Canonical Correlation Analysis

Max Turgeon

STAT 4690–Applied Multivariate Analysis

Introduction

- Canonical Correlation Analysis (CCA) is a dimension reduction method that is similar to PCA, but where we simultaneously reduce the dimension of **two** random vectors $\mathbf{Y}$ and $\mathbf{X}$.
- Instead of trying to explain overall variance, we try to explain the covariance $\mathrm{Cov}(\mathbf{Y}, \mathbf{X})$.
  - Note that this is a measure of **association** between $\mathbf{Y}$ and $\mathbf{X}$.
- Examples include:
  - Arithmetic speed and power ($\mathbf{Y}$) and reading speed and power ($\mathbf{X}$)
  - College performance metrics ($\mathbf{Y}$) and high-school achievement metrics ($\mathbf{X}$)

Population model i

- Let $\mathbf{Y}$ and $\mathbf{X}$ be p- and q-dimensional random vectors, respectively.
  - We will assume that $p \leq q$.
- Let μ_Y and μ_X be the mean of $\mathbf{Y}$ and $\mathbf{X}$, respectively.
- Let Σ_Y and Σ_X be the covariance matrix of $\mathbf{Y}$ and $\mathbf{X}$, respectively, and let $\Sigma_{YX} = \Sigma_{XY}^T$ be the covariance matrix $\mathrm{Cov}(\mathbf{Y}, \mathbf{X})$.
  - Assume Σ_Y and Σ_X are positive definite.
- Note that Σ_{YX} has pq entries, corresponding to all covariances between a component of $\mathbf{Y}$ and a component of $\mathbf{X}$.

Population model ii

- **Goal of CCA**: Summarise Σ_{YX} with p numbers.
    - These p numbers will be called the *canonical correlations*.

Dimension reduction i

- Let $U = a^T\mathbf{Y}$ and $V = b^T\mathbf{Y}$ be linear combinations of $\mathbf{Y}$ and $\mathbf{X}$, respectively.
- We have:
  - $\mathrm{Var}(U) = a^T\Sigma_Y a$
  - $\mathrm{Var}(V) = b^T\Sigma_X b$
  - $\mathrm{Cov}(U, V) = a^T\Sigma_{YX} b$.
- Therefore, we can write the correlation between U and V as follows:

$$\mathrm{Corr}(U, V) = \frac{a^T\Sigma_{YX} b}{\sqrt{a^T\Sigma_Y a}\sqrt{b^T\Sigma_X b}}.$$

Dimension reduction ii

- We are looking for vectors $a \in \mathbb{R}^p, b \in \mathbb{R}^q$ such that $\mathrm{Corr}(U, V)$ is **maximised**.

Definitions

- The *first pair of canonical variates* is the pair of linear combinations U_1, V_1 with unit variance such that $\mathrm{Corr}(U_1, V_1)$ is maximised.
- The k-**th pair of canonical variates** is the pair of linear combinations U_k, V_k with unit variance such that $\mathrm{Corr}(U_k, V_k)$ is maximised among all pairs that are uncorrelated with the previous $k-1$ pairs.
- When U_k, V_k is the k-th pair of canonical variates, we say that $\rho_k = \mathrm{Corr}(U_k, V_k)$ is the k-th *canonical correlation*.

Derivation of canonical variates i

- Make a change of variables:
  - $\tilde{a} = \Sigma_Y^{1/2} a$
  - $\tilde{b} = \Sigma_X^{1/2} b$
- We can then rewrite the correlation:

$$\begin{aligned}\mathrm{Corr}(U, V) &= \frac{a^T \Sigma_{YX} b}{\sqrt{a^T \Sigma_Y a}\sqrt{b^T \Sigma_X b}}\\ &= \frac{\tilde{a}^T \Sigma_Y^{-1/2} \Sigma_{YX} \Sigma_X^{-1/2} \tilde{b}}{\sqrt{\tilde{a}^T \tilde{a}}\sqrt{\tilde{b}^T \tilde{b}}}.\end{aligned}$$

Derivation of canonical variates ii

- Let $M = \Sigma_Y^{-1/2}\Sigma_{YX}\Sigma_X^{-1/2}$. We have

$$\max_{a,b} \mathrm{Corr}(a^T\mathbf{Y}, b^T\mathbf{Y}) \Longleftrightarrow \max_{\tilde{a},\tilde{b}:\|\tilde{a}\|=1,\|\tilde{b}\|=1} \tilde{a}^T M\tilde{b}$$

- The solution to this maximisation problem involves the **singular value decomposition** of M.
- Equivalently, it involves the **eigendecomposition** of MM^T, where

$$MM^T = \Sigma_Y^{-1/2}\Sigma_{YX}\Sigma_X^{-1}\Sigma_{XY}\Sigma_Y^{-1/2}.$$

CCA: Main theorem i

- Let $\lambda_1 \geq \cdots \geq \lambda_p$ be the eigenvalues of $\Sigma_Y^{-1/2}\Sigma_{YX}\Sigma_X^{-1}\Sigma_{XY}\Sigma_Y^{-1/2}$.
  - Let $e_1, \ldots, e_p$ be the corresponding eigenvector with unit norm.
- Note that $\lambda_1 \geq \cdots \geq \lambda_p$ are also the p largest eigenvalues of

$$M^T M = \Sigma_X^{-1/2}\Sigma_{XY}\Sigma_Y^{-1}\Sigma_{YX}\Sigma_X^{-1/2}.$$

  - Let $f_1, \ldots, f_p$ be the corresponding eigenvectors with unit norm.

CCA: Main theorem ii

- Then the k-th pair of canonical variates is given by

$$U_k = e_k^T \Sigma_Y^{-1/2} \mathbf{Y}, \qquad V_k = f_k^T \Sigma_X^{-1/2} \mathbf{X}.$$

- Moreover, we have

$$\rho_k = \mathrm{Corr}(U_k, V_k) = \sqrt{\lambda_k}.$$

Some vocabulary

1. **Canonical directions**: $(e_k^T \Sigma_Y^{-1/2}, f_k^T \Sigma_X^{-1/2})$
2. **Canonical variates**: $(U_k, V_k) = \left(e_k^T \Sigma_Y^{-1/2} \mathbf{Y}, f_k^T \Sigma_X^{-1/2} \mathbf{X}\right)$
3. **Canonical correlations**: $\rho_k = \sqrt{\lambda_k}$

Example i

```r
Sigma_Y <- matrix(c(1, 0.4, 0.4, 1), ncol = 2)
Sigma_X <- matrix(c(1, 0.2, 0.2, 1), ncol = 2)
Sigma_YX <- matrix(c(0.5, 0.3, 0.6, 0.4), ncol = 2)
Sigma_XY <- t(Sigma_YX)

rbind(cbind(Sigma_Y, Sigma_YX),
      cbind(Sigma_XY, Sigma_X))
```

Example ii

```
##      [,1] [,2] [,3] [,4]
## [1,]  1.0  0.4  0.5  0.6
## [2,]  0.4  1.0  0.3  0.4
## [3,]  0.5  0.3  1.0  0.2
## [4,]  0.6  0.4  0.2  1.0
```

Example iii

```r
library(expm)
sqrt_Y <- sqrtm(Sigma_Y)
sqrt_X <- sqrtm(Sigma_X)
M1 <- solve(sqrt_Y) %*% Sigma_YX %*% solve(Sigma_X)%*%
  Sigma_XY %*% solve(sqrt_Y)

(decomp1 <- eigen(M1))
```

Example iv

```
## eigen() decomposition
## $values
## [1] 0.5457180317 0.0009089525
##
## $vectors
##             [,1]       [,2]
## [1,] -0.8946536  0.4467605
## [2,] -0.4467605 -0.8946536
```

```
decomp1$vectors[,1] %*% solve(sqrt_Y)
```

Example v

```
##             [,1]       [,2]
## [1,] -0.8559647 -0.2777371
```

```
M2 <- solve(sqrt_X) %*% Sigma_XY %*% solve(Sigma_Y)%*%
  Sigma_YX %*% solve(sqrt_X)

decomp2 <- eigen(M2)
decomp2$vectors[,1] %*% solve(sqrt_X)
```

```
##            [,1]      [,2]
## [1,] 0.5448119 0.7366455
```

Example vi

```r
sqrt(decomp1$values)
```

```
## [1] 0.73872731 0.03014884
```

Sample CCA

- Let $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$ and $\mathbf{X}_1, \ldots, \mathbf{X}_n$ be random samples, and arrange them in $n \times p$ and $n \times q$ matrices $\mathbb{Y}, \mathbb{X}$, respectively.
  - Note that both sample sizes are equal.
  - Indeed, we assume that $(\mathbf{Y}_i, \mathbf{X}_i)$ are sampled jointly, i.e. on the **same** experimental unit.
- Let $\bar{\mathbf{Y}}$ and $\bar{\mathbf{X}}$ be the sample means.
- Let S_Y and S_X be the sample covariances.
- Define

$$S_{YX} = \frac{1}{n-1} \sum_{i=1}^{n} \left(\mathbf{Y}_i - \bar{\mathbf{Y}}\right) \left(\mathbf{X}_i - \bar{\mathbf{X}}\right)^T .$$

Sample CCA: Main theorem i

- Let $\hat{\lambda}_1 \geq \cdots \geq \hat{\lambda}_p$ be the eigenvalues of $S_Y^{-1/2} S_{YX} S_X^{-1} S_{XY} S_Y^{-1/2}$.
    - Let $\hat{e}_1, \ldots, \hat{e}_p$ be the corresponding eigenvector with unit norm.
- Note that $\hat{\lambda}_1 \geq \cdots \geq \hat{\lambda}_p$ are also the p largest eigenvalues of

$$S_X^{-1/2} S_{XY} S_Y^{-1} S_{YX} S_X^{-1/2}.$$

    - Let $\hat{f}_1, \ldots, \hat{f}_p$ be the corresponding eigenvectors with unit norm.

Sample CCA: Main theorem ii

- Then the k-th pair of *sample* canonical variates is given by
$$\hat{U}_k = \mathbb{Y} S_Y^{-1/2} \hat{e}_k, \qquad \hat{V}_k = \mathbb{X} S_X^{-1/2} \hat{f}_k.$$
- Moreover, we have that $\hat{\rho}_k = \sqrt{\hat{\lambda}_k}$ is the sample correlation of $\hat{U}_k$ and $\hat{V}_k$.

Example (cont'd) i

```r
# Let's generate data
library(mvtnorm)
Sigma <- rbind(cbind(Sigma_Y, Sigma_YX),
               cbind(Sigma_XY, Sigma_X))

YX <- rmvnorm(100, sigma = Sigma)
Y <- YX[,1:2]
X <- YX[,3:4]

decomp <- cancor(x = X, y = Y)
```

Example (cont'd) ii

```
U <- Y %*% decomp$ycoef
V <- X %*% decomp$xcoef

diag(cor(U, V))
```

```
## [1] 0.70084109 0.01977754
```

```
decomp$cor
```

```
## [1] 0.70084109 0.01977754
```

Example i

```r
library(tidyverse)
library(dslabs)

X <- olive %>%
  select(-area, -region) %>%
  as.matrix

Y <- olive %>%
  select(region) %>%
  model.matrix(~ region - 1, data = .)
```

Example ii

```r
head(unname(Y))
```

```
##      [,1] [,2] [,3]
## [1,]    0    0    1
## [2,]    0    0    1
## [3,]    0    0    1
## [4,]    0    0    1
## [5,]    0    0    1
## [6,]    0    0    1
```

Example iii

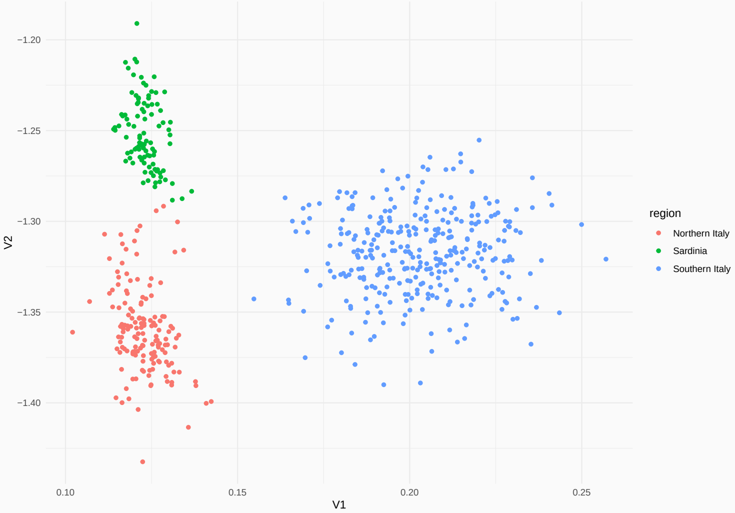
```r
decomp <- cancor(X, Y)

V <- X %*% decomp$xcoef
```

Example iv

```r
data.frame(
  V1 = V[,1],
  V2 = V[,2],
  region = olive$region
) %>%
  ggplot(aes(V1, V2, colour = region)) +
  geom_point() +
  theme_minimal()
```

Example v



−1.20
−1.25
−1.30
−1.35
−1.40
V2
0.10
0.15
0.20
0.25
V1
region
Northern Italy
Sardinia
Southern Italy

Comments i

- The main difference between CCA and Multivariate Linear Regression is that CCA treats $\mathbb{Y}$ and $\mathbb{X}$ *symmetrically*.
- As with PCA, you can use CCA and the covariance matrix or the correlation matrix.
  - The latter is equivalent to performing CCA on the standardised variables.
- Note that sample CCA involves inverting the sample covariance matrices S_Y and S_X:
  - This means we need to assume $p, q < n$.
  - In general, this is what drives most of the performance (or lack thereof) of CCA.

Comments ii

    - There may be gains in efficiency by directly estimating the inverse covariance.
- When one of the two datasets $\mathbb{Y}$ or $\mathbb{X}$ represent indicators variables for a categorical variables (cf. the olive dataset), CCA is equivalent to **Linear Discriminant Analysis**.
    - To learn more about this method, see a course/textbook on Statistical Learning.

Proportions of Explained Sample Variance i

- Just like in PCA, there is a notion of *proportion of explained variance* that may be helpful in determining the number of canonical variates to retain.
- Assume that $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$ and $\mathbf{X}_1, \ldots, \mathbf{X}_n$ have been **standardized**. The matrices A and B of canonical directions have the following properties:
  - The **rows** are the canonical directions (by definition!)
  - The **columns** of the inverses A^{-1}, B^{-1} are the sample correlations between the canonical variates and the standardized variables.

Proportions of Explained Sample Variance ii

- Moreover, we have
  - $\mathrm{Corr}(\mathbb{Y}) = A^{-1}A^{-T}$
  - $\mathrm{Corr}(\mathbb{X}) = B^{-1}B^{-T}$

- But recall that
  - $\mathrm{tr}\left(\mathrm{Corr}(\mathbb{Y})\right) = p$
  - $\mathrm{tr}\left(\mathrm{Corr}(\mathbb{X})\right) = q$

Proportions of Explained Sample Variance iii

- Putting this all together, we have that
  - Proportion of total standardized sample variance in $\mathbb{Y} = \begin{pmatrix} \mathbb{Y}_1 & \cdots & \mathbb{Y}_p \end{pmatrix}$ explained by $\hat{U}_1, \ldots, \hat{U}_r$:

$$R^2(\mathbf{Y} \mid \hat{U}_1, \ldots, \hat{U}_r) = \frac{\sum_{i=1}^{r} \sum_{j=1}^{p} \mathrm{Corr}\left(\hat{U}_i, \mathbb{Y}_k\right)^2}{p}$$

  - Proportion of total standardized sample variance in $\mathbb{X} = \begin{pmatrix} \mathbb{X}_1 & \cdots & \mathbb{X}_q \end{pmatrix}$ explained by $\hat{V}_1, \ldots, \hat{V}_r$:

$$R^2(\mathbf{X} \mid \hat{V}_1, \ldots, \hat{V}_r) = \frac{\sum_{i=1}^{r} \sum_{j=1}^{q} \mathrm{Corr}\left(\hat{V}_i, \mathbb{X}_k\right)^2}{q}$$

Example i

```r
# Olive data
X_sc <- scale(X)
Y_sc <- scale(Y)
decomp_sc <- cancor(X_sc, Y_sc)

V_sc <- X_sc %*% decomp_sc$xcoef
colnames(V_sc) <- paste0("CC", seq_len(ncol(V_sc)))

(prop_X <- rowMeans(cor(V_sc, X_sc)^2))
```

Example ii

```
##   CC1   CC2   CC3   CC4   CC5   CC6   CC7   CC8
## 0.340 0.153 0.124 0.081 0.134 0.039 0.067 0.061
```

```r
cumsum(prop_X)
```

```
##  CC1  CC2  CC3  CC4  CC5  CC6  CC7  CC8
## 0.34 0.49 0.62 0.70 0.83 0.87 0.94 1.00
```

Example iii

```r
# But since we are dealing with correlations
# We get the same with unstandardized variables
decomp <- cancor(X, Y)
V <- X %*% decomp$xcoef
colnames(V) <- paste0("CC", seq_len(ncol(V)))

(prop_X <- rowMeans(cor(V, X)^2))
```

```
##   CC1   CC2   CC3   CC4   CC5   CC6   CC7   CC8
## 0.340 0.153 0.124 0.081 0.134 0.039 0.067 0.061
```

Example iv

```r
cumsum(prop_X)
```

```
##  CC1  CC2  CC3  CC4  CC5  CC6  CC7  CC8
## 0.34 0.49 0.62 0.70 0.83 0.87 0.94 1.00
```

Interpreting the population canonical variates i

- To help interpretating the canonical variates, let's go back to the population model.
- Define

$$A = \begin{pmatrix} e_1^T \Sigma_Y^{-1/2} & \cdots & e_p^T \Sigma_Y^{-1/2} \end{pmatrix}^T,$$
$$B = \begin{pmatrix} f_1^T \Sigma_X^{-1/2} & \cdots & f_p^T \Sigma_X^{-1/2} \end{pmatrix}^T.$$

- In other words, both A and B are $p \times p$, and their *rows* are the canonical directions.

Interpreting the population canonical variates ii

- Using this notation, we can get all canonical variates using one linear transformation:

$$\mathbf{U} = A\mathbf{Y}, \qquad \mathbf{Y} = B\mathbf{X}.$$

- We then have

$$\mathrm{Cov}(\mathbf{U}, \mathbf{Y}) = \mathrm{Cov}(A\mathbf{Y}, \mathbf{Y}) = A\Sigma_Y.$$

- Since $\mathrm{Cov}(\mathbf{U}) = I_p$, we have

$$\mathrm{Corr}(U_k, Y_i) = \mathrm{Cov}(U_k, \sigma_i^{-1} Y_i),$$

where σ_i^2 is the variance of Y_i.

Interpreting the population canonical variates iii

- If we let D_Y be the diagonal matrix whose i-th diagonal element is $\sigma_i = \sqrt{\mathrm{Var}(Y_i)}$, we can write

$$\mathrm{Corr}(\mathbf{U}, \mathbf{Y}) = A\Sigma_Y D_Y^{-1}.$$

- Using similar computations, we get

$$\begin{aligned} \mathrm{Corr}(\mathbf{U}, \mathbf{Y}) &= A\Sigma_Y D_Y^{-1}, & \mathrm{Corr}(\mathbf{V}, \mathbf{Y}) &= B\Sigma_{XY} D_Y^{-1}, \\ \mathrm{Corr}(\mathbf{U}, \mathbf{X}) &= A\Sigma_{YX} D_X^{-1}, & \mathrm{Corr}(\mathbf{V}, \mathbf{X}) &= B\Sigma_X D_X^{-1}. \end{aligned}$$

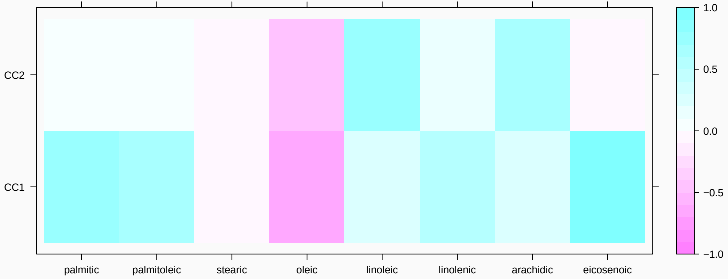
- **These quantities** (and their sample counterparts) **give us information about the contribution of the original variables to the canonical variates**.

Example i

```r
# Let's go back to the olive data
decomp <- cancor(X, Y)
V <- X %*% decomp$xcoef
colnames(V) <- paste0("CC", seq_len(8))

library(lattice)
levelplot(cor(X, V[,1:2]),
          at = seq(-1, 1, by = 0.1),
          xlab = "", ylab = "")
```

Example ii

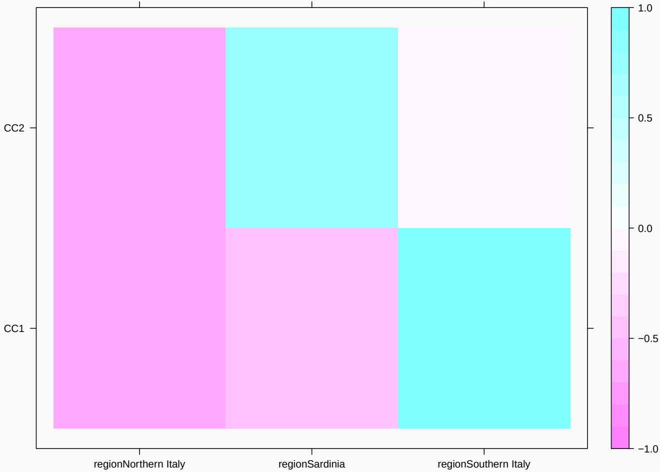


CC2
CC1
palmitic
palmitoleic
stearic
oleic
linoleic
linolenic
arachidic
eicosenoic
1.0
0.5
0.0
−0.5
−1.0

Example iii

```
levelplot(cor(Y, V[,1:2]),
          at = seq(-1, 1, by = 0.1),
          xlab = "", ylab = "")
```

Example iv



CC2
CC1
regionNorthern Italy
regionSardinia
regionSouthern Italy
1.0
0.5
0.0
−0.5
−1.0

Generalization of Correlation coefficients i

- The canonical correlations can be seen as a generalization of many notions of "correlation".
- If both $\mathbf{Y}, \mathbf{X}$ are one dimensional, then

$$\mathrm{Corr}(a^T\mathbf{Y}, b^T\mathbf{X}) = \mathrm{Corr}(\mathbf{Y}, \mathbf{X}), \quad \text{for all } a, b.$$

- In other words, the canonical correlation generalizes the **univariate correlation coefficient**.
- Then assume $\mathbf{Y}$ is one-dimensional, but $\mathbf{X}$ is q-dimensional. Then CCA is equivalent to (univariate) linear regression, and the first canonical correlation is equal to the **multiple correlation coefficient**.

Generalization of Correlation coefficients ii

- Now, let's go back to full-generality: $\mathbf{Y} = (Y_1, \ldots, Y_p)$, $\mathbf{X} = (X_1, \ldots, X_q)$. Let a be all zero except for a one in position i, and let b be all zero except for a one in position j. We have

$$\begin{aligned} |\mathrm{Corr}(Y_i, X_j)| &= |\mathrm{Corr}(a^T\mathbf{Y}, b^T\mathbf{X})| \\ &\leq \max_{a,b} \mathrm{Corr}(a^T\mathbf{Y}, b^T\mathbf{X}) \\ &= \rho_1. \end{aligned}$$

Generalization of Correlation coefficients iii

- In other words, the **first canonical correlation is larger than any entry** (in absolute value) **in the matrix** $\mathrm{Corr}(\mathbf{Y}, \mathbf{X})$.
- Finally, the k-th canonical correlation ρ_k can be interpreted as the **multiple correlation coefficient** of two different univariate linear regression model:
  - U_k against $\mathbf{X}$;
  - V_k against $\mathbf{Y}$.

Example (cont'd) i

```r
# Canonical correlations
decomp$cor
```

```
## [1] 0.95 0.84
```

```r
# Maximum value in correlation matrix
max(abs(cor(Y, X)))
```

```
## [1] 0.89
```

Example (cont'd) ii

```r
# Multiple correlation coefficients
sqrt(summary(lm(V[,1] ~ Y))$r.squared)
```

```
## [1] 0.95
```

```r
sqrt(summary(lm(V[,2] ~ Y))$r.squared)
```

```
## [1] 0.84
```

Geometric interpretation i

- Let's look at a geometric interpretation of CCA.
- First, some notation:
  - Let A be the matrix whose k-th row is the k-th canonical direction $e_k^T\Sigma_Y^{-1/2}$.
  - Let E be the matrix whose k-th *column* is the eigenvector e_k. Note that $E^TE = I_p$.
  - We thus have $A = E^T\Sigma_Y^{-1/2}$.
- We get all canonical variates U_k by transforming $\mathbf{Y}$ using A:

$$\mathbf{U} = A\mathbf{Y}.$$

Geometric interpretation ii

- Now, using the spectral decomposition of Σ_Y, we can write

$$A = E^T \Sigma_Y^{-1/2} = E^T P_Y \Lambda_Y^{-1/2} P_Y^T,$$

where P_Y contains the eigenvectors of Σ_Y and Λ_Y is the diagonal matrix with its eigenvalues.

- Therefore, we can see that

$$\mathbf{U} = A\mathbf{Y} = E^T P_Y \Lambda_Y^{-1/2} P_Y^T \mathbf{Y}.$$

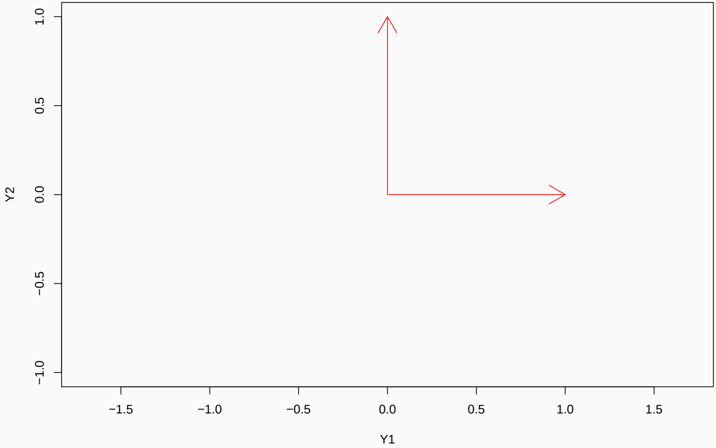
Geometric interpretation iii

- Let's look at this expression in stages:
  - $P_Y^T\mathbf{Y}$: This is the matrix of **principal components** of $\mathbf{Y}$.
  - $\Lambda_Y^{-1/2}\left(P_Y^T\mathbf{Y}\right)$: We standardize the principal components to have unit variance.
  - $P_Y\left(\Lambda_Y^{-1/2}P_Y^T\mathbf{Y}\right)$: We rotate the standardized PCs using a transformation that **only involves** Σ_Y.
  - $E^T\left(P_Y\Lambda_Y^{-1/2}P_Y^T\mathbf{Y}\right)$: We rotate the result using a transformation that **involves the whole covariance matrix** Σ.

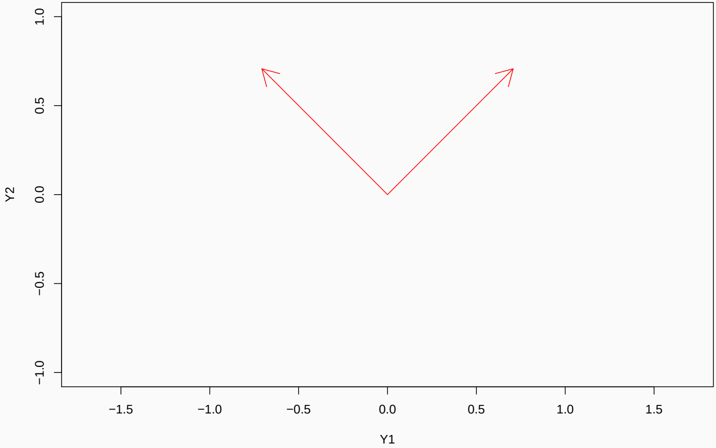
Example i

- Let's go back to the covariance matrix at the beginning of this slide deck:

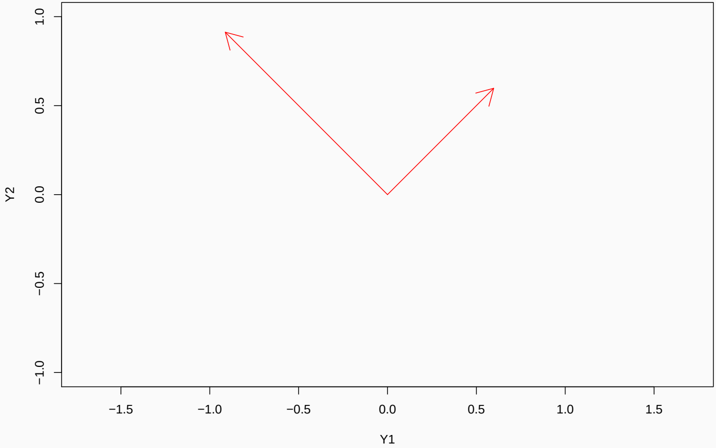
$$\Sigma = \begin{pmatrix} 1.0 & 0.4 & 0.5 & 0.6 \\ 0.4 & 1.0 & 0.3 & 0.4 \\ 0.5 & 0.3 & 1.0 & 0.2 \\ 0.6 & 0.4 & 0.2 & 1.0 \end{pmatrix}.$$



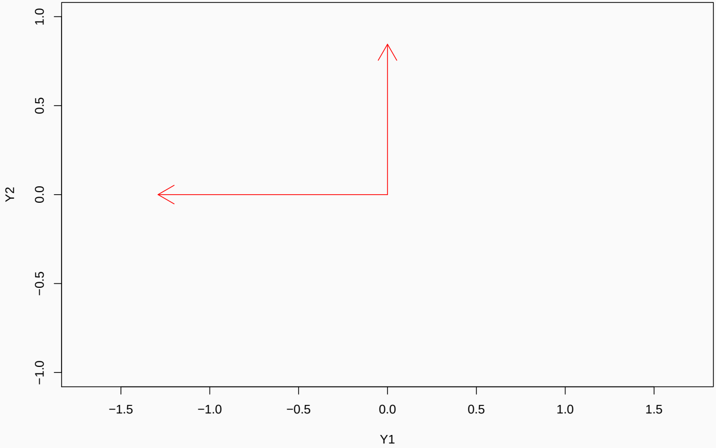
1.0
0.5
0.0
−0.5
−1.0
Y2
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
Y1

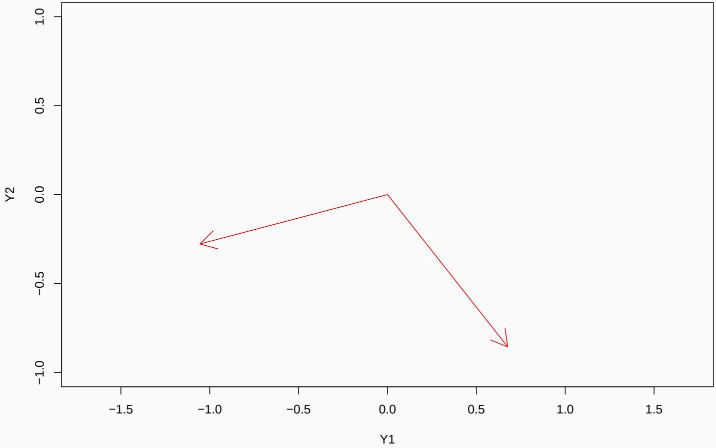


1.0
0.5
0.0
−0.5
−1.0
Y2
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
Y1



Y2
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
Y1


Y2
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
Y1


Y2
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
Y1

Large sample inference

Test of independence i

- Recall what we said at the outset: CCA trys to explain the covariance $\mathrm{Cov}(\mathbf{Y}, \mathbf{X})$.
- If there is no correlation between $\mathbf{Y}, \mathbf{X}$, then $\Sigma_{YX} = 0$.
  - In particular, $a^T \Sigma_{YX} b = 0$ for any choice of $a \in \mathbb{R}^p, b \in \mathbb{R}^q$, and therefore all canonical correlations are equal to 0.
- To test for independence between $\mathbf{Y}$ and $\mathbf{X}$, we will use a **likelihood ratio test**.

LRT for $\Sigma_{YX} = 0$ i

Let $(\mathbf{Y}_i, \mathbf{X}_i)$, $i = 1, \ldots, n$, be a random sample from a normal distribution $N_{p+q}(\mu, \Sigma)$, with

$$\Sigma = \begin{pmatrix} \Sigma_Y & \Sigma_{YX} \\ \Sigma_{XY} & \Sigma_X \end{pmatrix}.$$

Let S_Y, S_X be the sample covariances of $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$, respectively, and let S_n be the $p+q$-dimensional sample covariance of $(\mathbf{Y}_i, \mathbf{X}_i)$.

LRT for $\Sigma_{YX} = 0$ ii

Then the likelihood ratio test for $H_0 : \Sigma_{YX} = 0$ rejects H_0 for large values of

$$-2 \log \Lambda = n \log \left(\frac{|S_Y||S_X|}{|S_n|} \right) = -n \log \prod_{i=1}^{p} (1 - \hat{\rho}_i^2),$$

where $\hat{\rho}_1, \ldots, \hat{\rho}_p$ are the sample canonical correlations.

Null distribution

1. For large n, the statistic $-2\log\Lambda$ is approximately chi-square with degrees of freedom equal to

$$\left(\frac{(p+q)(p+q+1)}{2}\right) - \left(\frac{p(p+1)}{2} + \frac{q(q+1)}{2}\right) = pq.$$

2. Bartlett's correction uses a different statistic (but the same null distribution):

$$-\left(n-1-\frac{1}{2}(p+q+1)\right)\log\prod_{i=1}^{p}(1-\hat{\rho}_i^2).$$

Example i

- We will look at a different example, this time from the field of vegetation ecology.
- We have two datasets:
  - `varechem`: 14 chemical measurements from the soil.
  - `varespec`: 44 estimated cover values for lichen species.
- The data has 24 observations.
- For more details, see Väre, H., Ohtonen, R. and Oksanen, J. (1995) *Effects of reindeer grazing on understorey vegetation in dry Pinus sylvestris forests*. Journal of Vegetation Science 6, 523–530.

Example ii

```r
library(vegan)

data(varespec)
data(varechem)

# There are too many variables in varespec
# Let's pick first 10
Y <- varespec %>%
  select(Callvulg:Diphcomp) %>%
  as.matrix
```

Example iii

```
# The help page in `vegan` suggests a better
# chemical model
X <- varechem %>%
  model.matrix( ~ Al + P*(K + Baresoil) - 1,
               data = .)
```

```
decomp <- cancor(x = X, y = Y)

n <- nrow(X)
(LRT <- -n*log(prod(1 - decomp$cor^2)))
```

Example iv

```
## [1] 156
```

```r
p <- min(ncol(X), ncol(Y))
q <- max(ncol(X), ncol(Y))
LRT > qchisq(0.95, df = p*q)
```

```
## [1] TRUE
```

Example v

```
LRT_bart <- -(n - 1 - 0.5*(p + q + 1)) *
  log(prod(1 - decomp$cor^2))

c("Large Sample" = LRT,
  "Bartlett" = LRT_bart)
```

```
## Large Sample     Bartlett
##          156           94
```

```
LRT_bart > qchisq(0.95, df = p*q)
```

```
## [1] TRUE
```

Sequential inference i

- The LRT above was for independence, i.e. $\Sigma_{YX} = 0$.
- Given our description of CCA above, this test is equivalent to having all canonical correlations being equal to 0.

$$\Sigma_{YX} = 0 \iff \rho_1 = \cdots = \rho_p = 0.$$

- If we reject the null hypothesis, it is natural to ask how many canonical correlations are nonzero.
- Recall that by design $\rho_1 \geq \cdots \geq \rho_p$. We thus get a sequence of null hypotheses:

$$H_0^k : \rho_1 \neq 0, \ldots, \rho_k \neq 0, \rho_{k+1} = \cdots = \rho_p = 0.$$

Sequential inference ii

- We can test the k-th hypothesis using a *truncated* version of the likelihood ratio test statistic:

$$LRT_k = -\left(n - 1 - \frac{1}{2}(p + q + 1)\right) \log \prod_{i=k+1}^{p} (1 - \hat{\rho}_i^2),$$

where its null distribution is approximately chi-square on $(p-k)(q-k)$ degrees of freedom.

Example (cont'd) i

```
# We can get the truncated LRTs in one go
(log_ccs <- rev(log(cumprod(1 - rev(decomp$cor)^2))))
```

```
## [1] -6.513 -4.002 -2.259 -1.011 -0.262 -0.073
```

```
(LRTs <- -(n - 1 - 0.5*(p + q + 1)) * log_ccs)
```

```
## [1] 94.4 58.0 32.7 14.7  3.8  1.1
```

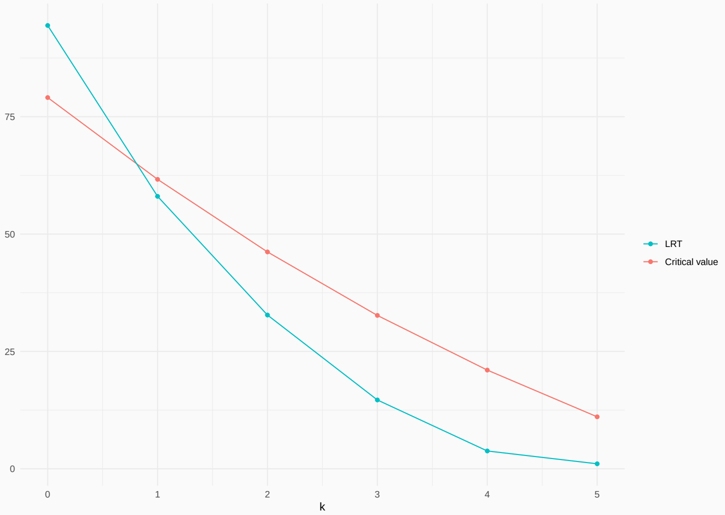
Example (cont'd) ii

```r
k_seq <- seq(0, p - 1)
LRTs > qchisq(0.95,
              df = (p - k_seq)*(q - k_seq))
```

```
## [1]  TRUE FALSE FALSE FALSE FALSE FALSE
```

```r
# We only reject the first null hypothesis
# of independence
```

Example (cont'd) iii



Summary

- CCA is a dimension reduction method like PCA
  - But we are reducing the dimension of two datasets **jointly**.
  - Instead of maximising variance, we maximise **correlation**.
- The goal is to explain the association between $\mathbf{Y}$ and $\mathbf{X}$.
  - Unlike MLR, both datasets are treated equally.
- All visualization methods we discussed in the context of PCA (e.g. component plots, loading plots, biplots) are available for CCA.
  - See the `R` package `vegan`.
- **Limitation**: CCA performs poorly when p and/or q are close to n.