Multivariate Analysis Lecture 7: Hotelling's T2

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Outline of Lecture 07

- Review of Wishart and the Hotelling's \mathcal{T}^2 distribution for one-sample problems
- 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



Review

Subsection 1

Wishart Distribution

Wishart Distribution

Definition of Wishart Distribution

- A Wishart distribution can be defined in the following way
- Let \mathbf{W} be a $p \times p$ random matrix. We say \mathbf{W} follows $Wishart_p(k, \mathbf{\Sigma})$ if \mathbf{W} can be written as $\mathbf{W} = \mathbf{X}^T \mathbf{X}$ where \mathbf{X} denotes the random matrix formed by a random sample of size k from MVN $N(\mathbf{0}, \mathbf{\Sigma})$.
- 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: $E[\mathbf{W}] = k\Sigma$.

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

Review ○ ○ ○ ○ ○ ○

Wishart vs Chi-squared (continued)

• When p=1,

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

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

[,1] [,2]

[1] 4 A -2 8

Wishart Distribution

##

A Simulation Study to 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,,]=(n-1)*cov(X)
apply(wmat.array, c(2,3), mean)
##
             [,1] \qquad [,2]
## [1.] 4.090403 -2.833826
## [2,] -2.833826 3.933867
Sigma*(n-1)
```

Hotelling's T^2

Review

Subsection 2

Hotelling's T^2

Definition of Hotelling's T^2

- Hotelling generalized the student's t, which is for univarite, to Hotelling's \mathcal{T}^2 , 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

 - $\mathbf{0} \mathbf{W} \sim \hat{W}_{p}(\nu, \mathbf{\Sigma})$
 - Z ⊥ W

Section 2

One-Sample Hotelling T^2

One-Sample Hotelling T^2

Review

- 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 X̄ and S̄, respectively.
- ullet The null hypothesis of interest $H_0: \mu = \mu_0$
- The one-sample Hotelling T^2 is defined as

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

ullet 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.

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

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=cov(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))
}
```

- 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

```
library (MASS) #the library "MASS" is required
my.cov=4*(diag(4) + 0.3* rep(1,4)%o%rep(1,4))
n=60;p=4
my.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
```

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 $cov(\bar{\mathbf{X}}) = \frac{\Sigma}{2}$

```
## meat dairy veg other ## 24.034032 15.928361 7.660490 7.738634
```

```
cov(protein)/n
```

Example of Multivariate One-Sample Problem: Protein Intake

 \bullet Use Hotelling's T^2 to quantify uncertainties. Recall that

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

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

The result indicates that

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

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

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

Example of Multivariate One-Sample Problem: Protein Intake

- The confidence region has exactly $(1-\alpha)100\%$ confidence; however
- In many situations, we would like to construct confidence intervals, which are in the form of

estimate \pm critical value \times standard error

- 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 from source *j*?
 - 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. for μ_j by using $t_{n-1,1-\frac{\alpha}{2}}$ as the critical value

Section 3

Simultaneous C.I.

The Coverage of simultaneous C.I.s

• Let $A_j = \{\mu_j \text{ is in the constructed C.I. }\}$. The C.I. in the previous slide has $(1-\alpha)100\%$ coverage for a specific μ_j , i.e.,

$$Pr(A_j) = 1 - \alpha$$

• If we are interested in all the parameters, which are $\mu_1, \mu_2, \mu_3, \mu_4$ in the protein intake example. The coverage for the mean vector is

$$Pr(A_1 \cap A_2 \cap A_3 \cap A_4)$$

- Clearly $Pr(A_1 \cap A_2 \cap A_3 \cap A_4) < 1 \alpha$
- Thus, if we use $t_{n-1,1-\frac{\alpha}{2}}$ as the critical value, we do not have enough coverage for all the parameters in μ simultaneously
- What we need to construct are simultaneous confidence intervals

Methods for Simultaneous Confidence Intervals

• Method 1 for simultaneous C.I. T^2 . 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

$$a^Tar{\mathbf{X}} \pm \sqrt{rac{(n-1)p}{n-p}F_{p,n-p,1-lpha}} \mathsf{se}(a^Tar{\mathbf{X}})$$

• Method 2 Bonferroni's correction: simply replace α with α/k where k is the total number of linear functions of the mean parameters: $t_{n-1,1-\alpha/(2k)}$, where k is the number of parameters of interest.

#sample means

Simultaneous C.I.s using T^2 : Protein Intake

```
colMeans(protein)
##
                                    other
       meat.
                dairy
                          veg
## 24.034032 15.928361 7.660490 7.738634
#standard errors
sqrt(diag(cov(protein)/n))
##
                dairy veg
                                    other
       meat
## 0.2675706 0.2709643 0.2935580 0.2747341
#critical value based on T2
cv=sqrt((n-1)*p/(n-p)*qf(0.95, p, n-p))
#lower hounds
low.bound=colMeans(protein) - cv *sqrt(diag(cov(protein)/n))
#upper bounds
up.bound=colMeans(protein) + cv *sqrt(diag(cov(protein)/n))
```

Simultaneous C.I.s using T^2 : 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
```

#sample means

Simultaneous C.I.s using Bonferroni: Protein Intake

```
colMeans(protein)
##
                                     other
        meat.
                 dairy
                             veg
## 24.034032 15.928361 7.660490 7.738634
#standard errors
sqrt(diag(cov(protein)/n))
##
                 dairy
                                     other
        meat
                             veg
## 0.2675706 0.2709643 0.2935580 0.2747341
#critical value based on T2
cv=qt(1-0.05/p/2, n-1)
#lower hounds
low.bound=colMeans(protein) - cv *sqrt(diag(cov(protein)/n))
#upper bounds
up.bound=colMeans(protein) + cv *sqrt(diag(cov(protein)/n))
```

Simultaneous C.I.s using Bonferroni: Protein Intake

```
## lower mean upper
## meat 23.344613 24.034032 24.723451
## dairy 15.230198 15.928361 16.626524
## veg 6.904112 7.660490 8.416868
## other 7.030758 7.738634 8.446511
```

Comparison of Different Critical Values

- Three choices of critical 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

Comparison of Different Critical Values 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)
```

Section 4

Two-Sample Hotellings T^2

One-Sample vs Two-Sample

Review

- In the one-sample problem, the goal is to make inference of
 - univariate: a population mean (one-sample t-test problem) or
 - ullet multivariate: a population mean vector (one-sample Hotelling \mathcal{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:

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

• Sample 2 is from population 2:

$$X_{21}, \cdots, X_{2,n_2} \stackrel{iid}{\sim} N(\mu_2, \sigma^2)$$

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

Univariate Two-Sample Problems

Pooled sample variance

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

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

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

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

• Sample 2 is from population 2:

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

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

Pooled sample covariance matrix

$$\mathbf{S}_{p} = \frac{(n_{1}-1)\mathbf{S}_{1} + (n_{2}-1)\mathbf{S}_{2}}{n_{1} + n_{2} - 2}$$

where

Review

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

• Two-sample Hotelling's T^2

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

• Null distribution:

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

• 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 th
    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: Write an R Function

- The built-in function "t.test" serves a dual-purpose function for univariate analyis
- We will write a dual-purpose 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)
}
```

Multivariate Two-Sample Problems: Iris setosa vs versicolor

```
## $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
##
        [,1]
## [1,]
```

Hotelling.T2.2sample(iris[1:50,1:4], iris[51:100,1:4])

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
##
        [,1]
## [1,]
```

Linear Functions of Differences: Iris Setosa vs Versicolor

- 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

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

Linear Functions of Differences: Iris Setosa vs Versicolor

```
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)
```

Linear Functions of Differences: Iris Setosa vs Versicolor

• Method 1: T^2

Review

```
## diff se CI.lower CI.upper
## 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
```

Review

Method 2: Bonferroni

```
cv=qt(1-0.05/p/2, n1+n2-2)
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)
```

```
## 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
```

Section 5

Assess MVN

The assumption of MVN

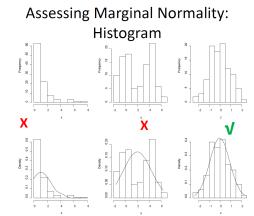
Review

- \bullet We assume each observation \mathbf{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

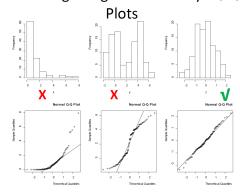
- Useful visual tools:
 - histogram
 - QQ plot
 - scatter plot
- Less useful tools (formal tests)
 - Kolmogorov-Smironov test
 - Shapiro-Wilk test (correlation coefficient between data and normal scores)

Thotograms



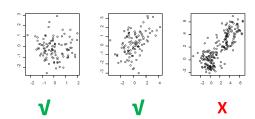
QQ plots

Assessing Marginal Normality: Q-Q



Bivariate Scatter Plots

Assessing Bivariate Normality



Review

Multivariate CLT

$$\begin{split} & \sqrt{n}(\bar{\mathbf{X}} - \boldsymbol{\mu}) \overset{\mathbf{D}}{\to} \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}) \\ \Rightarrow & n(\bar{\mathbf{X}} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{S}^{-1}(\bar{\mathbf{X}} - \boldsymbol{\mu}) \to \chi_p^2 \end{split}$$

- When n-p is large, we replace $\frac{(n-1)p}{n-p}F_{p,n-p}$ 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^2_p

Assignment 2: Due on Monday, April 28

- Problem 1: Choose a 3 − by − 3 covariance matrix with non-zero covariances. Also choose a sample size n (e.g., n=100, 500, 1000, etc). 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.
- Problem 2: Find a good data example to conduct a two-sample Hotelling's T² test. Do not use the data example discussed in this course. Please (1) include visualizations as exploratory methods and (2) make conclusion in the context of the data example.
- R Code should be included as appendices.