STAT 3690 Lecture Note

Week One (Jan 9, 11, & 13, 2023)

Zhiyang Zhou (zhiyang.zhou@umanitoba.ca, zhiyanggeezhou.github.io)

2023/Jan/11 19:10:30

IN THE CASE OF A FIRE ALARM:

- · Remain calm
 - · if it is safe, evacuate the classroom or lab
 - · go to the closest fire exit
 - · do not use the elevators
- If you need assistance to evacuate the building, inform your professor or instructor immediately.
- If you need to report an incident or a person left behind during a building evacuation, report it to a fire warden or call security services 204-474-9341.
 - Do not reenter the building until the "all clear" is declared by a fire warden, security services or the fire department.
- Important: only those trained in the use of a fire extinguisher should attempt to operate one!





Syllabus

Contact

- Instructor: Zhiyang (Gee) Zhou, PhD, Asst. Prof.
 - Email: zhiyang.zhou@umanitoba.ca
 - Homepage: zhiyanggeezhou.github.io
- Marker: Mr. Masudul Islam
 - Email: islamm8@myumanitoba.ca

Timeline

- Lectures
 - Mon/Wed/Fri 9:30–10:20 am
- · Office Hour
 - Wed 10:30-11:20 am
- Assessments
 - Assignments (4/5 times)
 - Midterm
 - Final project

Grading

- Assignments (30%)
 - Scanned/photographed and submitted to Crowdmark
 - Attaching both outputs and source codes (if applicable)
 - Including necessary interpretation
 - Organized in a clear and readable way
 - Accepting NO late submission
- Midterm (35%)
 - Open-book
 - In-person on Mar 10 6-8 pm OR take-home (webcam-invigilated) NOT later than Mar. 20
- Final project (35%)
 - Individual report analying recently collected datasets
 - See the Project Guideline posted at UM Learn

Materials

- Reading list (recommended but not required)
 - [J&W] R. A. Johnson & D. W. Wichern. (2007). Applied Multivariate Statistical Analysis, 5/6th Ed. London: Pearson Education.
 - * 2HR print reserve in the Sciences and Technology Library
 - [R&C] A. C. Rencher & W. F. Christensen. (2012). Methods of Multivariate Analysis, 3rd Ed. Hoboken: Wiley.
 - * Digital copy accessible via the library
 - D. Salsburg (2001). The Lady Tasting Tea: How Statistics Revolutionized Science in the Twentieth Century. New York: WH Freeman.
- Lecture notes and beyond
 - zhiyanggeezhou.github.io
 - UM Learn

Outline

- Topics to be covered
 - Matrix manipulation
 - Basics of statistical modeling
 - Multivariate normal distribution
 - Inference on a mean vector
 - Comparisons of several multivariate means
 - Multivariate linear regression
 - Principal component analysis
 - Factor analysis
 - Canonical correlation analysis
 - and so forth

R basics

- Installation
 - -download and install BASE ${\cal R}$ from https://cran.r-project.org
 - download and install Rstudio from https://www.rstudio.com
 - download and install packages via Rstudio
- Working directory
 - When you ask R to open a certain file, it will look in the working directory for this file.
 - When you tell R to save a data file or figure, it will save it in the working directory.

```
getwd()
mainDir <- "c:/"</pre>
subDir <- "stat3690"</pre>
dir.create(file.path(mainDir, subDir), showWarnings = FALSE)
setwd(file.path(mainDir, subDir))
   • Packages
       installation: install.packages()
        loading: library()
install.packages('nlme')
library(nlme)
   • Help manual: help(), ?, google, stackoverflow, etc.
   • R is free but not cheap
        - Open-source
        - Citing packages
       - NO quality control
        - Requiring statistical sophistication
        - Time-consuming to become a master
   • References for R
        - M. L. Rizzo (2019) Statistical Computing with R, 2nd Ed. (forthcoming)
       - O. Jones, R. Maillardet, A. Robinson (2014) Introduction to Scientific Programming and Simulation
          Using R, 2nd Ed.
        - .....
   • Courses online
        - https://www.pluralsight.com/search?q=R
   • Data types: let str() or class() tell you
        - numbers (integer, real, or complex)
        - characters ("abc")
        - logical (TRUE or FALSE)
       - date & time
        - factor (commonly encountered in this course)
       - NA (different from Inf, " '', 0, NaN etc.)
   • Data structures: let str() or class() tell you
       - vector: an ordered collection of the same data type
       - matrix: two-dimensional collection of the same data type
       - array: more than two dimensional collection of the same data type
       - data frame: collection of vectors of same length but of arbitrary data types
        - list: collection of arbitrary objects
   • Data input and output
        - create
            * vector: c(), seq(), rep()
            * matrix: matrix(), cbind(), rbind()
            * data frame
```

```
output: write.table(), write.csv(), write.xlsx()
import: read.table(), read.csv(), read.xlsx()
* header: whether or not assume variable names in first row
* stringsAsFactors: whether or not convert character string to factors
- scan(): a more general way to input data
- save.image() and load(): save and reload workspace
- source(): run R script
```

• Parenthesis in R

- paenthesis () to enclose inputs for functions
- square brackets [], [[]] for indexing
- braces {} to enclose for loop or statements such as if or if else

```
# Create numeric vectors
v1 = c(1,2,3); v1
v2 = seq(4,6,by=0.5); v2
v3 = c(v1, v2); v3
v4 = rep(pi, 5); v4
v5 = rep(v1,2); v5
v6 = rep(v1, each=2); v6
# Create Character vector
v7 <- c("one", "two", "three"); v7
# Select specific elements
v1[c(1,3)]
v7[2]
# Create matrices
m1 = matrix(-1:4, nrow=2); m1
m2 = matrix(-1:4, nrow=2, byrow=TRUE); m2
m3 = cbind(m1, m2); m3
(m4 = cbind(m1, m2))
# Create a data frame
e \leftarrow c(1,2,3,4)
f <- c("red", "white", "black", NA)</pre>
g <- c(TRUE,TRUE,TRUE,FALSE)</pre>
mydata <- data.frame(e,f,g)</pre>
names(mydata) <- c("ID", "Color", "Passed") # name variable</pre>
mydata
# Output
write.csv(mydata, file='mydata.csv', row.names=F)
# Import
(simple = read.csv('mydata.csv', header=TRUE, stringsAsFactors=TRUE))
class(simple)
class(simple[[1]])
class(simple[[2]])
class(simple[[3]])
(simple = read.csv('mydata.csv', header=FALSE, stringsAsFactors=FALSE))
class(simple[[3]])
# EXERCISE
# Create a matrix with 2 rows and 6 columns such that it contains the numbers 1,4,7,...,34.
```

```
# Make sure the numbers are increasing row-wise; ie, 4 should be in the second column. # Use the seq() function to generate the numbers. Do NOT type them out by hand!
```

```
# ANSWER
matrix(seq(from=1, to=34, by=3), nrow=2)
```

- Elementary arithmetic operators
 - +, -, *, /, ^
 - $-\log$, exp, sin, cos, tan, sqrt
 - FALSE and TRUE becoming 0 and 1, respectively
 - $-\operatorname{sum}(), \operatorname{mean}(), \operatorname{median}(), \operatorname{min}(), \operatorname{max}(), \operatorname{var}(), \operatorname{sd}(), \operatorname{summary}()$
- Matrix calculation
 - element-wise multiplication: A * B
 - matrix multiplication: A %[∗]% B
 - singlar value decomposition: eigen(A)
- Loops: for() and while()
- Probabilities
 - normal distribution: dnorm(), pnorm(), qnorm(), rnorm()
 - uniform distribution: dunif(), punif(), qunif(), runif()
 - multivariate normal distribution: dmvnorm(), rmvnorm()

```
# Generate two datasets
set.seed(100)
x = rnorm(250, mean=0, sd=1)
y = runif(250, -3, 3)
```

- Basic plots
 - strip chart, histogram, box plot, scatter plot
 - Package ggplot2 (RECOMMENDED)

```
# Strip chart
stripchart(x)

# Histogram
hist(x)

# Box plot
boxplot(x)

# Side-bu-side box plot
xy = data.frame(normal=x, uniform=y)
boxplot(xy)

# Scatter Plot with fitted line
plot(x, y ,xlab="x", ylab = "y", main = "scatter plot between x and y")
abline(lm(y~x))
```

```
# EXERCISE
# Play with a data set called "Gasoline" included in the package "nlme".
# 1. How many variables are contained in this data set? What are they?
# 2. Generate a histogram of yield and calculate the five number summary for it.
  What is the shape of the histogram?
# 3. Generate side-by-side boxplots,
# comparing the temperature at which all the gasoline is vaporized (endpoint) to sample.
# Does it seem that the temperatures at which all the gasoline is vaporized differ by sample?
# 4. Generate a plot that illustrates the relationship between yield and endpoint.
  Describe the relationship between these two variables.
# 5. What if the plot created in Q4 were separated by sample?
  Generate a plot of yield v.s. endpoint, separated by sample.
# ANSWER
attach(nlme::Gasoline)
# 1. Six variables: yield, endpoint, sample, API, vapor, ASTM
summary(yield)
hist(yield, nclass=50)
boxplot(endpoint ~ Sample)
anova(lm(endpoint ~ Sample))
# 4.
plot(x=endpoint, y=yield, xlab="endpoint",ylab = "yield",
      main = "scatter plot between endpoint and yield")
abline(lm(yield~endpoint))
# 5.
par(mfrow=c(2,5))
for (i in 1:10){
  plot(x=endpoint[Sample==i], y=yield[Sample==i], xlab='', ylab='', main=paste('Sample=', i))
  abline(lm(yield[Sample==i]~endpoint[Sample==i]))
# Do not forget to detach the dataset after using it.
detach(nlme::Gasoline)
```

Matrix basics

Matrix decomposition

```
• Eigen-decomposition (for square matrix \mathbf{A}_{n \times n}): \mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^{-1}

-\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_n)

*\lambda_1 \geq \dots \geq \lambda_n are the eigenvalues of \mathbf{A}, i.e., n roots of characteristic equation \det(\lambda \mathbf{I}_n - \mathbf{A}) = 0

-\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_n]_{n \times n}

*\mathbf{v}_1, \dots, \mathbf{v}_n are (right) eigenvectors of \mathbf{A}, i.e., \mathbf{A}\mathbf{v}_i = \lambda_i \mathbf{v}_i

-\operatorname{Implementation} in R: eigen()
```

- Spectral decomposition (for symmetric \mathbf{A}): $\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^{\top}$ - \mathbf{V} is orthogonal, i.e., $\mathbf{V}^{\top} = \mathbf{V}^{-1}$
- Singular value decomposition (SVD) for $n \times p$ matrix $\mathbf{B} : \mathbf{B} = \mathbf{U}\mathbf{S}\mathbf{W}^{\top}$ - $\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_n]_{n \times n}$ with \mathbf{u}_i the *i*th eigenvector of $\mathbf{B}\mathbf{B}^{\top}$

```
* U is orthogonal

- \mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_p]_{p \times p} with \mathbf{w}_i the ith eigenvector of \mathbf{B}^{\top} \mathbf{B}

* \mathbf{W} is orthogonal

- \mathbf{S} = \begin{bmatrix} \mathbf{S}_1 & \mathbf{0}_{n \times (p-n)} \end{bmatrix}_{n \times p} if n \leq p AND \begin{bmatrix} \mathbf{S}_1 & \mathbf{0}_{n-p} & \mathbf{0}_{n-p} \end{bmatrix}_{n \times p} if n > p

* \mathbf{S}_1 = \operatorname{diag}(s_1, \dots, s_n) if n \leq p and \operatorname{diag}(s_1, \dots, s_p) if n > p

* s_1 \geq \dots \geq s_n are squre roots of eigenvalues of \mathbf{B} \mathbf{B}^{\top}

* s_1 \geq \dots \geq s_p are squre roots of eigenvalues of \mathbf{B}^{\top} \mathbf{B}

- Thin/compact SVD for n \times p matrix \mathbf{B}:

\mathbf{B} = [\mathbf{u}_1, \dots, \mathbf{u}_r] \operatorname{diag}(s_1, \dots, s_r) [\mathbf{w}_1, \dots, \mathbf{w}_r]^{\top} = s_1 \mathbf{u}_1 \mathbf{w}_1^{\top} + \dots + s_r \mathbf{u}_r \mathbf{w}_r^{\top}

* r = \operatorname{rank}(\mathbf{B}) \leq \min\{n, p\}

* s_1 \geq \dots \geq s_r > 0 are square roots of non-zero eigenvalues of \mathbf{B}^{\top} \mathbf{B} or \mathbf{B} \mathbf{B}^{\top}

* Implementation via R: svd()
```

• The connection of decompositions

```
Spectral decomposition (for symmetric matrices) Eigen-decomposition (for square matrices)

(Thin) SVD
(for any matrices)
```

```
options(digits = 4) # control the number of significant digits
set.seed(1)
# Generate a symmetric matrix
A = matrix(runif(12), nrow = 2, ncol = 6)
B = t(A) %*% A # guaranteed to be symmetric
isSymmetric(B) # check symmetry
# Eigen-decomposition
(res_eigen = eigen(B))
res_eigen$vectors %*% diag(res_eigen$values) %*% t(res_eigen$vectors) - B # diff between B and decompos
(res svd = svd(B))
res_svd$u %*% diag(res_svd$d) %*% t(res_svd$v) - B # diff between B and decomposed B
# Thin SVD
r = qr(B) $rank # rank
res_svd$u[,1:r] %*% diag(res_svd$d[1:r]) %*% t(res_svd$v[,1:r]) - B # diff between B and decomposed B
# Comparing eigen-decomposition and SVD
res_eigen$values - res_svd$d
res_eigen$vectors - res_svd$u
res_eigen$vectors - res_svd$v
```

Square root of positive (semi-)definite matrix

- **A** is positive semi-definite (say $\mathbf{A} \geq 0$) iff **A** is symmetric and its eigenvalues are all non-negative Equiv., $\mathbf{u}^{\top} \mathbf{A} \mathbf{u} \geq 0$ for any non-zero real *n*-vector \mathbf{u} (i.e., $n \times 1$ real matrix, say $\mathbf{u} \in \mathbb{R}^{n \times 1}$ OR $\mathbf{u} \in \mathbb{R}^n$)
- A is positive definite (say A > 0) iff A is symmetric and its eigenvalues are all positive
 - Equiv., $\mathbf{u}^{\top} \mathbf{A} \mathbf{u} > 0$ for all non-zero $\mathbf{u} \in \mathbb{R}^n$

- If $\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^{\top}$ is the spectral decomposition of positive semi-definite \mathbf{A} , then $\mathbf{A}^{1/2} = \mathbf{V}\Lambda^{1/2}\mathbf{V}^{\top}$ satisfies
 - $\begin{array}{l} -\ \Lambda^{1/2} = \operatorname{diag}(\lambda_1^{1/2}, \dots, \lambda_n^{1/2}) \\ -\ \mathbf{A}^{1/2} \mathbf{A}^{1/2} = \mathbf{A} \end{array}$
- If $\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^{\top}$ is the spectral decomposition of positive definite \mathbf{A} , then $\mathbf{A}^{-1/2} = \mathbf{V}\Lambda^{-1/2}\mathbf{V}^{\top}$ satisfies
 - $\begin{array}{l} -\ \Lambda^{-1/2} = \mathrm{diag}(\lambda_1^{-1/2}, \dots, \lambda_n^{-1/2}) \\ -\ \mathbf{A}^{-1/2} \mathbf{A}^{-1/2} = \mathbf{A}^{-1} \end{array}$

 - $-\mathbf{A}^{1/2}\mathbf{A}^{-1/2}=\mathbf{I}_n$

Determinant and trace

- Applicable only to square matrices
- Properties for determinant

 - $\begin{aligned} & \det(\mathbf{A}) = \prod_i \lambda_i \\ & \det(\mathbf{A}^\top) = \det(\mathbf{A}) \\ & \det(\mathbf{A}^{-1}) = 1/\det(\mathbf{A}) \end{aligned}$
 - $-\det(c \cdot \mathbf{A}) = c^n \det(\mathbf{A})$ for $n \times n$ matrix **A** and scalar c
 - $-\det(\mathbf{AB}) = \det(\mathbf{A})\det(\mathbf{B})$ if **A** and **B** are square matrices of the identical dimension
- Properties for trace

 - $-\operatorname{tr}(\mathbf{A}) = \sum_{i} \lambda_{i}$ $-\operatorname{tr}(c \cdot \mathbf{A}) = c \cdot \operatorname{tr}(\mathbf{A}) \text{ for scalar } c$
 - $-\operatorname{tr}(\mathbf{A} + \mathbf{B}) = \operatorname{tr}(\mathbf{A}) + \operatorname{tr}(\mathbf{B})$ if **A** and **B** are square matrices of the identical dimension
 - $-\operatorname{tr}(\mathbf{AB}) = \operatorname{tr}(\mathbf{BA})$ for $m \times n$ matrix \mathbf{A} and $n \times m$ matrix \mathbf{B}
- Remark:det(A) and tr(A) can be taken as measures of the size of A when A is positive definite (i.e., its eigenvalues are all positive).
- Exercise: Prove that
 - 1. $tr(\mathbf{AB}) = tr(\mathbf{BA})$ for $m \times n \mathbf{A}$ and $n \times m \mathbf{B}$.
 - 2. (The trace trick) $\operatorname{tr}(\mathbf{A}_1 \cdots \mathbf{A}_k) = \operatorname{tr}(\mathbf{A}_{k'+1} \cdots \mathbf{A}_k \mathbf{A}_1 \cdots \mathbf{A}_{k'})$ for 1 < k' < k.
 - 3. $\operatorname{tr}(\mathbf{A}) = \sum_{i} \lambda_{i}$.
 - 4. $\det(\mathbf{A}) = \prod_{i} \lambda_{i}$. Hint: Jordan matrix decomposition, i.e., there exists a Jordan normal (or canonical) form **J** and invertible **U** such that $\mathbf{A} = \mathbf{U}\mathbf{J}\mathbf{U}^{-1}$ for any square **A**.

Block/partitioned matrix

• A partition of matrix: Suppose \mathbf{A}_{11} is of $p \times r$, \mathbf{A}_{12} is of $p \times s$, \mathbf{A}_{21} is of $q \times r$ and \mathbf{A}_{22} is of $q \times s$. Make a new $(p+q)\times(r+s)$ -matrix by organizing \mathbf{A}_{ij} 's in a 2 by 2 way:

$$\mathbf{A} = \left[egin{array}{c|c} \mathbf{A}_{11} & \mathbf{A}_{12} \ \hline \mathbf{A}_{21} & \overline{\mathbf{A}}_{22} \end{array}
ight.$$

e.g.,

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 2 \\ 0 & 1 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

if

$$\mathbf{A}_{11} = \left[\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right], \quad \mathbf{A}_{12} = \left[\begin{array}{c} 2 \\ 3 \end{array} \right], \quad \mathbf{A}_{21} = \left[\begin{array}{cc} 4 & 5 \end{array} \right], \quad \text{and} \quad \mathbf{A}_{22} = \left[\begin{array}{cc} 6 \end{array} \right].$$

- Operations with block matrices
 - Working with partitioned matrices just like ordinary matrices

- Matrix addition: if dimensions of \mathbf{A}_{ij} and \mathbf{B}_{ij} are quite the same, then

$$\mathbf{A} + \mathbf{B} = \left[\begin{array}{cc} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{array} \right] + \left[\begin{array}{cc} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{array} \right] = \left[\begin{array}{cc} \mathbf{A}_{11} + \mathbf{B}_{11} & \mathbf{A}_{12} + \mathbf{B}_{12} \\ \mathbf{A}_{21} + \mathbf{B}_{21} & \mathbf{A}_{22} + \mathbf{B}_{22} \end{array} \right]$$

- Matrix multiplication: if $\mathbf{A}_{ij}\mathbf{B}_{jk}$ makes sense for each i, j, k, then

$$\mathbf{AB} = \left[\begin{array}{ccc} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{array} \right] \left[\begin{array}{ccc} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{array} \right] = \left[\begin{array}{ccc} \mathbf{A}_{11} \mathbf{B}_{11} + \mathbf{A}_{12} \mathbf{B}_{21} & \mathbf{A}_{11} \mathbf{B}_{12} + \mathbf{A}_{12} \mathbf{B}_{22} \\ \mathbf{A}_{21} \mathbf{B}_{11} + \mathbf{A}_{22} \mathbf{B}_{21} & \mathbf{A}_{21} \mathbf{B}_{12} + \mathbf{A}_{22} \mathbf{B}_{22} \end{array} \right]$$

– Inverse: if $\mathbf{A}, \, \mathbf{A}_{11}$ and \mathbf{A}_{22} are all invertible, then

$$\mathbf{A}^{-1} = \left[\begin{array}{cc} \mathbf{A}_{11.2}^{-1} & -\mathbf{A}_{11.2}^{-1} \mathbf{A}_{12} \mathbf{A}_{22}^{-1} \\ -\mathbf{A}_{22}^{-1} \mathbf{A}_{21} \mathbf{A}_{11.2}^{-1} & \mathbf{A}_{22.1}^{-1} \end{array} \right]$$

- $\begin{array}{l} * \;\; \mathbf{A}_{11.2} = \mathbf{A}_{11} \mathbf{A}_{12} \mathbf{A}_{22}^{-1} \mathbf{A}_{21} \\ * \;\; \mathbf{A}_{22.1} = \mathbf{A}_{22} \mathbf{A}_{21} \mathbf{A}_{11}^{-1} \mathbf{A}_{12} \end{array}$