Canonical Correlation

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Discriminant Analysis

Exploring Redundancy In Sets of Variables

- Previously, we studied factor analytic methods as an approach to understanding the key sources of variation within sets of variables.
- There are situations in which we have several sets of variables, and we seek an understanding of key dimensions that are correlated across sets.
- Canonical correlation analysis is the one of the oldest and best known methods for discovering and exploring dimensions that are correlated across sets, but uncorrelated within set.

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An Example – Personality and Achievement

- The relationship between personality and achievement is of interest.
- Suppose the x variables are a set of personality scale scores, and the y variables are a set of academic achievement scores.
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Basic Properties of Canonical Variates

- Canonical Correlation Analysis (CCA) is, in a sense, a combination of the ideas of principal component analysis and multiple regression.
- In CCA, we have two sets of variables, $\boldsymbol{x}$ and $\boldsymbol{y}$, and we seek to understand what aspects of the two sets of variables are redundant.
- The CCA approach seeks to find *canonical variates*, linear combinations of the variables in $\boldsymbol{x}$ and $\boldsymbol{y}$.
- There are canonical variates within each set. If there are q_1 variables in $\boldsymbol{x}$ and q_2 variables in $\boldsymbol{y}$, then there are at most $k = \min(q_1, q_2)$ canonical variates in either set. These are $u_i = \boldsymbol{a}_i'\boldsymbol{x}$, and $v_i = \boldsymbol{b}_i'\boldsymbol{y}$, with i ranging from 1 to k.

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- Within each set, the k distinct canonical variates are uncorrelated.
- Across each set, $\boldsymbol{u}_i$ and $\boldsymbol{v}_j$ are uncorrelated, unless $i = j$.
- The correlation between corresponding canonical variates $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$ is the ith *canonical correlation*.
- An alternate view of the *first* canonical variate is that it is the linear combination of variables in one set that has the highest possible multiple correlation with the variables in the other set.

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Calculating Canonical Variates

- Defining the canonical variates is tantamount to deriving expressions for $\boldsymbol{a}_i$ and $\boldsymbol{b}_i$.
- Clearly, since correlations are invariant under linear transformations, there are infinitely many ways we might define canonical variates.
- It is important to realize that textbooks, in general, are very confused (or at least very confusing) in their treatments of canonical correlation.
- In particular, there are different meanings of the same term, depending on which book you read.

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The Fundamental Result

- A number of textbooks books derive the fact that the linear weights producing canonical variates with maximum possible correlation can be computed as an eigenvector problem.
- Specifically, $\boldsymbol{a}_i$ may be computed as the ith eigenvector of $\boldsymbol{S}_{xx}^{-1}\boldsymbol{S}_{xy}\boldsymbol{S}_{yy}^{-1}\boldsymbol{S}_{yx}$.
- The squared canonical correlation r_i^2 is the corresponding eigenvalue.
- Likewise, $\boldsymbol{b}_i$ is the ith eigenvector of $\boldsymbol{S}_{yy}^{-1}\boldsymbol{S}_{yx}\boldsymbol{S}_{xx}^{-1}\boldsymbol{S}_{xy}$.

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Different Kinds of Canonical Weights

- You don't have to look at many textbook presentations of canonical correlation to realize that the canonical weights presented do not necessarily agree with those produced by various computer programs.
- In some cases, the discrepancies are the result of error, but you should also be aware that there are several different kinds of canonical weights:
  - *Completely Raw.* These weights are, in fact, the eigenvectors described on the previous slide, computed from the covariance matrices.
  - *Partially Standardized.* These weights are multiplied by a constant, so the the resulting canonical variates have unit variance.
  - *Fully Standardized.* These weights are computed on standardized variables (i.e., correlation matrices), then multiplied by a constant so that the resulting canonical variates have unit variance.

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Partially Standardized Weights

- Let $\boldsymbol{A}$ and $\boldsymbol{B}$ contain the raw canonical weights obtained via eigenvector decompositions.
- Then the canonical variates are $\boldsymbol{U} = \boldsymbol{X}\boldsymbol{A}$ and $\boldsymbol{V} = \boldsymbol{Y}\boldsymbol{B}$.
- To standardize the canonical variates, we recall that $\text{Var}(\boldsymbol{U}) = \boldsymbol{A}'\boldsymbol{S}_{xx}\boldsymbol{A}$, and $\text{Var}(\boldsymbol{V}) = \boldsymbol{B}'\boldsymbol{S}_{yy}\boldsymbol{B}$.
- Consequently, we need only postmultiply $\boldsymbol{U}$ and $\boldsymbol{V}$ by the symmetric inverse square root of their covariance matrices.
- Thus, we have

$$\boldsymbol{U}^* = \boldsymbol{X}\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{S}_{xx}\boldsymbol{A})^{-1/2}$$
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which may be expressed as $\boldsymbol{U}^* = \boldsymbol{X}\boldsymbol{A}^*$, $\boldsymbol{V}^* = \boldsymbol{Y}\boldsymbol{B}^*$, with

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- To add to the confusion, SAS refers to these partially standardized weights as "raw canonical weights."

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Fully Standardized Weights

- In fully standardized canonical correlation analysis, we operate on Z scores instead of raw scores for both $\boldsymbol{x}$ and $\boldsymbol{y}$ variables.
- In score notation, the canonical weights $\boldsymbol{A}_s$ and $\boldsymbol{B}_s$ are the first k eigenvectors of $\boldsymbol{R}_{xx}^{-1}\boldsymbol{R}_{xy}\boldsymbol{R}_{yy}^{-1}\boldsymbol{R}_{yx}$ and $\boldsymbol{R}_{yy}^{-1}\boldsymbol{R}_{yx}\boldsymbol{R}_{xx}^{-1}\boldsymbol{R}_{xy}$, respectively, restandardized as in the previous slide.
- The canonical variate scores themselves are obtained by applying the canonical weights to $\boldsymbol{Z}_x$ and $\boldsymbol{Z}_y$, the sample Z-scores.
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A Simple Example

Suppose we have an $\boldsymbol{X}$ and $\boldsymbol{Y}$ given by

$$\boldsymbol{X} = \begin{pmatrix} 1 & 1 & 3 \\ 2 & 3 & 2 \\ 1 & 1 & 1 \\ 1 & 1 & 2 \\ 2 & 2 & 3 \\ 3 & 3 & 2 \\ 1 & 3 & 2 \\ 4 & 3 & 5 \\ 5 & 5 & 5 \end{pmatrix}, \quad \boldsymbol{Y} = \begin{pmatrix} 4 & 4 & -1.07846 \\ 3 & 3 & 1.214359 \\ 2 & 2 & 0.307180 \\ 2 & 3 & -0.385641 \\ 2 & 1 & -0.078461 \\ 1 & 1 & 1.61436 \\ 1 & 2 & 0.814359 \\ 2 & 1 & -0.0641016 \\ 1 & 2 & 1.535900 \end{pmatrix} \tag{3}$$

A Simple Example

- In this highly artificial example, I constructed the third column of $\boldsymbol{Y}$ from the columns of $\boldsymbol{X}$ with the linear weights $\boldsymbol{a}_1' = [.4, .6, -\sqrt{.48}]$.
- Here are some questions:
- What should the first vector of canonical weights for the $\boldsymbol{Y}$ variates be?
- What should the first canonical correlation be?

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- In our simple example, one of the variates in $\boldsymbol{Y}$ can be reproduced exactly as a linear combination of the three variates in $\boldsymbol{X}$.
- Canonical correlation analysis (if it is working properly) will simply select y_3 as the first canonical variate in the $\boldsymbol{Y}$ set, with canonical weights $\boldsymbol{b}_1' = [001]$, and recover the linear combination of the variables in the first group that was used to generate $\boldsymbol{y}_3$ by giving $\boldsymbol{a}_1' = [.4, .6, -\sqrt{.48}]$ as the canonical weights for the $\boldsymbol{X}$ set.
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- To answer the two questions on the preceding slide, recall that the purpose of canonical correlation analysis is to (a) *find* and (b) *characterize* the linear redundancy between two sets of variates.
- In our simple example, one of the variates in $\boldsymbol{Y}$ can be reproduced exactly as a linear combination of the three variates in $\boldsymbol{X}$.
- Canonical correlation analysis (if it is working properly) will simply select y_3 as the first canonical variate in the $\boldsymbol{Y}$ set, with canonical weights $\boldsymbol{b}_1' = [001]$, and recover the linear combination of the variables in the first group that was used to generate $\boldsymbol{y}_3$ by giving $\boldsymbol{a}_1' = [.4, .6, -\sqrt{.48}]$ as the canonical weights for the $\boldsymbol{X}$ set.
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Basic Calculations in R

- We have discussed three different ways of performing canonical correlation analysis:
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  - *Partially Standardized.*
  - *Fully Standardized.*
- Let's perform the calculations in R.
- We'll start with the "Completely Raw" calculation. Much of the work will simply involve setting up the data and calculating correlation and covariance matrices that we need.

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Basic Calculations in R

Completely Raw Weights

- To begin, open R and establish a working directory.
- Then download and copy into R the R Utility Functions routines, available in the *R Code and Support Materials* section of the course website.
- Next, copy into R the *data* file included with these lecture slides, or copy the code below:

```
> source("R Library Functions.txt")
> X <- matrix(c( 1,1,3,2,3,2,1,1,1,
+ 1,1,2,2,2,3,3,3,2,1,3,2,
+ 4,3,5,5,5,5),9,3,byrow=T)
> Y <- matrix(c( 4,4,-1.07846,3,3,1.214359,
+ 2,2,0.307180,2,3,-0.385641,
+ 2,1,-0.078461,1,1,1.61436,
+ 1,2,0.814359,2,1,-0.0641016,
+ 1,2,1.535900 ),9,3,byrow=T)
```

Completely Raw Weights

- To calculate the completely raw weights, we need the variance-covariance matrices for $\boldsymbol{X}$ and $\boldsymbol{Y}$, as well as the cross-covariance matrices.

```
> S.xy <- cov(X,Y)
> S.xx <- var(X)
> S.yx <- cov(Y,X)
> S.yy <- var(Y)
```

- Now that we have these matrices, it is easy to calculate the "completely raw" canonical weights and canonical correlations in R.

```
> A <- eigen(solve(S.xx) %*% S.xy %*%
+     solve(S.yy) %*% S.yx)$vectors
> B <- eigen(solve(S.yy) %*% S.yx %*%
+     solve(S.xx) %*% S.xy)$vectors
> R <- sqrt(eigen(solve(S.yy) %*% S.yx
+     %*% solve(S.xx) %*% S.xy)$values)
```

Completely Raw Weights

The resulting weights for the first canonical variates are what we expected, and the first canonical correlation is 1.

```
> A

           [,1]       [,2]       [,3]
[1,]  0.4000005  0.7960601 -0.5776411
[2,]  0.5999997 -0.5837796  0.4286259
[3,] -0.6928203 -0.1596549  0.6947018

> B

              [,1]        [,2]       [,3]
[1,]  1.940668e-07  0.53653086  0.8347746
[2,] -4.335515e-07 -0.84377041 -0.1385922
[3,]  1.000000e+00 -0.01364310  0.5328635

> R

[1] 1.00000000 0.51938306 0.09103064
```

Partially Standardized Weights

To standardize the weights so that the canonical variances have variances of 1, we need to apply the correction shown earlier.

```
> ## Singly standardized weights (SAS "raw")
> A.single <- A %*% solve(sqrt(diag(diag(var(X %*% A)))))
> B.single <- B %*% solve(sqrt(diag(diag(var(Y %*% B)))))
> A.single

           [,1]       [,2]       [,3]
[1,]  0.4323655  1.4467842 -0.8180369
[2,]  0.6485470 -1.0609791  0.6070064
[3,] -0.7488779 -0.2901618  0.9838146

> B.single

              [,1]        [,2]       [,3]
[1,]  2.097691e-07  0.84865163  1.5199701
[2,] -4.686311e-07 -1.33462432 -0.2523508
[3,]  1.080912e+00 -0.02157982  0.9702457
```

Fully Standardized Weights

- To compute fully standardized weights, we need to calculate Z-scores for our data. We begin by using the $\boldsymbol{Q}$ operator to convert the scores into deviation scores.
- Recall that we learned that $\boldsymbol{Q}_1$, the complementary orthogonal projector for a vector of 1's, will convert a column of scores into deviation score form. The R library functions include a `UnitVector` function and a `Q` function that make this easy.

```
> ##Deviation score X,Y
> X.dev <- Q(UnitVector(9)) %*% X
> Y.dev <- Q(UnitVector(9)) %*% Y
```

Fully Standardized Weights

Calculating Z-Scores

- To convert the deviation scores to Z-scores, we multiply each column by the inverse standard deviation of the scores in that column.
- There are lots of ways we can do this. I'm using the matrix algebra approach of post-multiplying by a diagonal matrix with diagonal entries equal to the inverse standard deviation.

```
> ##Z-score X,Y
> ## Create diagonal matrices with standard deviations
> ## Then invert using solve
> D.x <- solve(sqrt(diag(diag(var(X)))))
> D.y <- solve(sqrt(diag(diag(var(Y)))))
> ## Postmultiply the deviation score matrix
> ## to create Z-scores
> Z.x <- X.dev %*% D.x
> Z.y <- Y.dev %*% D.y
```

- Finally, we apply the identical method used to compute the singly standardized ("SAS Raw") canonical variates, except that we use Z-scores and correlation matrices instead of raw scores and covariance matrices.

```
> R.xy <- cor(X,Y)
> R.xx <- cor(X)
> R.yx <- cor(Y,X)
> R.yy <- cor(Y)
> A.s <- eigen(solve(R.xx) %*%
+   R.xy %*% solve(R.yy) %*% R.yx)$vectors
> B.s <- eigen(solve(R.yy) %*%
+   R.yx %*% solve(R.xx) %*% R.xy)$vectors
> A.fully <- A.s %*%
+   solve(sqrt(diag(diag(var(Z.x %*% A.s)))))
> B.fully <- B.s %*%
+   solve(sqrt(diag(diag(var(Z.y %*% B.s)))))
```

Fully Standardized Weights

```
> A.fully

           [,1]       [,2]       [,3]
[1,]  0.6404914  2.1432165 -1.2118119
[2,]  0.8647293 -1.4146388  0.8093419
[3,] -1.0442604 -0.4046112  1.3718640

> B.fully

              [,1]        [,2]       [,3]
[1,]  2.097691e-07  0.84865163  1.5199701
[2,] -4.939805e-07 -1.40681755 -0.2660011
[3,]  9.999999e-01 -0.01996446  0.8976176
```