# Lecture 11

# **Canonical Correlation Analysis**

Reading: Johnson & Wichern 2007, Chapter 10; Zelterman Chapter 13.2; Izenman Chapter 7.3

DSA 8070 Multivariate Analysis

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## Agenda

- Background
- 2 Canonical Variates & Canonical Correlations
- **3** Sales Data Example



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### Overview

Canonical correlation analysis (CCA, Hotelling, 1936) is a method for exploring the relationships between two sets of multivariate variables  $\boldsymbol{X}=(X_1,X_2,\cdots,X_p)^T$  and  $\boldsymbol{Y}=(Y_1,Y_2,\cdots,Y_q)^T$ 

# RELATIONS BETWEEN TWO SETS OF VARIATES\*.

By HAROLD HOTELLING, Columbia University.

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16. Further Problems

 The Correlation of Vectors. The Most Predictable Criterion and the Tetrad Difference. Concepts of correlation and regression may be applied not only to ordinary one-dimensional variates but also to variates of two or more dimensions.

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#### **Relating Two Random Vectors**

#### **Examples:**

- $X = (X_1, X_2)$  represents two **reading** test scores, and  $\boldsymbol{Y} = (Y_1, Y_2)$  represents two **arithmetic** test
- X is a vector of variables associated with environmental health: species diversity, total biomass, and environmental productivity, while  $oldsymbol{Y}$ represents concentrations of heavy metals, pesticides, and dioxin, which measure environmental toxins

Goal: CCA relates two sets of variables  $\boldsymbol{X}$  and  $\boldsymbol{Y}$  by finding linear combinations of variables that maximally correlated

**Motivation**: relates X and Y using a small number of linear combinations for ease of interpretation



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#### **Linear Combinations of Two Sets of Variables**

Recall we have  $\pmb{X}=(X_1,X_2,\cdots,X_p)^T$  and  $\pmb{Y}=(Y_1,Y_2,\cdots,Y_q)^T.$  Without loss of generality, let's assume  $p \leq q$ .

Similar to PCA, we define a set of linear combinations

$$U_1 = a_{11}X_1 + a_{12}X_2 + \dots + a_{1p}X_p$$

$$U_2 = a_{21}X_1 + a_{22}X_2 + \dots + a_{2p}X_p$$

$$\vdots = \dots$$

$$U_p = a_{p1}X_1 + a_{p2}X_2 + \dots + a_{pp}X_p$$

and

$$V_1 = b_{11}Y_1 + b_{12}Y_2 + \dots + b_{1q}Y_q$$

$$V_2 = b_{21}Y_1 + b_{22}Y_2 + \dots + b_{2q}Y_q$$

$$\vdots = \dots$$

$$V_p = b_{p1}Y_1 + b_{p2}Y_2 + \dots + b_{pq}Y_q$$

We want to find linear combinations that maximize the correlation of  $(U_i, V_i), \quad i = 1, \dots, p$ 



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#### **Defining Canonical Variates**

We call  $(U_i, V_i)$  be the  $i^{th}$  canonical variate pair. One can compute the variance of  $U_i$  with the following expression:

$$\operatorname{Var}(U_i) = \sum_{k=1}^{p} \sum_{\ell=1}^{p} a_{ik} a_{i\ell} \operatorname{Cov}(X_k, X_\ell), \quad i = 1, \dots, p.$$

Similarly, we compute the variance of  $\mathcal{V}_j$  with the following expression:

$$\mathrm{Var}(V_j) = \sum_{k=1}^q \sum_{\ell=1}^q b_{jk} b_{j\ell} \mathrm{Cov}(Y_k,Y_\ell), j=1,\cdots,p.$$

The covariance between  $U_i$  and  $V_i$  is:

$$Cov(U_i, V_j) = \sum_{k=1}^{p} \sum_{\ell=1}^{q} a_{ik} b_{j\ell} Cov(X_k, Y_\ell).$$

The canonical correlation for the  $i^{th}$  canonical variate pair is simply the correlation between  $U_i$  and  $V_i$ :

$$\rho_i^* = \frac{\text{Cov}(U_i, V_i)}{\sqrt{\text{Var}(U_i)\text{Var}(V_i)}}$$

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#### **Finding Canonical Variates**

Let us look at each of the  $\boldsymbol{p}$  canonical variates pair one by one

First canonical variable pair  $(U_1,V_1)$ : The coefficients  $a_{11},a_{12},\cdots,a_{1p}$  and  $b_{11},b_{12},\cdots,b_{1q}$  are chosen to maximize the canonical correlation  $\rho_1^*$ . As in PCA, this is subject to the constraint that  $\mathrm{Var}(U_1)=\mathrm{Var}(V_1)=1$ 

Second canonical variable pair  $(U_2,V_2)$ : Similarly we want to find  $a_{21},a_{22},\cdots,a_{2p}$  and  $b_{21},b_{22},\cdots,b_{2q}$  that maximize  $\rho_2^*$  under the following constraints:

$$Var(U_2) = Var(V_2) = 1,$$
  
 $Cov(U_1, U_2) = Cov(V_1, V_2) = 0,$   
 $Cov(U_1, V_2) = Cov(U_2, V_1) = 0.$ 

This procedure is repeated for each pair of canonical variates



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#### **Finding Canonical Variates Cont'd**

Let  $\mathrm{Var}(X)=\Sigma_X$  and  $\mathrm{Var}(Y)=\Sigma_Y$  and let  $Z^T=(X^T,Y^T).$  Then the covariance matrix of Z is

$$\begin{bmatrix} \operatorname{Var}(\boldsymbol{X}) & \operatorname{Cov}(\boldsymbol{X}, \boldsymbol{Y}) \\ \operatorname{Cov}(\boldsymbol{Y}, \boldsymbol{X}) & \operatorname{Var}(\boldsymbol{Y}) \end{bmatrix} = \begin{bmatrix} \underbrace{\boldsymbol{\Sigma}_{\boldsymbol{X}}}_{p \times p} & \underbrace{\boldsymbol{\Sigma}_{\boldsymbol{X}\boldsymbol{Y}}}_{p \times q} \\ \underbrace{\boldsymbol{\Sigma}_{\boldsymbol{Y}\boldsymbol{X}}}_{q \times p} & \underbrace{\boldsymbol{\Sigma}_{\boldsymbol{Y}}}_{q \times q} \end{bmatrix}$$

The  $i^{th}$  pair of canonical variates is given by

$$U_i = \underbrace{\boldsymbol{u}_i^T \boldsymbol{\Sigma}_X^{-1/2}}_{\boldsymbol{a}_i^T} \boldsymbol{X} \text{ and } V_i = \underbrace{\boldsymbol{v}_i^T \boldsymbol{\Sigma}_Y^{-1/2}}_{\boldsymbol{b}_i^T} \boldsymbol{Y},$$

where

- $m{u}_i$  is the  $i^{th}$  eigenvector of  $m{\Sigma}_{m{X}}^{-1/2}m{\Sigma}_{m{X}m{Y}}m{\Sigma}_{m{Y}}^{-1}m{\Sigma}_{m{Y}m{X}}m{\Sigma}_{m{X}}^{-1/2}$
- ullet  $v_i$  is the  $i^{th}$  eigenvector of  $oldsymbol{\Sigma}_{oldsymbol{Y}}^{-1/2} oldsymbol{\Sigma}_{oldsymbol{X}} oldsymbol{\Sigma}_{oldsymbol{X}}^{-1/2} oldsymbol{\Sigma}_{oldsymbol{X}} oldsymbol{\Sigma}_{oldsymbol{Y}}^{-1/2}$
- The  $i^{th}$  canonical correlation is given by,  $\operatorname{Cor}(U_i,V_i)=\rho_i^*$ , where  $\rho_i^{*2}$  is the  $i^{th}$  eigenvalue of  $\Sigma_X^{-1/2}\Sigma_{XY}\Sigma_Y^{-1}\Sigma_{YX}\Sigma_X^{-1/2}$



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### Likelihood Ratio Test: Is CCA Worthwhile?

Note that if  $\Sigma_{XY} = 0$ , then  $Cov(U, V) = a^T \Sigma_{XY} b = 0$  for all a and  $b \Rightarrow$  all canonical correlations must be zero and there is no point in pursuing CCA.

For large n, we reject  $H_0: \Sigma_{XY} = \mathbf{0}$  in favor of  $H_1: \Sigma_{XY} \neq \mathbf{0}$  if

$$-2\log(\Lambda) = n\log\left(\frac{|\hat{\mathbf{\Sigma}}_{\boldsymbol{X}}||\hat{\mathbf{\Sigma}}_{\boldsymbol{Y}}|}{|\hat{\mathbf{\Sigma}}|}\right) = -n\sum_{j=1}^p\log(1-\hat{\rho}_j^{*2})$$

is larger than  $\chi^2_{pg}(\alpha)$ 

For an improvement to the  $\chi^2$  approximation, Bartlett suggested using the following test statistic:

$$-2\log(\Lambda) = -[n-1 - \frac{1}{2}(p+q+1)] \sum_{i=1}^{p} \log(1 - \hat{\rho}_{j}^{*2})$$

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#### Example: Sales Data [Source: PSU STAT 505]

The example data comes from a firm that surveyed a random sample of n=50 of its employees in an attempt to determine which factors influence sales performance. Two collections of variables were measured:

- Sales Performance: Sales Growth, Sales Profitability, New Account Sales  $\Rightarrow p=3$
- Intelligence Test Scores: Creativity, Mechanical Reasoning, Abstract Reasoning, Mathematics  $\Rightarrow q=4$

We are going to carry out a canonical correlation analysis using  $\ensuremath{\mathbb{R}}$ 



# Likelihood Ratio Test: Is CCA Worthwhile?

Let's first determine if there is any relationship between the two sets of variables at all.

rho <- cc(sales, intelligence)\$cor
n <- dim(sales)[1]
p <- length(sales); q <- length(intelligence)
## Calculate | p-values using the F-approximations library(CCP)
p.asym(rho, n, p, q, tstat = "Wilks")</pre>

$H_0$	Approximate $F$ value	p-value
$\rho_1^* = \rho_2^* = \rho_3^* = 0$	87.39	$\sim 0$
$\rho_2^* = \rho_3^* = 0$	18.53	$8.25 \times 10^{-14}$
$\rho_3^* = 0$	3.88	0.028

All three canonical variate pairs are significantly correlated and dependent on one another. This suggests that we may summarize all three pairs.



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# **Estimates of Canonical Correlation**

Since we rejected the hypotheses of independence, the next step is to obtain estimates of canonical correlation

i	Canonical Correlation $(\rho_i^*)$	$\rho_i^{*2}$
1	0.9945	0.9890
2	0.8781	0.7711
3	0.3836	0.1472

98.9% of the variation in  $U_1$  is explained by the variation in  $V_1$ , 77.11% of the variation in  $U_2$  is explained by  $V_2$ , only 14.72% of the variation in  $U_3$  is explained by  $V_3$ 

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# **Obtain the Canonical Coefficients**

	$U_1$	$U_2$	$U_3$
Growth	0.0624	-0.1741	-0.3772
Profit	0.0209	0.2422	0.1035
New	0.0783	-0.2383	0.3834

The first canonical variable for sales is

 $U_1 = 0.0624X_{growth} + 0.0209X_{profit} + 0.0783X_{new}$ 

	$V_1$	$V_2$	$V_3$
Creativity	0.0697	-0.1924	0.2466
Mechanical	0.0307	0.2016	-0.1419
Abstract	0.08956	-0.4958	-0.2802
Math	0.0628	0.0683	-0.0113

The first canonical variable for test scores is

 $V_1 = 0.0697Y_{create} + 0.0307Y_{mech} + 0.0896Y_{abstract} + 0.0628Y_{math}$ 



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# Correlations Between Each Variable and The Corresponding Canonical Variate

## Correlations Between X's and U's

	$U_1$	$U_2$	$U_3$
Growth	0.9799	0.0006	-0.1996
Profit	0.9464	0.3229	0.0075
New	0.9519	-0.1863	0.2434

#### Correlations Between Y's and V's

	$V_1$	$V_2$	$V_3$
Creativity	0.6383	-0.2157	0.6514
Mechanical	0.7212	0.2376	-0.0677
Abstract	0.6472	-0.5013	-0.5742
Math	0.9441	0.1975	-0.0942



# **Correlations Between Each Set of Variables and The Opposite Group of Canonical Variates**

# Correlations Between X's and V's

	$V_1$	$V_2$	$V_3$
Growth	0.9745	0.0006	-0.0766
Profit	0.9412	0.2835	0.0029
New	0.9466	-0.1636	0.0934

### Correlations Between Y's and U's

	$U_1$	$U_2$	$U_3$
Creativity	0.6348	-0.1894	0.2499
Mechanical	0.7172	0.2086	-0.0260
Abstract	0.6437	-0.4402	-0.2203
Math	0.9389	0.1735	-0.0361

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# **Summary**

# Concepts to know:

- The main idea of canonical correlation analysis (CCA)
- How to compute the canonical variates from the data
- How to determine the number of significant canonical variate pairs
- How to use the results of CCA to describe the relationships between two sets of variables

# $\ensuremath{\mathbb{R}}$ functions to know

- cc from the CCA library
- p.asym from the CCP library

In the next lecture, we will learn about Classification



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