

Displays for Statistics 5401/8401

Lecture 19

October 19, 2005

Christopher Bingham, Instructor

612-625-1024, kb@umn.edu

372 Ford Hall

Class Web Page

<http://www.stat.umn.edu/~kb/classes/5401>

© 2005 by Christopher Bingham

All tests of multivariate linear hypotheses are derived from different ways of comparing  $\mathbf{H}$  and  $\mathbf{E}$ . A particularly important class of tests are based on  $\mathbf{E}^{-1}\mathbf{H}$ . Such tests have the following form:

- Reject  $H_0$  when  $\mathbf{E}^{-1}\mathbf{H}$  is "too large" compared to  $(f_h/f_e)\mathbf{I}_p$ ,

or equivalently

- Reject  $H_0$ : when the "multivariate F"  $(f_e/f_h)\mathbf{E}^{-1}\mathbf{H}$  is too large compared to  $\mathbf{I}_p$

**Here's a problem:**

$\mathbf{E}^{-1}\mathbf{H}$  is a  $p$  by  $p$  matrix. What number or numbers measure how large it is?

- $\det(\mathbf{E}^{-1}\mathbf{H})$  is **not** a useful number because

$$\det(\mathbf{E}^{-1}\mathbf{H}) = \det(\mathbf{E}^{-1})\det(\mathbf{H}) = \det(\mathbf{H})/\det(\mathbf{E})$$

But when  $f_h < p$ ,  $\det(\mathbf{H}) = 0$ , making  $\det(\mathbf{E}^{-1}\mathbf{H}) = 0$  so this is *not* helpful.

What are helpful are measures computed from the *eigenvalues* of  $\mathbf{H}$  relative to  $\mathbf{E}$ , that is the *relative eigenvalues*.

See the handout for a fairly complete explanation.

**Vocabulary**

The relative eigenvalues of  $\mathbf{H}$  relative to  $\mathbf{E}$  are the ordinary eigenvalues of  $\mathbf{E}^{-1}\mathbf{H}$

$$\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \dots \geq \hat{\lambda}_p \geq 0$$

You can use relative eigenvalues to express and compute several standard test statistics for multivariate linear hypothesis .

The relative eigenvectors  $\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_2, \dots, \hat{\mathbf{u}}_p$  of  $\mathbf{H}$  relative to  $\mathbf{E}$  are the ordinary eigenvectors of  $\mathbf{E}^{-1}\mathbf{H}$ . They satisfy

$$\mathbf{E}^{-1}\mathbf{H}\hat{\mathbf{u}}_j = \hat{\lambda}_j\hat{\mathbf{u}}_j$$

The standard normalization, which I always assume, is  $\hat{\mathbf{u}}_j'\mathbf{E}\hat{\mathbf{u}}_j = 1$  .

These are all measure that *are* helpful:

- **Hotelling's generalized  $T^2$**  (trace test) based on  $\text{tr } \mathbf{E}^{-1}\mathbf{H} = \sum_i \hat{\lambda}_i$
- **Roy's maximum root test** based on  $\hat{\lambda}_{\max} = \hat{\lambda}_1$ .
- **Likelihood ratio test** (Wilks' or Rao's test) based on  $1/\det(\mathbf{I}_p + \mathbf{E}^{-1}\mathbf{H}) = 1/\prod_i(1 + \hat{\lambda}_i)$  or  $\log(\det(\mathbf{I}_p + \mathbf{E}^{-1}\mathbf{H})) = \sum_i \log(1 + \hat{\lambda}_i)$
- **Pillai's trace test** based on  $\text{tr}((\mathbf{H} + \mathbf{E})^{-1}\mathbf{H}) = \text{tr}(\mathbf{I} + \mathbf{E}^{-1}\mathbf{H})^{-1}\mathbf{E}^{-1}\mathbf{H} = \sum_i \hat{\lambda}_i / (1 + \hat{\lambda}_i)$

When  $p = 1$ , there is only one  $\hat{\lambda}$  so they are functions of  $\hat{\lambda}_1 = SS_h/SS_e = (f_h/f_e)F$ . In particular  $\hat{\lambda}_1/(1 + \hat{\lambda}_1) = SS_h/(SS_h + SS_e)$ .

When  $p > 1$  and  $f_h > 1$  they are all different.

### Hotelling's generalized T<sup>2</sup>

$$T_0^2 = f_e \sum_i \hat{\chi}_i = f_e \text{tr}(\mathbf{E}^{-1}\mathbf{H}) = \text{tr}(\mathbf{S}^{-1}\mathbf{H})$$

where  $\mathbf{S} = (1/f_e)\mathbf{E} = \hat{\Sigma}$ .

When  $H_0$  is true, in large samples,  $T_0^2$  is approximately  $\chi_r^2$ , where  $f = f_h p$ .

$f = f_h p$  is the total number of *scalar* parameters (or linear combinations of *scalar* parameters) under test. There are  $f_h$  for each of  $p$  dimensions.

- 1-way MANOVA with  $g$  groups  
 $f_h = g-1, f = (g-1)p$
- Testing two-way interaction in MANOVA, with  
 $f_h = (a-1)(b-1), f = (a-1)(b-1)p$   
 where  $a$  and  $b$  are the numbers of levels in the two factors.
- Testing  $\beta_1 = \beta_2 = 0, f_h = 2$  and  $f = 2p$ .

You get a match to  $\chi_r^2$  if you replace  $f_e$  by  $m_2 \equiv f_e - p - 1$ , so the usual form of this test is

$T = (f_e - p - 1)\text{tr}(\mathbf{E}^{-1}\mathbf{H}) = (1 - (p+1)/f_e)T_0^2$ .  
 Note that the  $1 - (p+1)/f_e \rightarrow 1$  as  $f_e \rightarrow \infty$ , so with large enough  $f_e$  using  $m_2$  makes little difference.

For an example I created some artificial data with  $g = 4$  groups and  $p = 4$  variables. You can download the data from [www.stat.umn.edu/~kb/classes/5401/datafiles.html](http://www.stat.umn.edu/~kb/classes/5401/datafiles.html)

```
Cmd> data <- read("manovadata.txt","data")
data      50      5 LABELS
) Artificial one-way MANOVA data with p = 4 variables and
) g = 4 groups
) n_1 = 3, n_2 = 11, n_3 = 16, n_4 = 10
) Col. 1: Factor group with levels 1, 2, 3, 4
) Col. 2: Response Y1
) Col. 3: Response Y2
) Col. 4: Response Y3
) Col. 5: Response Y4
Read from file "TPl:Stat5401:Stat5401F05:Data:manovadata.txt"
Cmd> addmacrofile("") # get new version of mulvar.mac
Cmd> group <- factor(data[,1])
Cmd> Y <- data[,-1] # 50 by 4 matrix of response variables
Cmd> p <- ncols(Y) # number of dimensions
```

```
Cmd> manova("Y=group")
Model used is Y=group
WARNING: summaries are sequential
          SS and SP Matrices
          DF
CONSTANT 1
          Y1      Y2      Y3      Y4
Y1      48157    47709    47960    47828
Y2      47709    47265    47514    47383
Y3      47960    47514    47765    47633
Y4      47828    47383    47633    47501
group    3
          Y1      Y2      Y3      Y4
Y1      4.9987    5.3629    5.6136    3.7318
Y2      5.3629    7.2951    9.5705    7.042 = H
Y3      5.6136    9.5705    15.473   12.081
Y4      3.7318    7.042    12.081    9.578
ERROR1  46
          Y1      Y2      Y3      Y4
Y1      42.715    6.0666    1.1321    -8.952
Y2      6.0666    42.181    -5.4086    7.4368 = E
Y3      1.1321    -5.4086    51.907    2.5298
Y4      -8.952    7.4368    2.5298    44.303
```

Extract  $\mathbf{H}$  and  $\mathbf{E}$  and compute univariate F-statistics, their Bonferronized P-values and  $\mathbf{E}^{-1}\mathbf{H}$ .

```
Cmd> h <- matrix(SS[2,,]); fh <- DF[2]
Cmd> e <- matrix(SS[3,,]); fe <- DF[3]
Cmd> fstats <- (fe/fh)*diag(h)/diag(e); fstats
(1) 1.7944 2.6519 4.5706 3.315
Cmd> p*cumF(fstats,fh,fe,upper:T) # Bonferronized P-values
(1) 0.64589 0.23903 0.027837 0.11202
```

1 P-value < .05 so reject  $H_0$  at 5% level

```
Cmd> e_inv_h <- solve(e,h); e_inv_h # E^(-1)H
          Y1      Y2      Y3      Y4
Y1      0.11565    0.13005    0.14767    0.10174
Y2      0.11045    0.1524    0.20021    0.14761
Y3      0.11311    0.19017    0.30346    0.23624
Y4      0.082606    0.14879    0.2516    0.19848
```

Now find eigenvalues. Not this way:

```
Cmd> eigvals <- eigenvals(e_inv_h) # doesn't work
ERROR: 1st argument to eigenvals() must be symmetric REAL matrix
```

You *can't* use `eigen()` or `eigenvals()` since they work only with symmetric matrices and  $\mathbf{E}^{-1}\mathbf{H}$  is not symmetric. Use `releigen()` and `releigenvals()` instead.

```
Cmd> eigs <- releigen(h,e); eigs
component: values      eigs$values or eigs[1]
(1) 0.69325 0.073323 0.0034282 1.4755e-16
component: vectors      eigs$vectors or eigs[2]
          (1)      (2)      (3)      (4)
Y1 0.051256 -0.10812 0.10376 -0.017947
Y2 0.064869 -0.053316 -0.13646 -0.0099296
Y3 0.091838 0.038661 -0.0010638 0.098878
Y4 0.074768 0.057023 0.061523 -0.11043
```

```
Cmd> eigvals <- eigs$values;
Cmd> lambdamax <- eigs$values[1]; lambdamax
(1) 0.69325
Cmd> trace(e_inv_h) # sum of diagonals of E^(-1)H
(1) 0.77
Cmd> sum(eigvals) # same as trace(e_inv_h)
(1) 0.77
Cmd> t0sq <- fe*trace(e_inv_h); t0sq # Hotelling's T_0^2
(1) 35.42
```

$t0sq = T_0^2$  tests

$$H_0: \mu_1 = \mu_2 = \mu_3 = \mu_4$$

which is the same as

$$H_0: \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0$$

```
Cmd> cumchi(t0sq,p*fh,upper:T) # chi-squared(12) P-value
(1) 0.00040136 Very small P-value => Reject H_0
```

Compute the modified value which has the more accurate  $\chi^2$  approximation.

```
Cmd> m2 <- fe - p - 1; m2 # optimal replacement for fe = 147
(1) 41
Cmd> m2*trace(e_inv_h) # Improved Trace test statistic
(1) 31.57
Cmd> cumchi(m2*trace(e_inv_h),p*fh,upper:T)#chi-sq(12) P-val
(1) 0.0016117 Better large sample P-value
```

cumtrace() in the new version of Mulvar.mac uses an asymptotic series to find a yet more accurate P-value.

```
Cmd> cumtrace(trace(e_inv_h),fh,fe,p,upper:T)
(1) 0.0047263
```

Note this is about 10 times larger than crudest P-value from  $f_e \text{tr} \mathbf{E}^{-1} \mathbf{H}$  and about 3 times larger than the "better" large sample P-value from  $m_2 \text{tr} \mathbf{E}^{-1} \mathbf{H}$ .

A better multiplier of  $-\log \Lambda$  than N

$$m_1 \equiv f_e - (p - f_h + 1)/2,$$

so the standard form for the likelihood ratio test statistic is

$$\begin{aligned} & (f_e - (p - f_h + 1)/2) \log \det(\mathbf{I}_p + \mathbf{E}^{-1} \mathbf{H}) \\ &= (f_e - (p - f + 1)/2) (\log(\det(\mathbf{H} + \mathbf{E})/\det(\mathbf{E}))) \\ &= (f_e - (p - f + 1)/2) \sum_i \log(1 + \hat{\lambda}_i) \\ &\quad \approx \chi_{f_h p}^2 \end{aligned}$$

There are other approximations described in the handout on MANOVA tests and implemented in macro cumwilks()..

```
Cmd> N <- nrow(Y) # sample size
Cmd> I_p <- dmat(p,1) # identity matrix
Cmd> N * log(det(I_p + e_inv_h))
(1) 30.041
Cmd> N*sum(log(1 + eigvals))
(1) 30.041
Cmd> m1 <- (fe - (p - fh + 1)/2); m1
(1) 45
Cmd> wilks <- m1*log(det(I_p + e_inv_h)); wilks
(1) 27.037
Cmd> m1*sum(log(1 + eigvals)) # from eigenvalues
(1) 27.037
Cmd> cumchi(wilks,fh*p,upper:T) # approximate P-value
(1) 0.0076322
```

### Likelihood Ratio test (Wilks or Rao)

When errors are  $N_p(\mathbf{0}, \Sigma)$ , the likelihood ratio statistic to test  $H_0$  vs  $H_1$  is

$$\begin{aligned} \lambda &= \det(\mathbf{E}^{-1}(\mathbf{E} + \mathbf{H}))^{-N/2} = (\Lambda^*)^{N/2} \\ \Lambda^* &\equiv 1/\det(\mathbf{I}_p + \mathbf{E}^{-1} \mathbf{H}) = \det(\mathbf{E})/\det(\mathbf{H} + \mathbf{E}) \end{aligned}$$

Then

$$\begin{aligned} -2 \log \lambda &= N \log \det(\mathbf{I}_p + \mathbf{E}^{-1} \mathbf{H}) = -N \log \Lambda^* \\ &= N \sum_{1 \leq i \leq p} \log(1 + \hat{\lambda}_i) \end{aligned}$$

The theory of LR tests says

$$-2 \log \lambda = N \log \det(\mathbf{I}_p + \mathbf{E}^{-1} \mathbf{H})$$

should be approximately  $\chi_r^2$  in large samples when  $H_0$  is true, where  $f = f_h p$ .

This is **Wilks' or Rao's test**.

Note  $f = f_h p$  is the same as for Hotelling's trace test.

cumwilks() computes a more accurate P-value based on an F-statistic computed from a power of  $\Lambda^*$ . See the handout for details.

```
Cmd> cumwilks(det(e)/det(h+e),fh,fe,p)
(1) 0.0077151
Cmd> cumwilks(1/prod(1+eigvals),fh,fe,p)
(1) 0.0077151
```

This is very close to the P-value 0.00763 computed from  $\chi_r^2$ .

$H_0$  may be rejected at the 1% level of significance.

### Important facts

- p by p matrix **H** has rank  $s \equiv \min(f_h, p)$ .  
 $f_h = 1 \Rightarrow s = 1$ .  
 $p = 1 \Rightarrow s = 1$ .
- There are only s non-zero relative eigenvalues of **H** relative to **E**.
- When  $p > f_h$ ,  $s = f_h$  and  $\hat{\lambda}_{f_h+1} = \hat{\lambda}_{f_h+2} = \dots = \hat{\lambda}_p = 0$ .
- When  $p > f_h$ , **H** is singular.
- A *relative* eigenvalue  $\hat{\lambda}$  satisfies  $\mathbf{H}\hat{\mathbf{u}} = \hat{\lambda}\mathbf{E}\hat{\mathbf{u}}$  for some vector  $\hat{\mathbf{u}}$  which implies  $\mathbf{E}^{-1}\mathbf{H}\hat{\mathbf{u}} = \hat{\lambda}\hat{\mathbf{u}}$
- $\hat{\mathbf{u}}$  is a *relative eigenvector* of **H** relative to **E** with relative eigenvalues  $\hat{\lambda}$ .

### Example continued

```

Cmd> u_1 <- eigs$vector[1,]; z1 <- Y %>% u_1 # Canonical var
Cmd> u_2 <- eigs$vector[2,]; z2 <- Y %>% u_2
Cmd> u_3 <- eigs$vector[3,]; z3 <- Y %>% u_3
Cmd> anova("z1 = group", silent=T); SS
CONSTANT group ERROR1
3809.1 0.69325 1
Cmd> anova("z2 = group", silent=T); SS
CONSTANT group ERROR1
208.54 0.073323 1
Cmd> anova("z3 = group", silent=T); SS
CONSTANT group ERROR1
39.422 0.0034282 1
Cmd> eigvals
(1) 0.69325 0.073323 0.0034282 1.4755e-16
    
```

Note:

- $SS_h$  in the analyses of the  $\hat{z}_j$ 's match the relative eigenvalues in eigvals.
- $SS_e$  are all 1

Define  $\hat{z}_j = \hat{\mathbf{u}}_j' \mathbf{y}$  where  $\hat{\mathbf{u}}_j = j^{\text{th}}$  relative eigenvector.

$\hat{z}_j$  is the  $j^{\text{th}}$  MANOVA canonical variable associated with hypothesis  $H_0$ .

- $\hat{z}_j = \sum_{1 \leq l \leq p} \hat{u}_{lj} y_l$  is a linear combination of the response variables  $y_1, y_2, \dots, y_p$  with coefficients from the relative eigenvector  $\hat{\mathbf{u}}_j$ .
- $\hat{\mathbf{u}}_j' \mathbf{H} \hat{\mathbf{u}}_j = \hat{\lambda}_j = SS_h(\hat{z}_j) = \text{ANOVA hypothesis SS}$  computed from  $\hat{z}_j$  as if it were a new response variable.
- $\hat{\mathbf{u}}_j' \mathbf{E} \hat{\mathbf{u}}_j = 1 = SS_e(\hat{z}_j) = \text{ANOVA error SS}$  computed from  $\hat{z}_j$

Do MANOVA computations on matrix of all 4 canonical variables:

```

Cmd> z <- Y %>% eigs$vector; list(z) # all 4 canvar
z REAL 50 4 (labels)
Cmd> manova("z = group", silent=T)
• Diagonal elements  $\hat{\mathbf{u}}_j' \mathbf{H} \hat{\mathbf{u}}_j = \hat{\lambda}_j$ 
• Off diagonal elements  $\hat{\mathbf{u}}_j' \mathbf{H} \hat{\mathbf{u}}_k = 0, j \neq k$ 
Cmd> round(SS[2,,],12) # H for z to 12 decimals
group (1) (2) (3) (4)
(1) 0.69325 0 0 0
(2) 0 0.073323 0 0
(3) 0 0 0.0034282 0
(4) 0 0 0 0
    
```

(round(SS[2,,],12) suppresses small numbers like 1.242e-16 which are really zeros in disguise.)

- Diagonal elements  $\hat{\mathbf{u}}_j' \mathbf{E} \hat{\mathbf{u}}_j = 1$
- Off diagonal elements  $\hat{\mathbf{u}}_j' \mathbf{E} \hat{\mathbf{u}}_k = 0, j \neq k$

```

Cmd> round(SS[3,,],12) # E for z to 12 decimals
ERROR1 (1) (2) (3) (4)
(1) 1 0 0 0
(2) 0 1 0 0
(3) 0 0 1 0
(4) 0 0 0 1
    
```

The canonical correlations have 0 within group correlation.

An important fact is

- $\hat{\lambda}_1 = SS_h(\hat{z}_j)/SS_e(\hat{z}_j)$   
 $= \max_u SS_h(\mathbf{u}'\mathbf{y})/SS_e(\mathbf{u}'\mathbf{y})$
- $(f_h/f_e)\hat{\lambda}_1 = F_{\max}$  = largest possible F-statistic computed from any linear combination  $y_u = \mathbf{u}'\mathbf{y}$ .

That is, for *any* vector  $\mathbf{u}$  defining a linear combination of the variables in  $\mathbf{y}$ , in a univariate ANOVA of  $y_u = \mathbf{u}'\mathbf{y}$ , the ANOVA F-statistic must satisfy

$$F = (SS_h(\mathbf{u}'\mathbf{y})/f_h)/(SS_e(\mathbf{u}'\mathbf{y})/f_e) \leq f_e \hat{\lambda}_1 / f_h$$

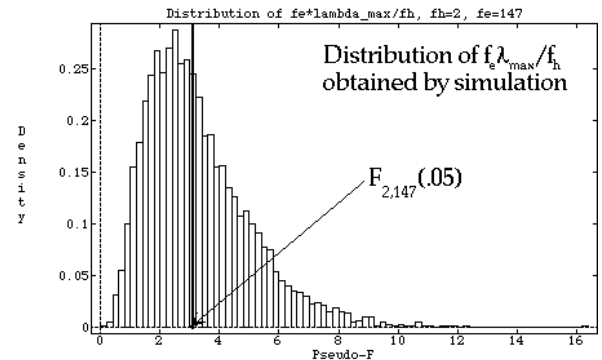
This suggests that the "pseudo-F-statistic"  $f_e \hat{\lambda}_1 / f_h$  or even just  $\hat{\lambda}_1$  might be a good candidate for a statistic to test  $H_0$ .

**Warning:** When  $p > 1$ ,  $(f_h/f_e)\hat{\lambda}_1$  does *not* have a F-distribution.

I did a small simulation of the null distribution (distribution when  $H_0$  is true) of  $(f_h/f_e)\hat{\lambda}_1$  that shows this clearly.

lambda\_max is a vector of  $\hat{\lambda}_1$ 's computed from  $M = 5,000$  simulated samples .

```
Cmd> hist(fe*lambda_max/fh,vector(0,.2),xlab:"Pseudo-F",\
title:"Distribution of fe*lambda_max/fh, fh=2, fe=147")
Cmd> addlines(rep(invF(.05,fh,fe,upper:T),2),vector(0,.3),\
thickness:2)
```



$F_{2,147}(.05)$  is closer to the median of simulated values than to the upper 5% point.

### Roy's maximum root test

Reject  $H_0$  when  $\hat{\lambda}_1 = \hat{\lambda}_{\max}$  is "large"  
 I found estimates of  $\hat{\lambda}_{\max}(.10)$ ,  $\hat{\lambda}_{\max}(.05)$  and  $\hat{\lambda}_{\max}(.01)$  from the 5000 simulated values in lambda\_max.

```
Cmd> lambda_max[round(vector(.90,.95,.99)*M)]
(1) 0.076562 0.090821 0.12154
```

Actually **Roy** proposed the canonical correlation form of the statistic

$$\hat{\theta}_1 = \hat{\theta}_{\max}$$

where  $\hat{\theta}_j = \hat{\lambda}_j / (1 + \hat{\lambda}_j)$ ,  $j = 1, \dots, p$

```
Cmd> theta_max <- lambda_max/(1 + lambda_max)
Cmd> theta_max[round(vector(.90,.95,.99)*M)] # critical vals
(1) 0.071117 0.083259 0.10837 10%, 5%, 1%
```

These last are estimated critical values for  $\hat{\theta}_{\max}$ .

This approach by simulation is always available with the right software.