

Comparisons of Several Multivariate Populations

Edps/Soc 584, Psych 594

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Spring 2017



Overview

- ▶ 1-way ANOVA
 - ▶ Classic Treatment
 - ▶ As a general linear model
- ▶ 1-way MANOVA
 - ▶ The Model: Generalization of ANOVA to multivariate.
 - ▶ Hypothesis Testing
 - ▶ Example 1: Massed vs distributed practice
- ▶ Multivariate General Linear Model and Example 2: Increased survival
- ▶ Following up to a significant result
 - ▶ Multivariate contrasts
 - ▶ Simultaneous confidence intervals
 - ▶ Discriminant function
- ▶ Summary of PCA, MANOVA, DA
- ▶ SAS IML and PROC GLM.

Reading: Johnson & Wichern pages 296–323.



Generalizing 1-way ANOVA to Multivariate Data

and Generalizing multivariate T^2 to more than two populations.

Suppose that we have random samples from g populations and measures on p variables:

$$\begin{array}{ll}
 \text{Population 1:} & \mathbf{x}_{11}, \mathbf{x}_{12}, \dots, \mathbf{x}_{1n_1} \\
 \text{Population 2:} & \mathbf{x}_{21}, \mathbf{x}_{22}, \dots, \mathbf{x}_{2n_2} \\
 & \vdots \\
 \text{Population } g: & \mathbf{x}_{g1}, \mathbf{x}_{g2}, \dots, \mathbf{x}_{gn_g}
 \end{array}$$

where each \mathbf{x}_{lj} is a $(p \times 1)$ vector.



Examples:

- ▶ 5 standardized tests scores the same for high school students who attend different high school programs (i.e., general, vo/tech, academic).
- ▶ Survival times measured in two ways different between those treated with supplemental vitamin C the over six types of cancer?
- ▶ Others?



Basic Assumptions

Assumptions needed for Statistical Inference.

- ▶ $\mathbf{X}_{j1}, \mathbf{X}_{j2}, \dots, \mathbf{X}_{jn_j}$ is a random sample of size n_j from a population with means $\boldsymbol{\mu}_j$ for $j = 1, \dots, g$ (i.e., **observations within populations are independent** and representative of their populations).
- ▶ Random samples from **different populations are independent**.
- ▶ All populations have the **same covariance matrix, $\boldsymbol{\Sigma}$** .
- ▶ $\mathbf{X}_{j_j} \sim \mathcal{N}(\boldsymbol{\mu}_j, \boldsymbol{\Sigma})$; that is, **each population is multivariate normal**.

If a population is **not** multivariate normal, then for large n_j central limit theorem may “kick-in”.



One-way ANOVA Review

- ▶ The univariate case where $p = 1$
- ▶ **Assumptions:** $X_{ij} \sim \mathcal{N}(\mu_l, \sigma^2)$ *i.i.d* for $j = 1, \dots, n_l$ and $l = 1, \dots, g$.
- ▶ **Hypotheses:**

$$H_o : \mu_1 = \mu_2 = \dots = \mu_g \quad \text{versus} \quad H_a : \text{not } H_o$$

- ▶ We usually express μ_l as the sum of a grand mean and deviations from the grand mean

$$\begin{aligned} \underbrace{\mu_l}_{l^{\text{th}} \text{ pop. mean}} &= \underbrace{\mu}_{\text{grand mean}} + \underbrace{\mu_l - \mu}_{l^{\text{th}} \text{ pop. treatment effect}} \\ &= \mu + \tau_l \end{aligned}$$

- ▶ If $\mu_1 = \mu_2 = \dots = \mu_g$, then an equivalent way to write the null hypothesis is

$$H_o : \tau_1 = \tau_2 = \dots = \tau_g = 0$$



The Model for an Observation

$$X_{lj} = \mu + \tau_l + \epsilon_{lj}$$

where $\epsilon_{lj} \sim \mathcal{N}(0, \sigma^2)$ and independent.

- ▶ ϵ_{lj} is “random error”.
- ▶ We typically impose the condition $\sum_{l=1}^g \tau_l = 0$ as an **identification constraint**.
- ▶ The decomposition of an observation is

$$\underbrace{X_{lj}}_{\text{observation}} = \underbrace{\bar{X}}_{\text{overall sample mean}} + \underbrace{(\bar{X}_l - \bar{X})}_{\text{estimated treatment effect}} + \underbrace{(X_{lj} - \bar{X}_l)}_{\text{residual “error”}}$$

- ▶ \bar{X} is the estimator of μ
- ▶ $\hat{\tau}_l = (\bar{X}_l - \bar{X})$ is the estimator of τ_l
- ▶ $(X_{lj} - \bar{X}_l)$ is the estimator of ϵ_{lj} .



The Sums of Squares

The sum of squared observations

$$SS_{obs} = SS_{total} = \sum_{l=1}^g \sum_{j=1}^{n_l} X_{lj}^2$$

We also take the three components of X_{lj} and form sums of squares

$$SS_{mean} = \sum_{l=1}^g \sum_{j=1}^{n_l} \bar{X}^2 = \left(\sum_{l=1}^g n_l \right) \bar{X}^2$$

$$SS_{treatment} = \sum_{l=1}^g \sum_{j=1}^{n_l} \hat{\tau}_l^2 = \sum_{l=1}^g \sum_{j=1}^{n_l} (\bar{X}_l - \bar{X})^2 = \sum_{l=1}^g n_l (\bar{X}_l - \bar{X})^2$$

$$SS_{res} = \sum_{l=1}^g \sum_{j=1}^{n_l} \hat{\epsilon}_{lj}^2 = \sum_{l=1}^g \sum_{j=1}^{n_l} (X_{lj} - \bar{X}_l)^2$$



Sums of Squared Decomposition & Geometry

$$SS_{obs} = SS_{mean} + SS_{tr} + SS_{res}$$

or

$$SS_{corrected} = SS_{obs} - SS_{mean} = SS_{tr} + SS_{res}$$

This works because the components (sums of squares) are orthogonal.

Geometry: Consider the $n = (\sum_{l=1}^g n_l)$ dimensional **observation space** where each observation defines a dimension.

- ▶ We break this space into three orthogonal sub-spaces corresponding to each component.
- ▶ The dimensionality of the sub-space corresponds to the degrees of freedom for the corresponding SS .

(see text for more details).



ANOVA Summary Table

Let $n_+ = \sum_{l=1}^g n_l$, the total sample size

Source of Variation	Sum of Squares	df
Treatment	$SS_{tr} = (\sum_{l=1}^g n_l) \bar{X}_l^2$	$g - 1$
Residual	$SS_{res} = \sum_{l=1}^g \sum_{j=1}^{n_l} (X_{lj} - \bar{X}_l)^2$	$n_+ - g$
Total (corrected for mean)	$(SS_{obs} - SS_{mean})$ $= \sum_{l=1}^g \sum_{j=1}^{n_l} (X_{lj} - \bar{X})^2$	$n_+ - 1$

Test statistic for $H_o : \mu_1 = \dots = \mu_g$ (or $H_o : \tau_1 = \dots = \tau_g$) and its sampling distribution are

$$F = \frac{SS_{tr}/(g-1)}{SS_{res}/(n_+ - g)} \sim \mathcal{F}_{(g-1), (n_+ - g)}$$

Reject H_o for

- ▶ “large” values of SS_{tr}/SS_{res} .
- ▶ “large” values of $1 + SS_{tr}/SS_{res}$.
- ▶ “small” values of $(1 + SS_{tr}/SS_{res})^{-1} = \frac{SS_{res}}{SS_{tr} + SS_{res}}$



One-Way ANOVA as a GLM

$$\begin{pmatrix} X_{11} \\ \vdots \\ X_{1n_1} \\ X_{21} \\ \vdots \\ X_{2n_2} \\ \vdots \\ X_{g1} \\ \vdots \\ X_{gn_g} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & -1 & -1 & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & -1 & -1 & \cdots & -1 \end{pmatrix} \begin{pmatrix} \mu \\ \tau_1 \\ \vdots \\ \tau_1 \\ \tau_2 \\ \vdots \\ \tau_2 \\ \vdots \\ \tau_{g-1} \\ \vdots \\ \tau_{g-1} \end{pmatrix} + \begin{pmatrix} \epsilon_{11} \\ \vdots \\ \epsilon_{1n_1} \\ \epsilon_{21} \\ \vdots \\ \epsilon_{2n_2} \\ \vdots \\ \epsilon_{g1} \\ \vdots \\ \epsilon_{gn_g} \end{pmatrix}$$

$\underbrace{\mathbf{X}_{n_+ \times 1}}$ "Dependent" = $\underbrace{\mathbf{A}_{n_+ \times g}}$ Design Matrix $\underbrace{\boldsymbol{\beta}_{g \times 1}}$ Parameters + $\underbrace{\boldsymbol{\epsilon}_{n_+ \times 1}}$ Residuals



Least Squares Estimates of GLM

How we get parameter estimates depends on how the design matrix is set up. There are multiple ways of setting up the design matrix. We'll use the rank g matrix \mathbf{A} on the previous slide.

$$\begin{aligned}\hat{\boldsymbol{\beta}} &= (\mathbf{A}'\mathbf{A})^{-1}\mathbf{A}'\mathbf{X} \\ \hat{\mathbf{x}} &= \mathbf{A}\hat{\boldsymbol{\beta}} = \{\bar{\mathbf{x}}_I\}_{n_+ \times 1} \\ \hat{\boldsymbol{\epsilon}} &= \mathbf{X} - \hat{\mathbf{X}} \\ &= \mathbf{X} - \mathbf{A}(\mathbf{A}'\mathbf{A})^{-1}\mathbf{A}'\mathbf{X} \\ &= (\mathbf{I} - \mathbf{A}(\mathbf{A}'\mathbf{A})^{-1}\mathbf{A}')\mathbf{X}\end{aligned}$$

Our hypothesis test of equal population means,

$$H_o : \mu_1 = \mu_2 = \cdots = \mu_g \Leftrightarrow \tau_1 = \tau_2 = \cdots = \tau_g = 0$$

can be expressed as $H_o : \mathbf{C}\boldsymbol{\beta} = \mathbf{0}$ where \mathbf{C} is a contrast matrix.



Testing Using C

For example,

$$C_{(g-1) \times g} = \begin{pmatrix} 0 & 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -1 \end{pmatrix}$$

So

$$H_o : C\beta = \mathbf{0} = \begin{pmatrix} \tau_1 - \tau_2 \\ \tau_2 - \tau_3 \\ \vdots \\ \tau_{g-2} - \tau_{g-1} \end{pmatrix}$$

Our F -test (given before) tests $H_o : C\beta = \mathbf{0}$.

- ▶ From GLM framework, you can introduce “continuous” (numerical) variables.
- ▶ ANOVA and multiple regression are essentially the same.
- ▶ We can generalize the GLM to the multivariate GLM.
- ▶ SAS PROC GLM will make more sense.



One-Way MANOVA

MANOVA model for comparing g population mean vectors parallels univariate ANOVA:

$$\underbrace{\begin{pmatrix} \mathbf{X}_{lj} \\ \text{observation} \\ \text{vector} \\ p \times 1 \end{pmatrix}}_{\text{Random}} = \underbrace{\begin{pmatrix} \boldsymbol{\mu} \\ \text{overall} \\ \text{mean} \\ \text{vector} \\ p \times 1 \end{pmatrix}}_{\text{Fixed}} + \underbrace{\begin{pmatrix} \boldsymbol{\tau}_l \\ l^{\text{th}} \text{ treatment} \\ \text{effect vector} \\ p \times 1 \end{pmatrix}}_{\text{Fixed}} + \underbrace{\begin{pmatrix} \epsilon_{lj} \\ \text{residual for} \\ l^{\text{th}} \text{ group,} \\ j^{\text{th}} \text{ case} \\ p \times 1 \end{pmatrix}}_{\text{Random}}$$

where $\epsilon_{lj} \sim \mathcal{N}_p(\mathbf{0}, \boldsymbol{\Sigma})$ and all independent.

for $j = 1, \dots, n_l$ cases per group, and $l = 1, \dots, g$ groups.

For Identification, $\sum_{l=1}^g n_l \boldsymbol{\tau}_l = \mathbf{0}$.



Observation Vectors

Each component of \mathbf{X}_{lj} satisfies the 1-way ANOVA model, but now the model includes covariances among the component parts.

The covariances are assumed to be equal across populations.

A vector of observations can be decomposed as

$$\begin{aligned}
 \begin{pmatrix} \mathbf{X}_{lj} \\ \text{(Observation)} \end{pmatrix} &= \begin{pmatrix} \bar{\mathbf{X}} \\ \text{overall} \\ \text{sample} \\ \text{mean} \end{pmatrix} + \begin{pmatrix} (\bar{\mathbf{X}}_l - \bar{\mathbf{X}}) \\ \text{estimated} \\ \text{treatment} \\ \text{effect} \end{pmatrix} + \begin{pmatrix} (\mathbf{X}_{lj} - \bar{\mathbf{X}}_l) \\ \text{(residual)} \end{pmatrix} \\
 &= \hat{\boldsymbol{\mu}} + \hat{\boldsymbol{\tau}}_l + \hat{\boldsymbol{\epsilon}}_{lj}
 \end{aligned}$$

We also have a decomposition of **sums-of-squares** and **crossproducts**, or “SSCP” for short.



Sums-of-Squares and Cross-Products (SSCP)

First we'll find the total corrected squares and cross-products.

$$\begin{aligned}
 (\mathbf{x}_{lj} - \bar{\mathbf{x}})(\mathbf{x}_{lj} - \bar{\mathbf{x}})' &= [(\mathbf{x}_{lj} - \bar{\mathbf{x}}_l) + (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})] [(\mathbf{x}_{lj} - \bar{\mathbf{x}}_l) + (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})]' \\
 &= \underbrace{(\mathbf{x}_{lj} - \bar{\mathbf{x}}_l)(\mathbf{x}_{lj} - \bar{\mathbf{x}}_l)' + (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})(\bar{\mathbf{x}}_l - \bar{\mathbf{x}})'}_{\text{squares \& cross-products}} \\
 &\quad + \underbrace{(\mathbf{x}_{lj} - \bar{\mathbf{x}}_l)(\bar{\mathbf{x}}_l - \bar{\mathbf{x}})' + (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})(\mathbf{x}_{lj} - \bar{\mathbf{x}}_l)'}_{\text{cross-products}}
 \end{aligned}$$

Next sum all of this over cases and groups.

Since addition is distributive, we'll do this in pieces looking just at cross-product first. . .



Sum of Cross-Products

$$\begin{aligned}
 \sum_{j=1}^{n_l} (\mathbf{x}_{lj} - \bar{\mathbf{x}}_l)(\bar{\mathbf{x}}_l - \bar{\mathbf{x}})' &= \left(\sum_{j=1}^{n_l} (\mathbf{x}_{lj} - \bar{\mathbf{x}}_l) \right) (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})' \\
 &= \left(\left(\sum_{j=1}^{n_l} \mathbf{x}_{lj} \right) - n_l \bar{\mathbf{x}}_l \right) (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})' \\
 &= \underbrace{n_l (\bar{\mathbf{x}}_l - \bar{\mathbf{x}}_l)}_{\mathbf{0}} (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})' = \mathbf{0}
 \end{aligned}$$



Sum of Squares

Now summing the rest over j and l we get

$$\sum_{l=1}^g \sum_{j=1}^{n_l} (\mathbf{x}_{lj} - \bar{\mathbf{x}})(\mathbf{x}_{lj} - \bar{\mathbf{x}})' = \sum_{l=1}^g n_l (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})(\bar{\mathbf{x}}_l - \bar{\mathbf{x}})' + \sum_{l=1}^g \sum_{j=1}^{n_l} (\mathbf{x}_{lj} - \bar{\mathbf{x}}_l)(\mathbf{x}_{lj} - \bar{\mathbf{x}}_l)'$$

Total (corrected) SSCP	=	Treatment	+	Residual
	=	<u>B</u> etween Groups	+	<u>W</u> ithin Groups
	=	<u>H</u> ypothesis	+	<u>E</u> rror



A Closer Look at Within Groups SSCP

$$\begin{aligned}
 \mathbf{W} = \mathbf{E} &= \sum_{l=1}^g \sum_{j=1}^{n_l} (\mathbf{x}_{lj} - \bar{\mathbf{x}}_l)(\mathbf{x}_{lj} - \bar{\mathbf{x}}_l)' \\
 &= \sum_{j=1}^{n_1} (\mathbf{x}_{1j} - \bar{\mathbf{x}}_1)(\mathbf{x}_{1j} - \bar{\mathbf{x}}_1)' + \sum_{j=1}^{n_2} (\mathbf{x}_{2j} - \bar{\mathbf{x}}_2)(\mathbf{x}_{2j} - \bar{\mathbf{x}}_2)' \\
 &\quad \cdots + \sum_{j=1}^{n_g} (\mathbf{x}_{gj} - \bar{\mathbf{x}}_g)(\mathbf{x}_{gj} - \bar{\mathbf{x}}_g)' \\
 &= \mathbf{W}_1 + \mathbf{W}_2 + \cdots + \mathbf{W}_g \\
 &= (n_1 - 1)\mathbf{S}_1 + (n_2 - 1)\mathbf{S}_2 + \cdots + (n_g - 1)\mathbf{S}_g
 \end{aligned}$$

\mathbf{S}_l is the sample covariance matrix for the l^{th} group (treatment, condition, etc).

\mathbf{W} (“ \mathbf{E} ”) is proportional to a pooled estimated of the common Σ .



Between Groups SSCP & Test Statistic

With respect to between groups SSCP,

$$\mathbf{B} = \mathbf{H} = \sum_{l=1}^g n_l (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})(\bar{\mathbf{x}}_l - \bar{\mathbf{x}})' = \sum_{l=1}^g n_l \hat{\boldsymbol{\tau}}_l \hat{\boldsymbol{\tau}}_l'$$

- ▶ If $H_0 : \boldsymbol{\tau}_1 = \boldsymbol{\tau}_2 = \dots = \boldsymbol{\tau}_g = \mathbf{0}$ is true, Then \mathbf{B} (or “ \mathbf{H} ”) should be “close” to $\mathbf{0}$.
- ▶ To test H_0 , we consider the ratio of **generalized SSCPs**,

$$\Lambda^* = \frac{|\mathbf{W}|}{|\mathbf{W} + \mathbf{B}|} = \frac{|\mathbf{W}|}{|\mathbf{T}|}$$

where $\mathbf{T} = \mathbf{W} + \mathbf{B}$ (i.e., the total corrected SSCP).

- ▶ Λ^* is known as “Wilk’s Lambda”.
- ▶ It’s equivalent to likelihood ratio statistic.



Hypothesis Testing with Λ^*

Λ^* is a ratio of generalized sampling variances

$$\Lambda^* = \frac{|\mathbf{W}|}{|\mathbf{T}|} = \frac{\prod_{i=1}^p \lambda_i}{\prod_{i=1}^p \lambda_i^*}$$

- ▶ Where λ_i 's are eigenvalues of \mathbf{W} , and λ_i^* 's are eigenvalues of \mathbf{T} .
- ▶ If $H_0 : \tau_1 = \tau_2 = \dots = \tau_g = \mathbf{0}$ is **true** then \mathbf{B} is close to $\mathbf{0}$
 - ▶ $\implies \mathbf{T} \approx \mathbf{W}$
 - ▶ $\implies \lambda_i \approx \lambda_i^*$
 - ▶ $\implies \Lambda^*$ close to 1.
- ▶ If $H_0 : \tau_1 = \tau_2 = \dots = \tau_g = \mathbf{0}$ is **false** then \mathbf{B} is not close $\mathbf{0}$
 - ▶ \implies values on diagonals of \mathbf{T} , which will be positive, will be large.
 - ▶ $\implies \lambda_i < \lambda_i^*$
 - ▶ $\implies \Lambda^*$ is "small".
- ▶ The exact **distribution of Λ^*** can be derived for special cases of p and g .



Distribution of Wilk's Lambda Λ^*

$$\text{Wilk's } \Lambda^* = \frac{|SSCP_e|}{|SSCP_e + SS CP_h|}$$

Number variables	<i>df</i> for Hypothesis	Sampling distribution for multivariate data
$p = 1$	$\nu_h \geq 1$	$\left(\frac{\nu_e}{\nu_h}\right) \left(\frac{1-\Lambda^*}{\Lambda^*}\right) \sim \mathcal{F}_{\nu_h, \nu_e}$
$p = 2$	$\nu_h \geq 1$	$\left(\frac{\nu_e-1}{\nu_h}\right) \left(\frac{1-\sqrt{\Lambda^*}}{\sqrt{\Lambda^*}}\right) \sim \mathcal{F}_{2\nu_h, 2(\nu_e-1)}$
$p \geq 1$	$\nu_h = 1$	$\left(\frac{\nu_e+\nu_h-p}{p}\right) \left(\frac{1-\Lambda^*}{\Lambda^*}\right) \sim \mathcal{F}_{p, (\nu_e+\nu_h-p)}$
$p \geq 2$	$\nu_h = 2$	$\left(\frac{\nu_e+\nu_h-p-1}{p}\right) \left(\frac{1-\sqrt{\Lambda^*}}{\sqrt{\Lambda^*}}\right) \sim \mathcal{F}_{2p, 2(\nu_e+\nu_h-p-1)}$

where ν_h = degrees of freedom for hypothesis, and

ν_e = degrees of freedom for error (residual).



Other Test Statistics

There are more than one way to combine the information in \mathbf{B} and \mathbf{W} (or \mathbf{H} and \mathbf{E}).

- ▶ Wilk's Λ^*

$$\Lambda^* = \frac{|\mathbf{W}|}{|\mathbf{W} + \mathbf{B}|} = \frac{|\mathbf{E}|}{|\mathbf{E} + \mathbf{H}|} = \frac{\prod_{i=1}^p \lambda_i}{\prod_{i=1}^p \lambda_i^*}$$

where λ_i are eigenvalues of \mathbf{E} , and λ_i^* are eigenvalues of $(\mathbf{E} + \mathbf{H})$.

- ▶ Hotelling-Lawley Trace Criteria

$$= \text{trace}(\mathbf{E}^{-1}\mathbf{H}) = \text{tr}(\mathbf{H}\mathbf{E}^{-1}) = \sum_{i=1}^g \tilde{\lambda}_i$$

where $\tilde{\lambda}_i$ is eigenvalue of $\mathbf{H}\mathbf{E}^{-1}$.

- ▶ Reject H_o when $\text{tr}(\mathbf{H}\mathbf{E}^{-1})$ is large.
- ▶ When H_o is true, $\text{tr}(\mathbf{H}\mathbf{E}^{-1}) \sim \chi_{p(g-1)}^2$.
- ▶ Note: $df = \text{rank of design matrix (GLM approach)}$.



Pillai's Trace and Roy's Largest Root

► Pillai's Trace Criterion

$$= \text{trace}(\mathbf{B}(\mathbf{B} + \mathbf{W})^{-1}) = \text{trace}(\mathbf{H}(\mathbf{H} + \mathbf{E})^{-1}) = \sum_{i=1}^p \frac{\tilde{\lambda}_i}{1 + \tilde{\lambda}_i}$$

where $\tilde{\lambda}_i$ is the eigenvalue (root) of $\mathbf{H}\mathbf{E}^{-1}$.

► Roy's Largest Root Criterion

$$\begin{aligned} \theta &= \text{largest root of } (\mathbf{E} + \mathbf{H})^{-1}\mathbf{H} \\ &= \text{largest root of } \mathbf{H}(\mathbf{E} + \mathbf{H})^{-1} \\ &= \left(\frac{\tilde{\lambda}_1}{1 + \tilde{\lambda}_1} \right) \end{aligned}$$

where $\tilde{\lambda}_1$ is the largest root of $\mathbf{E}^{-1}\mathbf{H} = \mathbf{H}\mathbf{E}^{-1}$.



How They are All Related to Wilk's Λ^*

Let $\tilde{\lambda}_i$ be root of \mathbf{HE}^{-1} ("eigenvalue of \mathbf{H} relative to \mathbf{E} ") and if all $\tilde{\lambda}_i$'s > 0 (i.e., $\tilde{\lambda}_1 \geq \tilde{\lambda}_2 \geq \dots \geq \tilde{\lambda}_p \geq 0$),

Then we can write

$$\begin{aligned}
 \Lambda^* &= \frac{|\mathbf{E}|}{|\mathbf{E} + \mathbf{H}|} = \frac{|\mathbf{E}|}{|\mathbf{E}||\mathbf{I}_p + \mathbf{E}^{-1}\mathbf{H}|} \\
 &= \frac{|\mathbf{E}||\mathbf{E}|^{-1}}{|\mathbf{I}_p + \mathbf{HE}^{-1}|} \\
 &= \frac{1}{|\mathbf{I} + \mathbf{HE}^{-1}|} \quad \text{because various theorems} \\
 &= \frac{1}{\prod_{i=1}^p (1 + \tilde{\lambda}_i)}
 \end{aligned}$$

So Λ^* is a decreasing function of $\tilde{\lambda}_i$.



Which Test Statistic to Use

- ▶ Wilk's Λ^* = likelihood ratio statistic.
- ▶ If all statistics lead to the same conclusion, use Λ^* .
- ▶ If statistics lead to different conclusion, need to figure out why.
- ▶ From Simulation studies (power & robustness):
 - ▶ Roy's largest root found to be the least useful, except when the population structure is such that groups differ in one dimension and one group is much more different from the rest.
 - ▶ Others all do pretty good w/rt power (they use more information in **E** and **H** than Roy's).
 - ▶ Pillai's trace criterion is
 - ▶ Least affected by departures from usual population model (i.e., more robust against departures from normality).
 - ▶ Better for "diffuse" alternative hypotheses versus sharper ones.
 - ▶ When roots are approximately equal, it has best power.
 - ▶ Wilk's and Hotwelling-Lawley have about the same power for a wider-range (spectrum) of alternative hypotheses.



Other Cases and Summary MANOVA

For cases not covered. . . If H_o is true and $\sum_{l=1}^g n_l = n$ is **Large**, then

$$-\ln \Lambda^* \left(n - 1 - \frac{1}{2}(p + g) \right) = \left(\frac{|\mathbf{W}|}{|\mathbf{B} + \mathbf{W}|} \right) \left(n - 1 - \frac{1}{2}(p + g) \right) \approx \chi_{p(g-1)}^2$$

You should examine the residual vectors for normality and outliers (i.e., $\hat{\epsilon}_{jl}$'s) . . . maybe use PCA or methods mentioned in the text.

Source of variation	SSCP	df	Wilk's Λ^*
Treatment (Between)	$\mathbf{B} = \sum_{l=1}^g n_l (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})(\bar{\mathbf{x}}_l - \bar{\mathbf{x}})'$	$g - 1$	$\frac{ \mathbf{W} }{ \mathbf{T} }$
Residual (Within)	$\mathbf{W} = \sum_{l=1}^g \sum_{j=1}^{n_l} (\mathbf{x}_{jl} - \bar{\mathbf{x}}_l)(\mathbf{x}_{jl} - \bar{\mathbf{x}}_l)'$	$n - g$	
Total (corrected for mean)	$\mathbf{T} = \mathbf{W} + \mathbf{B}$ $= \sum_{l=1}^g \sum_{j=1}^{n_l} (\mathbf{x}_{jl} - \bar{\mathbf{x}})(\mathbf{x}_{jl} - \bar{\mathbf{x}})'$	$n - 1$	



Example 1: Distributed vs Massed Practice

1-Way MANOVA: Data from Tatsuoka (1988), *Multivariate Analysis: Techniques for Educational and Psychological Research*, pp 273–279.

(up-dated story) An experiment was conducted for comparing 2 methods (A & B) of teaching computer programming to 60 female seniors in a technical training high school program. Also of interest were the effects of distributed versus massed practice

C_1 : 2 hours of instruction/day for 6 weeks

C_2 : 3 hours of instruction/day for 4 weeks

C_3 : 4 hours of instruction/day for 3 weeks

Each subject received a total of 12 hours of instruction. For now, we'll just look the effect of distributed versus massed practice.

Note: $n_l = 20$ for $l = 1, 2, 3$

Two variables (dependent measures):

$X_1 = \text{speed}$ and $X_2 = \text{accuracy}$



Descriptive Statistics

The overall mean vector and mean vectors for each condition:

$$\bar{\mathbf{x}} = \begin{pmatrix} 33.62 \\ 18.25 \end{pmatrix} \quad \bar{\mathbf{x}}_1 = \begin{pmatrix} 38.55 \\ 23.70 \end{pmatrix} \quad \bar{\mathbf{x}}_2 = \begin{pmatrix} 34.00 \\ 18.20 \end{pmatrix} \quad \bar{\mathbf{x}}_3 = \begin{pmatrix} 28.30 \\ 12.85 \end{pmatrix}$$

The treatment effect vectors (i.e., $\hat{\boldsymbol{\tau}}_i = \bar{\mathbf{x}}_i - \bar{\mathbf{x}}$)

$$\hat{\boldsymbol{\tau}}_1 = \begin{pmatrix} 4.93 \\ 5.45 \end{pmatrix} \quad \hat{\boldsymbol{\tau}}_2 = \begin{pmatrix} 0.38 \\ -0.05 \end{pmatrix} \quad \hat{\boldsymbol{\tau}}_3 = \begin{pmatrix} -5.32 \\ -5.40 \end{pmatrix}$$

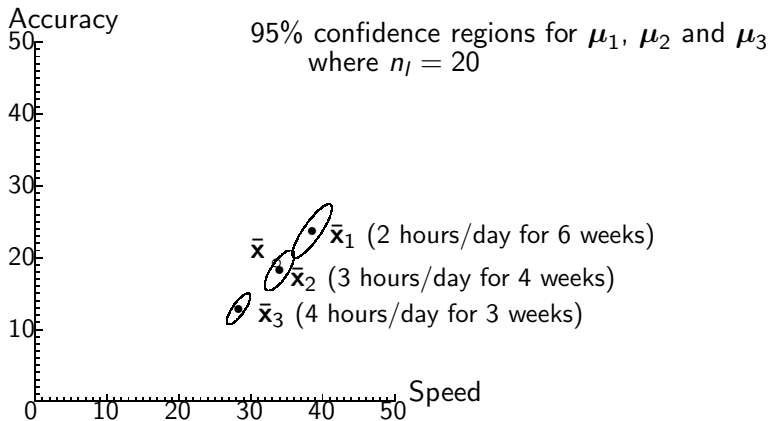
Sample covariance matrices:

$$\mathbf{S}_1 = \begin{pmatrix} 49.52 & 13.17 \\ 13.17 & 7.59 \end{pmatrix} \quad \mathbf{S}_2 = \begin{pmatrix} 27.47 & 4.21 \\ 4.21 & 4.48 \end{pmatrix}$$

$$\mathbf{S}_3 = \begin{pmatrix} 16.33 & 4.42 \\ 4.42 & 3.19 \end{pmatrix}$$



Means and Confidence Regions





Hypothesis Test

No difference between massed versus distributed practice on either speed or accuracy:

$$H_o : \tau_1 = \tau_2 = \tau_3 = \mathbf{0} \quad \text{versus} \quad H_a : \tau_l \neq \mathbf{0} \quad \text{for all } l = 1, 2, 3$$

The within groups (residual) sums of squares and cross-products matrix

$$\begin{aligned} \mathbf{W} &= (n_1 - 1)\mathbf{S}_1 + (n_2 - 1)\mathbf{S}_2 + (n_3 - 1)\mathbf{S}_3 \\ &= 19 \begin{pmatrix} 49.52 & 13.17 \\ 13.17 & 7.59 \end{pmatrix} + 19 \begin{pmatrix} 27.47 & 4.21 \\ 4.21 & 4.48 \end{pmatrix} \\ &\quad + 19 \begin{pmatrix} 16.33 & 4.42 \\ 4.42 & 3.19 \end{pmatrix} \\ &= \begin{pmatrix} 1773.15 & 414.20 \\ 414.20 & 289.95 \end{pmatrix} \end{aligned}$$



Hypothesis Test continued

The between groups SSCP matrix:

$$\begin{aligned}
 \mathbf{B} &= \sum_{l=1}^3 n_l (\bar{\mathbf{x}}_l - \bar{\mathbf{x}})(\bar{\mathbf{x}}_l - \bar{\mathbf{x}})' \\
 &= 20 \begin{pmatrix} 4.93 \\ 5.45 \end{pmatrix} (4.93, 5.45) + 20 \begin{pmatrix} 0.38 \\ -0.05 \end{pmatrix} (0.38, -0.05) \\
 &\quad + 20 \begin{pmatrix} -5.32 \\ -5.40 \end{pmatrix} (-5.32, -5.40) \\
 &= \begin{pmatrix} 1055.033 & 1111.55 \\ 1111.55 & 1177.30 \end{pmatrix}
 \end{aligned}$$

$$\mathbf{T} = \mathbf{W} + \mathbf{B} = \begin{pmatrix} 2828.18 & 1525.75 \\ 1525.75 & 1467.25 \end{pmatrix}$$

Or $\mathbf{T} = (n - 1)\mathbf{S}$ where \mathbf{S} is the covariance matrix computed over all groups and n is the total sample. Then $\mathbf{B} = \mathbf{T} - \mathbf{W}$.



Test Statistic & Distribution

$$|\mathbf{W}| = (1773.15)(289.95) - (414.20)^2 = 342563.2$$

$$|\mathbf{T}| = (2828.18)(1467.25) - (1525.75)^2 = 1821738.9$$

$$\Lambda^* = \frac{|\mathbf{W}|}{|\mathbf{T}|} = \frac{342563.2}{1821738.9} = 0.188$$

For $p = 2$ and $g = 3$, we can use the exact sample distribution:

$$\left(\frac{n-g-1}{g-1} \right) \left(\frac{1-\sqrt{\Lambda^*}}{\sqrt{\Lambda^*}} \right) = \left(\frac{n-p-2}{p} \right) \left(\frac{1-\sqrt{\Lambda^*}}{\sqrt{\Lambda^*}} \right) \sim \mathcal{F}_{2(g-1), 2(n-g)}$$



Test Statistic & Distribution

For this example,

$$\frac{(60 - 3 - 1)}{(3 - 1)} \left(\frac{1 - \sqrt{.188}}{\sqrt{.188}} \right) = \frac{56}{2} \left(\frac{.566}{.434} \right) = 36.568$$

Since $\mathcal{F}_{4,112}(\alpha = .05) \sim \mathcal{F}_{4,120}(\alpha = .05) = 2.45$, reject H_0 that treatment vectors are all equal to $\mathbf{0}$.

The data support the conclusion that there is an effect of massed versus distributed. practice.



Following up a Significant Result

- ▶ Multivariate contrasts & confidence regions
- ▶ “Tests” on individual variables (simultaneous confidence intervals for group/treatment differences).
- ▶ Discriminant Analysis.

Multivariate Contrasts

- ▶ We need the multivariate generalization of the general linear model:

$$\mathbf{X}_{gn \times p} = \mathbf{A}_{gn \times (g+1)} \mathbf{B}_{(g+1) \times p} + \mathcal{E}_{gn \times p}$$

where \mathbf{A} is the design matrix (it could have g or $g + 1$ columns depending on the parameterization), and \mathbf{B} is a matrix of coefficients (model parameters). . . some examples. . .



A is $n_+ \times g$ with dummy codes

$$\mathbf{X}_{n_+ \times p} = \begin{pmatrix} 1 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix} \begin{pmatrix} \beta_{o1} & \beta_{o2} & \cdots & \beta_{op} \\ \beta_{11} & \beta_{12} & \cdots & \beta_{1p} \\ \beta_{21} & \beta_{22} & \cdots & \beta_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{g-1,1} & \beta_{g-1,2} & \cdots & \beta_{g-1,p} \end{pmatrix} + \mathcal{E}_{n_+ \times p}$$

Given the design matrix above, $\beta_{ok} = \mu_{gk}$, and $\beta_{lk} = \mu_{lk} - \mu_{gk}$.

If $p = 1$, we would have 1-way ANOVA.



SAS PROC GLM design: A is $gn \times (g + 1)$

An alternative design matrix and parameter vector:

$$\mathbf{X}_{n_+ \times p} = \begin{pmatrix} 1 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \cdots & 1 \end{pmatrix} \begin{pmatrix} \beta_{o1} & \beta_{o2} & \cdots & \beta_{op} \\ \beta_{11} & \beta_{12} & \cdots & \beta_{1p} \\ \beta_{21} & \beta_{22} & \cdots & \beta_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{g-1,1} & \beta_{g-1,2} & \cdots & \beta_{g-1,p} \\ \beta_{g,1} & \beta_{g,2} & \cdots & \beta_{g,p} \end{pmatrix} + \mathcal{E}_{n_+ \times p}$$

$n_+ \times (g+1)$

Normally, $\hat{\beta} = (\mathbf{A}'\mathbf{A})^{-1}\mathbf{A}'\mathbf{X}$; however, the rank of \mathbf{A} defined above (and hence $\mathbf{A}'\mathbf{A}$) is only g

\Rightarrow There's no unique solution to $\mathbf{A}'\mathbf{X} = \mathbf{A}'\mathbf{A}\beta$.



What's Interesting

We're interested in differences between group means; that is,

$$\mu_i - \mu_k = (\mu + \tau_i)_{p \times 1} - (\mu + \tau_k)_{p \times 1} = \tau_i - \tau_k$$

Even if we can't get unique estimates of elements of \mathcal{B} , we can get unique estimates of differences between parameter estimates, which correspond to differences between group means regardless of what inverse of $(\mathbf{A}'\mathbf{A})$ is used.

Moore-Penrose inverses of non-full rank square matrix $(\mathbf{A}'\mathbf{A})$ is denoted by $(\mathbf{A}'\mathbf{A})^-$.

SAS PROC GLM uses the Moore-Penrose inverse of $(\mathbf{A}'\mathbf{A})$.

In SAS/PROC IML, the Moore-Penrose inverse is obtained by the command `ginv()`, for example

```
giAA = ginv(A'*A);
```



Estimable and Testable

What we can do is test linear combinations of elements of \mathcal{B} if the linear combination is a **contrast**.

- ▶ **Estimable**: A linear function $\mathbf{c}'\mathcal{B}$ is estimable if

$$(\mathbf{A}'\mathbf{A})(\mathbf{A}'\mathbf{A})^{-}\mathbf{c} = \mathbf{c}.$$

- ▶ **Testable**: A linear function is testable if it only involves the estimable **functions** of \mathcal{B} .
- ▶ Contrasts of elements of \mathcal{B} are estimable and therefore testable. These correspond to differences between means.
- ▶ We'll demonstrate multivariate General linear model by example. . .



Example: Cameron & Pauling Data

Increase in survival of cancer patients given supplemental treatment with vitamin C.

“Increase in survival” = the number of days a patient survives minus the number of days matched control survives.

- ▶ $x_1 = d_1$ = increase in survival measured as days from first hospitalization.
- ▶ $x_2 = d_2$ = increase in survival measured days from un-treatability.
- ▶ type = type of cancer (1 =stomach, 2 =bronchus, 3 =colon, 4 =rectum, 5 =bladder, 6 =kidney).



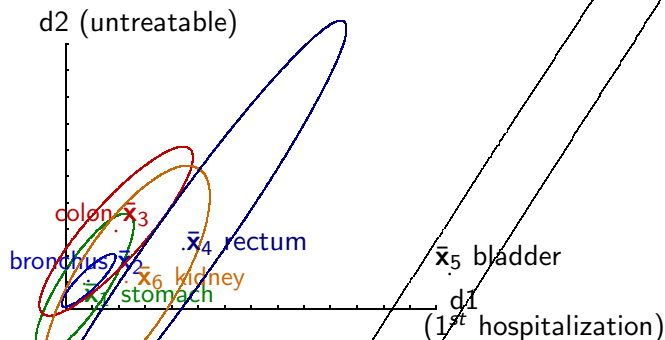
Example: Descriptive statistics

l	Type	n_l	$\bar{\mathbf{x}}_l = \bar{\mathbf{d}}_l$	\mathbf{S}_l	
1	Stomach	12	70.67	125869.88	15206.70
			94.92	15206.70	12235.36
2	Bronchus	16	49.50	23915.07	17461.47
			106.88	17461.47	16619.45
3	Colon	16	117.19	252027.76	147884.76
			293.19	147884.76	118274.56
4	Rectum	7	297.43	508715.62	155250.05
			226.57	155250.05	56340.62
5	Bladder	5	1304.20	3747663.20	214071.05
			129.80	214071.05	14697.70
6	Kidney	7	118.86	129018.48	3344.62
			101.71	3344.62	17392.91

$$S_{pool} = \sum_{l=1}^5 (n_l - 1) \mathbf{S}_l = \begin{pmatrix} 419668.42 & 76815.85 \\ 76815.85 & 45848.122 \end{pmatrix}$$



Plot of Means and 95% Confidence Regions

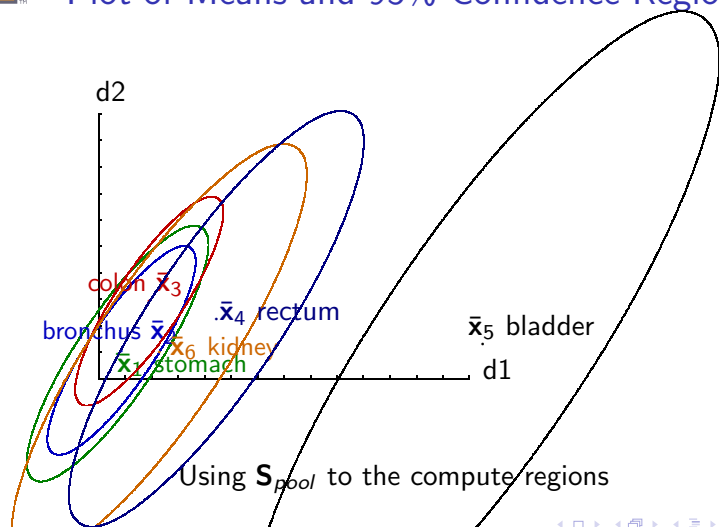


Using S_i to compute the regions

$$n_1 = 12, n_2 = 16, n_3 = 16, n_4 = 7, n_5 = 5, n_6 = 7$$



Plot of Means and 95% Confidence Regions





Results of MANOVA Hypothesis Test

$$H_0 : \mu_{stomach} = \mu_{bronchus} = \mu_{colon} = \mu_{rectum} = \mu_{bladder} = \mu_{kidney}$$

or equivalently

$$H_0 : \tau_{stomach} = \tau_{bronchus} = \tau_{colon} = \tau_{rectum} = \tau_{bladder} = \tau_{kidney}$$

- ▶ df type of cancer (hypothesis) $\nu_h = g - 1 = 6 - 1 = 5$
- ▶ df within (error) $= \nu_e = \sum_I n_I - g = 63 - 6 = 57$



Results of MANOVA Hypothesis Test continued

- ▶ Wilk's $\Lambda^* = \det(\mathbf{W}) / \det(\mathbf{T}) = 0.5817749$
- ▶ Since $p = 2$ dependent variables, Wilk's Λ^* has an exact sampling distribution that is \mathcal{F} , in particular

$$F = \left(\frac{(\nu_e - 1)}{\nu_h} \right) \left(\frac{1 - \sqrt{\Lambda^*}}{\sqrt{\Lambda^*}} \right) \sim \mathcal{F}_{2\nu_h, 2\nu_e}$$

- ▶ $F = 3.4838$ and $p\text{-value} = .0005$.
- ▶ Reject H_0 . The data support the conclusion that not all of the means (or τ 's are equal).



Estimated MANOVA parameters

$$\hat{\boldsymbol{\mu}} = \begin{pmatrix} 205.56 \\ 166.46 \end{pmatrix}$$

Type		hospitalization	untreatable
Stomach	$\hat{\tau}'_1 =$	(-134.888,	-71.543)
Bronchus	$\hat{\tau}'_2 =$	(156.055,	-59.585)
Colon	$\hat{\tau}'_3 =$	(-88.368,	126.727)
Rectum	$\hat{\tau}'_4 =$	(91.873,	60.111)
Bladder	$\hat{\tau}'_5 =$	(1098.644,	-36.660)
Kidney	$\hat{\tau}'_6 =$	(-86.698,	-64.746)

Recall that $\boldsymbol{\mu}_j = \boldsymbol{\mu} + \boldsymbol{\tau}_j$



MANOVA as a multivariate GLM

A main effect and six dummy variables (this is what PROC GLM does). So the design matrix looks like

$$\mathbf{A}_{n_+ \times 7} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{array}{l} \} n_{stomach} \\ \} n_{bronchus} \\ \} n_{colon} \\ \} n_{rectum} \\ \} n_{bladder} \\ \} n_{kidney} \end{array}$$

MANOVA (multivariate general linear model):

$$\mathbf{y}_{n_+ \times 2} = \mathbf{A}_{n_+ \times 7} \mathbf{B}_{7 \times 2} + \boldsymbol{\epsilon}_{n_+ \times 2}$$

$$\text{Estimation: } \mathbf{B} = (\mathbf{A}'\mathbf{A})^{-1} \mathbf{A}'\mathbf{y}$$

$$\text{Predicted values: } \hat{\mathbf{y}} = \mathbf{AB} \quad \text{where } \hat{\mathbf{y}}'_{jl} = (\bar{x}_{1l}, \bar{x}_{2l})'$$



MANOVA as a multivariate GLM (continued)

For $\hat{\mathbf{y}}'_{jl} = (\bar{x}_{1l}, \bar{x}_{2l})'$, it is the the case that

$$\bar{x}_{j1l} = b_{o1} + b_{l1} \quad \text{and} \quad \bar{x}_{j2l} = b_{o2} + b_{l2}$$

So to compare two groups (types of cancer),

$$\bar{x}_{il} - \bar{x}_{il^*} = (b_{oi} + b_{li}) - (b_{oi} + b_{l^*i}) = b_{li} - b_{l^*i}$$

Consider a contrast between means for two types of cancer, for example, stomach and bronchial,

$$\mathbf{c}'\mathbf{B} = (0, 1, -1, 0, 0, 0, 0) \begin{pmatrix} b_{o1} & b_{o2} \\ b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \\ b_{41} & b_{42} \\ b_{51} & b_{52} \\ b_{61} & b_{62} \end{pmatrix}$$



MANOVA as a multivariate GLM (continued)

$$\begin{aligned}\mathbf{c}'\mathbf{B} &= ((b_{11} - b_{21}), (b_{12} - b_{22})) \\ &= ((\bar{x}_{11} - \bar{x}_{21}), (\bar{x}_{12} - \bar{x}_{22}))\end{aligned}$$

$$H_o : \mathbf{c}'\mathbf{B} = \mathbf{0}$$



With the Parameter Estimates

$$\mathbf{B} = \begin{pmatrix} 326.31 & 158.84 \\ -255.64 & -63.93 \\ -276.81 & -51.97 \\ -209.12 & 134.34 \\ -28.88 & 67.73 \\ 977.89 & -29.04 \end{pmatrix}$$

$$\text{stomach: } \bar{x}_{11} = b_{o1} + b_{11} = 326.31 + (-255.64) = 70.67$$

$$\bar{x}_{12} = b_{o2} + b_{12} = 158.84 + (-63.93) = 94.91$$

$$\text{bronchus: } \bar{x}_{21} = b_{o1} + b_{21} = 326.31 + (-276.81) = 49.50$$

$$\bar{x}_{22} = b_{o2} + b_{22} = 158.84 + (-51.97) = 106.87$$

$$\begin{aligned} H_0 : (0, 1, -1, 0, 0, 0, 0)\mathbf{B} &= ((-255.64 + 276.81), (-63.93 - 51.97)) \\ &= (21.17, -11.96) = ((\bar{x}_{11} - \bar{x}_{21}), (\bar{x}_{12} - \bar{x}_{22})) = \mathbf{0}' \end{aligned}$$



Testing $H_0 : \mathbf{CBM} = \mathbf{0}$

Our hypothesis tests can be of the form

$$H_0 : \mathbf{C}_{r \times g} \mathbf{B}_{g \times p} \mathbf{M}_{p \times s} = \mathbf{0}_{r \times s}$$

- ▶ \mathbf{C} defines hypotheses (contrasts) on the elements of columns of \mathbf{B} ; that is, comparison between the means on the **same variables over groups**.
- ▶ \mathbf{M} defines hypotheses (contrasts) on the elements of rows of \mathbf{B} ; that is, comparison between the means on the **same group over variables**.

For now $\mathbf{M} = \mathbf{I}$ and we'll consider hypotheses of the form

$$H_0 : \mathbf{CB} = \mathbf{0}_{r \times p}$$

Specifically, we want to consider (for example)

$$H_0 : 0b_{0k} + c_1b_{1k} + c_2b_{2k} + \cdots + c_gb_{gk} \Leftrightarrow c_1\tau_1 + c_2\tau_2 + \cdots + c_g\tau_g$$

where $\sum_{l=1}^g c_l = 0$.



Testing Contrasts: The H matrix

For a simple contrast, such as

$$\mathbf{c} = (0, 1, -1, 0, \dots, 0),$$

we could do this as a multivariate T^2 test for independent groups; however, we'll stay within the MANOVA and multivariate linear model framework (so we can test multiple ones).

Suppose that we have a contrast matrix $\mathbf{C}_{r \times (g+1)}$ where the rows are r orthogonal contrasts, the hypothesis matrix equals

$$\mathbf{H} = (\mathbf{CB})'(\mathbf{C}(\mathbf{A}'\mathbf{A})^{-1}\mathbf{C}')^{-1}(\mathbf{CB})$$

For a balanced design (i.e., $n_1 = n_2 = \dots = n_g = n$) and a single contrast (i.e., $r = 1$), this reduces to

$$H = \frac{n}{\sum_{l=1}^g c_l} \left(\sum_{l=1}^g c_l \bar{\mathbf{x}}_l \right) \left(\sum_{l=1}^g c_l \bar{\mathbf{x}}_l \right)'$$



Testing Contrasts

The “Error” matrix is \mathbf{W} ; that is,

$$\begin{aligned}\mathbf{E} = \mathbf{W} &= \sum_{\ell=1}^g \sum_{j=1}^n (\mathbf{x}_j - \bar{\mathbf{x}}_{\ell})(\mathbf{x}_{j\ell} - \bar{\mathbf{x}}_{\ell})' \\ &= \mathbf{X}'\mathbf{X} - \mathbf{B}'(\mathbf{A}'\mathbf{A})\mathbf{B}\end{aligned}$$

Wilk's Lambda for the test $H_o : \mathbf{C}\mathbf{B} = \mathbf{0}$ is

$$\Lambda^* = \frac{\det(\mathbf{E})}{\det(\mathbf{H} + \mathbf{E})}.$$

To find the transformation of this to an \mathcal{F} distribution:

- ▶ $p =$ anything
- ▶ $\nu_{\text{hypothesis}} = r$
- ▶ $\nu_{\text{error}} = \sum_{\ell} n_{\ell} - p$



Example: Five types the same?

Three equivalent forms for Hypothesis 1:

$$H_o : \quad \boldsymbol{\mu}_{bronchus} = \boldsymbol{\mu}_{colon} = \boldsymbol{\mu}_{kidney} = \boldsymbol{\mu}_{rectum} = \boldsymbol{\mu}_{stomach}$$

$$H_o : \quad \boldsymbol{\tau}_{bronchus} = \boldsymbol{\tau}_{colon} = \boldsymbol{\tau}_{kidney} = \boldsymbol{\tau}_{rectum} = \boldsymbol{\tau}_{stomach}$$

$$H_o : \quad \boldsymbol{\beta}_{bronchus} = \boldsymbol{\beta}_{colon} = \boldsymbol{\beta}_{kidney} = \boldsymbol{\beta}_{rectum} = \boldsymbol{\beta}_{stomach}$$

where $\boldsymbol{\beta}_\ell$ is a $p \times 1$ column vector of \boldsymbol{B}' (i.e., a row of \boldsymbol{B} written as a column).

For the contrast matrix we need to know the order of the effects in the GLM.

- ▶ I re-order them so that they are in alphabetical order, because
- ▶ PROC GLM puts them in alphabetical order (or numerical if groups are coded this way).



H_0 : Four types the same?

$$H_0 : \mathbf{CB} = \mathbf{0} = \begin{pmatrix} 0 & 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \beta_{01} & \beta_{02} \\ \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \\ \beta_{31} & \beta_{32} \\ \beta_{41} & \beta_{42} \\ \beta_{51} & \beta_{52} \\ \beta_{61} & \beta_{61} \end{pmatrix} \begin{array}{l} \text{intercept} \\ \text{bladder} \\ \text{bronchus} \\ \text{colon} \\ \text{kidney} \\ \text{rectum} \\ \text{stomach} \end{array}$$

So

$$H_0 : \begin{pmatrix} (\beta_{21} - \beta_{31}) & (\beta_{22} - \beta_{32}) \\ (\beta_{21} - \beta_{41}) & (\beta_{22} - \beta_{42}) \\ (\beta_{21} - \beta_{51}) & (\beta_{22} - \beta_{52}) \\ (\beta_{21} - \beta_{61}) & (\beta_{22} - \beta_{62}) \end{pmatrix} = \begin{pmatrix} (\tau_{21} - \tau_{31}) & (\tau_{22} - \tau_{32}) \\ (\tau_{21} - \tau_{41}) & (\tau_{22} - \tau_{42}) \\ (\tau_{21} - \tau_{51}) & (\tau_{22} - \tau_{52}) \\ (\tau_{21} - \tau_{61}) & (\tau_{22} - \tau_{62}) \end{pmatrix} = \mathbf{0}$$



Hypothesis Matrices

$$\mathbf{H} = (\mathbf{CB})'(\mathbf{C}(\mathbf{A}'\mathbf{A})(ns + nb + nc + nr + nd + nk - 6)\mathbf{C}')^{-1}(\mathbf{CB})$$

$$\begin{pmatrix} 324369.92785 & 180717.48204 \\ 180717.48204 & 429243.40815 \end{pmatrix}$$

The \mathbf{E} error SSCP is the same as \mathbf{W} that we used before, which equals

$$\begin{aligned} \mathbf{E} = \mathbf{W} &= \mathbf{X}'\mathbf{X} - \mathbf{B}(\mathbf{A}'\mathbf{A})\mathbf{B}' \\ &= \begin{pmatrix} 24340768.476 & 4455319.3042 \\ 4455319.3042 & 2659191.047 \end{pmatrix} \end{aligned}$$

Wilk's Lambda,

$$\Lambda^* = \frac{\det(\mathbf{E})}{\det(\mathbf{H} + \mathbf{E})} = \frac{4.4877E13}{5.4684E13} = 0.820661$$



Results

- ▶ $\nu_h =$ number of rows of $\mathbf{C} = 4$
- ▶ $\nu_e =$ number of rows of $\mathbf{X} - p = 57$

Referring to the table for transformations of Λ^* that have sampling distributions that are \mathcal{F} , we use the one for $p = 2$ and $\nu_h \geq 1$, which is

$$F = \left(\frac{\nu_e - 1}{\nu_h} \right) \left(\frac{1 - \sqrt{\Lambda^*}}{\sqrt{\Lambda^*}} \right) = \left(\frac{56}{4} \right) \left(\frac{1 - \sqrt{0.820661}}{\sqrt{0.820661}} \right) = 1.4541861$$

If the null is true, then this should have a $\mathcal{F}_{2\nu_h, 2(\nu_e-1)}$ sampling distribution.

Comparing $F = 1.45$ to the $\mathcal{F}_{4,112}$, we find that the p -value is .18. Retain the null hypothesis. The data suggest no difference in increased survival of patients over different types of cancer (except bladder).



Five versus the Rest

$$H_o : \tau_{bladder} = (\tau_{bronchus} + \tau_{colon} + \tau_{kidney} + \tau_{rectum} + \tau_{stomach})/5$$

or equivalently

$$H_o : \mathbf{CB} = \mathbf{0} = (0, -5, 1, 1, 1, 1, 1)$$

(β_{01}	β_{02})	intercept
	β_{11}	β_{12}		bladder
	β_{21}	β_{22}		bronchus
	β_{31}	β_{32}		colon
	β_{41}	β_{42}		kidney
	β_{51}	β_{52}		rectum
	β_{61}	β_{61}		stomach

E is the same as before, but now

$$\mathbf{H} = \begin{pmatrix} 6266038.6574 & -186105.9247 \\ -186105.9247 & 5527.481893 \end{pmatrix}$$



The Test and Result

$$\Lambda^* = \frac{4.4877E13}{6.3332E13} = 0.7085934$$

- ▶ $\nu_e = \sum_{l=1}^g n_l - g = 57$.
- ▶ $\nu_h = 1$, the number of rows of \mathbf{C} .

So, for $\nu_h = 1$, use

$$F = \left(\frac{\nu_e + \nu_h - p}{p} \right) \left(\frac{1 - \Lambda^*}{\Lambda^*} \right) = 11.514901,$$

which if the null is true (and assumptions valid), F should have a sampling distribution that is $\mathcal{F}_{p,(\nu_e + \nu_h - p)}$. Comparing F to $\mathcal{F}_{2,56}$, we get a p -value $< .01$. Reject H_0 .

Summary: The mean survival of patients with bladder cancer differs from that of those with other types of cancer; however, no support for differences between the other types.

Question: Are there differences for survival from first hospitalization



Simultaneous Confidence Intervals

We can construct simultaneous confidence intervals for components of differences

$$\tau_I - \tau_{I'} \quad (\text{which equal } \mu_I - \mu_{I'})$$

or other linear combinations such as

$$\tau_1 - (\tau_2 + \tau_3)/2$$

There are at least three ways of doing this

- ▶ Specify a matrix \mathbf{M} in the hypothesis test $H_0 : \mathbf{CBM} = \mathbf{0}$ that is a $(p \times 1)$ vector with all

$$\mathbf{M}' = (0, \dots, \underbrace{1}_{j^{th}}, \dots, 0)$$

- ▶ **Bonferroni-type**: Same as above but split the α into pieces, on part for each of the **planned** comparisons.
- ▶ **Roys' method**, which is based on the “union-intersection” principle.



Using $CBM = 0$

- ▶ **C** picks out which two (or more groups to compare).
e.g., want to compare bladder with the rest,

$$\mathbf{C} = (0, 1, -.2, -.2, -.2, -.2, -.2)$$

- ▶ **M** picks out which variable (or linear combination of variables).
e.g., Just compare d_1 , increase in survival from first hospitalization,

$$\mathbf{M}' = (1, 0)$$

Putting these together in our example gives us

$$(0, 1, -.2, -.2, -.2, -.2, -.2) \begin{pmatrix} \beta_{01} & \beta_{02} \\ \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \\ \beta_{31} & \beta_{32} \\ \beta_{41} & \beta_{42} \\ \beta_{51} & \beta_{52} \\ \beta_{61} & \beta_{61} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \left(\beta_{11} - \frac{1}{5} \sum_{l=2}^6 \beta_{l1} \right)$$



Confidence interval for CBM

$$\beta_{11} - \frac{1}{5} \sum_{l=2}^6 \beta_{l1} = \tau_{11} - \sum_{l=2}^6 \tau_{l1}$$

We need two things:

- ▶ A “fudge-factor” — a value from a probability distribution
- ▶ An estimate of the standard error

A $(1 - \alpha)100\%$ confidence statement given vectors $\mathbf{C}_{1 \times (g+1)}$ and $\mathbf{M}_{p \times 1}$ is

$$CBM \pm \sqrt{\mathcal{F}_{1,ve}(\alpha)} \sqrt{(\mathbf{M}'\mathbf{S}_{pool}\mathbf{M})(\mathbf{C}(\mathbf{A}'\mathbf{A})^{-1}\mathbf{C})}$$

Note: Consider two columns of \mathcal{B} , β_i and β_k , the covariance matrix between them is

$$\text{cov}(\beta_i, \beta_k) = s_{pool,ik}(\mathbf{A}'\mathbf{A})^{-1}$$



Our example: CI for CBM

$$\beta_{11} - \frac{1}{5} \sum_{l=2}^6 \beta_{l1} = 1304.20 - \frac{1}{5}(49.50 + 117.19 + 118.86 + 297.43 + 70.67) = 1173.47$$

$$\begin{aligned} (\mathbf{M}'\mathbf{S}_{pool}\mathbf{M})(\mathbf{C}(\mathbf{A}'\mathbf{A})^{-1}\mathbf{C}') &= s_{pool,11}(0.2197619) \\ &= (427031.03)(0.2197619) = 93845.152 \end{aligned}$$

And $\mathcal{F}_{1,57}(.05) = 4.01$. So our 95% confidence interval is

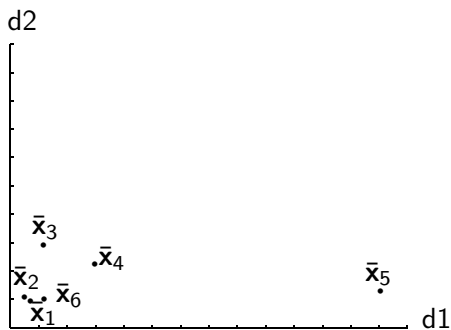
$$\begin{aligned} 1304.20 \pm \sqrt{4.01} \sqrt{93845.152} \\ 1304.20 \pm \sqrt{4.01}(306.34) \longrightarrow (560.03, 1786.91) \end{aligned}$$

Since 0 is not in the interval, the mean increase in survival from first hospitalization due to bladder cancer is larger than the average of the others means.

Should we test whether the same is true for increase in survival from time of untreatability?



Plot of Means





Notes about These CIs

- ▶ If you're only looking (testing) the difference between two means, e.g.,

$$\tau_{ji} - \tau_{j'i}$$

Then the standard error is just $s_{pool,ii} \sqrt{1/n_j + 1/n_{j'}}$

- ▶ When looking at a difference for a variable (e.g., above), these confidence statements are equivalent to what you would get from 1-way ANOVA using Fisher's least significant differences; that is, they are univariate CIs.
- ▶ When considering a linear combination of variables, these CIs are equivalent to univariate CIs where you've analyzed a new or composite variable defined by the linear combination.
- ▶ In our example, we don't have to worry too much about inflated Type I error rate, because we only did one CI after rejecting the overall test and using multivariate contrasts to narrow down where differences exist.
- ▶ If you do all pairwise differences, there are $g(g-1)/2$ pairs times p variables. (e.g., $2(6)(5)/2 = 30$).



Bonferroni Intervals

If you have planned to look at all pairwise comparisons before looking at the data (i.e., $m = pg(g - 1)/2$), then you can use

$$t_{\nu_e}(\alpha/(2m))$$

as your fudge factor.

Let $n_+ = \sum_{l=1}^g n_l$. For the model $\mathbf{X}_{lj} = \boldsymbol{\mu} + \boldsymbol{\tau}_l + \boldsymbol{\epsilon}_{lj}$ with $j = 1, \dots, n_l$ and $l = 1, \dots, g$ with confidence at least $(1 - \alpha)$, $(\tau_{li} - \tau_{l'i})$ belongs to

$$(\bar{x}_{li} - \bar{x}_{l'i}) \pm t_{\nu_e}(\alpha/(2m)) \sqrt{s_{pool,ii} \left(\frac{1}{n_l} + \frac{1}{n_{l'}} \right)}$$

for all components (variables) $i = 1, \dots, p$ and all differences $l < l' = 1, \dots, g$.



Roy's Method

- ▶ This is based on the union intersection principle.
- ▶ This is more like the first method that we considered (i.e., **CBM**); however, we use a different distribution for our “fudge factor”.
- ▶ We use Greatest Root of $|\mathbf{H} - \theta(\mathbf{E} + \mathbf{H})| = 0$ where \mathbf{H} (between groups or hypothesis SSCP matrix) and $\mathbf{E} = \mathbf{W}$ (error or within groups SSCP matrix) are independent Wishart matrices.
- ▶ To apply this result, we need percentiles of the greatest root distribution of the largest root λ of the equation $|\mathbf{H} - \lambda\mathbf{E}| = 0$. Percentile can be found in tables.
- ▶ This distribution does not depend on Σ but only on $df = n - g - p - 1$.



Roy's Method

Tables and charts of greatest root distribution exist; however, these are difficult to read (can find them in older literature).

Recommendation: I'd suggest using Scheffé's method where you do 1-way ANOVA on a linear combination of variables and then specify the contrast that you want.



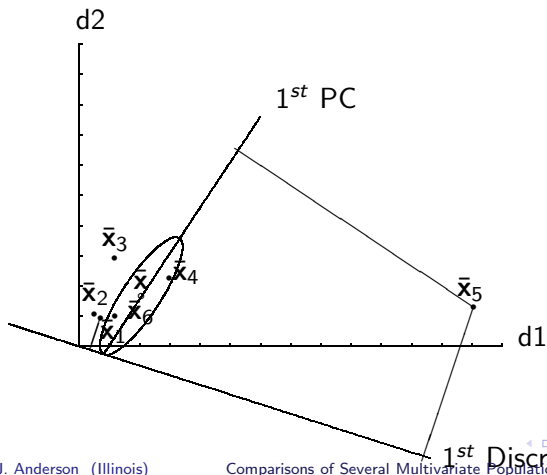
A Truly Multivariate Follow-Up

Discriminate Analysis

- ▶ The first discriminate function gives a linear combination of the p variables that yields the greatest differences between the means of the groups.
- ▶ You can get $p - 1$ functions.
- ▶ They equal the characteristic roots of $\mathbf{E}^{-1}\mathbf{H}$.
- ▶ For now, we'll just get them from SAS/PROC GLM.



Summary: PCA, MANOVA, DA





SAS IML and GLM

- ▶ SAS IML code using “traditional” approach & GLM one.
- ▶ PROC GLM data=vitC;

```
class type ;
```

```
model d1 d2 = type /solution;
```

* Note: The order of the values in the contrast are alphabetical, in this case order is bladder bronchus colon kidney rectum stomach;

```
contrast 'bronchus=colon=kidney=rectum=stomach'
```

```
    type 0 1 0 0 0 -1,      type 0 0 1 -1 0 0,
```

```
    type 0 1 -1 -1 0 1,     type 0 1 1 1 -4 1;
```

```
contrast 'bladder vs others' type -5 1 1 1 1 1 ;
```

```
manova h=type /printh printe;
```

```
estimate 'b vs o' type 1 -.2 -.2 -.2 -.2 -.2;
```

```
lsmeans type;
```

```
title 'MANOVA of vitamin C and Cancer';
```

- ▶ Alternate MANOVA statement where \mathbf{M} is entered as \mathbf{M}' :

```
manova h=type M=(1 0);
```



SAS GLM Output

- ▶ Univariate ANOVAs for each dependent variable.
- ▶ If requested, **E** (printe) and **H** (printh) SSCP matrices.
- ▶ p characteristic roots and vectors of $\mathbf{E}^{-1}\mathbf{H}$ (i.e., discriminant functions).
- ▶ Other requested statistics:
 - ▶ contrasts
 - ▶ estimates of contrasts
 - ▶ cell means
 - ▶ etc.
- ▶ Test statistics for “no overall effect” specified in MANOVA statement.
- ▶ Show SAS program and output.