Multivariate Analysis Lecture 7: Hotelling's T2

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2023-04-25

Outline of Lecture 07

- Review of Wishart and the Hotelling's \mathcal{T}^2 distribution for one-sample problems
- \bullet Examples of one-sample Hotelling's T^2
- Two-sample Hotelling's T^2
- Examples of two-sample Hotelling's T^2
- The multivariate normality (MVN) assumption



Section 1

Review

Wishart Distribution

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Subsection 1

Wishart Distribution

Wishart Distribution

Definition of Wishart Distribution

- A Wishart distribution can be defined in the following way
- Let **W** be a $p \times p$ random matrix. We say **W** follows $Wishart_p(k, \Sigma)$ if **W** can be written as $\mathbf{W} = \mathbf{X}^T \mathbf{X}$ where **X** denotes the random matrix formed by a random sample of size k from MVN $N(\mathbf{0}, \Sigma)$.
- The definition indicates that if we have a random sample $\mathbf{X}_1, \cdots \mathbf{X}_k$ from $N(\mathbf{0}, \mathbf{\Sigma})$, then $\mathbf{X}^T \mathbf{X} = \sum_{i=1}^k \mathbf{X}_i \mathbf{X}_i^T \sim Wishart_p(k, \mathbf{\Sigma})$.
- Remark: $E[\mathbf{W}] = k\Sigma$.

Review

Wishart Distribution

Wishart vs Chi-squared

• Wishart: If $X_1, \dots X_k \stackrel{iid}{\sim} N(0, \Sigma)$, then

$$\mathbf{X}^T\mathbf{X} = \sum_{i=1}^k \mathbf{X}_i \mathbf{X}_i^T \sim Wishart_p(k, \mathbf{\Sigma}), \text{ where } \mathbf{X}_{k \times p} = \begin{pmatrix} X_1' \\ \vdots \\ X_k^T \end{pmatrix}$$

• Chi-squared: If $X_1, \dots, X_k \stackrel{iid}{\sim} N(0,1)$, then

$$\mathbf{X}^T\mathbf{X} = \sum_{i=1}^k X_i^2 \sim \chi_k^2$$
, where $\mathbf{X}_{k \times 1} = \begin{pmatrix} X_1 \\ \vdots \\ X_k \end{pmatrix}$

Wishart Distribution

Wishart vs Chi-squared (continued)

• When p = 1,

$$W = \sum_{i=1}^{k} X_i^2 = \sigma^2 \sum_{i=1}^{k} \left(\frac{X_i}{\sigma}\right)^2 \sim \sigma^2 \chi_k^2$$

Review

The Sample Covariance Matrix

• Let X_1, \dots, X_n be a random sample from $N(\mu, \Sigma)$. The $X_{n \times p}$ follows a matrix normal distribution:

$$X \sim N(\mathbf{1}_n \otimes \boldsymbol{\mu}^T, \boldsymbol{\Sigma}, \mathbf{I}_n)$$

We have shown that

$$(n-1)$$
S $\sim Wishart_p(n-1, \Sigma)$

Hotelling's T^2

Review

Subsection 2

Hotelling's T^2

Review

Definition of Hotelling's T^2

- Hotelling generalized the student's t, which is for univarite, to Hotelling's T2, which is the multivariate version
- Definition. We say a random variable follows Hotelling's $T_{\rho,\nu}^2$ if the random variable can be written as $\mathbf{Z}^T \left(\frac{W}{\nu} \right)^{-1} \mathbf{Z}$ where

 - $\mathbf{O} \mathbf{W} \sim W_p(\nu, \mathbf{\Sigma})$
 - \bigcirc Z \perp W

Section 2

One-Sample Hotelling T^2

One-Sample Hotelling T^2

- Let $X_1, X_2, ..., X_n$ be a random sample from a multivariate normal distribution with mean vector μ and covariance matrix Σ .
- The sample mean vector and sample covariance matrix are denoted by X and S, respectively.
- ullet The null hypothesis of interest $H_0: \mu = \mu_0$
- The one-sample Hotelling T^2 is defined as

$$T^2 = (\hat{\mu} - \mu_0)^T (Cov(\hat{\mu}))^{-1} (\hat{\mu} - \mu_0)$$

• We have shown that $T^2 \sim T_{p,n-1}^2$ when $H_0: \mu = \mu_0$.

Hotelling's T^2 Distribution vs F Distribution

Hotelling's T^2

Claim: $T_{p,\nu}^2 \sim \frac{\nu p}{\nu+1-p} F_{p,\nu+1-p}.$

For the T^2 statistic, we have $T^2 \stackrel{H_0}{\sim} \frac{(n-1)p}{n-p} F_{p,n-p}$. We reject H_0 at significance level α when $T^2 > \frac{(n-1)p}{n-p} F_{p,n-p,1-\alpha}$.

Corollary.

$$\frac{n-p}{p}(\bar{X}-\mu_0)^T(\hat{\Sigma})^{-1}(\bar{X}-\mu_0) \stackrel{H_0}{\sim} F_{p,n-p}$$

where $\hat{\Sigma} = \frac{1}{n} X^T H X = \frac{1}{n} \sum_{i=1}^n (X_i - \bar{X}) (X_i - \bar{X})^T = \frac{(n-1)S}{n}$.

Subsection 1

A Simulation Study

Understand the Wishart Distribution

• Recall that if $W \sim Wishart_p(k, \Sigma)$, then $E[\mathbf{W}] = k\Sigma$.

```
library(MASS)
p=2; n=5; B=1000; rho=0.7
Sigma=diag(1+rho, p, p) - matrix(rho, p, p)
wmat.array=array(0, c(B, p, p)) #wishart-distributed
for(b in 1:B){
    X=mvrnorm(n, rep(0,p), Sigma)
    wmat.array[b,,]=cov(X)}
apply(wmat.array, c(2,3), mean)

## [,1] [,2]
## [1,] 0.9583646 -0.6909337
## [2,] -0.6909337 1.0107182

Sigma*(n-1)
```

```
## [,1] [,2]
## [1,] 4.0 -2.8
## [2,] -2.8 4.0
```

Review

Write an R function to conduct Hotelling's T^2

- There is no R base function for conducting Hotelling's T^2 test
- We will write an R function

```
#Hotelling's T^2 for testing HO: mu=muO vs mu != muO
Hotelling.T2.1sample=function(X, muO)
{
    n=dim(X)[1]
    p=dim(X)[2]
    X.bar=colMeans(X)
    X.S=colMeans(X)
    T2=n*t(X.bar=muO)%*%solve(X.S)%*%(X.bar=muO)
    p.value=1-pf(T2/((n-1)*p/(n-p)),p,n-p)
    return(list(X.bar=X.bar, X.cov=X.S, T2=T2, p.value=p.value))
}
```

Review

Example of Multivariate One-Sample Problem: Protein Intake

- For the protein intake data, it might be more interesting to estimate the means than conducting hypothesis testing
- Suppose we are interested in estimating the means of the daily protein intake from different sources

```
my.cov=4*(diag(4) + 0.3* rep(1,4)%o%rep(1,4))
n=60:p=4
mv.mean=8*c(3,2,1,1)
eigen(my.cov) #to check whether the cov matrix is p.d.
## eigen() decomposition
## $values
## [1] 8.8 4.0 4.0 4.0
##
## $vectors
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                   [,2]
                              [.3]
                                         [.4]
## [1,] -0.5 0.8660254 0.0000000 0.0000000
## [2,] -0.5 -0.2886751 -0.5773503 -0.5773503
## [3.] -0.5 -0.2886751 -0.2113249 0.7886751
## [4,] -0.5 -0.2886751 0.7886751 -0.2113249
```

library(MASS)#the library "MASS" is required

Example of Multivariate One-Sample Problem: Protein Intake

- Estimate the mean vector using the sample mean vector
- Estimate covariance of the sample mean vector. Recall that $cov(\bar{\mathbf{X}}) = \frac{\mathbf{\Sigma}}{n}$

```
## meat 0.07159404 0.013584596 0.018824131 0.009220700
## dairy 0.01358460 0.073421655 0.005829816 0.003895500
## veg 0.01882413 0.005829816 0.086176323 0.009828535
## other 0.00922070 0.003895500 0.009828535 0.075478822
```

Example of Multivariate One-Sample Problem: Protein Intake

ullet Use Hotelling's \mathcal{T}^2 to quantify uncertainties. Recall that

$$T^2 = (\bar{\mathbf{X}} - \boldsymbol{\mu})^T \left(Cov(\bar{\mathbf{X}}) \right)^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}) \sim \frac{(n-1)p}{n-p} F_{p,n-p}$$

where $Cov(\bar{\mathbf{X}}) = \frac{\mathbf{S}}{n}$.

• The result indicates that

$$Pr[(\bar{\mathbf{X}} - \boldsymbol{\mu})^T \left(Cov(\bar{\mathbf{X}}) \right)^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}) \le \frac{(n-1)p}{n-p} F_{p,n-p,1-\alpha}] = 1 - \alpha$$

• Thus, a $(1-\alpha)100\%$ confidence region for μ is

$$\{\mu: (\bar{\mathbf{X}} - \boldsymbol{\mu})^T \left(Cov(\bar{\mathbf{X}}) \right)^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}) \leq \frac{(n-1)p}{n-p} F_{p,n-p,1-\alpha} \}$$

Example of Multivariate One-Sample Problem: Protein Intake

- \bullet Confidence intervals, which are in the form of ${\sf estimate} \pm {\sf critical} \ {\sf value} \times {\sf standard} \ {\sf error}$ are often preferred
- If there is only one parameter of interest, we can construct a C.I. using t-distribution, just as in univariate analysis
- Example. What is the mean protein intake? We have discussed the problem in Lecture 04.
 - Lecture 04: we constructed a large-sample C.I. by using 1.96 as the critical value. (See the protein intake example)
 - This lecture: we construct a C.I. by using $t_{n-1,1-\frac{\alpha}{2}}$ as the critical value

$$\bar{X}_{(j)} \pm t_{n-1,1-\frac{\alpha}{2}} \sqrt{\frac{s_{X_{(j)}}^2}{n}} \text{ for } j = 1, \cdots, p.$$

Review

Example of Multivariate One-Sample Problem: Protein Intake

- The confidence region has exactly $(1-\alpha)100\%$ confidence; however
- In many situations, we would like to construct confidence intervals for multiple parameters
- This is known as simultaneous intervals
- If we use the conventional method to construct individual C.I.s, we will have lower than $(1-\alpha)100\%$ confidence to cover all the parameters simultaneously

Review

Example of Multivariate One-Sample Problem: Protein Intake

• Some linear algebra result ensures that the following method gives $(1-\alpha)100\%$ confidence to cover all linear combinations of the parameters (in the form of $a^T\mu$) simultaneously

$$a^T \mathbf{\bar{X}} \pm \sqrt{\frac{(n-1)p}{n-p}} F_{p,n-p,1-\alpha} se(a^T \mathbf{\bar{X}})$$

• Example, consider the individual means $\mu_j, j=1,\cdots,4$ in the protein intake example, the following intervals are 95% simultaneous C.I. for the mean protein intake from the four sources

Review

Example of Multivariate One-Sample Problem: Protein Intake

```
#sample means
colMeans(protein)
                 dairy
        meat
                                      other
## 24 034032 15 928361 7 660490 7 738634
#standard errors
sqrt(diag(cov(protein)/n))
                 dairy
        meat.
                                      other
## 0.2675706 0.2709643 0.2935580 0.2747341
#critical value based on T2
sart((n-1)*p/(n-p)*af(0.95, p, n-p))
## [1] 3.269537
#lower hounds
low.bound = colMeans(protein) - sqrt((n-1)*p/(n-p)*qf(0.95, p, n-p)) *sqrt(diag(cov(protein)/n)) \\
#upper bounds
up.bound=colMeans(protein) + sqrt((n-1)*p/(n-p)*qf(0.95, p, n-p)) *sqrt(diag(cov(protein)/n))
```

Example of Multivariate One-Sample Problem: Protein Intake

```
## lower mean upper
## meat 23.159200 24.034032 24.908864
## dairy 15.042433 15.928361 16.814289
## veg 6.700691 7.660490 8.620288
## other 6.840381 7.738634 8.636887
```

Review

Example of Multivariate One-Sample Problem: Protein Intake

- Three choices of critic values
 - unadjusted: $t_{n-1,1-\alpha/2}$. Should NOT be used if multiple linear functions need to be estimated
 - T^2 : $\sqrt{\frac{(n-1)p}{n-p}}F_{p,n-p,1-\alpha}$
 - Bonferroni's correction: simply replace α with α/k where k is the total number of linear functions of the mean parameters:

$$t_{n-1,1-\alpha/(2k)}$$

 Example: the critical values for the individual means from four protein sources

[1] 2.576588

Example of Multivariate One-Sample Problem: Protein Intake

```
#unadjusted, shouldn't be used when constructing simultaneous C.I.s
qt(1-0.05/2, n-1)

## [1] 2.000995

#T^2
sqrt((n-1)*p/(n-p)*qf(0.95, p, n-p))

## [1] 3.269537

#Bonferroni correction
qt(1-0.05/p/2, n-1)
```

Two-Sample Hotellings T^2

Two-Sample Hotellings T^{2}

One-Sample vs Two-Sample

- In the one-sample problem, the goal is to make inference of
 - univariate: a population mean (one-sample t-test problem) or

Two-Sample Hotellings T^2

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- multivariate: a population mean vector (one-sample Hotelling T^2 problem)
- In the two-sample problem
 - univariate: compare two population means
 - multivariate: compare two population mean vectors

Univariate Two-Sample Problems

- Two independent samples
 - Sample 1 is from population 1:

$$X_{11}, \cdots, X_{1,n_1} \stackrel{iid}{\sim} N(\mu_1, \sigma^2)$$

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• Sample 2 is from population 2:

$$X_{21}, \cdots, X_{2,n_1} \stackrel{iid}{\sim} N(\mu_2, \sigma^2)$$

• Null hypothesis: $H_0: \mu_1 = \mu_2$

Univariate Two-Sample Problems

Pooled sample variance

$$s_p^2 = \frac{(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2}{n_1 + n_2 - 2}$$

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where

$$s_i^2 = \frac{\sum_{j=1}^{n_i} X_{ij}^2 - (\sum_{j=1}^{n_i} X_{ij})^2 / n_i}{n_i - 1}$$

• Two-sample t-statistic

$$t = \frac{\bar{x}_1 - \bar{x}_2}{\sqrt{s_p^2(\frac{1}{n_1} + \frac{1}{n_2})}}$$

• Null distribution: $t \stackrel{H_0}{\sim} t_{n_1+n_2-2}$.

Multivarite Two-Sample Problems

- Two independent samples
 - Sample 1 is from population 1:

$$\mathbf{X}_{11},\cdots,\mathbf{X}_{1,n_1}\stackrel{\mathit{iid}}{\sim} \mathit{N}(\mu_1,\mathbf{\Sigma})$$

Two-Sample Hotellings T^2

Sample 2 is from population 2:

$$\mathbf{X}_{21}, \cdots, \mathbf{X}_{2,n_2} \stackrel{iid}{\sim} N(\boldsymbol{\mu}_2, \boldsymbol{\Sigma})$$

• Null and alternative hypotheses: H_0 : $\mu_1 = \mu_2$ vs $H_1: \mu_1 \neq \mu_2$

Two-Sample Hotellings T^2

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Multivarite Two-Sample Problems

SPooled sample variance

$$\mathbf{S}_p = \frac{(n_1 - 1)\mathbf{S}_1 + (n_2 - 1)\mathbf{S}_2}{n_1 + n_2 - 2}$$

where

$$\mathbf{S}_i = rac{1}{n_i - 1} \sum_{i=1}^{n_i} (\mathbf{X}_{ij} - \bar{\mathbf{X}}_i) (\mathbf{X}_{ij} - \bar{\mathbf{X}}_i)'$$

• Two-sample Hotelling's T^2

$$T^2 = (\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}_2)^T \{ \mathbf{S}_p (\frac{1}{n_1} + \frac{1}{n_2}) \}^{-1} (\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}_2)$$

• Null distribution:

$$T^2 \stackrel{H_0}{\sim} \frac{(n_1 + n_2 - 2)p}{n_1 + n_2 - p - 1} F_{p, n_1 + n_2 - p - 1}$$

Multivariate Two-Sample Problems: Write an R Function

Two-Sample Hotellings T^2

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No existing base function in R.

```
Hotelling.T2.2sample=function(X, Y){
 n=dim(X)[1]; m=dim(Y)[1]; p=dim(X)[2]
 if(p!= dim(Y)[2]) return("Error: the dimensions of X and Y are not the same")
 X.bar=colMeans(X): Y.bar=colMeans(Y)
 X.S=cov(X); Y.S=cov(Y)
 pooled.S=((n-1)*X.S+(m-1)*Y.S)/(m+n-2)
 T2=t(X.bar-Y.bar)%*%solve((1/n+1/m)*pooled.S)%*%(X.bar-Y.bar)
 p.value=1-pf(T2/((n+m-2)*p/(n+m-1-p)),p,n+m-1-p)
 return(list(X.bar=X.bar, Y.bar=Y.bar, T2=T2, p.value=p.value))}
```

Multivariate Two-Sample Problems: Wite an R Function

- The built-in function "t.test" serves a dual function for univariate analyis
- We will write a dual function Hotelling.T2

```
Hotelling.T2=function(X, Y=NULL, mu0=NULL)
{
  if(is.null(Y) && is.null(mu0) )
    return("Error: mu0 is not specified")
  if(!is.null(X) && !is.null(mu0))
    obj=Hotelling.T2.1sample(X, mu0)
  if(!is.null(X) && !is.null(Y))
    obj=Hotelling.T2.2sample(X,Y)
  return(obj)
}
```

Two-Sample Hotellings T^2

Multivariate Two-Sample Problems: Iris setosa vs versicolor

```
Hotelling.T2.2sample(iris[1:50,1:4], iris[51:100,1:4])
## $X.bar
## Sepal.Length Sepal.Width Petal.Length Petal.Width
##
          5.006
                       3.428
                                    1.462
                                                  0.246
##
## $Y.bar
## Sepal.Length Sepal.Width Petal.Length Petal.Width
##
          5.936
                       2.770
                                    4.260
                                                  1.326
##
## $T2
##
            [,1]
## [1.] 2580.839
##
## $p.value
        Γ.17
## [1,]
```

Two-Sample Hotellings T^2 00000000000000000

Multivariate TWo-Sample Problems: Example

```
Hotelling.T2(iris[1:50,1:4], iris[51:100,1:4])
## $X.bar
## Sepal.Length Sepal.Width Petal.Length Petal.Width
##
          5.006
                       3.428
                                    1.462
                                                  0.246
##
## $Y.bar
## Sepal.Length Sepal.Width Petal.Length Petal.Width
##
          5.936
                       2.770
                                    4.260
                                                  1.326
##
## $T2
##
            [,1]
## [1.] 2580.839
##
## $p.value
        Γ.17
## [1,]
```

Two-Sample Hotellings T^2

- We might be interested in the difference between iris setosa and versicolor in the four features
- Because we are interested all the four features, we do need to construct simultaneous C.I.s for the four features. Two methods to find critical values with adjustment for multiple C.I.s:
 - Method 1 T2:

$$\sqrt{\frac{(n_1+n_2-2)p}{n_1+n_2-p-1}}F_{p,n_1+n_2-p-1,1-\alpha}$$

• Method 2- Bonferroni's correction by replacing α with α/k , i.e., use the following critical value

$$t_{n_1+n_2-2,1-\alpha/(2k)}$$

Two-Sample Hotellings T^2

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```
n1=n2=50; p=4
mean1=matrix(colMeans(iris[1:50,1:p]), p, 1)
mean2=matrix(colMeans(iris[51:100,1:p]), p, 1)
mean.diff = mean1-mean2
S1=cov(iris[1:50,1:p]); S2=cov(iris[51:100,1:p]);
Sp=((n1-1)*S1+(n2-1)*S2)/(n1+n2-2)
```

Method 1: T²

```
cv=sqrt((n1+n2-2)*p/(n1+n2-p-1)*qf(1-0.05, p, n1+n2-p-1 ))
round(data.frame(diff=mean.diff, se=sqrt(diag((1/n1+1/n2)*Sp) ),
CI.lower=mean1-mean2-qt(1-0.05/(2*p), n1+n2-2)*sqrt(diag((1/n1+1/n2)*Sp) ),
CI.upper=mean1-mean2+qt(1-0.05/(2*p), n1+n2-2)*sqrt(diag((1/n1+1/n2)*Sp) )), 3)
```

```
## Sepal.Length -0.930 0.088 -1.155 -0.705
## Sepal.Width 0.658 0.070 0.481 0.835
## Petal.Length -2.798 0.071 -2.978 -2.618
## Petal.Width -1.080 0.032 -1.161 -0.999
```

Method 1 Bonferroni

```
cv=sqrt((n1+n2-2)*p/(n1+n2-p-1)*qf(1-0.05, p, n1+n2-p-1 ))
round(data.frame(diff=mean.diff, se=sqrt(diag((1/n1+1/n2)*Sp) ),
CI.lower=mean1-mean2-qt(1-0.05/(2*p), n1+n2-2)*sqrt(diag((1/n1+1/n2)*Sp) ),
CI.upper=mean1-mean2+qt(1-0.05/(2*p), n1+n2-2)*sqrt(diag((1/n1+1/n2)*Sp) )), 3)
```

```
## Sepal.Length -0.930 0.088 -1.155 -0.705
## Sepal.Width 0.658 0.070 0.481 0.835
## Petal.Length -2.798 0.071 -2.978 -2.618
## Petal.Width -1.080 0.032 -1.161 -0.999
```

Assess MVN

The assumption of MVN

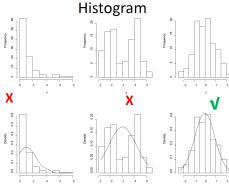
- We assume each observation X_i follows a MVN
- Assessing the assumption of multivariate normality is more difficult than assessing the assumption of normality (univariate)
- This is because univariate normality does not guarantee multivariate normality. Typically, we look at the following two items:
- It is difficult to examine joint normality in more than 2d. In practice, we do 1d and 2d
 - Marginal normality
 - Are pairs of variables show elliptical contours?
- Are there outliers in the data?

Assess Marignal Normality

- Useful visual tools:
 - histogram
 - QQ plot
 - scatter plot
- Less useful tools (formal tests)
 - Kolmogorov-Smironov test
 - Shapiro-Wilk test (correlation coefficient between data and normal scores)

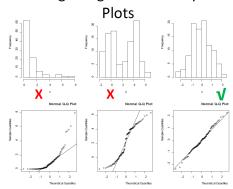
Histograms

Assessing Marginal Normality:



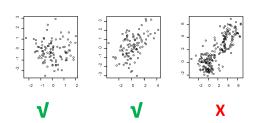
QQ plots

Assessing Marginal Normality: Q-Q



Bivariate Scatter Plots

Assessing Bivariate Normality



Large-Sample Results

Multivariate CLT

$$\begin{array}{ccc} \sqrt{n}(\bar{\mathbf{X}} - \boldsymbol{\mu}) \stackrel{\mathbf{D}}{\rightarrow} \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}) \\ \Rightarrow & n(\bar{\mathbf{X}} - \boldsymbol{\mu})^T \mathbf{S}^{-1}(\bar{\mathbf{X}} - \boldsymbol{\mu}) \rightarrow \chi_p^2 \end{array}$$

- When n-p is large, we replace $\frac{(n-1)p}{p-p}F_{p,n-p}$ with χ_p^2
- When $n_1 p$ and $n_2 p$ are large, we replace $\frac{(n_1+n_2-2)p}{n_1+n_2-p-1}F_{p,n_1+n_2-p-1}$ with χ_p^2

Assignment 2: Due on Monday, May 1st

- Problem 1: Choose a 3-by-3 covariance matrices with non-zero covariances. For each covariance matrix, simulate 1,000 data sets from a trivariate normal distribution.
 - O Hints:
 - Hint 1: the R library MASS provides a function to generate a random sample from a multivariate normal distribution.
 - Hint 2: Make sure that the covariance matrix you choose is positive definite. You can compute the eigenvalues by the "eigen" function in R and and check whether all the eigenvalues are positive.
 - Try to make sense of the covariance matrix by examining the pairwise scatter plots using the data you simulate.
 - Ouring the simulation, you will generate 1,000 Wishart distributed random matrices. Calculate the trace for each of them. Explain what distribution the traces should follow and examine their histogram.