

MAST 90138: MULTIVARIATE STATISTICAL TECHNIQUES

Assessment:

- Three assignments (15% each) due at dates TBD spread over the course.
- Final written examination (55%).

Got question about course material?

- Ask your peers on Ed discussion
- or ask instructor/tutor during office hours and tutorials
- Questions are **not to be asked by email**.

Office hours :

Regular weeks (subject to change, changes announced on LMS):

- Tu 3.00-4.00: room 189, Peter Hall building, start week 2,
- Wed 3.15-4.15: room 189, PHB
- Fri 11.00-12.00: Zoom, meeting ID 81136149049.

Aug 4-11: see subject overview on LMS.

Other comments

- The tutorials will involve the software R.
- You need to attend the tutorial that was assigned to you as the lists have been designed based on the computer rooms capacity.
- The official slides of the course will be the ones posted AFTER the class.
- I will try to post a version of the slides BEFORE the class. This will NOT be the official version of the slides.

I will often replace those slides after the class to post the official version of the slides.

MAST 90138: MULTIVARIATE STATISTICAL TECHNIQUES

1 INTRODUCTION

Goal of the course: Describe, understand and discover properties of data in $p > 1$ dimensions. 多维数据 多维

- We are interested in analysing a sample of n random vectors X_1, \dots, X_n , also denoted by X_i for $i = 1, \dots, n$, where X_1, X_2 , etc all belong to \mathbb{R}^p :
 分析 n 个向量 每个向量是 p 维

$$X_1 = (X_{11}, \dots, X_{1p}) \in \mathbb{R}^p$$

$$X_2 = (X_{21}, \dots, X_{2p}) \in \mathbb{R}^p$$

\vdots

$$X_n = (X_{n1}, \dots, X_{np}) \in \mathbb{R}^p.$$

- This means that we have a sample of n individuals, and that for each individual we observe p variables (sometimes called features).

- $X_i = (X_{i1}, \dots, X_{ip})$ is a row vector

$$X_i^T = \begin{pmatrix} X_{i1} \\ \dots \\ X_{ip} \end{pmatrix} \text{ is a column vector.}$$

Example:

- We consider a health study involving $n = 100$ patients.
- On each patient we measure $p = 4$ quantities: age, weight, body mass index, systolic blood pressure.
- For the i th individual, where $i = 1, \dots, 100$ we observe the vector

$$X_i = (X_{i1}, X_{i2}, X_{i3}, X_{i4}).$$

- X_{i1} =age of i th patient
 X_{i2} =weight of i th patient
 X_{i3} = body mass index of i th patient
 X_{i4} =systolic blood pressure of i th patient.

Often we gather all the observations into a single $n \times p$ matrix

$$\mathcal{X} = \begin{pmatrix} X_{11} & \dots & X_{1p} \\ X_{21} & \dots & X_{2p} \\ \vdots & & \\ X_{n1} & \dots & X_{np} \end{pmatrix}$$

- ➡ Each X_{ij} , for $i = 1, \dots, n$ and $j = 1, \dots, p$ is a random variable.
 - ➡ \mathcal{X} has n rows and p columns.
 - ➡ The i th row represents the p variables corresponding to the i th individual,
 - ➡ the j th column represents the j th variable for all n individuals.
- We call the value taken by $X_i = (X_{i1}, \dots, X_{ip})$ the observed value or realisation.
 - Often we use a lower case to denote the observed value: $x_i = (x_{i1}, \dots, x_{ip})$ is the observed value (or realisation) of the random vector X_i .

What we will do in the course:

- The technique learned in basic statistics courses are not focused on multivariate data.
- For ex, how would we do a scatterplot in more than $p = 2$ dimensions?
How to represent graphically multivariate data?
- In this course we will learn techniques especially designed for multivariate data.
- This course will introduce various **CORE statistical methods** for analysing and describing multivariate data.
- Topics such as neural networks, support vector machine, graphical models, etc **will NOT** be covered in this course.

MATERIAL COVERED IN THE COURSE:

- Revision of basic matrix results and multivariate data needed in the course (tentative schedule: weeks 1 and 2).
 - 👉 As this is just a revision, we won't spend much time on examples but the reference book has examples.
- Principal component analysis, factor analysis, partial least squares.
- Classification (linear and quadratic discriminant, regression-based, including trees and forest).
- Clustering (K -means, K -medoids, hierarchical).
- If time permits, other topics such as correspondence analysis or more techniques for above topics.

Main reference books:

- Härdle, W. and Simar, L (2015). Applied multivariate statistical analysis, 4th edition.

Available for download at the unimelb library website.

- Hastie, T. Tibshirani, R. and Friedman, J. (2009). The elements of statistical learning, 2nd edition (available online):
<https://hastie.su.domains/Papers/ESLII.pdf>

We might also use

- Koch, I. (2013). Analysis of Multivariate and High-Dimensional Data. Cambridge University Press.
- K. V. Mardia, J. T. Kent, & J. M. Bibby (1979). Multivariate Analysis. New York: Academic Press.
- Other resources as needed.

2 REVIEW OF MATRIX PROPERTIES

Sections 2.1, 2.2, 2.3, 2.4 and 2.6 in Härdle and Simar (2015).

2.1 ELEMENTARY OPERATIONS

- Let $A = (a_{ij}) = (a_{ij})_{1 \leq i \leq n, 1 \leq j \leq p}$ be an $n \times p$ matrix (matrix with n rows and p columns):

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1p} \\ a_{21} & a_{22} & \dots & a_{2p} \\ \vdots & & & \\ a_{n1} & a_{n2} & \dots & a_{np} \end{pmatrix}$$

- We use A^T to denote the transpose of the matrix A :

$$A^T = \begin{pmatrix} a_{11} & a_{21} & \dots & a_{n1} \\ a_{12} & a_{22} & \dots & a_{n2} \\ \vdots & & & \\ a_{1p} & a_{2p} & \dots & a_{np} \end{pmatrix}$$

(rows become columns and columns become rows).

- Product of two matrices A , an $n \times p$ matrix, and B , a $p \times m$ matrix:

$$AB = C,$$

where C is an $n \times m$ matrix whose (i, j) th element is given by:

$$c_{ij} = \sum_{k=1}^p a_{ik} b_{kj}$$

- Scalar product of two p dimensional vectors $x = (x_1, \dots, x_p)^T$ and $y = (y_1, \dots, y_p)^T$:

$$x^T y = \sum_{j=1}^p x_j y_j.$$

- Norm of a p dimensional vector $x = (x_1, \dots, x_p)^T$ or $x = (x_1, \dots, x_p)$:

$$\|x\| = \sqrt{\sum_{j=1}^p x_j^2} = \begin{cases} \sqrt{x^T x} & \text{if } x = (x_1, \dots, x_p)^T \\ \sqrt{xx^T} & \text{if } x = (x_1, \dots, x_p) \end{cases}$$

Some properties:

$$A + B = B + A$$

$$A(B + C) = AB + AC$$

$$A(BC) = (AB)C$$

$$(A^T)^T = A$$

$$(AB)^T = B^T A^T$$

BUT :

$$AC \neq CA$$

乘法
交换律

乘法
消去律
没有

Special matrices (taken from Härdle and Simar):

Table 2.1 Special matrices and vectors

Name	Definition	Notation	Example
Scalar	$p = n = 1$	a	3
Column vector	$p = 1$	a	$\begin{pmatrix} 1 \\ 3 \end{pmatrix}$
Row vector	$n = 1$	a^\top	$\begin{pmatrix} 1 & 3 \end{pmatrix}$
Vector of ones	$\underbrace{(1, \dots, 1)}_n^\top$	1_n	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$
Vector of zeros	$\underbrace{(0, \dots, 0)}_n^\top$	0_n	$\begin{pmatrix} 0 \\ 0 \end{pmatrix}$
Square matrix	$n = p$	$\mathcal{A}(p \times p)$	$\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$
Diagonal matrix	$a_{ij} = 0, i \neq j, n = p$	$\text{diag}(a_{ii})$	$\begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$

Identity matrix	$\text{diag}(\underbrace{1, \dots, 1}_p)$	\mathcal{I}_p	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
Unit matrix	$a_{ij} = 1, n = p$	$\mathbf{1}_n \mathbf{1}_n^\top$	$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$
Symmetric matrix	$a_{ij} = a_{ji}$		$\begin{pmatrix} 1 & 2 \\ 2 & 3 \end{pmatrix}$
Null matrix	$a_{ij} = 0$	0	$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$
Upper triangular matrix	$a_{ij} = 0, i < j$		$\begin{pmatrix} 1 & 2 & 4 \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{pmatrix}$
Idempotent matrix	$\mathcal{A}\mathcal{A} = \mathcal{A}$		$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
Orthogonal matrix	$\mathcal{A}^\top \mathcal{A} = \mathcal{I} = \mathcal{A}\mathcal{A}^\top$ $A^\top = A^{-1}$		$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$

各列范数为1
各列正交
点积=0

- A set of k rows (or columns) a_1, \dots, a_k of A are said to be linearly independent if none of them can be expressed as a nontrivial linear combination of the other $k - 1$ rows (or columns). It is not possible to write

$$a_j = \sum_{i \neq j} c_i a_i,$$

对任意列(或行)都没法表示为其他列(或行)的线性组合.

where the c_i 's are all different from zero, or equivalently

$$\sum_{i=1}^k c_i a_i = 0 \Rightarrow c_1, \dots, c_k = 0.$$

对一个矩阵我随便找一组vector, 使等式成立的唯一解是 $c_1, \dots, c_k = 0$

- Rank: The **rank** of an $n \times p$ matrix A , denoted by **rank**(A) is defined as the maximum number of linearly independent rows (or columns).

最大线性独立行的数量.

We always have

$$\text{rank}(A) \leq \min(n, p).$$

n, p 的最小值
行列

- **Trace:** The trace of a **square** $p \times p$ matrix A , denoted by $\text{tr}(A)$, is the sum of its diagonal elements:

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

- **Determinant:** The determinant of a **square** $p \times p$ matrix A , denoted by $\det(A)$ or $|A|$, is a number computed from the matrix and which plays an important role in all sorts of problems. For a 2×2 matrix

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

it is computed by

$$|A| = a_{11}a_{22} - a_{21}a_{12} .$$

For larger matrices, we compute this recursively. If you forgot how a determinant is computed, see

<https://en.wikipedia.org/wiki/Determinant>

- If rank of ^{square matrix} $p \times p$ matrix A not full ($\text{rank}(A) < p$) then $\det(A) = 0$. 不足秩 $\det(A)=0$
- **Inverse:** If $|A| \neq 0$, the inverse of a **square** $p \times p$ matrix A exists. It is denoted by A^{-1} and is such that
full rank $\Rightarrow |A| \neq 0 \Rightarrow \det(A) \neq 0 \Rightarrow$ non singular.

$$AA^{-1} = A^{-1}A = I_p$$

($I_p = p \times p$ identity matrix).

See Härdle and Simar, page 57, for how to compute the inverse.

We have

$$\star \boxed{|A^{-1}| = 1/|A|} \star$$

- A non invertible square matrix is also said to be **singular**.

// not full rank matrix // $\det(A)=0$

- Eigenvalues and eigenvectors of a **square** $p \times p$ matrix A :

The (non zero) $p \times 1$ vector v is an eigenvector of A with eigenvalue λ if it is such that

$$Av = \lambda v .$$

Note that λ is a real number (not a vector).

☞ If A is symmetric then there are p eigenvalues and eigenvectors.

☞ All eigenvalues satisfy

$$|A - \lambda I_p| = 0$$

解方程

(they are the p roots of the above polynomial of order p in λ).

☞ The eigenvalues are not necessarily all different from each other.

eigenvalue 不-相同

☞ Constant multiples of an eigen vector v with eigenvalue λ are also eigenvectors with eigenvalue λ . 特征向量的数量是无限的

☞ It is common to work with scaled version of eigenvectors that have norm 1:

$$\|v\| = \sqrt{v^T v} = 1.$$

$$|v| = \sqrt{|v|} \quad \text{开根}$$

☞ In practice we often compute them with a software, e.g. R .

- Suppose the ^{方阵} **square** $p \times p$ matrix A has eigenvalues $\lambda_1, \dots, \lambda_p$.

Let Λ be the diagonal matrix $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_p)$ with the λ_i 's on the diagonal and 0 everywhere else.

$$A \text{ 的对角矩阵 } \Lambda = \text{diag}(\lambda_1, \dots, \lambda_p)$$

Then we have

$$\det(A) = \underbrace{(|A| = |\Lambda|)}_{\text{product of eigenvalues}} = \prod_{i=1}^p \lambda_i \quad (\text{连乘}) = \det(A).$$

and

$$\text{tr}(A) = \text{tr}(\Lambda) = \sum_{i=1}^p \lambda_i.$$

- If A and B are two invertible matrices of the same dimension, then

$$(A \cdot B)^{-1} = B^{-1} A^{-1}.$$

Some other properties of matrix characteristics (from Härdle and Simar):

$$\mathcal{A}(n \times p), \mathcal{B}(p \times q), \mathcal{C}(q \times n)$$

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

$$\mathcal{A}(n \times n), \mathcal{B}(n \times n), c \in \mathbb{R}$$

$$\text{tr}(\mathcal{A} + \mathcal{B}) = \text{tr} \mathcal{A} + \text{tr} \mathcal{B}$$

$$\text{tr}(c \mathcal{A}) = c \text{tr} \mathcal{A}$$

$$|cA| = c^n |A|$$

$$|AB| = |BA| = |A||B|$$

$$A(n \times p), B(p \times n)$$

$$\text{tr}(A \cdot B) = \text{tr}(B \cdot A)$$

$$\text{rank}(A) \leq \min(n, p)$$

$$\text{rank}(A) \geq 0$$

$$\text{rank}(A) = \text{rank}(A^T)$$

$$\text{rank}(A^T A) = \text{rank}(A)$$

有时候算 $A^T A$ might be easier.

$$\text{rank}(A + B) \leq \text{rank}(A) + \text{rank}(B)$$

$$\text{rank}(AB) \leq \min\{\text{rank}(A), \text{rank}(B)\}$$

Errata: The dimensions of A and B have to match for $A + B$ to be defined in

$$\text{rank}(A + B) \leq \text{rank}(A) + \text{rank}(B),$$

2.2 SPECTRAL DECOMPOSITIONS

Spectral decomposition

- **Spectral decomposition**: Suppose A is a square and symmetric $p \times p$ matrix and let

$\lambda_1, \dots, \lambda_p$ denote its p eigenvalues and *每个 eigenvalue 不一定全不同*

v_1, \dots, v_p denote the associated $p \times 1$ eigenvectors of norm 1 and orthogonal to each other (each v_k is the eigenvector associated to λ_k).

Note: two $p \times 1$ column vectors v and w are orthogonal if

$$v^T w = \sum_{i=1}^p v_i w_i = 0.$$

列向量点积得0.

Then we can always express A in the following way, which is called spectral decomposition of A :

matrix $\left\{ \begin{array}{l} \text{symmetric} \\ \text{square} \end{array} \right.$ p

有特征值, 特征记
我们都能将矩阵表示成

$$A = \sum_{j=1}^p \lambda_j v_j v_j^T$$

λ_j eigenvalue
 v_j eigenvector

This can also be written in matrix form, if we let

$$\Lambda = \text{diag}(\lambda_1, \dots, \lambda_p)$$

and

Gamma eigenvector set

$$\Gamma = (v_1, \dots, v_p)$$

the $p \times p$ orthogonal matrix whose columns are the p eigenvectors standardised to be of norm 1: (标准特征向量) 每个特征向量 norm

$$A = \Gamma \Lambda \Gamma^T$$

Γ norm 1


- In the above notation, if $A = \Gamma \Lambda \Gamma^T$ then if we take an integer **power of A** , for example A^α , we find


$$\underline{A^\alpha = \Gamma \Lambda^\alpha \Gamma^T.} \quad A^2 = \Gamma \Lambda^2 \Gamma^T$$


This is because the v_j 's are orthonormal (i.e. orthogonal and of norm 1).

For example

$$A^2 = \Gamma \Lambda \Gamma^T \Gamma \Lambda \Gamma^T = \Gamma \Lambda^2 \Gamma^T.$$







This also works for **negative powers** if A is **invertible** (which happens if and only if the eigenvalues are all **nonzero**). For example,

$$A^{-1} = \Gamma \Lambda^{-1} \Gamma^T$$

满秩矩阵

(A^{-1} : the inverse of the matrix A).

Singular value decomposition

More generally, a similar **decomposition** exists for matrices that are **not especially square** matrices. In particular, any $n \times p$ matrix A with rank r can be decomposed as

$$A = \Gamma \Lambda \Delta^T$$

不同矩阵
 $n \times p$ $n \times r$ $r \times p$

$\text{rank} \leq \min(3, 2)$
 rank: # of non-zero eigenvalues of matrix

where the $n \times r$ matrix Γ and the $p \times r$ matrix Δ are **column orthonormal**, i.e. their columns are orthonormal (i.e., orthogonal and of norm 1), that is

$$\Gamma^T \Gamma = \Delta^T \Delta = I_r$$

Γ, Δ 都正交

and

$$\Lambda = \text{diag}(\lambda_1^{1/2}, \dots, \lambda_r^{1/2})$$

where each $\lambda_i > 0$.

$A, A^T A$ 非零特征值的平方

The λ_i 's are the **nonzero eigenvalues** of the matrices AA^T or $A^T A$; the columns of Γ and Δ are the corresponding r **eigenvectors** of those matrices, respectively.

Δ : eigenvectors of $A^T A$
 Γ : eigenvectors of AA^T

$$A = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}_{2 \times 3}$$

$\text{rank}(A) = 2$ because it's impossible to express $(1, 1, 0) = c \cdot (0, 1, 1)$

$$AA^T = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 0 & 1 \end{pmatrix}_{\substack{2 \times 3 \\ 3 \times 2}} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

\rightarrow # of eigenvalues $= 2$

$$\text{rank}(A^T A) = \text{rank}(A) \Rightarrow 2$$

$$\det(AA^T - \lambda I) = \begin{vmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{vmatrix} = (2-\lambda)^2 - 1 = \lambda^2 - 4\lambda + 3 = 0$$

$$\lambda^2 - 4\lambda + 3 = 0$$

$$(\lambda - 2)^2 = 1$$

$$\begin{cases} \lambda - 2 = 1 & \lambda_1 = 3 \\ \lambda - 2 = -1 & \lambda_2 = 1 \end{cases}$$

$$V_1 = \begin{pmatrix} v_{11} \\ v_{12} \end{pmatrix} \text{ associated to } \lambda_1 = 3$$

$$AA^T \cdot V_1 = \lambda_1 \cdot V_1$$

$$\Rightarrow \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} v_{11} \\ v_{12} \end{pmatrix} = 3 \begin{pmatrix} v_{11} \\ v_{12} \end{pmatrix}$$

$$\begin{vmatrix} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} & \begin{pmatrix} v_{11} \\ v_{12} \end{pmatrix} \end{vmatrix} = 3 \begin{pmatrix} v_{11} \\ v_{12} \end{pmatrix}$$

... $\lambda_3 v_{11}, \lambda_3 v_{12}$

2x2x2x1

$$\begin{pmatrix} 2V_{11} + V_{12} \\ V_{11} + 2V_{12} \end{pmatrix} = \begin{pmatrix} V_{11} \\ V_{12} \end{pmatrix}$$

$$\begin{cases} V_{12} = -V_{11} \\ V_{11} = -V_{12} \end{cases} \Rightarrow \begin{pmatrix} -V_{12} \\ V_{12} \end{pmatrix} \Rightarrow \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\|V_1\| = \sqrt{1+1} = \sqrt{2}$$

normalize: $V_1 = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$

$$P = \begin{pmatrix} \pi_1 & \pi_2 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

(orthogonal matrix)

$$A^T A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

3x2x2x3

rank 相同

非零 $r(A^T A) = r(AA^T) \Rightarrow$ 非零特征个数相同

$$\begin{bmatrix} 1 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix} \begin{pmatrix} V_{11} \\ V_{12} \\ V_{13} \end{pmatrix} = \lambda \begin{pmatrix} V_{11} \\ V_{12} \\ V_{13} \end{pmatrix}$$

$$V_1 = \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix}$$

$$V_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

$$V_3 = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$$

$$1+4+1=6$$

$$\pi_1 = 3$$

$$\text{norm} = \frac{1}{\sqrt{6}}$$

$$\pi_2 = 1$$

$$\text{norm} = \frac{1}{\sqrt{2}}$$

$$\pi_3 = 0$$

$$\text{norm} = \frac{1}{\sqrt{3}}$$

$$\Delta = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{2}{\sqrt{6}} & 0 & -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \end{pmatrix}$$

$$\pi_1 \quad \pi_2 \quad \pi_3$$

$$\Lambda = \begin{bmatrix} \sqrt{6} & & \\ & \sqrt{2} & \\ & & \sqrt{3} \\ & & & 0 \end{bmatrix}$$

A 的特征向量

$$P \Lambda P^T$$

$$A = \Gamma \Lambda \Delta^T$$