STAT 3690 Lecture Note

Part I: R and matrix basics

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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!**

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Syllabus

Contact

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Timeline

- Lectures
  - Mon/Wed/Fri 9:30–10:20 am
- Office Hour
  - Wed 10:30–11:30 am
- Assessments
  - 4 or 5 Assignments
  - 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 *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:/"
subDir <- "stat3690"
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 forloop or statements such as if or ifelse

---

```r
# 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]
```

```r
# 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))
```

```r
# Create a data frame
e <- c(1,2,3,4)
f <- c("red", "white", "black", NA)
g <- c(TRUE,TRUE,TRUE,FALSE)
mydata <- data.frame(e,f,g)
names(mydata) <- c("ID", "Color", "Passed") # name variable
mydata
```

```r
# Output
write.csv(mydata, file='mydata.csv', row.names=F)
```

```r
# 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]])
```

```r
# EXERCISE
# Create a matrix with 2 rows and 6 columns such that it contains the numbers 1,4,7,...,34.
```

```r
# 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!
```

```r
# 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
  - sum(), mean(), median(), min(), max(), var(), sd(), 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()

```r
# 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)

```r
# 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))
```

```r
# 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.
```

```r
# ANSWER
attach(nlme::Gasoline)
# 1. Six variables: yield, endpoint, sample, API, vapor, ASTM
# 2.
summary(yield)
hist(yield, nclass=50)
# 3.
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 $\mathbf{A}_{n\times n}$): $\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^{-1}$
  - $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$
    - $\lambda_1 \geq \cdots \geq \lambda_n$ are the eigenvalues of $\mathbf{A}$, i.e., n roots of characteristic equation $\det(\lambda\mathbf{I}_n - \mathbf{A}) = 0$
  - $\mathbf{V} = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n]_{n\times n}$
    - $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n$ are (right) eigenvectors of $\mathbf{A}$, i.e., $\mathbf{A}\boldsymbol{v}_i = \lambda_i\boldsymbol{v}_i$
  - 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 $\mathbf{B}$: $\mathbf{B} = \mathbf{U}\mathbf{S}\mathbf{W}^\top$
  - $\mathbf{U} = [\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n]_{n\times n}$ with $\boldsymbol{u}_i$ the ith eigenvector of $\mathbf{B}\mathbf{B}^\top$

    - $\mathbf{U}$ is orthogonal
  - $\mathbf{W} = [\boldsymbol{w}_1, \ldots, \boldsymbol{w}_p]_{p \times p}$ with $\boldsymbol{w}_i$ the ith eigenvector of $\mathbf{B}^\top \mathbf{B}$
    - $\mathbf{W}$ is orthogonal
  -
$$\mathbf{S} = \left[\begin{array}{c:c} \mathbf{S}_1 & \mathbf{0}_{n \times (p-n)} \end{array}\right]_{n \times p} \text{ if } n \leq p \text{ AND } \left[\begin{array}{c} \mathbf{S}_1 \\ \hdashline \mathbf{0}_{(n-p) \times p} \end{array}\right]_{n \times p} \text{ if } n > p$$
    - $\mathbf{S}_1 = \text{diag}(s_1, \ldots, s_n)$ if $n \leq p$ and $\text{diag}(s_1, \ldots, s_p)$ if $n > p$
    - $s_1 \geq \cdots \geq s_n$ are squre roots of eigenvalues of $\mathbf{B}\mathbf{B}^\top$
    - $s_1 \geq \cdots \geq s_p$ are squre roots of eigenvalues of $\mathbf{B}^\top \mathbf{B}$
  - Thin/compact SVD for $n \times p$ matrix $\mathbf{B}$:
$$\mathbf{B} = [\boldsymbol{u}_1, \ldots, \boldsymbol{u}_r] \text{diag}(s_1, \ldots, s_r) [\boldsymbol{w}_1, \ldots, \boldsymbol{w}_r]^\top = s_1 \boldsymbol{u}_1 \boldsymbol{w}_1^\top + \cdots + s_r \boldsymbol{u}_r \boldsymbol{w}_r^\top$$
    - $r = \text{rank}(\mathbf{B}) \leq \min\{n, p\}$
    - $s_1 \geq \cdots \geq s_r > 0$ 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

$$\begin{array}{ccc} \text{Spectral decomposition} & \Leftarrow & \text{Eigen-decomposition} \\ \text{(for symmetric matrices)} & & \text{(for square matrices)} \\ \Uparrow & & \\ \text{(Thin) SVD} & & \\ \text{(for any matrices)} & & \end{array}$$

```r
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$vectors) - B # diff between B and decompos
# SVD
(res_svd = svd(B))
res_svd$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 and inverse of positive (semi-)definite matrix

- $\mathbf{A}$ is positive semi-definite (say $\mathbf{A} \geq 0$) iff $\mathbf{A}$ is symmetric and its eigenvalues are all non-negative
  - Equiv., $\boldsymbol{u}^\top \mathbf{A} \boldsymbol{u} \geq 0$ for any non-zero real n-vector $\boldsymbol{u}$ (i.e., $n \times 1$ real matrix, say $\boldsymbol{u} \in \mathbb{R}^{n \times 1}$ OR $\boldsymbol{u} \in \mathbb{R}^n$)
- If $\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^\top$ is the spectral decomposition of positive semi-definite $\mathbf{A}$, then $\mathbf{A}^{1/2} = \mathbf{V}\Lambda^{1/2}\mathbf{V}^\top$, where

- $\Lambda^{1/2} = \text{diag}(\lambda_1^{1/2}, \dots, \lambda_n^{1/2})$
  - $\mathbf{A}^{1/2}\mathbf{A}^{1/2} = \mathbf{A}$
- $\mathbf{A}$ is positive definite (say $\mathbf{A} > 0$) iff $\mathbf{A}$ is symmetric and its eigenvalues are all positive
  - Equiv., $\boldsymbol{u}^\top \mathbf{A}\boldsymbol{u} > 0$ for all non-zero $\boldsymbol{u} \in \mathbb{R}^n$
- If $\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^\top$ is the spectral decomposition of positive definite $\mathbf{A}$, then
  - $\mathbf{A}^{-1} = \mathbf{V}\Lambda^{-1}\mathbf{V}^\top$, where $\Lambda^{-1} = \text{diag}(\lambda_1^{-1}, \dots, \lambda_n^{-1})$
  - $\mathbf{A}^{-1/2} = \mathbf{V}\Lambda^{-1/2}\mathbf{V}^\top$ is the inverse of $\mathbf{A}^{1/2}$ and also the root of $\mathbf{A}^{-1}$, where $\Lambda^{-1/2} = \text{diag}(\lambda_1^{-1/2}, \dots, \lambda_n^{-1/2})$

```r
options(digits = 4) # control the number of significant digits
set.seed(1)
## Generate a demo of positive semi-definite matrices
A = matrix(runif(12), nrow = 2, ncol = 6)
B = t(A) %*% A # guaranteed to be positive semi-definite
# Get the root of B via the eigen-decomposition of B
res_eigen_B = eigen(B)
B_root1 = res_eigen_B$vectors %*%
  diag((res_eigen_B$values*(res_eigen_B$values>1e-6))^.5) %*%
  t(res_eigen_B$vectors)
# Get the root of B via an existing function
B_root2 = expm::sqrtm(B)
# Comparing
B_root1 - B_root2

## Generate a demo of positive definite matrices
C = A %*% t(A) # (almost surely) guaranteed to be positive definite
# Get the inverse of C via the eigen-decomposition of B
res_eigen_C = eigen(C)
C_inv1 = res_eigen_C$vectors %*%
  diag(res_eigen_C$values^-1) %*%
  t(res_eigen_C$vectors)
# Get the inverse of C via an existing function
C_inv2 = solve(C)
# Comparing
C_inv1 - C_inv2
```

Determinant and trace

- Merely applicable to square matrices
- Properties for determinant
  - $\det(\mathbf{A}) = \prod_i \lambda_i$
  - $\det(\mathbf{A}^\top) = \det(\mathbf{A})$
  - $\det(\mathbf{A}^{-1}) = 1/\det(\mathbf{A})$
  - $\det(c \cdot \mathbf{A}) = c^n \det(\mathbf{A})$ for $n \times n$ matrix $\mathbf{A}$ and scalar c
  - $\det(\mathbf{AB}) = \det(\mathbf{A})\det(\mathbf{B})$ if $\mathbf{A}$ and $\mathbf{B}$ are square matrices of the identical dimension
- Properties for trace
  - $\text{tr}(\mathbf{A}) = \sum_i \lambda_i$
  - $\text{tr}(c \cdot \mathbf{A}) = c \cdot \text{tr}(\mathbf{A})$ for scalar c
  - $\text{tr}(\mathbf{A} + \mathbf{B}) = \text{tr}(\mathbf{A}) + \text{tr}(\mathbf{B})$ if $\mathbf{A}$ and $\mathbf{B}$ are square matrices of the identical dimension

- (Trace trick) $\mathrm{tr}(\mathbf{A}_1 \cdots \mathbf{A}_k) = \mathrm{tr}(\mathbf{A}_{k'+1} \cdots \mathbf{A}_k \mathbf{A}_1 \cdots \mathbf{A}_{k'})$ for $1 < k' < k$.
    - Specifically, $\mathrm{tr}(\mathbf{AB}) = \mathrm{tr}(\mathbf{BA})$

- Remark: $\det(\mathbf{A})$ and $\mathrm{tr}(\mathbf{A})$ can be taken as measures of the size of $\mathbf{A}$ when $\mathbf{A} > 0$

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:

$$\mathbf{A} = \left[\begin{array}{c|c} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \hline \mathbf{A}_{21} & \mathbf{A}_{22} \end{array}\right]$$

  e.g.,

$$\mathbf{A} = \left[\begin{array}{cc|c} 1 & 0 & 2 \\ 0 & 1 & 3 \\ \hline 4 & 5 & 6 \end{array}\right]$$

  if

$$\mathbf{A}_{11} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{A}_{12} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}, \quad \mathbf{A}_{21} = \begin{bmatrix} 4 & 5 \end{bmatrix}, \quad \text{and} \quad \mathbf{A}_{22} = \begin{bmatrix} 6 \end{bmatrix}.$$

- 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

$$\mathbf{A} + \mathbf{B} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} + \begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{11} + \mathbf{B}_{11} & \mathbf{A}_{12} + \mathbf{B}_{12} \\ \mathbf{A}_{21} + \mathbf{B}_{21} & \mathbf{A}_{22} + \mathbf{B}_{22} \end{bmatrix}$$

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

$$\mathbf{AB} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{11}\mathbf{B}_{11} + \mathbf{A}_{12}\mathbf{B}_{21} & \mathbf{A}_{11}\mathbf{B}_{12} + \mathbf{A}_{12}\mathbf{B}_{22} \\ \mathbf{A}_{21}\mathbf{B}_{11} + \mathbf{A}_{22}\mathbf{B}_{21} & \mathbf{A}_{21}\mathbf{B}_{12} + \mathbf{A}_{22}\mathbf{B}_{22} \end{bmatrix}$$

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

$$\mathbf{A}^{-1} = \begin{bmatrix} \mathbf{A}_{11.2}^{-1} & -\mathbf{A}_{11.2}^{-1}\mathbf{A}_{12}\mathbf{A}_{22}^{-1} \\ -\mathbf{A}_{22}^{-1}\mathbf{A}_{21}\mathbf{A}_{11.2}^{-1} & \mathbf{A}_{22.1}^{-1} \end{bmatrix}$$

    - $\mathbf{A}_{11.2} = \mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21}$
    - $\mathbf{A}_{22.1} = \mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12}$

```r
options(digits = 4)
set.seed(1)
## Generate an (almost surely) invertible matrix
(A = matrix(runif(9), nrow = 3, ncol = 3)) #

# Verify the inverse of partition matrix
## Method 1: following the above formula
(A11 = A[1:2, 1:2])
(A12 = matrix(A[1:2, 3], nrow = 2, ncol = 1))
(A21 = matrix(A[3, 1:2], nrow = 1, ncol = 2))
(A22 = matrix(A[3, 3], nrow = 1, ncol = 1))
(A11.2 = A11 - A12 %*% solve(A22) %*% A21)
(A22.1 = A22 - A21 %*% solve(A11) %*% A12)
```

```
(Ainv1 = rbind(
  cbind(solve(A11.2), -solve(A11.2) %*% A12 %*% solve(A22)),
  cbind(-solve(A22) %*% A21 %*% solve(A11.2), solve(A22.1))
))

## Method 2: solve()
Ainv2 = solve(A)

## Comparison
Ainv2 - Ainv1
```

An example utilizing matrix basics: rephrasing the ridge estimator