

Preamble to Discriminant Analysis (part 2)

Predictive Modeling & Statistical Learning

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Introduction

About

In these slides we continue talking about the concept of Variance decomposition taking into account a group structure as well as variance matrices.

The idea is to layout a couple of foundational principles that should allow you to understand discriminant methods in a more comprehensive way.

BTW: this material is not in the textbooks *ISL* and *APM*.

Iris Data



Dataset iris in R

$n = 150$ Observations, i.e. iris flowers

$p = 4$ predictors

- ▶ Sepal.Length
- ▶ Sepal.Width
- ▶ Petal.Length
- ▶ Petal.Width

One response (categorical)

- ▶ Species (3 classes: setosa, versicolor, virginica)

Famous data set collected by Edgar Anderson (1935), and used by Ronald Fisher (1936) in his paper about Discriminant Analysis.

Dataset iris in R

```
head(iris)
```

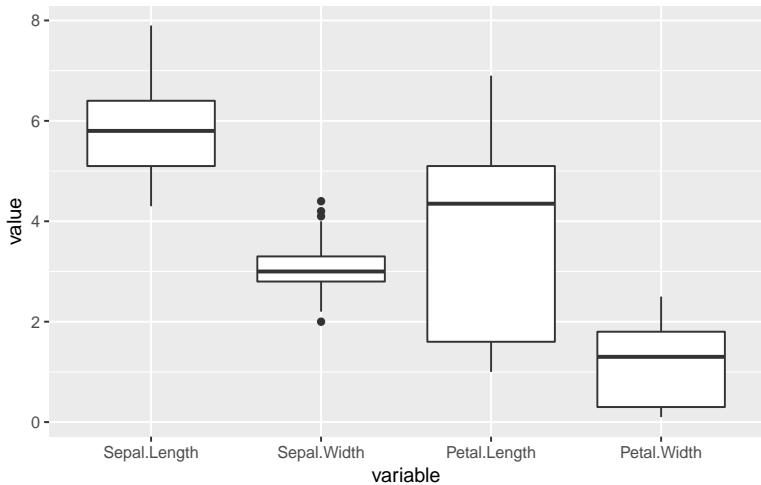
	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1	5.1	3.5	1.4	0.2	setosa
2	4.9	3.0	1.4	0.2	setosa
3	4.7	3.2	1.3	0.2	setosa
4	4.6	3.1	1.5	0.2	setosa
5	5.0	3.6	1.4	0.2	setosa
6	5.4	3.9	1.7	0.4	setosa

Dataset iris in R

```
summary(iris)
```

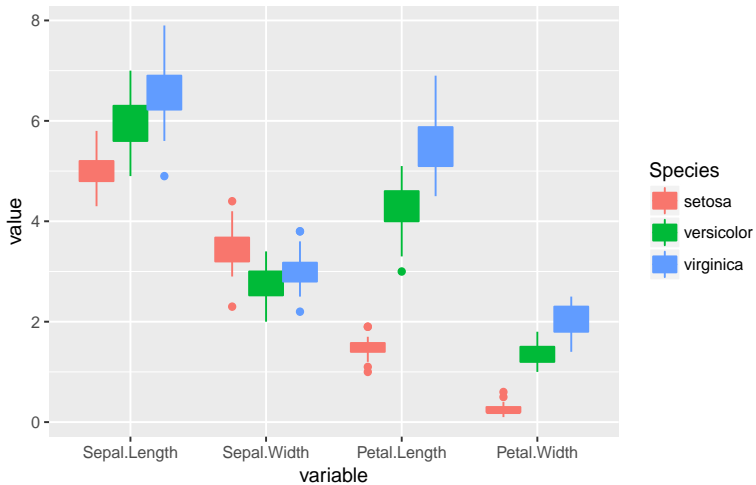
Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
Min. :4.300	Min. :2.000	Min. :1.000	Min. :0.100	setosa :50
1st Qu.:5.100	1st Qu.:2.800	1st Qu.:1.600	1st Qu.:0.300	versicolor:50
Median :5.800	Median :3.000	Median :4.350	Median :1.300	virginica :50
Mean :5.843	Mean :3.057	Mean :3.758	Mean :1.199	
3rd Qu.:6.400	3rd Qu.:3.300	3rd Qu.:5.100	3rd Qu.:1.800	
Max. :7.900	Max. :4.400	Max. :6.900	Max. :2.500	

Boxplot of predictors (iris data)

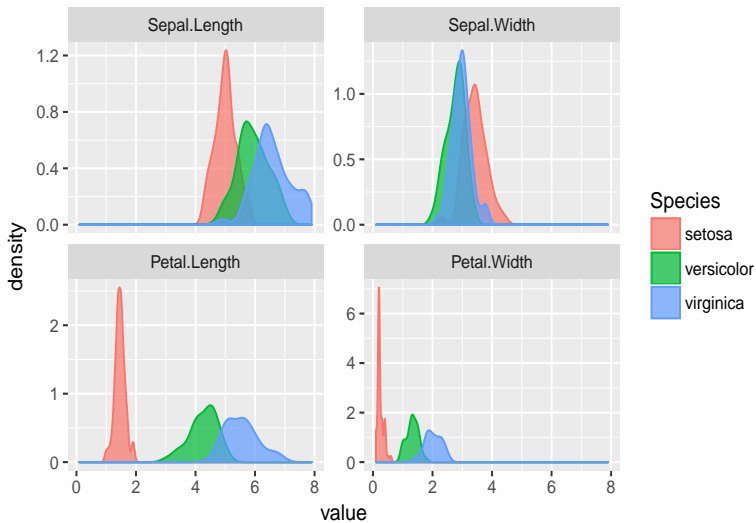


Let's take into account
the group structure

Boxplot of predictors (iris data)



Kernel densities of predictors (iris data)



```
library(reshape2)
library(ggplot2)

iris_melt <- melt(iris, id = "Species")

ggplot(data = iris_melt, aes(x = variable, y = value)) +
  geom_boxplot() +
  ggtitle("Boxplot of predictors (iris data)")

ggplot(data = iris_melt, aes(x = variable, y = value)) +
  geom_boxplot(aes(fill = Species, color = Species)) +
  ggtitle("Boxplot of predictors (iris data)")

ggplot(data = iris_melt, aes(x = value)) +
  geom_density(aes(fill = Species, color = Species),
              alpha = 0.7) +
  facet_wrap(~ variable, scales = 'free_y') +
  ggtitle("Kernel densities of predictors (iris data)")
```

More Notation: generalization
for more than 1 predictor

Predictors and Response

Consider the following assumptions:

- ▶ p predictors X_1, X_2, \dots, X_p
- ▶ One categorical response Y with K categories
- ▶ Y introduces a group or class structure
- ▶ Observations divided in K groups or classes

Caveat: messy notation

Here's some notation that I'll be using while covering classification methods:

Let n_k be the number of observations in the k -th group

Let x_{ijk} represent the i -th observation, of the j -th variable, in the k -th group.

Let x_{ik} represent i -th observation in group k

Let x_{jk} represent j -th variable in group k

I hope this doesn't create a lot of confusion

Caveat: messy notation

Let n_k be the number of observations in the k -th group G_k , then:

$$n = n_1 + n_2 + \cdots + n_K = \sum_{k=1}^K n_k$$

Caveat: messy notation

For a given variable X_j , represented with vector \mathbf{x}_j , we have:

Total or global mean:

$$\bar{x}_j = \frac{1}{n} \sum_{i=1}^n x_{ij}$$

Local mean of observations in group k :

$$\bar{x}_{jk} = \frac{1}{n_k} \sum_{i \in G_k} x_{ij}$$

where G_k represents the set of observations in group k

Caveat: messy notation

For a given variable X_j , represented with vector \mathbf{x}_j , we have:
Total Sum of Squared deviations

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

Assuming centered variables (mean = 0)

$$\text{tss}_j = \mathbf{x}_j^\top \mathbf{x}_j$$

Decomposition of sums-of-squares

An important aspect has to do with looking at the squared deviations: $(x_{ij} - \bar{x}_j)^2$ in terms of the group structure.

A useful trick is to rewrite the deviation terms $x_{ij} - \bar{x}_j$, as:

$$\begin{aligned}x_{ij} - \bar{x}_j &= x_{ij} - (\bar{x}_{jk} - \bar{x}_{jk}) - \bar{x}_j \\ &= (x_{ij} - \bar{x}_{jk}) + (\bar{x}_{jk} - \bar{x}_j)\end{aligned}$$

Decomposition of Sums-of-Squares

Using the previous format of deviations, the sum of squared deviations can be decomposed as:

$$\sum_{i=1}^n (x_{ij} - \bar{x}_j)^2 = \sum_{k=1}^K n_k (\bar{x}_{jk} - \bar{x}_k)^2 + \sum_{k=1}^K \sum_{i \in G_k} (x_{ijk} - \bar{x}_{jk})^2$$

What's this?

Decomposition of Sums-of-Squares

Using the previous format of deviations, the sum of squared deviations can be decomposed as:

$$\underbrace{\sum_{i=1}^n (x_{ij} - \bar{x}_j)^2}_{\text{Total SS}} = \underbrace{\sum_{k=1}^K n_k (\bar{x}_{jk} - \bar{x}_k)^2}_{\text{Between-groups SS}} + \underbrace{\sum_{k=1}^K \sum_{i \in G_k} (x_{ijk} - \bar{x}_{jk})^2}_{\text{Within-groups SS}}$$

Decomposition of Variance

The sums-of-squares decompositions can be put in terms of **population** variances:

$$\underbrace{\frac{1}{n} \sum_{i=1}^n (x_{ij} - \bar{x}_j)^2}_{\text{Total variance}} = \underbrace{\sum_{k=1}^K \frac{n_k}{n} (\bar{x}_{jk} - \bar{x}_k)^2}_{\text{Between-groups variance}} + \underbrace{\frac{1}{n} \sum_{k=1}^K \sum_{i \in G_k} n_k (x_{ijk} - \bar{x}_{jk})^2}_{\text{Within-groups variance}}$$

Formula from one-way analysis of variance (anova)

Decomposition of Variance

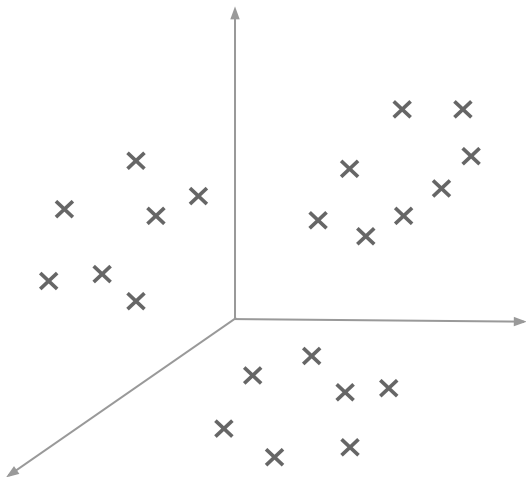
Alternatively, the sums-of-squares decompositions can also be put in terms of **sample** variances:

$$T = \underbrace{\frac{1}{n-1} \sum_{i=1}^n (x_{ij} - \bar{x}_j)^2}_{\text{Total variance}} =$$

$$\underbrace{\sum_{k=1}^K \frac{n_k}{n-1} (\bar{x}_{jk} - \bar{x}_j)^2}_{\text{Between-groups variance}} + \underbrace{\frac{1}{n-1} \sum_{k=1}^K \sum_{i \in G_k} (n_k - 1) (x_{ijk} - \bar{x}_{jk})^2}_{\text{Within-groups variance}}$$

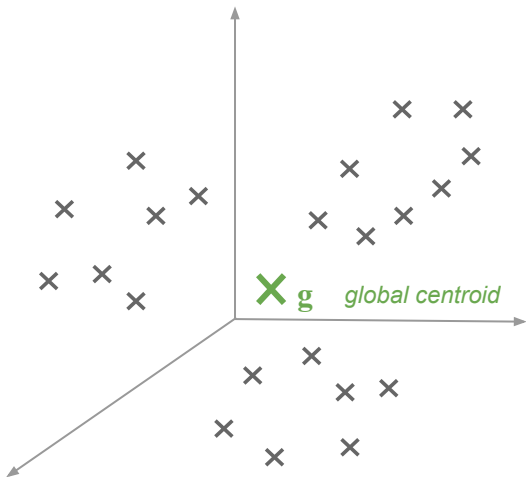
Geometric Perspective

Data as a cloud of points in p -dim space



Cloud of n points in p -dimensional space

Global centroid (center of gravity)



The *centroid* g is the point of averages

Global Centroid

The global centroid \mathbf{g} is the point of averages which consists of the point formed with all the variable means:

$$\mathbf{g} = [\bar{x}_1, \bar{x}_2, \dots, \bar{x}_p]$$

where:

$$\bar{x}_j = \frac{1}{n} \sum_{i=1}^n x_{ij}$$

If all variables are mean-centered, the centroid is the origin

$$\mathbf{g} = \underbrace{[0, 0, \dots, 0]}_{p \text{ times}}$$

Total Dispersion

Taking the global centroid as a point of reference, we can look at the amount of spread or dispersion in the data.

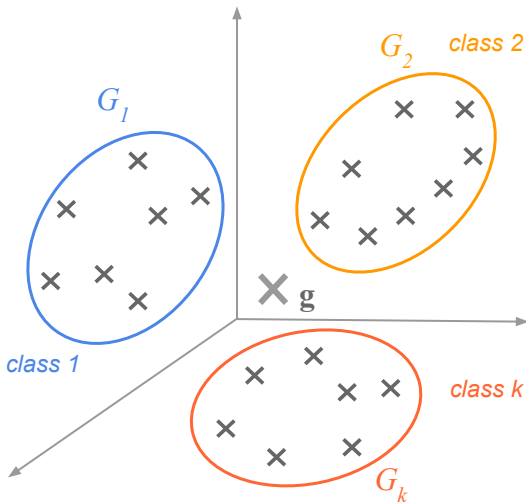
Assuming centered variables, a matrix of total dispersion is given by the *Total Sums of Squares* (TSS):

$$\text{TSS} = \mathbf{X}^T \mathbf{X}$$

Alternatively, we can get the variance-covariance matrix \mathbf{V} :

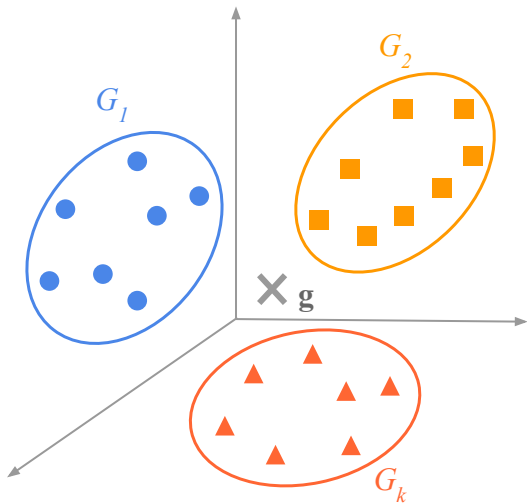
$$\mathbf{V} = \frac{1}{n-1} \mathbf{X}^T \mathbf{X}$$

Class (group) structure



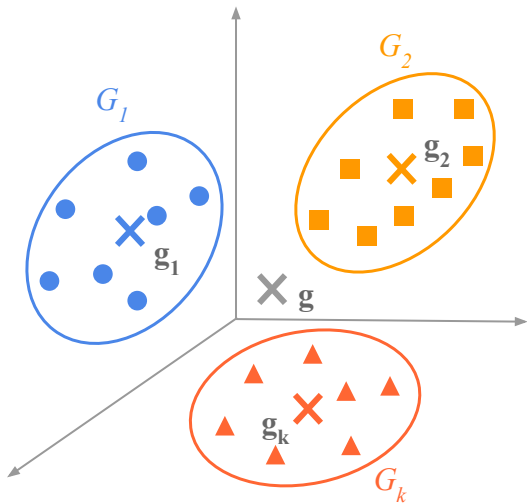
The objects are divided into classes or groups

Sub-cloud of points for each group



Each group G_k forms its own sub-cloud

Local or group centroids (one per class)



Each group G_k has its own centroid g_k

Group Centroids

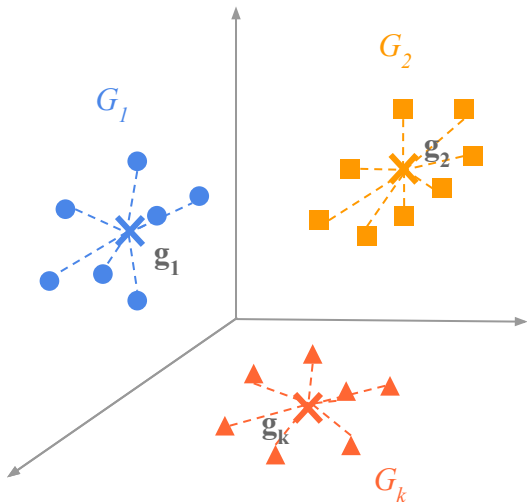
The group centroid \mathbf{g}_k is the point of averages for those observations in group k :

$$\mathbf{g}_k = [\bar{x}_{1k}, \bar{x}_{2k}, \dots, \bar{x}_{pk}]$$

where:

$$\bar{x}_{jk} = \frac{1}{n_k} \sum_{i \in G_k} x_{ij}$$

Within-groups dispersion



We can focus on the dispersion within the clouds

Dispersion inside a group

Each group will have an associated spread or dispersion matrix given by a *Group Sums of Squares* (GSS):

$$\text{GSS}_k = \mathbf{X}_k^T \mathbf{X}_k$$

Equivalently, there is an associated variance matrix \mathbf{W}_k for each group

$$\mathbf{W}_k = \frac{1}{n_k - 1} \mathbf{X}_k^T \mathbf{X}_k$$

where \mathbf{X}_k is the data matrix of the k -th group

Within-groups dispersion

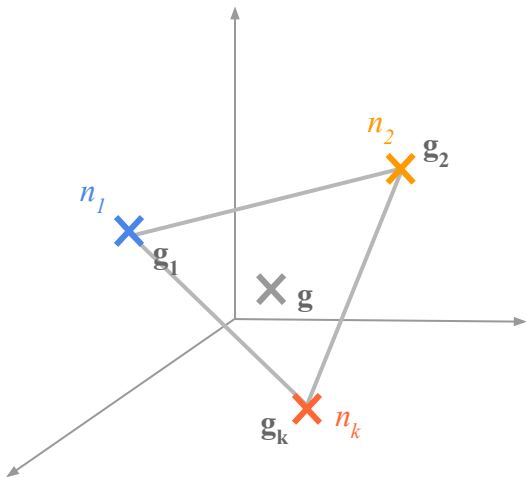
We can combine the groups dispersion to obtain a Within-groups Sums of Squares (WSS) matrix:

$$\text{WSS} = \sum_{k=1}^K \mathbf{X}_k^{\top} \mathbf{X}_k$$

Likewise, we can combine the group variances \mathbf{W}_k as a weighted average to get the **Within-groups** variance matrix \mathbf{W} :

$$\mathbf{W} = \sum_{k=1}^K \frac{n_k - 1}{n - 1} \mathbf{W}_k$$

Global and Group Centroids



What if we focus on just the centroids?

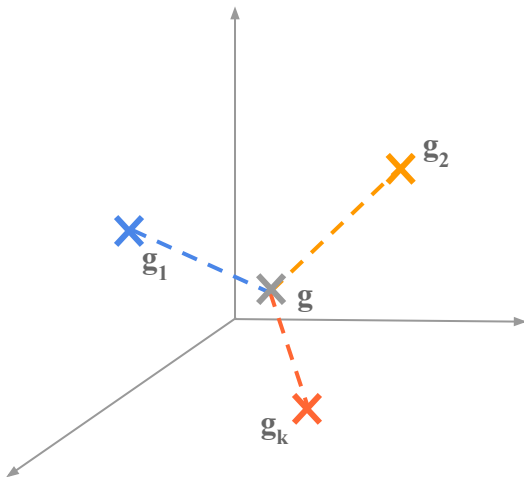
Global and Group Centroids

Note that the global centroid \mathbf{g} can be expressed as a weighted average of the group centroids:

$$\mathbf{g} = \frac{n_1}{n} \mathbf{g}_1 + \frac{n_2}{n} \mathbf{g}_2 + \cdots + \frac{n_K}{n} \mathbf{g}_K$$

$$\mathbf{g} = \sum_{k=1}^K \left(\frac{n_k}{n} \right) \mathbf{g}_k$$

Between-groups dispersion



We can focus on the dispersion between the centroids

Dispersion between groups

Focusing on just the centroids, we can get its corresponding matrix of dispersion given by the *Between Sums of Squares* (BSS):

$$\text{BSS} = \sum_{k=1}^K n_k (\mathbf{g}_k - \mathbf{g})(\mathbf{g}_k - \mathbf{g})^\top$$

Equivalently, there is an associated **Between-groups** variance matrix \mathbf{B}

$$\mathbf{B} = \sum_{k=1}^K \frac{n_k}{n-1} (\mathbf{g}_k - \mathbf{g})(\mathbf{g}_k - \mathbf{g})^\top$$

Three types of Dispersions

Let's recap. We have three types of sums-of-squares matrices:

- ▶ TSS: Total Sums of Squares
- ▶ WSS: Within-groups Sums of Squares
- ▶ BSS: Between-groups Sums of Squares

Alternatively, we also have three types of variance matrices:

- ▶ **V**: Total variance
- ▶ **W**: Within-groups variance
- ▶ **B**: Between-groups variance

Dispersion Decomposition

It can be shown (Huygens theorem) for both, sums-of-squares and variances, that the total dispersion (TSS or V) can be decomposed as:

- ▶ $TSS = BSS + WSS$
- ▶ $V = B + W$

Dispersion Decomposition

Let \mathbf{X} be the $n \times p$ mean-centered matrix of predictors, and \mathbf{Y} be the $n \times K$ dummy matrix of groups

- ▶ $\text{TSS} = \mathbf{X}^T \mathbf{X}$
- ▶ $\text{BSS} = \mathbf{X}^T \mathbf{Y} (\mathbf{Y}^T \mathbf{Y})^{-1} \mathbf{Y}^T \mathbf{X}$
- ▶ $\text{WSS} = \mathbf{X}^T (\mathbf{I} - \mathbf{Y} (\mathbf{Y}^T \mathbf{Y})^{-1} \mathbf{Y}^T) \mathbf{X}$

Bibliography

- ▶ **Principles of Multivariate Analysis: A User's Perspective** by W.J. Krzanowski (1988). *Chapter 11: Incorporating group structure: descriptive methods*. Wiley.
- ▶ **Practical Biostatistical Methods** by Steve Selvin (1995). *Chapter 1: General Concepts*. Duxbury Press.
- ▶ **Data Mining and Statistics for Decision Making** by Stephane Tuffery (2011). *Chapter 11: Classification and prediction methods*.
- ▶ **Multivariate Analysis** by Maurice Tatsuoka (1988). *Chapter 7: Discriminant Analysis and Canonical Correlation*.

French Literature

- ▶ **Statistique Exploratoire Multidimensionnelle** by Lebart et al (2004). *Chapter 3, section 3: Analyse factorielle discriminante.* Dunod, Paris.
- ▶ **Probabilites, analyse des donnees et statistique** by Gilbert Saporta (2011). *Chapter 18: Analyse discriminante et regression logistique.* Editions Technip, Paris.
- ▶ **Statistique explicative appliquee** by Nakache and Confais (2003). *Chapter 1: Analyse discriminante sur variables quantitatives.* Editions Technip, Paris.
- ▶ **Statistique: Methodes pour decrire, expliquer et prevoir** by Michel Tenenhaus (2008). *Chapter 10: L'analyse discriminante.* Dunod, Paris.