf{e}_n^T.$$

This is known as the spectral decomposition of \mathcal{A} .

- (p) The determinant of \mathcal{A} can be expressed as the product of its eigenvalues. That is,

$$|\mathcal{A}| = \prod_{i=1}^n \lambda_i$$

- (q) Positive Definite Matrix: The symmetric matrix \mathcal{A} is called a positive definite matrix provided

$$\mathbf{x}^T \mathcal{A} \mathbf{x} > 0 \quad \text{for} \quad \mathbf{x} \neq \mathbf{0}$$

If $\mathbf{x}^T \mathcal{A} \mathbf{x} \geq 0$ then \mathcal{A} is called nonnegative (or semipositive) definite.

- (r) The symmetric matrix \mathcal{A} is positive definite iff the eigenvalues of \mathcal{A} , $\lambda_i > 0$ for all i .
- (s) If \mathcal{A} is nonnegative definite then $\lambda_i \geq 0$ for all i .
- (t) If \mathcal{A} is positive definite, then the special decomposition of the inverse

$$\mathcal{A}^{-1} = \lambda_1^{-1} \mathbf{e}_1 \mathbf{e}_1^T + \lambda_2^{-1} \mathbf{e}_2 \mathbf{e}_2^T + \dots + \lambda_n^{-1} \mathbf{e}_n \mathbf{e}_n^T.$$

- (u) Square Root of a Positive Definite Matrix: Using the special decomposition, the square root of a positive matrix is given by

$$\mathcal{A}^{\frac{1}{2}} = \lambda_1^{\frac{1}{2}} \mathbf{e}_1 \mathbf{e}_1^T + \lambda_2^{\frac{1}{2}} \mathbf{e}_2 \mathbf{e}_2^T + \dots + \lambda_n^{\frac{1}{2}} \mathbf{e}_n \mathbf{e}_n^T.$$

3 Random Vectors

Reference: Johnson & Wichern (2002) *Applied Multivariate Statistical Analysis*, Chapter 2.

3.1 Moments of Random Vectors

A random vector is a vector whose elements are random variables. Let $\mathbf{X}^T = (X_1 \ X_2 \ \dots \ X_p)_{1 \times p}$ be a random vector. Then X_i ($i = 1, 2, \dots, p$) are random variables.

(a) Population Mean Vector, $\boldsymbol{\mu}$ is

$$\boldsymbol{\mu} = \boldsymbol{\mu}_{p \times 1} = \mathbf{E}(\mathbf{X}_{p \times 1}) = \begin{pmatrix} \mathbf{E}(X_1) \\ \mathbf{E}(X_2) \\ \vdots \\ \mathbf{E}(X_p) \end{pmatrix}_{p \times 1} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_p \end{pmatrix}_{p \times 1}$$

where $\mu_i = \mathbf{E}(X_i)$ for $i = 1, 2, \dots, p$.

(b) Population covariance matrix, Σ is given by

$$\Sigma = \Sigma_{p \times p} = \mathbf{Cov}(\mathbf{X}_{p \times 1}) = \mathbf{E}[(\mathbf{X} - \boldsymbol{\mu})(\mathbf{X} - \boldsymbol{\mu})^T].$$

This gives

$$\Sigma_{p \times p} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \dots & \sigma_{1p} \\ \sigma_{21} & \sigma_{22} & \dots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{p1} & \sigma_{p2} & \dots & \sigma_{pp} \end{pmatrix}_{p \times p}$$

where $\sigma_{ij} = \mathbf{Cov}(X_i, X_j) = \mathbf{E}[(X_i - \mu_i)(X_j - \mu_j)]$ and $\sigma_{ij} = \sigma_{ji}$. Note when $i = j$, $\sigma_{ii} = \sigma_i^2 = \mathbf{E}(X_i - \mu_i)^2 = \mathbf{Var}(X_i)$.

Note : Covariance matrix is a symmetric matrix, that is, $\Sigma^T = \Sigma$.

(c) Generalized Variance: The determinant of a covariance matrix is called the generalized variance, hence

$$\text{Generalized Variance} = \det(\Sigma).$$

- (d) Population Correlation Matrix $\boldsymbol{\rho}$: The correlation matrix of a random vector \mathbf{X} is given by

$$\boldsymbol{\rho} = \begin{pmatrix} 1 & \rho_{12} & \cdots & \rho_{1p} \\ \rho_{21} & 1 & \cdots & \rho_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{p1} & \rho_{p2} & \cdots & 1 \end{pmatrix}_{p \times p}$$

where

$$\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}}\sqrt{\sigma_{jj}}} \quad \text{for } i \neq j$$

(e) Let $\mathcal{V} = \begin{pmatrix} \sigma_{11} & 0 & \cdots & 0 \\ 0 & \sigma_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_{pp} \end{pmatrix}_{p \times p} = \text{diag}(\sigma_{11} \ \sigma_{22} \ \cdots \ \sigma_{pp})$ then, it is easily verified that

$$\boldsymbol{\rho} = \mathcal{V}^{-\frac{1}{2}} \Sigma \mathcal{V}^{-\frac{1}{2}}.$$

Note that $\mathcal{V}^{-\frac{1}{2}} = \text{diag}(1/\sqrt{\sigma_{11}} \ 1/\sqrt{\sigma_{22}} \ \cdots \ 1/\sqrt{\sigma_{pp}})$ and $\Sigma = \mathcal{V}^{\frac{1}{2}} \boldsymbol{\rho} \mathcal{V}^{\frac{1}{2}}$

3.2 Properties of Random Vectors

Let \mathbf{X} and \mathbf{Y} be two p -variate random vectors (not necessarily normal) such that

$$\begin{aligned} \mathbf{E}(\mathbf{X}) &= \boldsymbol{\mu}_x, & \mathbf{E}(\mathbf{Y}) &= \boldsymbol{\mu}_y, \\ \mathbf{Cov}(\mathbf{X}) &= \Sigma_x, & \mathbf{Cov}(\mathbf{Y}) &= \Sigma_y, \end{aligned}$$

and $\mathbf{Cov}(\mathbf{X}, \mathbf{Y}) = \Gamma$. Consider \mathbf{a}, \mathbf{b} and \mathbf{c} are vector constant and, \mathcal{A}, \mathcal{B} and \mathcal{C} are constant matrices. We can prove the following properties.

- (a) $\mathbf{E}(\mathbf{a}^T \mathbf{X}) = \mathbf{a}^T \boldsymbol{\mu}_x$
- (b) $\mathbf{E}(\mathcal{A}^T \mathbf{X} + \mathbf{c}) = \mathcal{A}^T \boldsymbol{\mu}_x + \mathbf{c}$
- (c) $\mathbf{Cov}(\mathbf{a}^T \mathbf{X}, \mathbf{b}^T \mathbf{X}) = \mathbf{a}^T \Sigma_x \mathbf{b} = \mathbf{b}^T \Sigma_x \mathbf{a}$
- (d) $\mathbf{Cov}(\mathbf{a}^T \mathbf{X}) = \mathbf{a}^T \Sigma_x \mathbf{a}$
- (e) $\mathbf{Cov}(\mathcal{D} \mathbf{X}) = \mathcal{D} \Sigma_x \mathcal{D}^T$
- (f) $\mathbf{Cov}(\mathbf{X}, \mathbf{Y}) = \mathbf{E}\{(\mathbf{X} - \mathbf{E}(\mathbf{X}))(\mathbf{Y} - \mathbf{E}(\mathbf{Y}))^T\} = \mathbf{Cov}(\mathbf{Y}, \mathbf{X})^T$

- (g) $\mathbf{Cov}(\mathcal{A}^T \mathbf{X}, \mathcal{B}^T \mathbf{X}) = \mathcal{A}^T \Sigma_x \mathcal{B}$
- (h) $\mathbf{Cov}(\mathbf{a}^T \mathbf{X}, \mathbf{b}^T \mathbf{Y}) = \mathbf{a}^T \mathbf{Cov}(\mathbf{X}, \mathbf{Y}) \mathbf{b}$
- (i) $\mathbf{Cov}(\mathcal{A}^T \mathbf{X}, \mathcal{B}^T \mathbf{Y}) = \mathcal{A}^T \mathbf{Cov}(\mathbf{X}, \mathbf{Y}) \mathcal{B}$

3.3 Linear combinations of random variables

Consider random variables X_1 and X_2 and a and b are constants, then

$$\mathbf{E}(aX_1 + bX_2) = a\mathbf{E}(X_1) + b\mathbf{E}(X_2) = a\mu_1 + b\mu_2$$

using additional properties, covariance of aX_1 and bX_2 is

$$\mathbf{Cov}(aX_1, bX_2) = \mathbf{E}[(aX_1 - a\mu_1)(bX_2 - b\mu_2)] = ab\mathbf{Cov}(X_1, X_2) = ab\sigma_{12}$$

and

$$\begin{aligned} \mathbf{Var}(aX_1 + bX_2) &= a^2\mathbf{Var}(X_1) + b^2\mathbf{Var}(X_2) + 2ab\mathbf{Cov}(X_1, X_2) \\ &= a^2\sigma_{11} + b^2\sigma_{22} + 2ab\sigma_{12} = a^2\sigma_1^2 + b^2\sigma_2^2 + 2ab\sigma_1\sigma_2\rho_{12} \end{aligned}$$

- (a) If X_1 and X_2 are independent random variable, then $\rho_{12} = 0$, hence

$$\mathbf{Var}(aX_1 + bX_2) = a^2\sigma_1^2 + b^2\sigma_2^2$$

- (b) Let $\mathbf{c}^T = (a \ b)$, $\boldsymbol{\mu}^T = (\mu_1 \ \mu_2)$ and $\mathbf{X}^T = (X_1 \ X_2)$ then

$$\mathbf{E}(\mathbf{c}^T \mathbf{X}) = \mathbf{E}(ab) \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = (ab) \begin{pmatrix} \mathbf{E}(X_1) \\ \mathbf{E}(X_2) \end{pmatrix} = \mathbf{E}(ab) \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} = \mathbf{c}^T \boldsymbol{\mu}$$

Note that $\mathbf{E}(\mathbf{c}^T \mathbf{X}) = \mathbf{E}(aX_1 + bX_2) = a\mu_1 + b\mu_2 = \mathbf{c}^T \boldsymbol{\mu}$.

- (c) Let

$$\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}$$

then

$$\mathbf{Var}(\mathbf{c}^T \mathbf{X}) = (a \ b) \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \mathbf{c}^T \Sigma \mathbf{c}$$

Note that $\mathbf{Var}(\mathbf{c}^T \mathbf{X}) = \mathbf{Var}(aX_1 + bX_2) = a^2\sigma_{11} + 2ab\sigma_{12} + b^2\sigma_{22} = \mathbf{c}^T \Sigma \mathbf{c}$.

(d) The linear combination $\mathbf{c}^T \mathbf{X} = c_1 X_1 + c_2 X_2 + \dots + c_p X_p$ has

$$\begin{aligned}\text{Mean} &= \mathbf{E}(\mathbf{c}^T \mathbf{X}) = \mathbf{c}^T \boldsymbol{\mu} \quad \text{and} \\ \text{Variance} &= \mathbf{Var}(\mathbf{c}^T \mathbf{X}) = \mathbf{c}^T \Sigma \mathbf{c}\end{aligned}$$

where $\boldsymbol{\mu} = \mathbf{E}(\mathbf{X})$ and $\Sigma = \mathbf{Cov}(\mathbf{X})$.

(e) In general consider the q linear combinations of the p random variables X_1, X_2, \dots, X_p .

$$\begin{aligned}Z_1 &= a_{11}X_1 + a_{12}X_2 + \dots + a_{1p}X_p \\ Z_2 &= a_{21}X_1 + a_{22}X_2 + \dots + a_{2p}X_p \\ &\vdots \\ Z_q &= a_{q1}X_1 + a_{q2}X_2 + \dots + a_{qp}X_p\end{aligned}$$

This linear combinations can be rewritten as $\mathbf{Z}_{q \times 1} = \mathcal{A}_{q \times p} \mathbf{X}_{p \times 1}$, therefore we obtain

$$\boldsymbol{\mu}_z = \mathbf{E}(\mathbf{Z}) = \mathbf{E}(\mathcal{A}\mathbf{X}) = \mathcal{A}\boldsymbol{\mu}_x$$

and

$$\Sigma_z = \mathbf{Cov}(\mathbf{Z}) = \mathbf{Cov}(\mathcal{A}\mathbf{X}) = \mathcal{A}\Sigma_x \mathcal{A}^T$$

where $\boldsymbol{\mu}_x$ and Σ_x are respectively the mean vector and covariance matrix of \mathbf{X} .