Workshop Multivariate General Linear Models (# 170, Richard F. Haase)

Jorge Tendeiro

18 May 2016



Overview

- Goals of today's talk
- 2 Chapter 1: Review of univariate GLMs
- 3 Chapter 2: Structure of multivariate GLMs
- Chapter 3: Estimating the parameters of the multivariate GLM
- 5 Chapter 4: Partitioning the SSCP, strength of association, test statistics
- 6 Chapter 5: Testing hypotheses in the multivariate GLM
- Chapter 6: Coding the design matrix and MANOVA
- 8 Conclusion

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Four main goals motivated the organization of this talk:

1. Provide insight into the generalization of <u>univariate</u> multiple regression (UMR) to <u>multivariate</u> multiple regression (MMR).

We will see that the model formulation, parameter estimation, and inferential procedures of MMR extend naturally from UMR.

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2. Look into the most popular multivariate test statistics in use (Pillai's trace V, Wilks's Λ, Hotteling's trace T, and Roy's greatest characteristic root θ).

We will relate each of these multivariate test statistics to common tools and concepts from UMR (namely, F tests, sr's, and pr's).

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4. (Briefly) Refer to MANOVA as a special case of MMR.

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Multiple regression model:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_q X_q + \varepsilon$$

 X_1, \ldots, X_q : Predictors (continuous and/or categorical).

 $(\beta_0), \beta_1, \ldots, \beta_q$: Regression coefficients.

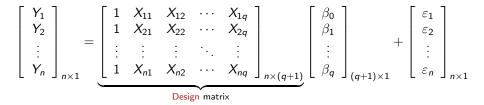
- Y: Dependent variable (only one in univariate MR).
- ε : Error term.

Expressing the same model in matrix algebraic terms:

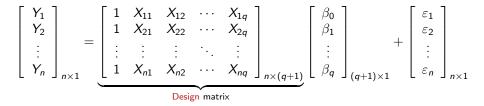
$$\mathbf{y}_{n imes 1} = \mathbf{X}_{n imes (q+1)} \ eta_{(q+1) imes 1} + egin{array}{c} \varepsilon_{n imes 1} \end{array}$$

- n: Sample size.
- q: Number of predictors.

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Four steps of GLM analysis:

- 1. Specify the model.
- 2. Estimate the model parameters.
- 3. Check goodness of fit of the model.
- 4. Test hypotheses about the model.

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 - Choose adequate predictors X_i (i = 1, 2, ..., q) and DV Y (choice is typically theory-driven, not statistics-driven).
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- Estimate the model parameters. The OLS solution consists of finding β that minimizes the sum of the squared residuals:

$$\sum_{i=1}^{n} \varepsilon_{i}^{2} = (\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta) = \varepsilon'\varepsilon.$$

The solution is:

• Unstandardized regression coefficients:

$$\left[\widehat{oldsymbol{eta}}_{(q+1) imes 1} = ({f X}'{f X})^{-1}{f X}'{f y}.
ight]$$

• Standardized regression coefficients ('beta' coefficients):

$$\widehat{\boldsymbol{\beta}}_{(q+1)\times 1}^{*} = (\mathbf{Z}_{\mathbf{X}}^{\prime}\mathbf{Z}_{\mathbf{X}})^{-1}\mathbf{Z}_{\mathbf{X}}^{\prime}\mathbf{Z}_{\mathbf{y}} = \mathbf{R}_{XX}^{-1}\mathbf{R}_{XY}.$$

3. Check goodness of fit of the model.

$$\begin{split} SS_{\text{Total}} &= SS_{\text{Model}} &+ SS_{\text{Error}} \\ \sum_{i=1}^{n} \left(Y_{i} - \overline{Y} \right)^{2} &= \sum_{i=1}^{n} \left(\widehat{Y}_{i} - \overline{Y} \right)^{2} + \sum_{i=1}^{n} \left(Y_{i} - \widehat{Y}_{i} \right)^{2} \end{split}$$

The most common measure of goodness of fit is

$$R^{2} = \frac{SS_{\text{Model}}}{SS_{\text{Total}}}$$

= $1 - \frac{SS_{\text{Error}}}{SS_{\text{Total}}}$
= $\hat{\beta}_{1}^{*} r_{Y \cdot X1} + \hat{\beta}_{2}^{*} r_{Y \cdot X2} + \dots + \hat{\beta}_{q}^{*} r_{Y \cdot Xq}.$

Other goodness of fit measures include the semipartial (sr) and partial (pr) correlation coefficients.

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- Semipartial correlation = Correlation between Y and the part of the predictor that is uncorrelated to all the remaining predictors.

Equivalently, it is the R^2 increment achieved by adding the predictor to a model that already includes the remaining (q - 1) predictors. E.g.,

$$sr_1^2 = r^2(Y, X_1 | X_2 \cdots X_q).$$

= $R_{Y \cdot X_1 \cdots X_q}^2 - R_{Y \cdot X_2 \cdots X_q}^2$
= $R_{\text{full}}^2 - R_{\text{restricted}}^2.$

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• Partial correlation = Correlation between the Y and a predictor, after the remaining predictors have been partialled out from both. E.g.,

$$pr_1 = r(Y|X_2\cdots X_q, X_1|X_2\cdots X_q).$$

- 4. Test hypotheses about the model. Under the usual regression assumptions (namely of normality) then:
 - *F* test associated to *R*²:

$$F = rac{SS_{ ext{Model}}/q}{SS_{ ext{Error}}/(n-q-1)} = rac{MS_{ ext{Model}}}{MS_{ ext{Error}}} pprox_{H_0} F(q,n-q-1).$$

• More generally, the F test associated to sr^2 (or β):

$$F=rac{(R_{ ext{full}}^2-R_{ ext{restricted}}^2)/(q-q_r)}{(1-R_{ ext{full}}^2)/(n-q-1)} \mathop\sim\limits_{ ext{H}_0} F(q-q_r,n-q-1),$$

where q_r = number of predictors in the restricted model.

Obs: Any test of interest in regression (i.e., any contrast) can be reexpressed as an F test as shown above. So there is only one type of test, really.

In general, any contrast of interest under the GLM can be written as follows:

$$H_0: \mathbf{L}_{c \times (q+1)} \beta_{(q+1) \times 1} = \mathbf{0}_{c \times 1},$$

where c = number of contrasts to be tested and **L** is a matrix of contrast coefficients.

Example:

•
$$H_0: \beta_1 = \dots = \beta_q = 0$$
 becomes $(c = q)$
$$H_0: \mathbf{L}\beta = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_q \end{bmatrix} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_q \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Example:

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$$H_0: \beta_1 = 0$$
 becomes $(c = 1)$

$$H_0: \mathbf{L}\boldsymbol{\beta} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_q \end{bmatrix} = \beta_1 = 0$$

• $H_0: \beta_1 = \beta_2$ becomes (c = 1)

$$H_0: \mathbf{L}\boldsymbol{\beta} = \begin{bmatrix} 0 & 1 & -1 & \cdots & 0 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_q \end{bmatrix} = \beta_1 - \beta_2 = 0$$

In general:

Any hypothesis of the type

$$H_0: \mathbf{L}_{c \times (q+1)} \boldsymbol{\beta}_{(q+1) \times 1} = \mathbf{0}_{c \times 1}$$

can be tested by means of the F test

$$\left(F = \frac{(R_{\text{full}}^2 - R_{\text{restricted}}^2)/c}{(1 - R_{\text{full}}^2)/(n - q - 1)} = \frac{SS_{\text{Hypothesis}}/c}{SS_{\text{Error}}/(n - q - 1)} \underset{H_0}{\sim} F(c, n - q - 1),$$

with R_{full}^2 and $R_{restricted}^2$ computed directly from **X**, $\hat{\beta}$, and suitable **L** matrices.

. . .

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Structure of multivariate GLMs

Extend the previous results to cases with more than one DV.

$$\left(\mathbf{Y}_{n\times p} = \mathbf{X}_{n\times (q+1)} \; \mathbf{B}_{(q+1)\times p} + \mathbf{E}_{n\times p}\right)$$

- n: Sample size.
- q: Number of predictors.
- *p*: Number of DVs.

The design matrix **X** is the same as before. **Y**, **B**, and **E** were extended to accomodate p columns.

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Estimating the parameters of the multivariate GLM

$$\left[\mathbf{Y}_{n\times p} = \mathbf{X}_{n\times (q+1)} \; \mathbf{B}_{(q+1)\times p} + \mathbf{E}_{n\times p}\right]$$

The OLS solution consists of finding ${\bf B}$ that minimizes the sum of the squared residuals:

$$tr(\mathbf{E}'\mathbf{E}) = tr\left[(\mathbf{Y} - \mathbf{X}\mathbf{B})'(\mathbf{Y} - \mathbf{X}\mathbf{B})
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The solution is:

• Unstandardized regression coefficients:

$$\widehat{\mathbf{B}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}.$$

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Recall that for univariate GLMs,

$$\left[\widehat{\mathbf{y}}_{n\times 1} = \mathbf{X}_{n\times (q+1)} \ \widehat{\boldsymbol{\beta}}_{(q+1)\times 1}\right]$$

with $\widehat{oldsymbol{eta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}.$

The SS partitioning is given by

$$SS_{\text{Total}} = SS_{\text{Model}} + SS_{\text{Error}}$$

$$\sum_{i=1}^{n} (Y_i - \overline{Y})^2 = \sum_{i=1}^{n} (\widehat{Y}_i - \overline{Y})^2 + \sum_{i=1}^{n} (Y_i - \widehat{Y}_i)^2$$

$$(\mathbf{y}'\mathbf{y} - n\overline{\mathbf{y}}'\overline{\mathbf{y}}) = (\widehat{\mathbf{y}}'\mathbf{y} - n\overline{\mathbf{y}}'\overline{\mathbf{y}}) + (\mathbf{y}'\mathbf{y} - \widehat{\mathbf{y}}'\mathbf{y})$$

Multivariate GLMs generalize these formulas to accomodate multiple DVs (say, p).

For multivariate GLMs,

$$\widehat{\mathbf{Y}}_{n \times p} = \mathbf{X}_{n \times (q+1)} \ \widehat{\mathbf{B}}_{(q+1) \times p}$$

with $\widehat{\mathbf{B}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}.$

The SSCP (matrices!) partitioning is given by

$$\underbrace{\left(\mathbf{Y}'\mathbf{Y} - n\overline{\mathbf{Y}}'\overline{\mathbf{Y}}\right)}_{p \times p} = \underbrace{\left(\widehat{\mathbf{Y}}'\mathbf{Y} - n\overline{\mathbf{Y}}'\overline{\mathbf{Y}}\right)}_{p \times p} + \underbrace{\left(\mathbf{Y}'\mathbf{Y} - \widehat{\mathbf{Y}}'\mathbf{Y}\right)}_{p \times p}$$

Recall that the R^2 measure of strength of association was, for univariate GLMs, given by

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The R^2 of each DV in multivariate GLMs is readily available using the same formula:

$$\left(R_{Y_1}^2, R_{Y_2}^2, \dots, R_{Y_p}^2\right) = \frac{\mathsf{Diag}(SSCP_{\mathsf{Model}})}{\mathsf{Diag}(SSCP_{\mathsf{Total}})} = 1 - \frac{\mathsf{Diag}(SSCP_{\mathsf{Error}})}{\mathsf{Diag}(SSCP_{\mathsf{Total}})}$$

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- Q: Is there such a measure?
- A: Well, yes... The problem is that there are several.

One first attempt for a multivariate measure of strength of association:

$$R_{dYX}^2 = \frac{R_{Y_1}^2 + R_{Y_2}^2 + \dots + R_{Y_p}^2}{p}.$$

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- Actually, it overestimates the proportion of joint variance in {Y₁,..., Y_p} that is predictable from {X₁,..., X_q} because it fails to adjust for multicollinearity among the Y_i variables. Not ideal.
- Another problem:

The redundancy index is asymmetric: $R_{dYX}^2 \neq R_{dXY}^2$ unless p = q. This is awkward.

(Think of overlapping areas in Venn diagrams.)

We want better measures of strength of association between ${\bf Y}$ and ${\bf X},$ in particular:

- Adjusted for multicollinearity among the Y_i variables.
- Symmetric.

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Motivation: Generalize the univariate idea of a sr^2 ,

$$sr^2 = R_{\text{full}}^2 - R_{\text{restricted}}^2,$$

and its associated F test:

$$F = rac{SS_{ ext{Hypothesis}}/(q-q_r)}{SS_{ ext{Error}}/(n-q-1)} \underset{H_0}{\sim} F(q-q_r,n-q-1).$$

Recall univariate

For full model (i.e., based on all q predictors X_1, \ldots, X_q):



For reduced model (i.e., based on only a subset of predictors):

$$\mathbf{Y} = \mathbf{X}_{R}\mathbf{B}_{R} + \mathbf{E}'$$

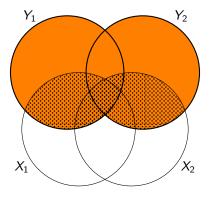
$$\underbrace{SSCP_{\text{Total}}}_{\mathbf{Q}_{T}} = \underbrace{SSCP_{\text{Restricted}}}_{\mathbf{Q}_{R}} + \underbrace{SSCP_{\text{Error}}}_{\mathbf{Q}_{E'}}$$

Thus, focus on the hypothesis SSCP matrix:

$$\left(\mathbf{Q}_{H}=\mathbf{Q}_{F}-\mathbf{Q}_{R}
ight)$$

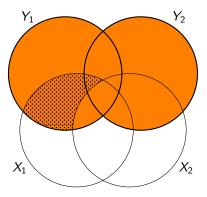
 $\mathbf{Q}_{H} =$ Incremental influence of the variables in the full model that are not in the restricted model.

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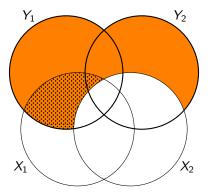
$$"R^2" = \frac{\mathbf{Q}_F}{\mathbf{Q}_T} = \frac{\mathbf{Q}_F}{\mathbf{Q}_F + \mathbf{Q}_E}$$





$$"sr_1^2" = \frac{\mathbf{Q}_H}{\mathbf{Q}_T} = \frac{\mathbf{Q}_H}{\mathbf{Q}_F + \mathbf{Q}_E}$$

where \mathbf{Q}_H represents the unique contribution of X_1 to explaining the total variance in \mathbf{Y} .



$$"pr_1^2" = \frac{\mathbf{Q}_H}{\mathbf{Q}_H + \mathbf{Q}_E}$$

where \mathbf{Q}_H represents the unique contribution of X_1 to explaining the variance in \mathbf{Y} not explained by X_2 .

A second attempt for a multivariate measure of strength of association: Hooper's squared trace correlation. From

$$``R^{2"} = \frac{\mathbf{Q}_F}{\mathbf{Q}_T}$$
Recall Venn's diagram

one derives

$$"R^2" = \mathbf{Q}_T^{-1}\mathbf{Q}_F,$$

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Hooper (1959) suggested the following (scalar) formula:

$$\overline{r}^2 = rac{1}{
ho} \mathrm{tr} \left(\mathbf{Q}_T^{-1} \mathbf{Q}_F
ight) = rac{1}{
ho} \mathrm{tr} \left(\mathbf{R}_{YY}^{-1} \mathbf{R}_{YX} \mathbf{R}_{XX}^{-1} \mathbf{R}_{XY}
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- \checkmark Unlike R^2_{dYX} (Recall , \overline{r}^2 does adjust for multicollinearity among the Ys and among the Xs.
- $\sqrt{r^2}$ reduces to the common R^2 measure in simple (p = q = 1) and multiple (p = 1, q > 1) linear regression.
- ✓ Straightforward interpretation:

 \overline{r}^2 is the proportion of the joint, nonredundant variance in $\{Y_1, \ldots, Y_p\}$ that is explained by the joint, nonredundant variance in $\{X_1, \ldots, X_q\}$.

About \overline{r}^2 :

- \checkmark Unlike R^2_{dYX} [Recall , \bar{r}^2 does adjust for multicollinearity among the Ys and among the Xs.
- $\sqrt{r^2}$ reduces to the common R^2 measure in simple (p = q = 1) and multiple (p = 1, q > 1) linear regression.
- ✓ Straightforward interpretation:

 \overline{r}^2 is the proportion of the joint, nonredundant variance in $\{Y_1, \ldots, Y_p\}$ that is explained by the joint, nonredundant variance in $\{X_1, \ldots, X_q\}$.

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We are finally led to present the "big four" R^2 -like measures of wide use nowadays, all of which are symmetric and adjusted for multicollinearity among the Ys:

- Pillai's trace V.
- Wilks' Λ.

- Lawley-Hotteling's trace *T*.
- Roy's GCR θ .

Test statistic	Multivariate test statistic	R_m^2	Univ. <i>R</i> ² conceptual equivalent	Multiv. <i>F</i> -test equivalent
Pillai's <i>V</i>	$V = \operatorname{tr}\left[(\mathbf{Q}_H + \mathbf{Q}_E)^{-1} \mathbf{Q}_H \right]$	$R_V^2 = \frac{V}{s}$	pr^2 Venn diag. (= R^2 if $\mathbf{Q}_F = \mathbf{Q}_H$)	(*)
Wilks' A	$\Lambda = \frac{ \mathbf{Q}_E }{ \mathbf{Q}_H + \mathbf{Q}_E }$	$R_{\Lambda}^2 = 1 - \Lambda^{\frac{1}{s}}$	$1 - pr^2$ (=1 - R^2 if $\mathbf{Q}_F = \mathbf{Q}_H$)	(*)
Hotelling's T	$\mathcal{T} = tr\left(\mathbf{Q}_{E}^{-1}\mathbf{Q}_{H} ight)$	$R_T^2 = \frac{T}{T+s}$	$ \begin{array}{l} \frac{\rho r^2}{1-\rho r^2} \\ (= \frac{R^2}{1-R^2} \text{ if } \mathbf{Q}_F = \mathbf{Q}_H) \end{array} $	(*)
Roy's θ	$ heta = max_{eigen} \left(\mathbf{Q}_E^{-1} \mathbf{Q}_H ight)$	$R_{ heta}^2 = rac{ heta}{1+ heta}$	<i>r</i> ²	(*)
$s = \min(p, q_h)$				

 $\rho_{\max}^2 = \max \operatorname{imum} \operatorname{squared} \operatorname{canonical} \operatorname{correlation} \operatorname{between} \mathbf{X}$ and \mathbf{Y} .

(*) = These F test are all similar to each other, and all are approximations of the exact tests based on V, Λ , T, and θ .

Example — **Personality and success in job application process** Based on Caldwell and Burger (1998).

Predictors					
Neurot	Neuroticism				
Extrav	Extraversion				
Consci	Conscientiousness				
Outcomes					
BackPrep	Background preparation for the interviews				
SociPrep	Social preparation for the interviews				
FollowUp	Number of follow-up interviews achieved				
Offers	Number of offers of employment received				

- Original data based on an observational study of 99 college students.
- I generated synthetic data based on the original means, SDs, and correlations for the seven variables above.

Multivariate tests								
Test	Test Stat.	R_m^2	Approx. F	Num Df	Den Df	<i>p</i> -value		
Pillai's V	0.470	$\frac{V}{s} = .156$	4.361	12	282	<.001		
Wilks' A	0.579	$1 - \Lambda^{\frac{1}{s}} = .166$	4.658	12	243.701	<.001		
Hotteling's T	0.645	$\frac{T}{T+s} = .177$	4.872	12	272	<.001		
Roy's θ	0.489	$\frac{ heta}{1+ heta} = .328$	11.492	4	94	<.001		
In this example, $s = \min(p, q_h) = \min(4, 3) = 3$.								

Obs.: R_m^2 values are typically not given by statistical software, so manual computation might be needed.

Some notes:

• The interpretation of R_m^2 for V, A, and T is more or less the same, namely:

"About $(100 \times R_m^2)$ % of the joint, nonredundant, variance of the DVs is accounted for by the joint variance of the predictors."

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- Very often, $(R_V^2 \simeq R_\Lambda^2 \simeq R_T^2) < R_{ heta}^2$.
- In cases where $R_{\theta}^2 \gg \{R_V^2, R_{\Lambda}^2, R_T^2\}$: Be careful not to put too much trust on R_{θ}^2 .

Both SPSS and R do not give the omnibus (approximate) F test results. One needs to explicitly ask for these:

In SPSS...

GLM BackPrep SociPrep FollowUp Offers WITH Neurot Extrav Consci /LMATRIX Neurot 1; Extrav 1; Consci 1.

(see output table Multivariate Test Results)

Recall omnibus contrast

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All (approximate!) multivariate F-tests have the same form, which is an extension from the common univariate F test for pr^2 :

$$F = rac{R_{
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The approximate multivariate *F*-tests ((*) in Recall multivariate tests) are a test of the partial R_m^2 :

$${\cal F}=rac{R_m^2/v_h}{(1-R_m^2)/v_e} \underset{{\cal H}_0}{\sim} {\cal F}(v_h,v_e),$$

with v_h , v_e specific to each test statistic (Pillai, Wilks, etc.).

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- The approximate multivariate *F* test for Roy's θ is too liberal, i.e., it overrejects H₀ (inflated Type I error rates). Be aware.
 Exact test is preferred (but not often provided by software).
- It is straightforward to adapt these approximate multivariate *F* tests to test any contrast of interest, similarly to what we saw for univariate models:

$$H_0: \mathbf{L}_{c \times (q+1)} \mathbf{B}_{(q+1) \times p} = \mathbf{0}_{c \times p}$$

with

$$\mathbf{Q}_{H} = (\mathbf{L}\widehat{\mathbf{B}})' \left(\mathbf{L} (\mathbf{X}'\mathbf{X})^{-1} \mathbf{L}' \right)^{-1} (\mathbf{L}\widehat{\mathbf{B}}).$$

For the running example (personality and success in job application process):

• H_0 : There is no overall effect of the three personality dimensions on the DVs (i.e., the omnibus test discussed before).

$$\mathbf{L} = \left[\begin{array}{rrrr} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right]$$

In R:

```
L <- cbind(0, diag(3))
linearHypothesis(res.CB, L)
```

• H_0 : Extraversion (2nd predictor) has no effect.

$$\mathbf{L} = \left[\begin{array}{cccc} \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} \end{array} \right],$$

so H_0 : **B**_{Extr. on the 4 DVs} = (0, 0, 0, 0). In R:

```
L <- c(0, 0, 1, 0)
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- The *p* univariate follow-up tests are based on DVs which are not adjusted for their mutual correlations. This may lead to univariate follow-up tests overestimating the contribution of single DVs to the multivariate relationship.
- The Roy-Bargman stepdown tests are one way to solve this issue related to correlated DVs.

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- Different coding systems lead to different regression coefficients **B**.
- The multivariate test of contrasts (e.g., omnibus test, test for individual predictors, ...) is performed as before:

$$[H_0:\mathbf{L}_{c\times(q+1)}\mathbf{B}_{(q+1)\times p}=\mathbf{0}_{c\times p},]$$

where the specific form of L will depend on B (i.e., on the coding system of choice).

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- Scalar multivariate R^2 s exist which can be computed and reported.
- MANOVA directly benefits from these insights.