CLEMSON UNIVERSITY

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

1. **Background**
2. **Canonical Variates & Canonical Correlations**
3. **Sales Data Example**

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.

CONTENTS.

1. *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.

Relating Two Random Vectors

Examples:

- $\boldsymbol{X} = (X_1, X_2)$ represents two **reading** test scores, and $\boldsymbol{Y} = (Y_1, Y_2)$ represents two **arithmetic** test scores
- $\boldsymbol{X}$ is a vector of variables associated with **environmental health**: species diversity, total biomass, and environmental productivity, while $\boldsymbol{Y}$ 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 $\boldsymbol{X}$ and $\boldsymbol{Y}$ using a small number of linear combinations for ease of interpretation

Linear Combinations of Two Sets of Variables

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

Similar to PCA, we define a set of linear combinations

$$\begin{aligned} U_1 &= a_{11}X_1 + a_{12}X_2 + \cdots + a_{1p}X_p \\ U_2 &= a_{21}X_1 + a_{22}X_2 + \cdots + a_{2p}X_p \\ \vdots &= \cdots \\ U_p &= a_{p1}X_1 + a_{p2}X_2 + \cdots + a_{pp}X_p \end{aligned}$$

and

$$\begin{aligned} V_1 &= b_{11}Y_1 + b_{12}Y_2 + \cdots + b_{1q}Y_q \\ V_2 &= b_{21}Y_1 + b_{22}Y_2 + \cdots + b_{2q}Y_q \\ \vdots &= \cdots \\ V_p &= b_{p1}Y_1 + b_{p2}Y_2 + \cdots + b_{pq}Y_q \end{aligned}$$

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

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:

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

Similarly, we compute the variance of V_j with the following expression:

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

The covariance between U_i and V_j is:

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

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

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

Finding Canonical Variates

Let us look at each of the 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 ρ_1^*. As in PCA, this is subject to the constraint that $\text{Var}(U_1) = \text{Var}(V_1) = 1$

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 ρ_2^* under the following constraints:

$$\begin{aligned}
\text{Var}(U_2) &= \text{Var}(V_2) = 1, \\
\text{Cov}(U_1, U_2) &= \text{Cov}(V_1, V_2) = 0, \\
\text{Cov}(U_1, V_2) &= \text{Cov}(U_2, V_1) = 0.
\end{aligned}$$

This procedure is repeated for each pair of canonical variates

Finding Canonical Variates Cont'd

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

$$\begin{bmatrix} \mathrm{Var}(\boldsymbol{X}) & \mathrm{Cov}(\boldsymbol{X}, \boldsymbol{Y}) \\ \mathrm{Cov}(\boldsymbol{Y}, \boldsymbol{X}) & \mathrm{Var}(\boldsymbol{Y}) \end{bmatrix} = \begin{bmatrix} \underbrace{\boldsymbol{\Sigma_X}}_{p\times p} & \underbrace{\boldsymbol{\Sigma_{XY}}}_{p\times q} \\ \underbrace{\boldsymbol{\Sigma_{YX}}}_{q\times p} & \underbrace{\boldsymbol{\Sigma_Y}}_{q\times q} \end{bmatrix}$$

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

- $\boldsymbol{u}_i$ is the i^{th} eigenvector of $\boldsymbol{\Sigma_X}^{-1/2}\boldsymbol{\Sigma_{XY}}\boldsymbol{\Sigma_Y}^{-1}\boldsymbol{\Sigma_{YX}}\boldsymbol{\Sigma_X}^{-1/2}$
- $\boldsymbol{v}_i$ is the i^{th} eigenvector of $\boldsymbol{\Sigma_Y}^{-1/2}\boldsymbol{\Sigma_{YX}}\boldsymbol{\Sigma_X}^{-1}\boldsymbol{\Sigma_{XY}}\boldsymbol{\Sigma_Y}^{-1/2}$
- The i^{th} canonical correlation is given by, $\mathrm{Cor}(U_i, V_i) = \rho_i^*$, where ρ_i^{*2} is the i^{th} eigenvalue of $\boldsymbol{\Sigma_X}^{-1/2}\boldsymbol{\Sigma_{XY}}\boldsymbol{\Sigma_Y}^{-1}\boldsymbol{\Sigma_{YX}}\boldsymbol{\Sigma_X}^{-1/2}$

Likelihood Ratio Test: Is CCA Worthwhile?

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

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

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

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

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

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

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 `R`

Likelihood Ratio Test: Is CCA Worthwhile?

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

```r
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")
```

H_0	Approximate F value	p-value
$\rho_1^* = \rho_2^* = \rho_3^* = 0$	87.39	~ 0
$\rho_2^* = \rho_3^* = 0$	18.53	8.25×10^{-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.

Estimates of Canonical Correlation

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

```
cc1 <- cc(sales, intelligence)
cc1$cor
```

i	Canonical Correlation (ρ_i^*)	ρ_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

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

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

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

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

`R` functions to know

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

In the next lecture, we will learn about Classification