#### Introduction to R

None

#### Matrix algebra

Matrix multiplication:

$$\mathbf{AB} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} & a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32} \\ a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} & a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} \end{bmatrix}$$

- Inverse: For  $\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$ ,  $\mathbf{A}^{-1} = \frac{1}{a_{11}a_{22} a_{12}a_{21}} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$
- Trace:  $tr(\mathbf{A}) = \sum_{i=1}^{p} a_{ii} = a_{11} + a_{22} + ... + a_{pp}$
- Determinant of  $2 \times 2$ :  $\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = a_{11}a_{22} a_{12}a_{21}$
- Eigenvalues: Roots of the polynomial equation  $|\mathbf{A} \lambda \mathbf{I}| = 0$  where **I** is an identity matrix
- Eigenvectors: Each eigenvalue of **A** has a corresponding nonzero vector **b** that satisfies  $\mathbf{Ab} = \lambda \mathbf{b}$
- For eigenvalues  $\lambda_i$  of **A**:  $tr(\mathbf{A}) = \sum_{i=1}^p \lambda_i$  and  $\left| \mathbf{A} \right| = \prod_{i=1}^p \lambda_i = \lambda_1 \lambda_2 \cdots \lambda_p$
- Quadratic formula: The roots of the equation  $ax^2 + bx + c = 0$  are  $\frac{-b \pm \sqrt{b^2 4ac}}{2a}$
- Vector length:  $\sqrt{\sum_{i=1}^{p} a_i^2}$
- Positive definite matrices have all eigenvalues greater than 0 and positive semidefinite matrices are the same but with at least one eigenvalue equal to 0

# Data, distributions, and correlation

• 
$$\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}} = \frac{\text{Cov}(x_i, x_j)}{\sqrt{\text{Var}(x_i)\text{Var}(x_j)}}$$

• 
$$\mu = E(\mathbf{x}) = \begin{bmatrix} E(x_1) \\ \vdots \\ E(x_p) \end{bmatrix} = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_p \end{bmatrix}$$

$$\bullet \quad \Sigma = \text{Cov}(\mathbf{x}) = \text{E}[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})'] = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{p1} & \sigma_{p2} & \cdots & \sigma_{pp} \end{bmatrix}$$

• 
$$\mathbf{P} = \text{Corr}(\mathbf{x}) = \begin{bmatrix} 1 & \rho_{12} & \cdots & \rho_{1p} \\ \rho_{21} & 1 & \cdots & \rho_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{p1} & \rho_{p2} & \cdots & 1 \end{bmatrix}$$

• Multivariate normal distribution, 
$$\mathbf{x} \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$
:  $f(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{p/2} |\boldsymbol{\Sigma}|^{1/2}} e^{-\frac{1}{2} \left[ (\mathbf{x} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right]}$  for  $-\infty < x_i < \infty$ ,

i=1,...,p, and  $|\Sigma|>0$ 

$$\bullet \quad \hat{\boldsymbol{\mu}} = \frac{1}{N} \sum_{r=1}^N \boldsymbol{x}_r = \frac{1}{N} \big( \boldsymbol{x}_1 + \boldsymbol{x}_2 + ... + \boldsymbol{x}_N \big)$$

$$\bullet \quad \hat{\Sigma} = \frac{1}{N-1} \sum_{r=1}^{N} (\mathbf{x}_r - \hat{\mu})(\mathbf{x}_r - \hat{\mu})'$$

• 
$$\hat{\sigma}_{ij} = Cov(x_i, x_j) = \frac{1}{N-1} \sum_{r=1}^{N} (x_{ri} - \overline{x}_i)(x_{rj} - \overline{x}_j)$$

$$\bullet \quad r_{ij} = Corr(x_i, x_j) = \frac{\hat{\sigma}_{ij}}{\sqrt{\hat{\sigma}_{ii}\hat{\sigma}_{jj}}} = \frac{\frac{1}{N-1}\sum\limits_{r=1}^{N}(x_{ri} - \overline{x}_i)(x_{rj} - \overline{x}_j)}{\sqrt{\left[\frac{1}{N-1}\sum\limits_{r=1}^{N}(x_{ri} - \overline{x}_i)^2\right]\left[\frac{1}{N-1}\sum\limits_{r=1}^{N}(x_{rj} - \overline{x}_j)^2\right]}} = \frac{\sum\limits_{r=1}^{N}(x_{ri} - \overline{x}_i)(x_{rj} - \overline{x}_j)}{\sqrt{\left[\sum\limits_{r=1}^{N}(x_{ri} - \overline{x}_i)^2\right]\left[\sum\limits_{r=1}^{N}(x_{rj} - \overline{x}_j)^2\right]}}$$

$$\bullet \quad R = \begin{bmatrix} 1 & r_{12} & \cdots & r_{1p} \\ r_{21} & 1 & \cdots & r_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ r_{p1} & r_{p2} & \cdots & 1 \end{bmatrix}$$

## **Graphics**

None

**PCA**  
• 
$$y_j = a'_i(x - \mu)$$
 for  $j = 1, ..., p$ 

• Total variance: 
$$tr(\Sigma) = \sum_{i=1}^{p} \sigma_{ii} = \sigma_{11} + \sigma_{22} + ... + \sigma_{pp}$$

• 
$$\hat{y}_j = \hat{a}'_j(\mathbf{x} - \hat{\mu})$$
 for  $j = 1, ..., p$ 

• 
$$\hat{y}_{rj}^* = \hat{a}_j^* \mathbf{z}_r$$
 and  $\hat{y}_{rj} = \hat{a}_j' (\mathbf{x}_r - \hat{\mu})$  for  $j = 1, ..., p$  and  $r = 1, ..., N$ 

• 
$$x_j = \mu_j + \lambda_{j1}f_1 + \lambda_{j2}f_2 + ... + \lambda_{jm}f_m + \eta_j$$
 for  $j = 1, ..., p$ 

$$\begin{array}{l} \underline{\textbf{FA}} \\ \bullet \quad x_j = \mu_j + \lambda_{j1}f_1 + \lambda_{j2}f_2 + \ldots + \lambda_{jm}f_m + \eta_j \text{ for } j = 1, \ldots, p \\ \bullet \quad \tilde{X}_j = \lambda_{j1}f_1 + \lambda_{j2}f_2 + \ldots + \lambda_{jm}f_m + \eta_j \text{ for } j = 1, \ldots, p; \quad \tilde{\textbf{x}} = \underset{p \times m}{\boldsymbol{\Lambda}} \underbrace{\textbf{f}}_{p \times m} + \underset{p \times 1}{\boldsymbol{\eta}} + \underset{p \times m}{\boldsymbol{\eta}} \\ \end{array}$$

• 
$$Var(ay_1+by_2) = a^2Var(y_1) + b^2Var(y_2) + 2abCov(y_1,y_2)$$

- $\Sigma = \Lambda \Lambda' + \psi$ ;  $Var(x_j) = \sum_{k=1}^{m} \lambda_{jk}^2 + \psi_j$  and  $Cov(x_j, x_{j'}) = \sum_{k=1}^{m} \lambda_{jk} \lambda_{j'k}$
- With standardized variables,  $\mathbf{P} = \Lambda \Lambda' + \psi$ ,  $\sum_{k=1}^{m} \lambda_{jk}^2 + \psi_j = 1$ , and  $Corr(z_j, f_k) = \lambda_{jk}$
- $LRT: \ A = (N-1-(2p+4m+5)/6)log\left(\frac{\mid \hat{\Lambda}\hat{\Lambda}'+\hat{\Psi}\mid}{\mid \lceil (N-1)/N \rceil \hat{\Sigma}\mid}\right) \ can \ be \ approximated \ by \ \chi^2_{\lceil (p-m)^2-p-m\rceil/2}$
- AIC:  $-2\log(L(\tilde{\mathbf{x}} \mid \hat{\Lambda}, \hat{\Psi})) + 2(\text{degrees of freedom for model})$
- Orthogonal matrix: Individual columns within a matrix are orthogonal to each other
- $\mathbf{B}_{\mathsf{p}\times\mathsf{m}} = \mathbf{\Lambda}_{\mathsf{p}\times\mathsf{m}} \mathbf{T}_{\mathsf{m}\times\mathsf{m}}$
- $V = \frac{1}{p^2} \sum_{q=1}^{m} \left( p \sum_{j=1}^{p} \frac{b_{jq}^4}{h_i^4} \left( \sum_{j=1}^{p} \frac{b_{jq}^2}{h_i^2} \right)^2 \right) \text{ where } h_j^2 = \sum_{k=1}^{m} \lambda_{jk}^2$
- Bartlett's method (a.k.a., weighted least-squares method):  $\hat{\mathbf{f}}_r = (\hat{\boldsymbol{\Lambda}}'\hat{\boldsymbol{\Psi}}^{-1}\hat{\boldsymbol{\Lambda}})^{-1}\hat{\boldsymbol{\Lambda}}'\hat{\boldsymbol{\Psi}}^{-1}\mathbf{z}_r$
- Thompson's method (a.k.a., regression method):  $\hat{\mathbf{f}}_r = \hat{\Lambda}'(\hat{\Lambda}\hat{\Lambda}' + \hat{\Psi})^{-1}\mathbf{z}_r$

### CA

- $\bullet \quad d_{rs} = \left[ \left( \boldsymbol{x}_r \boldsymbol{x}_s \right)' \left( \boldsymbol{x}_r \boldsymbol{x}_s \right) \right]^{r/2}$
- $d_{rs} = \left[ \left( \mathbf{z}_r \mathbf{z}_s \right)' \left( \mathbf{z}_r \mathbf{z}_s \right) \right]^{1/2}$
- $\bullet \quad d_{ab} = \frac{1}{\frac{1}{n_a} + \frac{1}{n_b}} \big(\overline{\boldsymbol{x}}_a \overline{\boldsymbol{x}}_b\big)' \big(\overline{\boldsymbol{x}}_a \overline{\boldsymbol{x}}_b\big)$
- $\bullet \qquad \sum_{k=1}^{K} \sum_{r=1}^{N} \sum_{i=1}^{p} (X_{rik} \overline{X}_{ik})^2$
- $W = \frac{\text{Within sum of squares}}{\text{Total sum of squares}}$

#### DA

- Choose  $\Pi_1$  if  $L(\mu_1, \Sigma_1 | \mathbf{x}) > L(\mu_2, \Sigma_2 | \mathbf{x})$  and choose  $\Pi_2$  otherwise
- Suppose  $\Sigma_1 = \Sigma_2$ . Choose  $\Pi_1$  if  $\mathbf{b}'\mathbf{x} \mathbf{k} > 0$  and choose  $\Pi_2$  otherwise, where  $\mathbf{b} = \Sigma^{-1}(\mu_1 \mu_2)$  and  $\mathbf{k} = \Sigma^{-1}(\mu_1 \mu_2)$  $(1/2)(\mu_1-\mu_2)'\Sigma^{-1}(\mu_1+\mu_2)$
- $d_i = (\mathbf{x} \mu_i)' \Sigma^{-1} (\mathbf{x} \mu_i)$
- $P(\Pi_i \mid \mathbf{x}) = \frac{e^{-\frac{1}{2}d_i}}{e^{-\frac{1}{2}d_i} + e^{-\frac{1}{2}d_2}}$
- $\hat{\Sigma} = \frac{(N_1 1)\hat{\Sigma}_1 + (N_2 1)\hat{\Sigma}_2}{N_1 + N_2 2}$
- $$\begin{split} p_1 * C(2|1) * P(2|1) + p_2 * C(1|2) * P(1|2) \\ p_1^* &= \frac{p_1 C(2|1)}{p_1 C(2|1) + p_2 C(1|2)}, \, p_2^* = \frac{p_2 C(1|2)}{p_1 C(2|1) + p_2 C(1|2)} \end{split}$$
- $d_i^{**} = \frac{1}{2}(\mathbf{x} \mathbf{\mu}_i)^2 \sum_{i=1}^{-1} (\mathbf{x} \mathbf{\mu}_i) + \frac{1}{2} \log(|\Sigma_i|) \log[p_i * C(i|i)]$

### **NNC**

None

• 
$$logit(\pi) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

### **Multinomial regression**

$$\bullet \quad \frac{n!}{\prod\limits_{j=1}^J n_j!} \prod\limits_{j=1}^J \pi_j^{n_j}$$

$$\bullet \quad \prod_{r=1}^{N} \frac{n_r \,!}{\prod\limits_{i=1}^{J} n_{rj} \,!} \prod\limits_{j=1}^{J} \pi_j^{n_{rj}}$$

• 
$$log(\pi_i/\pi_1) = \beta_{j0} + \beta_{j1}x_1 + ... + \beta_{jp}x_p$$
 for  $j = 2, ..., J$ 

$$\bullet \quad \pi_1 = \frac{1}{1 + \sum\limits_{j=2}^{J} e^{\beta_{j0} + \beta_{j1}x_1 + \cdots + \beta_{jp}x_p}}, \ \pi_j = \frac{e^{\beta_{j0} + \beta_{j1}x_1 + \cdots + \beta_{jp}x_p}}{1 + \sum\limits_{j=2}^{J} e^{\beta_{j0} + \beta_{j1}x_1 + \cdots + \beta_{jp}x_p}} \ \text{for } j = 2, \ \ldots, \ J$$

• 
$$logit[P(Y \le j)] = log \left\lceil \frac{P(Y \le j)}{1 - P(Y \le j)} \right\rceil = \beta_{j0} + \beta_1 x_1 + \dots + \beta_p x_p$$

$$\begin{split} \bullet \quad & \pi_1 = \ e^{\beta_{10} + \beta_1 x_1 + \dots + \beta_p x_p} \big/ \big( 1 + e^{\beta_{10} + \beta_1 x_1 + \dots + \beta_p x_p} \big) \,, \ \pi_J = 1 - e^{\beta_{J-1,0} + \beta_1 x_1 + \dots + \beta_p x_p} \big/ \big( 1 + e^{\beta_{J-1,0} + \beta_1 x_1 + \dots + \beta_p x_p} \big) \,, \ \text{and} \\ & \pi_j = \frac{e^{\beta_{j0} + \beta_1 x_1 + \dots + \beta_p x_p}}{1 + e^{\beta_{j0} + \beta_1 x_1 + \dots + \beta_p x_p}} - \frac{e^{\beta_{j-1,0} + \beta_1 x_1 + \dots + \beta_p x_p}}{1 + e^{\beta_{j-1,0} + \beta_1 x_1 + \dots + \beta_p x_p}} \ \ \text{for} \ j = 2, \ \dots, \ J-1 \end{split}$$

# <u>R functions</u> – These functions are listed mostly in the order they were introduced in the notes

## Introduction to R

Function	Description
pnorm()	Finds a cumulative probability from a univariate normal distribution
qnorm()	Finds a quantile from a univariate normal
	distribution
ls() and objects()	List items in R's database
c()	Combine items into a vector
sd()	Calculate a standard deviation
var()	Calculate a variance
sqrt()	Calculate a square root
read.table(file =	Read in a text data file with variable names in the
"c:\\chris\\datafile.txt",	first row and spaces separating the variable names
header = TRUE, sep = "")	and their values.
read.csv(file =	Read in a comma delimited data file.
"c:\\chris\\datafile.csv")	
summary()	Summarize information in a data frame or list
head()	Print the first few rows of a data frame
<pre>write.table(x = set1, file =</pre>	Save data in a data frame to a file. The data was in
"C:\\out_file.csv", quote =	the data frame set1 and it will be written as a
FALSE, row.names =	comma delimited file named out file.csv.
FALSE, sep=",")	_
plot(x = x, y = y)	Plots $y$ on the y-axis and $x$ on the x-axis
$lm(formula = y \sim x, data = set1)$	Find the sample regression model with the
	response (dependent) variable y and explanatory
	(independent) variable x within set1
names()	Provide the names of items in a list
class()	State the class of an object
dev.new(width = 6, height = 6,	Opens a new graphics window that is 6"x6" with
pointsize = 10)	font size of 10
segments()	Draw a line segment on a plot
curve()	Plot a function of x, like $f(x) = x^2$
expression()	Can be used to put Greek letters and mathematical
	symbols on a plot
axis()	Allows for finer control of an x or y-axis on a plot
methods()	List the method or generic functions

# Matrix algebra

Function	Description
matrix(data = c(1, 2, 3, 4, 5, 6),	Create a matrix of size 2×3 by row
nrow = 2, $ncol = 3$ , $byrow =$	·
TRUE)	
t()	Transpose a matrix
A+B	Matrix addition for matrices A and B
A%*%B	Matrix multiplication for <b>A</b> and <b>B</b>
A*B	Elementwise multiplication for A and B

cbind()	Combine elements by column
solve(A)	Find the inverse of <b>A</b>
diag(A)	Extract the diagonal elements of A
sum(A)	Sum the elements of A
det(A)	Determinant of <b>A</b>
eigen(A)	Find the eigenvalues and eigenvectors of A
abline(h = y)	Plots a horizontal line at y. A vertical line is plotted
	with the argument v.
arrows()	Draw an arrow on a plot

Data, distributions, and correlation

Function	Description
cov2cor()	Calculate a correlation matrix from a covariance matrix
dmvnorm()	f(x) for a multivariate normal distribution; this is in the mvtnorm package
seq()	Create a sequence of numbers
persp3d()	3D surface plot; this function is in the rgl package
contour()	Contour plot
cov()	Calculate estimated covariance matrix
cor()	Calculate estimated correlation matrix
colMeans()	Find the means of each column in a matrix
apply()	Apply a function to every row or column of a matrix
set.seed()	Set a seed number
rmvnorm()	Simulate random vectors from a multivariate normal distribution; this function is in the mytnorm package
points()	Add points to a plot
scale()	Standardize columns of data
expand.grid()	Create all possible combinations of items within separate vectors
par()	Graphics parameters; pty = "s" creates a
	square plot, $mfrow = c(2,2)$ creates a $2\times2$
	matrix of plots

**Graphics** 

Function	Description
pairs()	Side-by-side scatter plots
scatterplotMatrix()	Side-by-side scatter plots
symbols()	Bubble plot; circles argument specifies the third
	variable; inches argument controls the maximum
	size of the bubble
identify()	Interactively identifies points on a plot
text()	Puts text on a plot
plot3d()	3D scatter plot; this function is within the rgl
	package

grid3d()	Put gridlines on a plot created in the rgl package
stars()	Star plot
parcoord()	Parallel coordinate plot; this function is within the MASS package
reshape()	Changes a data frame from a wide to long format and vice versa
histogram()	Trellis histogram; this function is within the lattice package
xyplot()	Trellis scatter plot; this function is within the lattice package
cloud()	Trellis 3D scatter plot; this function is within the lattice package
equal.count()	Creates shingles for a trellis plot; this function is within the lattice package

# PCA

Function	Description
princomp()	Performs PCA; cor argument specifies whether to
	use the covariance (FALSE) or correlation (TRUE)
	matrix
summary()	This function can be used to summarize the
	information with an object created by
	princomp(); the argument values of loadings
	= TRUE and cutoff = 0.0 will lead to the
	printing of all the values within the eigenvectors
screeplot()	Creates a scree plot; this can also be done with the
	plot() function
predict()	Computes PC scores when using an object
	created by princomp(); see my programs for
	how to calculate the scores correctly

# FA

Function	Description
factanal()	<pre>Performs FA; the rotation = "varimax"</pre>
	argument specifies the varimax rotation method;
	the scores argument can be used to specify the
	type of scores ("regression" or "Bartlett")
	to be calculated
print()	This function can be used to summarize the
	information with an object created by
	<pre>factanal(); the argument value of cutoff =</pre>
	0.0 will lead to the printing of all common factor
	loadings

# CA

Function	Description
dist()	Calculates distances between observation pairs
hclust()	Performs agglomerative clustering
plot()	This function can be used with an object created
	by hclust() to create a hierarchical tree diagram
palette()	Provides a listing of eight colors corresponding to
	the numbers 1, 2,, 8
cutree()	Gives the cluster memberships when used with an
	object created by hclust(); the k argument
	specifies the number of clusters
rect.hclust()	Puts rectangles on a hierarchical tree diagram
	corresponding to clusters when used with an object
	<pre>created by hclust()</pre>
agnes()	Performs agglomerative clustering
kmeans()	Performs K-means clustering
aggregate()	Applies a desired function to groups of
	observations within a data frame

# DA

Function	Description
lda()	Linear discriminant analysis; use the cv = TRUE
	argument for cross-validation; this function is in the
	MASS package
<pre>predict()</pre>	The corresponding method function calculates
	posterior probabilities for resubstitution
<pre>summarize.class()</pre>	Calculates the accuracy of the classification
	methods; this function is written by your instructor,
	and it is available in PlacekickDA.R
qda()	Quadratic discriminant analysis; use the cv =
	TRUE argument for cross-validation; this function is
	in the MASS package
rbind()	Combine two or more data frames or matrices by
	rows
<pre>sample.int()</pre>	Randomly samples integers

# NNC

Function	Description
knn()	Nearest neighbor classification using
	resubstitution; this function is in the class
	package
knn.cv()	Nearest neighbor classification using cross-
	validation; this function is in the class package

Logistic regression

Logistic regression	
Function	Description
glm()	Estimate a logistic regression model when family
	= binomial(link = logit) is given as an
	argument
Anova()	Perform LRTs; this function is in the car package
predict()	The corresponding method function estimates $\pi$
	<pre>when type = "response" is given as an</pre>
	argument
CV()	Calculates the cross-validation estimates of $\pi$ ; this
	function is written by your instructor, and it is
	available in PlacekickLogisticReg.R
prediction()	Calculates the sensitivity and specificity for a
	number of cut-off probabilities; this function is in
	the ROCR package
performance()	Calculates the x and y-axis items for an ROC curve
	when the optional "sens" and "fpr" argument
	values are given; this function can also be used to
	calculate the area under the ROC curve by giving
	an optional "auc" argument value; this function is
	in the ROCR package
plot()	The corresponding method function plots the ROC
	curve; the print.cutoffs.at argument
	specifies the specific cut-off probabilities to include
	on a plot; this function is in the ROCR package
slotNames()	View components of an S4 object

**Multinomial regression** 

Function	Description
<pre>multinom()</pre>	Estimates a multinomial regression model; this function is in the nnet package
<pre>predict()</pre>	The corresponding method function estimates $\pi_j$ when type = "probs" is given as an argument, and it gives the classifications when type = "class" is given as an argument
cv2()	Calculates the cross-validation estimates of $\pi_j$ and the corresponding classifications; this function is written by your instructor, and it is available in WheatMultRegNoPlots.R