

**STATS 206**  
**Applied Multivariate Analysis**  
**Lecture 8: Canonical Correlation Analysis**

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## Agenda

- Population canonical variates and canonical correlations
- Sample canonical variates and canonical correlations

## Introduction

- Objective:
  - to identify and quantify the association between two sets of variables
- Focus:
  - Correlation between a linear combination of variables in set 1 and that in set 2.
- Procedure:
  - first, to find the pair of linear combinations yielding the largest correlation
  - then, to find the pair of linear combinations yielding the largest correlation but uncorrelated with the first pair
  - ...
- Thus:
  - Canonical variables: the pairs of linear combinations described above
  - Canonical correlations: correlations between these pairs

# Population Canonical Variates and Canonical Correlations

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- Assumptions:
  - Two groups of variables: represented by two random vectors

$$\mathbf{X}_{p \times 1}^{(1)} \text{ and } \mathbf{X}_{q \times 1}^{(2)}$$

- Without loss of generality: let  $p \leq q$
  - Let

$$E(\mathbf{X}^{(1)}) = \boldsymbol{\mu}^{(1)}, \quad \text{Cov}(\mathbf{X}^{(1)}) = \boldsymbol{\Sigma}_{11}$$

$$E(\mathbf{X}^{(2)}) = \boldsymbol{\mu}^{(2)}, \quad \text{Cov}(\mathbf{X}^{(2)}) = \boldsymbol{\Sigma}_{22}$$

$$\text{Cov}(\mathbf{X}^{(1)}, \mathbf{X}^{(2)}) = \boldsymbol{\Sigma}_{12} = \boldsymbol{\Sigma}_{21}'$$

- Consider  $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}$  jointly

$$\mathbf{X}_{(p+q) \times 1} = \begin{bmatrix} \mathbf{X}^{(1)} \\ \mathbf{X}^{(2)} \end{bmatrix} \quad E(\mathbf{X}) = \begin{bmatrix} \boldsymbol{\mu}^{(1)} \\ \boldsymbol{\mu}^{(2)} \end{bmatrix} \quad \text{Cov}(\mathbf{X}) = \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix}$$

# Population Canonical Variates and Canonical Correlations

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- Given coefficient vectors  $\mathbf{a}$ ,  $\mathbf{b}$ , set

$$U = \mathbf{a}'\mathbf{X}^{(1)}, V = \mathbf{b}'\mathbf{X}^{(2)}$$

to obtain

$$\text{Var}(U) = \mathbf{a}'\text{Cov}(\mathbf{X}^{(1)})\mathbf{a} = \mathbf{a}'\Sigma_{11}\mathbf{a}$$

$$\text{Var}(V) = \mathbf{b}'\text{Cov}(\mathbf{X}^{(2)})\mathbf{b} = \mathbf{b}'\Sigma_{22}\mathbf{b}$$

$$\text{Cov}(U, V) = \mathbf{a}'\text{Cov}(\mathbf{X}^{(1)}, \mathbf{X}^{(2)})\mathbf{b} = \mathbf{a}'\Sigma_{12}\mathbf{b}$$

and the correlation between  $U$  and  $V$

$$\text{Corr}(U, V) = \frac{\mathbf{a}'\Sigma_{12}\mathbf{b}}{\sqrt{\mathbf{a}'\Sigma_{11}\mathbf{a}}\sqrt{\mathbf{b}'\Sigma_{22}\mathbf{b}}}$$

# Population Canonical Variates and Canonical Correlations

- Definitions:

- First canonical variate pair:  $U_1 = \mathbf{a}'_1 \mathbf{X}^{(1)}, V_1 = \mathbf{b}'_1 \mathbf{X}^{(2)}$ ;  $\mathbf{a}_1, \mathbf{b}_1$  solves:

$$\max_{\mathbf{a}_1, \mathbf{b}_1} \text{Corr}(U_1, V_1) \quad \left[ \text{or} \quad \max_{\mathbf{a}_1, \mathbf{b}_1} \frac{\mathbf{a}'_1 \Sigma_{12} \mathbf{b}_1}{\sqrt{\mathbf{a}'_1 \Sigma_{11} \mathbf{a}_1} \sqrt{\mathbf{b}'_1 \Sigma_{22} \mathbf{b}_1}} \right]$$

subject to  $\mathbf{a}'_1 \Sigma_{11} \mathbf{a}_1 = 1, \mathbf{b}'_1 \Sigma_{22} \mathbf{b}_1 = 1$

- Second canonical variate pair:  $U_2 = \mathbf{a}'_2 \mathbf{X}^{(1)}, V_2 = \mathbf{b}'_2 \mathbf{X}^{(2)}$ ;  
 $(\mathbf{a}_2, \mathbf{b}_2)$  is the solution to: (given  $\mathbf{a}_1, \mathbf{b}_1$ )

$$\max_{\mathbf{a}_2, \mathbf{b}_2} \frac{\mathbf{a}'_2 \Sigma_{12} \mathbf{b}_2}{\sqrt{\mathbf{a}'_2 \Sigma_{11} \mathbf{a}_2} \sqrt{\mathbf{b}'_2 \Sigma_{22} \mathbf{b}_2}}$$

subject to  $\mathbf{a}'_2 \Sigma_{11} \mathbf{a}_2 = 1, \mathbf{b}'_2 \Sigma_{22} \mathbf{b}_2 = 1$   
 $\mathbf{a}'_2 \Sigma_{11} \mathbf{a}_1 = 0, \mathbf{b}'_2 \Sigma_{22} \mathbf{b}_1 = 0, \mathbf{a}'_1 \Sigma_{12} \mathbf{b}_2 = 0, \mathbf{a}'_2 \Sigma_{12} \mathbf{b}_1 = 0$

# Population Canonical Variates and Canonical Correlations

- Definitions:

3.  $k$ -th canonical variate pair:  $U_k = \mathbf{a}'_k \mathbf{X}^{(1)}$ ,  $V_k = \mathbf{b}'_k \mathbf{X}^{(2)}$ , where  $U_k, V_k$ :

- having unit variances
- having the maximum correlation  $\text{Corr}(U_k, V_k)$
- uncorrelated with the previous  $(k - 1)$  canonical variable pairs

- Results: see next page

# Population Canonical Variates and Canonical Correlations

- Results: (to be cont'd on next page)

Let  $p \leq q$  and  $\mathbf{X} = \begin{bmatrix} \mathbf{X}^{(1)}_{p \times 1} \\ \mathbf{X}^{(2)}_{q \times 1} \end{bmatrix}$  with  $\text{Cov}(\mathbf{X}) = \Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$  (here  $\Sigma$  has full-rank). For coefficient vectors  $\mathbf{a}, \mathbf{b}$ , form linear combinations  $U = \mathbf{a}'\mathbf{X}^{(1)}, V = \mathbf{b}'\mathbf{X}^{(2)}$ . Then

$$\max_{\mathbf{a}, \mathbf{b}} \text{Corr}(U, V) = \rho_1^*$$

is attained by the linear combinations (first canonical variate pair)

$$U_1 = \underbrace{\mathbf{e}_1' \Sigma_{11}^{-1/2}}_{\mathbf{a}_1'} \mathbf{X}^{(1)}, \quad V_1 = \underbrace{\mathbf{f}_1' \Sigma_{22}^{-1/2}}_{\mathbf{b}_1'} \mathbf{X}^{(2)}.$$



# Population Canonical Variates and Canonical Correlations

- Results: (Cont'd and to be cont'd on next page)

The  $k$ -th canonical variate pairs,  $k = 2, 3, \dots, p$ ,

$$U_k = \mathbf{e}_k' \Sigma_{11}^{-1/2} \mathbf{X}^{(1)}, \quad V_k = \mathbf{f}_k' \Sigma_{22}^{-1/2} \mathbf{X}^{(2)}$$

maximizes

$$\text{Corr}(U_k, V_k) = \rho_k^*$$

among all linear combinations uncorrelated with  $\{(U_j, V_j)\}_{j=1}^{k-1}$ .

Here  $\rho_1^{*2} \geq \dots \geq \rho_p^{*2}$  are eigenvalues of  $\Sigma_{11}^{-1/2} \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \Sigma_{11}^{-1/2}$  and  $\mathbf{e}_1, \dots, \mathbf{e}_p$  are the corresponding eigenvectors.

$\rho_1^{*2} \geq \dots \geq \rho_p^{*2}$  are also eigenvalues of  $\Sigma_{22}^{-1/2} \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \Sigma_{22}^{-1/2}$  and  $\mathbf{f}_1, \dots, \mathbf{f}_p$  are the associated eigenvectors. Each  $\mathbf{f}_i$  is proportional to  $\Sigma_{22}^{-1/2} \Sigma_{21} \Sigma_{11}^{-1/2} \mathbf{e}_i$  (i.e.,  $\mathbf{f}_i \propto \Sigma_{22}^{-1/2} \Sigma_{21} \Sigma_{11}^{-1/2} \mathbf{e}_i$ ).

# Population Canonical Variates and Canonical Correlations

- Results: (Cont'd)

$\rho_k^*$ : the canonical correlation of  $(U_k, V_k)$ ,  $k = 1, \dots, p$

The canonical variates have the following properties:

$$\text{Var}(U_k) = \text{Var}(V_k) = 1$$

$$\text{Cov}(U_k, U_l) = \text{Corr}(U_k, U_l) = 0, k \neq l$$

$$\text{Cov}(V_k, V_l) = \text{Corr}(V_k, V_l) = 0, k \neq l$$

$$\text{Cov}(U_k, V_l) = \text{Corr}(U_k, V_l) = 0, k \neq l$$

for  $k, l = 1, \dots, p$ .

## Example 1 – (1)

Calculating canonical variates/correlations for standardized variables

- Given:  $\mathbf{Z}^{(1)} = \begin{bmatrix} Z_1^{(1)} \\ Z_2^{(1)} \end{bmatrix}$ ,  $\mathbf{Z}^{(2)} = \begin{bmatrix} Z_1^{(2)} \\ Z_2^{(2)} \end{bmatrix}$ : **standardized**;  $\mathbf{Z} = \begin{bmatrix} \mathbf{Z}^{(1)} \\ \mathbf{Z}^{(2)} \end{bmatrix}$

$$\text{Cov}(\mathbf{Z}) = \left[ \begin{array}{c|c} \rho_{11} & \rho_{12} \\ \hline \rho_{21} & \rho_{22} \end{array} \right] = \left[ \begin{array}{cc|cc} 1 & 0.4 & 0.5 & 0.6 \\ 0.4 & 1 & 0.3 & 0.4 \\ \hline 0.5 & 0.3 & 1 & 0.2 \\ 0.6 & 0.4 & 0.2 & 1 \end{array} \right]$$

- Then

$$\rho_{11}^{-1/2} = \begin{bmatrix} 1.0681 & -0.2229 \\ -0.2229 & 1.0681 \end{bmatrix}, \quad \rho_{22}^{-1} = \begin{bmatrix} 1.0417 & -0.2083 \\ -0.2083 & 1.0417 \end{bmatrix}$$

$$\rho_{11}^{-1/2} \rho_{12} \rho_{22}^{-1} \rho_{21} \rho_{11}^{-1/2} = \begin{bmatrix} 0.4370 & 0.2178 \\ 0.2178 & 0.1097 \end{bmatrix}$$

From the above, we can obtain  $\rho_1^{*2} = 0.5457$ ,  $\rho_2^{*2} = 0.0009$

## Example 1 – (2)

The eigenvector  $\mathbf{e}_1$  of  $\rho_{11}^{-1/2} \rho_{12} \rho_{22}^{-1} \rho_{21} \rho_{11}^{-1/2}$  associated with  $\rho_1^{*2}$  is

$$\mathbf{e}_1 = \begin{bmatrix} 0.8947 \\ 0.4468 \end{bmatrix} \Rightarrow \mathbf{a}_1 = \rho_{11}^{-1/2} \mathbf{e}_1 = \begin{bmatrix} 0.8560 \\ 0.2777 \end{bmatrix}$$

The eigenvector  $\mathbf{f}_1$  of  $\rho_{22}^{-1/2} \rho_{21} \rho_{11}^{-1} \rho_{12} \rho_{22}^{-1/2}$  associated with  $\rho_1^{*2}$  is

$$\mathbf{f}_1 = \begin{bmatrix} 0.6161 \\ 0.7877 \end{bmatrix} \Rightarrow \mathbf{b}_1 = \rho_{22}^{-1/2} \mathbf{f}_1 = \begin{bmatrix} 0.5448 \\ 0.7366 \end{bmatrix}$$

- $\mathbf{f}_1$  above was obtained using the eigenvalue decomposition of  $\rho_{22}^{-1/2} \rho_{21} \rho_{11}^{-1} \rho_{12} \rho_{22}^{-1/2}$ .
- Alternatively, use the fact that  $\mathbf{f}_1 \propto \rho_{22}^{-1/2} \rho_{21} \rho_{11}^{-1/2} \mathbf{e}_1$ ,  $\mathbf{b}_1 = \rho_{22}^{-1/2} \mathbf{f}_1$

$$\mathbf{b}_1 \propto \rho_{21} \mathbf{a}_1 = \rho_{22}^{-1} \rho_{21} \mathbf{a}_1 = \begin{bmatrix} 0.3959 & 0.2292 \\ 0.5209 & 0.3542 \end{bmatrix} \begin{bmatrix} 0.8560 \\ 0.2777 \end{bmatrix} = \begin{bmatrix} 0.4026 \\ 0.5443 \end{bmatrix}$$

## Example 1 – (3)

(Cont'd)

We must scale  $\mathbf{b}_1$  such that  $\text{Var}(V_1) = \text{Var}(\mathbf{b}_1' \mathbf{Z}^{(2)}) = \mathbf{b}_1' \boldsymbol{\rho}_{22} \mathbf{b}_1 = 1$

The vector  $[0.4026 \ 0.5443]'$  yields:

$$[0.4026 \ 0.5443] \begin{bmatrix} 1 & 0.2 \\ 0.2 & 1 \end{bmatrix} \begin{bmatrix} 0.4026 \\ 0.5443 \end{bmatrix} = 0.5460$$

$$\Rightarrow \mathbf{b}_1 = \frac{1}{\sqrt{0.5460}} \begin{bmatrix} 0.4026 \\ 0.5443 \end{bmatrix} = \begin{bmatrix} 0.5448 \\ 0.7366 \end{bmatrix}$$

- Therefore, the 1st pair of canonical variates is

$$U_1 = \mathbf{a}_1' \mathbf{Z}^{(1)} = 0.86Z_1^{(1)} + 0.28Z_2^{(1)}, \quad V_1 = \mathbf{b}_1' \mathbf{Z}^{(2)} = 0.54Z_1^{(2)} + 0.74Z_2^{(2)}$$

with their canonical correlation being  $\rho_1^* = \sqrt{\rho_1^{*2}} = \sqrt{0.5457} = 0.74$

- The 2nd canonical correlation  $\rho_2^* = \sqrt{0.0009} = 0.03$  (very small, conveying little info. about the association between sets)

## Sample Canonical Variates and Canonical Correlations

- In applications, sample mean and covariances are used instead.
- Random sample of  $n$  observations of each of the  $(p + q)$  variables  $\mathbf{X}_{n \times p}^{(1)}, \mathbf{X}_{n \times q}^{(2)}$

$$\mathbf{X}_{n \times (p+q)} = \begin{bmatrix} \mathbf{X}^{(1)} & \mathbf{X}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1^{(1)'} & \mathbf{x}_1^{(2)'} \\ \vdots & \vdots \\ \mathbf{x}_n^{(1)'} & \mathbf{x}_n^{(2)'} \end{bmatrix}$$

# Sample Canonical Variates and Canonical Correlations

- Given  $\mathbf{X}_{n \times (p+q)}$ :

$$\underbrace{\bar{\mathbf{x}}}_{\text{sample mean}} = \begin{bmatrix} \bar{\mathbf{x}}^{(1)} \\ \bar{\mathbf{x}}^{(2)} \end{bmatrix} = \begin{bmatrix} \frac{1}{n} \sum_{j=1}^n \mathbf{x}_j^{(1)} \\ \frac{1}{n} \sum_{j=1}^n \mathbf{x}_j^{(2)} \end{bmatrix}, \quad \underbrace{\mathbf{S}}_{\substack{(p+q) \times (p+q) \\ \text{sample covariance matrix}}} = \begin{bmatrix} \underbrace{\mathbf{S}_{11}}_{p \times p} & \underbrace{\mathbf{S}_{12}}_{p \times q} \\ \underbrace{\mathbf{S}_{21}}_{q \times p} & \underbrace{\mathbf{S}_{22}}_{q \times q} \end{bmatrix}$$

$$\mathbf{S}_{kl} = \frac{1}{n-1} \sum_{j=1}^n (\mathbf{x}_j^{(k)} - \bar{\mathbf{x}}^{(k)}) (\mathbf{x}_j^{(l)} - \bar{\mathbf{x}}^{(l)})', \quad k, l = 1, 2$$

- Linear combinations  $\hat{U} = \hat{\mathbf{a}}' \mathbf{x}^{(1)}$ ,  $\hat{V} = \hat{\mathbf{b}}' \mathbf{x}^{(2)}$  have sample correlation

$$r_{\hat{U}, \hat{V}} = \frac{\hat{\mathbf{a}}' \mathbf{S}_{12} \hat{\mathbf{b}}}{\sqrt{\hat{\mathbf{a}}' \mathbf{S}_{11} \hat{\mathbf{a}}} \sqrt{\hat{\mathbf{b}}' \mathbf{S}_{22} \hat{\mathbf{b}}}}$$

## Sample Canonical Variates and Canonical Correlations

- The first pair of sample canonical variates is the pair of linear combinations  $\hat{U}_1, \hat{V}_1$ 
  - having unit sample variances
  - and having maximum  $r_{\hat{U}, \hat{V}}$
- In general, the  $k$ -th pair of sample canonical variates is the pair of linear combinations  $\hat{U}_k, \hat{V}_k$ 
  - having unit sample variances
  - having maximum  $r_{\hat{U}, \hat{V}}$
  - and uncorrelated with the previous  $(k - 1)$  sample canonical variates
- Results: see next page



## Sample Canonical Variates and Canonical Correlations

$\hat{\rho}_1^{*2} \geq \dots \geq \hat{\rho}_p^{*2}$ : the  $p$  ordered eigenvalues of  $\mathbf{S}_{11}^{-1/2} \mathbf{S}_{12} \mathbf{S}_{22}^{-1} \mathbf{S}_{21} \mathbf{S}_{11}^{-1/2}$

$\hat{\mathbf{e}}_1, \dots, \hat{\mathbf{e}}_p$ : the corresponding eigenvectors;

$\hat{\mathbf{f}}_1, \dots, \hat{\mathbf{f}}_p$ : the eigenvectors of  $\mathbf{S}_{22}^{-1/2} \mathbf{S}_{21} \mathbf{S}_{11}^{-1} \mathbf{S}_{12} \mathbf{S}_{22}^{-1/2}$

Then the  $k$ -th sample canonical variate pair is

$$\hat{U}_k = \underbrace{\hat{\mathbf{e}}_k' \mathbf{S}_{11}^{-1/2}}_{\hat{\mathbf{a}}_k'} \mathbf{x}^{(1)}, \quad \hat{V}_k = \underbrace{\hat{\mathbf{f}}_k' \mathbf{S}_{22}^{-1/2}}_{\hat{\mathbf{b}}_k'} \mathbf{x}^{(2)}$$

$(\mathbf{x}^{(1)}, \mathbf{x}^{(2)})$ : values of  $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}$  for a particular experiment unit)

The first sample canonical variate pair has the maximum sample correlation  $r_{\hat{U}_1, \hat{V}_1} = \hat{\rho}_1^*$ ; and for the  $k$ -th pair,  $r_{\hat{U}_k, \hat{V}_k} = \hat{\rho}_k^*$  is the largest possible correlation among linear combinations uncorrelated with the preceding  $(k - 1)$  sample canonical variates.

$\hat{\rho}_1^*, \dots, \hat{\rho}_p^*$ : sample canonical correlations

## Example 2 – (1)

### Canonical Correlation Analysis of Chicken-bone Data

- The chicken-bone measurements used here:

$$\underbrace{\mathbf{X}^{(1)}}_{\text{Head}} : \begin{cases} X_1^{(1)} = \text{skull length} \\ X_2^{(1)} = \text{skull breadth} \end{cases} \quad \underbrace{\mathbf{X}^{(2)}}_{\text{Leg}} : \begin{cases} X_1^{(2)} = \text{femur length} \\ X_2^{(2)} = \text{tibia length} \end{cases}$$

Standardizing the data to obtain  $\mathbf{Z}^{(1)}$ ,  $\mathbf{Z}^{(2)}$ , and  $\mathbf{Z} = [\mathbf{Z}^{(1)} | \mathbf{Z}^{(2)}]$

The sample correlation matrix  $\mathbf{R}$  (in place of  $\mathbf{S}$ ) is given by

$$\mathbf{R} = \left[ \begin{array}{c|c} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \hline \mathbf{R}_{21} & \mathbf{R}_{22} \end{array} \right] = \left[ \begin{array}{cc|cc} 1 & 0.505 & 0.569 & 0.602 \\ 0.505 & 1 & 0.422 & 0.467 \\ \hline 0.569 & 0.422 & 1 & 0.926 \\ 0.602 & 0.467 & 0.926 & 1 \end{array} \right]$$

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See the textbook, p. 552, Example 10.4.

## Example 2 – (2)

- Thus,  $\mathbf{R}_{11}^{-1/2}\mathbf{R}_{12}\mathbf{R}_{22}^{-1}\mathbf{R}_{21}\mathbf{R}_{11}^{-1/2} = \begin{bmatrix} 0.2844 & 0.1789 \\ 0.1789 & 0.1170 \end{bmatrix}$   
and  $\hat{\rho}_1^{*2} = 0.3893, \hat{\rho}_2^{*2} = 0.0032$ . The eigenvector  $\hat{\mathbf{e}}_1$  (associated with  $\hat{\rho}_1^{*2}$ ) of  $\mathbf{R}_{11}^{-1/2}\mathbf{R}_{12}\mathbf{R}_{22}^{-1}\mathbf{R}_{21}\mathbf{R}_{11}^{-1/2}$  is

$$\hat{\mathbf{e}}_1 = \begin{bmatrix} 0.8437 \\ 0.5468 \end{bmatrix} \implies \hat{\mathbf{a}}_1 = \mathbf{R}_{11}^{-1/2}\hat{\mathbf{e}}_1 = \begin{bmatrix} 0.7808 \\ 0.3445 \end{bmatrix}$$

The eigenvector  $\hat{\mathbf{f}}_1$  (associated with  $\hat{\rho}_1^{*2}$ ) of  $\mathbf{R}_{22}^{-1/2}\mathbf{R}_{21}\mathbf{R}_{11}^{-1}\mathbf{R}_{12}\mathbf{R}_{22}^{-1/2}$  is

$$\hat{\mathbf{f}}_1 = \begin{bmatrix} 0.5766 \\ 0.8170 \end{bmatrix} \implies \hat{\mathbf{b}}_1 = \mathbf{R}_{22}^{-1/2}\hat{\mathbf{f}}_1 = \begin{bmatrix} 0.0603 \\ 0.9439 \end{bmatrix}$$

- The 1st sample canonical variate pair and  $\hat{\rho}_1^*$  are obtained:

$$\hat{U}_1 = 0.781z_1^{(1)} + 0.345z_2^{(1)}, \hat{V}_1 = 0.060z_1^{(2)} + 0.944z_2^{(2)}, \hat{\rho}_1^* = 0.631$$

Similarly, we can work out the 2nd pair and their sample canonical correlation.