Lab 10: Canonical Discriminant Analysis

Stat 154, Spring 2018

Introduction

In this lab you will be working with the `iris` data set. The main purpose is to work around the concepts of how total dispersion (i.e. total sum of squares) can be broken down into between-groups and within-groups dispersion. These concepts are the root of linear discriminant analysis and quadratic discriminant analysis (to be reviewed in HW5).

1) Sum-of-Squares Dispersion Functions

Consider a variable X and a categorical variable Y. Assume that Y represents the class (or group) of each observation. Let k be an index for the classes: $k = 1, \dots, K$; each class is of size n_k; and $n = n_1 + \cdots + n_K$

Function `tss()`: write a function `tss()` that computes the total sum of squares of a given variable:

$$\text{tss} = \sum_{i=1}^{n} (x - \bar{x})^2$$

The function `tss()` should take one argument `x`, the input vector.

Here's how you should be able to call `tss()`

```
tss(iris$Sepal.Length)
```

```
## [1] 102.1683
```

Function `bss()`: write a function `bss()` that computes the between groups sum of squares:

$$\text{bss} = \sum_{k=1}^{K} n_k (\bar{x}_k - \bar{x})^2$$

where:

- n_k is the number of individuals in class k
- $\bar{x}_k$ is the average of class k

The function `bss()` takes two arguments:

- `x` = vector for the predictor variable

- y = vector (or factor) for the response variable
- check that x and y have equal length, otherwise stop() execution

Here's how you should be able to call bss()

```r
bss(iris$Sepal.Length, iris$Species)
```

```
## [1] 63.21213
```

Function wss(): write a function wss() that computes the wetween groups sum of squares:

$$\text{wss} = \sum_{k=1}^{K} \sum_{i \in G_k} (x_{ik} - \bar{x}_k)^2$$

where:

- x_{ik} is the i-th individual in class k
- $\bar{x}_k$ is the average of group k
- G_k represents the group of individuals in class k

The function wss() takes two arguments:

- x = vector for the predictor variable
- y = vector (or factor) for the response variable
- check that x and y have equal length, otherwise stop() execution

Here's how you should be able to call wss()

```r
wss(iris$Sepal.Length, iris$Species)
```

```
## [1] 38.9562
```

2) Sum-of-Squares Ratio Functions

Function cor_ratio(): use bss() and tss() to write a function cor_ratio() that computes the correlation ratio η^2 between a variable x and a response y.

$$\eta^2(x, y) = \frac{\text{bss}}{\text{tss}}$$

Here's how you should be able to call cor_ratio()

```r
cor_ratio(iris$Sepal.Length, iris$Species)
```

```
## [1] 0.6187057
```

Function F_ratio(): use bss() and tss() to write a function F_ratio() that computes the F-ratio between a variable x and a response y.

$$F = \frac{\text{bss}/(K-1)}{\text{wss}/(n-K)}$$

Here's how you should be able to call `F_ratio()`

```
F_ratio(iris$Sepal.Length, iris$Species)
```

```
## [1] 119.2645
```

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3) Discriminant Power of Predictors

For this part of the lab, you will rank the predictors (e.g. `Sepal.Length`, `Sepal.Width`, `Petal.Length`, and `Petal.Width`) using two approaches: 1) correlation ratios, and 2) F-ratios.

The first approach consists of computing correlation ratios:

- Calculate correlation ratios for each predictor and the response.
- Make a table (e.g. data frame) with the predictors ranked by η^2 value in increasing order. The largest the η^2, the more discriminant the predictor.
- Display the η^2's in a barchart.

The second approach consists of computing F-ratios:

- Calculate F-ratios for each predictor and the response.
- Make a table (e.g. data frame) with the predictors ranked by F-value in increasing order. The largest the F, the more discriminant the predictor.
- Display the F-values in a barchart.

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4) Variance functions

Function `total_variance()`: Write a function `total_variance()` that takes a matrix of predictors, and returns the (sample) variance-covariance matrix $\mathbf{V}$. Do NOT use `var()` to create `total_variance()`.

Here's how yo should be able to invoke `total_variance()`, and compare it with the `var()` function.

```
# test total_variance()
total_variance(iris[ ,1:4])
```

```
##              Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length    0.6856935  -0.0424340    1.2743154   0.5162707
```

```
## Sepal.Width    -0.0424340   0.1899794  -0.3296564  -0.1216394
## Petal.Length    1.2743154  -0.3296564   3.1162779   1.2956094
## Petal.Width     0.5162707  -0.1216394   1.2956094   0.5810063
```

```r
# compare with var()
var(iris[ ,1:4])
```

```
##              Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length    0.6856935  -0.0424340    1.2743154   0.5162707
## Sepal.Width    -0.0424340   0.1899794   -0.3296564  -0.1216394
## Petal.Length    1.2743154  -0.3296564    3.1162779   1.2956094
## Petal.Width     0.5162707  -0.1216394    1.2956094   0.5810063
```

Function `between_variance()`: Write a function `between_variance()` that takes a matrix of predictors, and a response vector (or factor), and returns the (sample) Between-variance matrix $\mathbf{B}$. Do NOT use `var()` to create `between_variance()`.

Here's how yo should be able to invoke `between_variance()` on `iris` data

```r
# test between_variance()
between_variance(iris[ ,1:4], iris$Species)
```

```
##              Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length    0.4242425 -0.13391051    1.1090497   0.4783848
## Sepal.Width    -0.1339105  0.07614049   -0.3841584  -0.1539105
## Petal.Length    1.1090497 -0.38415839    2.9335758   1.2535168
## Petal.Width     0.4783848 -0.15391051    1.2535168   0.5396868
```

Function `within_variance()`: Write a function `within_variance()` that takes a matrix of predictors, and a response vector (or factor), and returns the (sample) Within-variance matrix $\mathbf{W}$. Do NOT use `var()` to create `within_variance()`.

Here's how yo should be able to invoke `within_variance()` on `iris` data

```r
# test within_variance()
within_variance(iris[ ,1:4], iris$Species)
```

```
##              Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length   0.26145101  0.09147651   0.16526577  0.03788591
## Sepal.Width    0.09147651  0.11383893   0.05450201  0.03227114
## Petal.Length   0.16526577  0.05450201   0.18270201  0.04209262
## Petal.Width    0.03788591  0.03227114   0.04209262  0.04131946
```

Confirm that $\mathbf{V} = \mathbf{B} + \mathbf{W}$

```r
# confirm V = B + W
Viris <- total_variance(iris[ ,1:4])
Viris
```

```
##              Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length    0.6856935  -0.0424340    1.2743154   0.5162707
## Sepal.Width    -0.0424340   0.1899794   -0.3296564  -0.1216394
## Petal.Length    1.2743154  -0.3296564    3.1162779   1.2956094
## Petal.Width     0.5162707  -0.1216394    1.2956094   0.5810063
```

```
# B + W
Biris <- between_variance(iris[ ,1:4], iris$Species)
Wiris <- within_variance(iris[ ,1:4], iris$Species)
Biris + Wiris
```

```
##              Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length    0.6856935  -0.0424340    1.2743154   0.5162707
## Sepal.Width    -0.0424340   0.1899794   -0.3296564  -0.1216394
## Petal.Length    1.2743154  -0.3296564    3.1162779   1.2956094
## Petal.Width     0.5162707  -0.1216394    1.2956094   0.5810063
```

5) Canonical Discriminant Analysis (CDA)

As we saw in class, CDA involves looking for vectors $\mathbf{u}$ such that:

$$max \left\{ \frac{\mathbf{u^\mathsf{T} B u}}{\mathbf{u^\mathsf{T} V u}} \right\} \Longleftrightarrow max \{ \mathbf{u^\mathsf{T} B u} \} \quad \text{s.t.} \quad \mathbf{u^\mathsf{T} V u} = 1$$

It can be shown that $\mathbf{u}$ is eigenvector of $\mathbf{W^{-1} B}$

$$\mathbf{W^{-1} B u} = \rho \mathbf{u}$$

The problem is that, in general, $\mathbf{W^{-1} B}$ is not symmetric. So what can we do? We can factorize $\mathbf{B}$ as:

$$\mathbf{B} = \mathbf{C C^\mathsf{T}}$$

where $\mathbf{C}$ has general term:

$$c_{jk} = \sqrt{\frac{n_k}{n-1}} \left(\bar{x}_{kj} - \bar{x}_j \right)$$

The $p \times p$ matrix $\mathbf{W^{-1} B}$ and the $k \times k$ matrix $\mathbf{C^\mathsf{T} W^{-1} C}$ have the same eigenvalues.

Their eigenvectors are related by:

$$\mathbf{u} = \mathbf{W^{-1} C w}$$

Thus, we can diagonalize (EVD) the following symmetric matrix:

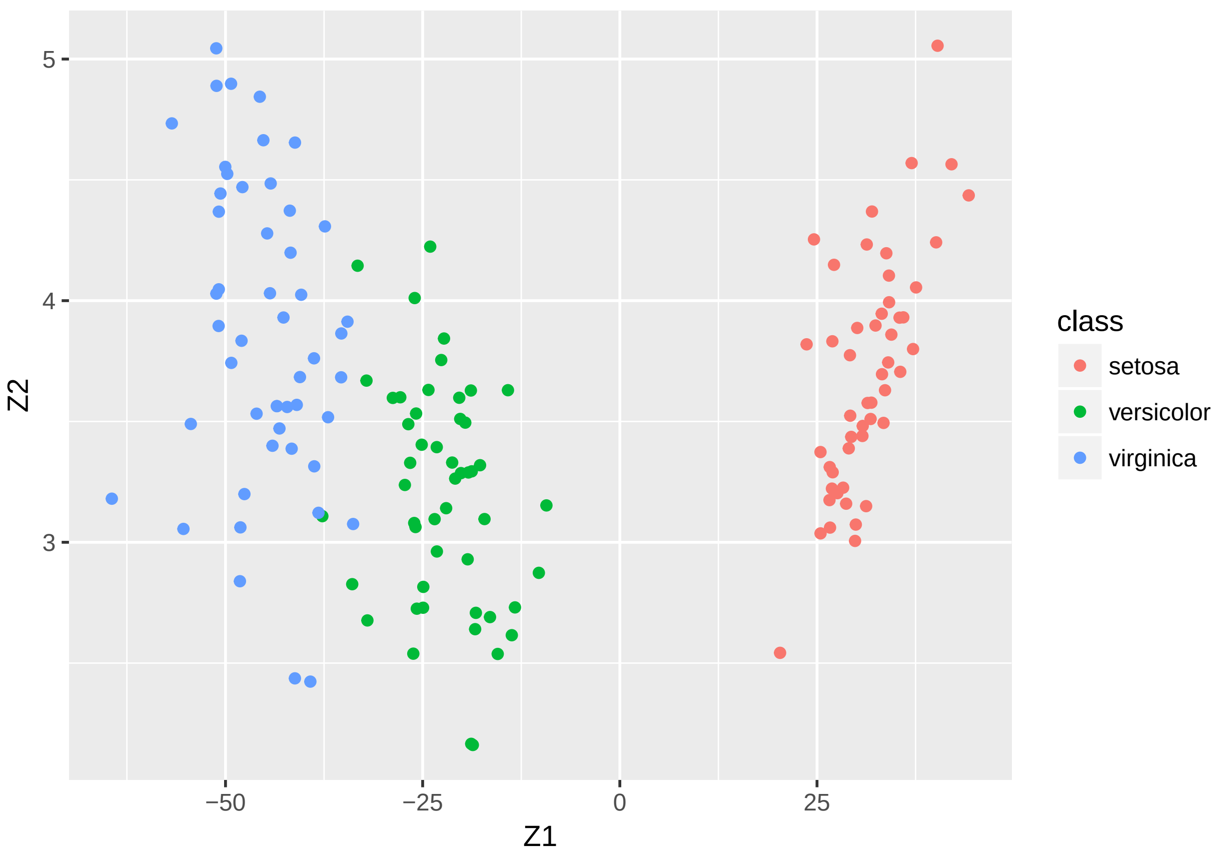
$$\mathbf{C}^\mathsf{T}\mathbf{W}^{-1}\mathbf{C}$$

and then use the eigenvector $\mathbf{w}$ to recover $\mathbf{u}$

Your Turn

Use the predictors and response of the `iris` data, to write code in R that allows you to find the eigenvectors $\mathbf{u_k}$. In other words:

- Create the matrix $\mathbf{C}$
- Obtain EVD of $\mathbf{C}^\mathsf{T}\mathbf{W}^{-1}\mathbf{C}$; this will give you eigenvectors $\mathbf{w}$. Use eigenvectors $\mathbf{w}$ to obtain eigevectors $\mathbf{u} = \mathbf{W}^{-1}\mathbf{C}\mathbf{w}$
- Compute canonical variables $\mathbf{Z} = \mathbf{X}\mathbf{u}$, and use them to plot the `iris` data: i.e. get a scatterplot in which iris classes are best separated.



It is possible that the scale of your scatterplot is different, or even that the shape is different (e.g. you may have an inverted image of my plot). The important thing is the relative position of the cloud of points.

- Obtain a scatterplot of the `iris` data but this time using the first two principal components on the standardized predictors. Add color to the dots indicating the different classes. How does this compare to the previous scatterplot?