Preamble to Discriminant Analysis

Predictive Modeling & Statistical Learning

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Introduction

Introduction

In these slides I'll talk about the concept of Variance decomposition taking into account a group structure.

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

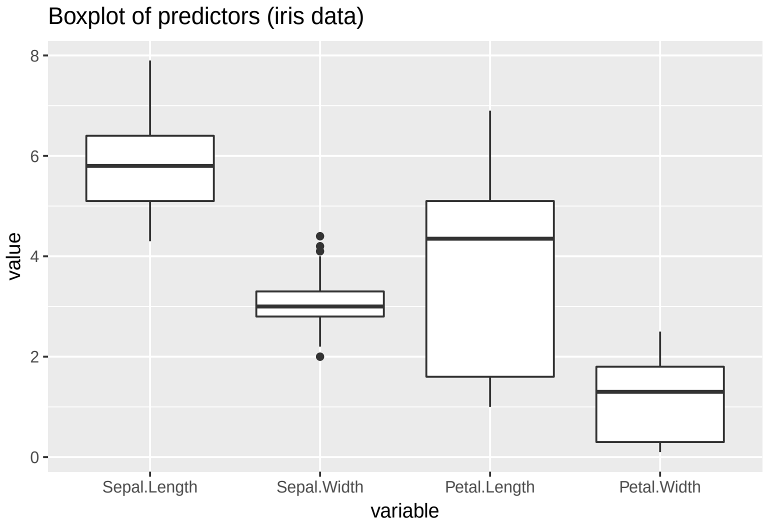
```r
head(iris)
```

```
  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
```



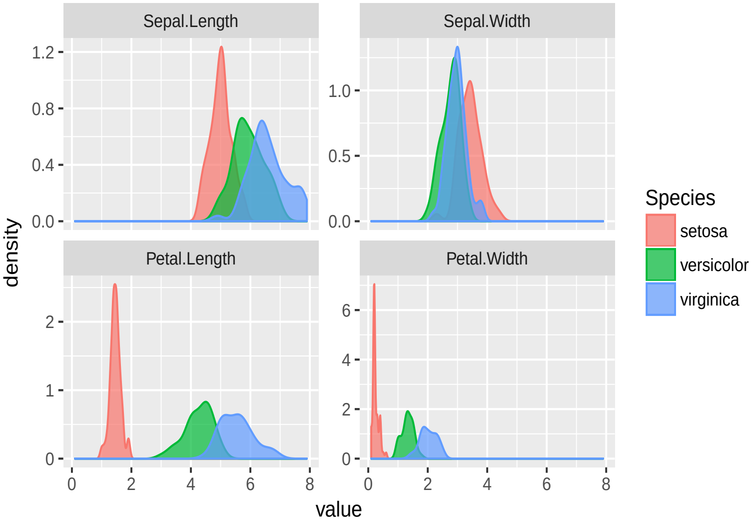
Boxplot of predictors (iris data)
8
6
4
2
0
value
Sepal.Length
Sepal.Width
Petal.Length
Petal.Width
variable

Let's take into account

the group structure

Boxplot of predictors (iris data)

Kernel densities of predictors (iris data)



```r
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)")
```

Which predictor provides the "best" distinction between Species?

Caveat: messy notation

In regression problems we've been using two indices i and j

- i for objects, $i = 1, \ldots, n$
- j for predictors, $j = 1, \ldots, p$

New index k

Now we have a new index k for groups or classes, $k = 1, \ldots, K$.

Sum of Squares

Consider a single predictor X and a categorical response Y

Ignoring the respone, we can obtain the mean $\bar{x}$ and the total sum of squares (TSS) of X as:

$$\bar{x} = \sum_{i=1}^{n} x_i$$

$$\mathsf{TSS} = \sum_{i=1}^{n} (x_i - \bar{x})^2$$

Group (or class) structure

Let's take into account the group structure conveyed by Y

- Let G_k represent the k-th group in Y
- Let n_k be the number of observations in group G_k,
- Then:

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

Between Sum of Squares

Each group k will have its mean $\bar{x}_k$:

$$\bar{x}_k = \sum_{i \in G_k} x_{ik}$$

We can obtain the *Between-Groups Sum of Squares* (BSS)

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

Within Sum of Squares

Each group k will also have its own sum-of-squares SS_k

$$\mathsf{SS}_k = \sum_{i \in G_k} (x_{ik} - \bar{x}_k)^2$$

We can obtain the *Within-Groups Sum of Squares* (WSS)

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

Decomposition of sums-of-squares

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

A useful trick is to rewrite the deviation terms $x_i - \bar{x}$ as:

$$\begin{aligned} x_i - \bar{x} &= x_i - (\bar{x}_k - \bar{x}_k) - \bar{x} \\ &= (x_i - \bar{x}_k) + (\bar{x}_k - \bar{x}) \end{aligned}$$

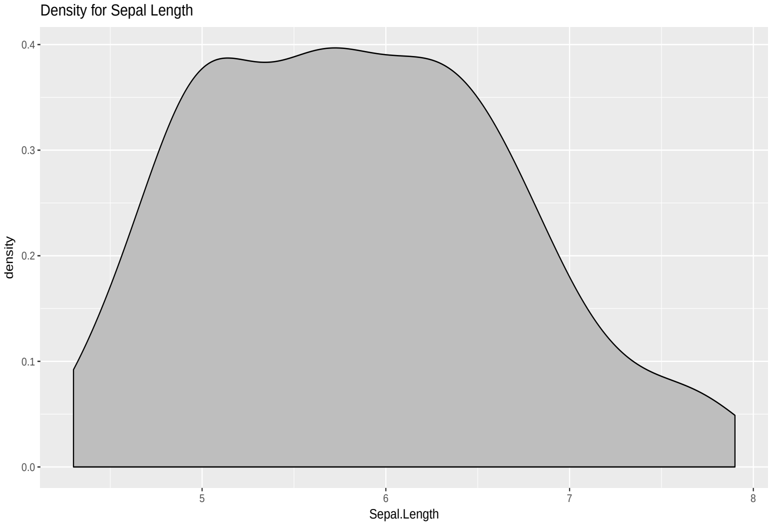
Sum of Squares Decomposition

We can decompose TSS in terms of BSS and WSS:

$$\underbrace{\sum_{k=1}^{K} \sum_{i \in G_k} (x_{ik} - \bar{x})^2}_{\text{TSS}} = \underbrace{\sum_{k=1}^{K} n_k (\bar{x}_k - \bar{x})^2}_{\text{BSS}} + \underbrace{\sum_{i \in G_k} (x_{ik} - \bar{x}_k)^2}_{\text{WSS}}$$

In summary:

$$\text{TSS} = \text{BSS} + \text{WSS}$$




```r
ggplot(data = iris, aes(x = Sepal.Length)) +
geom_density(fill = 'gray') +
ggtitle('Density for Sepal Length')
```

TSS for Sepal.Length

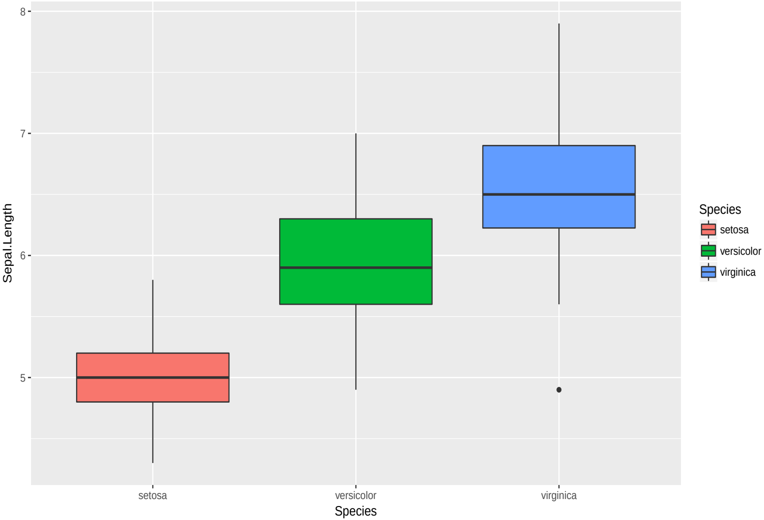
```
x <- iris$Sepal.Length

# overall mean
x_bar <- mean(x)
x_bar
```

```
## [1] 5.843333
```

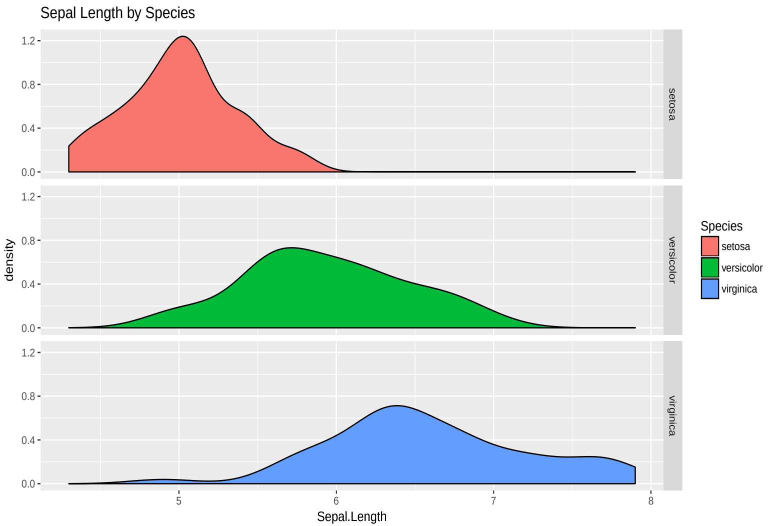
```
# total sums-of-squares
tss <- sum((x - x_bar)^2)
tss
```

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

Let's consider the group structure




```r
ggplot(data = iris, aes(x = Species, y = Sepal.Length)) +
  geom_boxplot(aes(fill = Species))
```




```r
ggplot(data = iris, aes(x = Sepal.Length, group = Species)) +
  geom_density(aes(fill = Species)) +
  facet_grid(Species ~ .) +
  ggtitle('Sepal Length by Species')
```

BSS for Sepal.Length

```
# Sepal Length group means
x_means <- tapply(x, iris$Species, mean)

# between sums-of-squares
bss <- sum(50 * (x_means - x_bar)^2)
bss
```

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

WSS for Sepal.Length

```r
# Sepal Length group sum of squares
w1 <- sum((x[1:50] - x_means[1])^2)
w2 <- sum((x[51:100] - x_means[2])^2)
w3 <- sum((x[101:150] - x_means[3])^2)

# within sums-of-squares
wss <- w1 + w2 + w3
wss
```

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

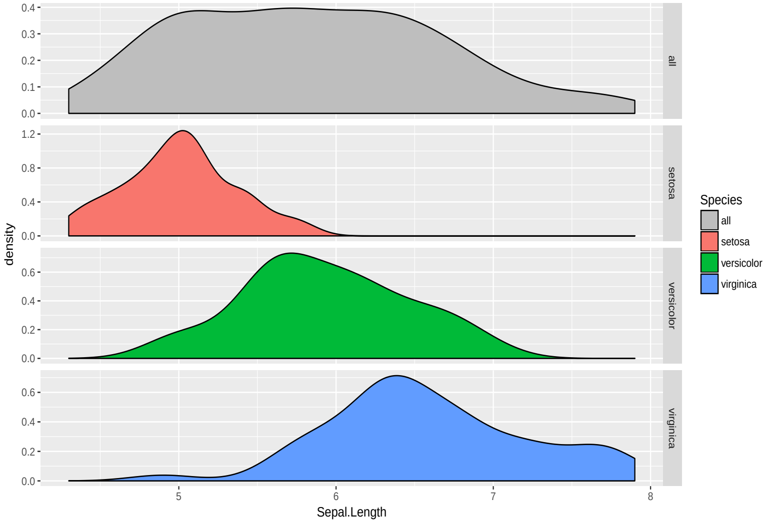
TSS Decomposition

Let's check that we have:

$$\text{TSS} = \text{BSS} + \text{WSS}$$

```
# tss
tss

## [1] 102.1683

# bss + wss
bss + wss

## [1] 102.1683
```

Dispersion in Sepal.Length



Derived Ratios from $\text{TSS} = \text{BSS} + \text{WSS}$

Correlation Ratio

Correlation ratio η^2 (proposed by K. Pearson):

$$\eta^2(X,Y) = \frac{\text{BSS}}{\text{TSS}}$$

- η^2 takes vaues between 0 and 1
- $\eta^2 = 0$ represents the special case of no dispersion among the means of the different categories
- $\eta^2 = 1$ refers to no dispersion within the respective categories.

The correlation ratio is a measure of the relationship between the dispersion within categories and the dispersion across all individuals.

F Ratio

With $\text{TSS} = \text{BSS} + \text{WSS}$, we can also calculate:

F ratio (proposed by R.A. Fisher):

$$F = \frac{\text{BSS}/(k-1)}{\text{WSS}/(n-k)}$$

The larger the value of both ratios, the more variability is there between groups than within groups.

Ratios for Sepal.Length

```r
# correlation ratio
eta_sqr <- bss / tss
eta_sqr

## [1] 0.6187057

# F ratio
F_ratio <- (bss / (3 - 1)) / (wss / (150 - 3))
F_ratio

## [1] 119.2645
```

Ratios for all Variables

Let's compute the decompositions for all predictors, and obtain the correlation ratios and F ratios

```
etas

## Sepal.Length  Sepal.Width Petal.Length  Petal.Width
##    0.6187057    0.4007828    0.9413717    0.9288829

Fs

## Sepal.Length  Sepal.Width Petal.Length  Petal.Width
##    119.26450     49.16004   1180.16118    960.00715
```

More Notation: generalization for more than 1 predictor

Predictors and Response

- p predictors $X_1, X_2, \ldots, X_p$
- 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 confussion

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, representeded with vector $\mathbf{x_j}$, we have:
Total Sum of Squared deviations

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

Assuming centered variables (mean $= 0$)

$$\mathsf{TSS}_j = \mathbf{x_j}^\mathsf{T} \mathbf{x_j}$$

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

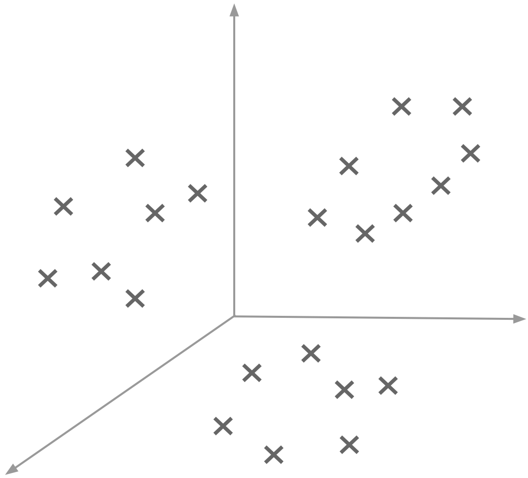
Alternatively, the sums-of-squares decompositions can also be put in terms of **sample** variances:

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

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

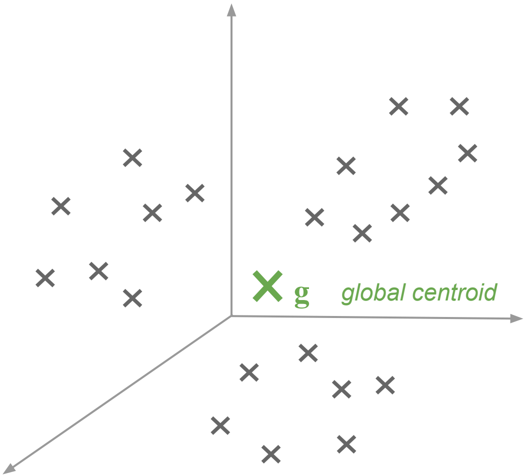
Geometric Perspective

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.

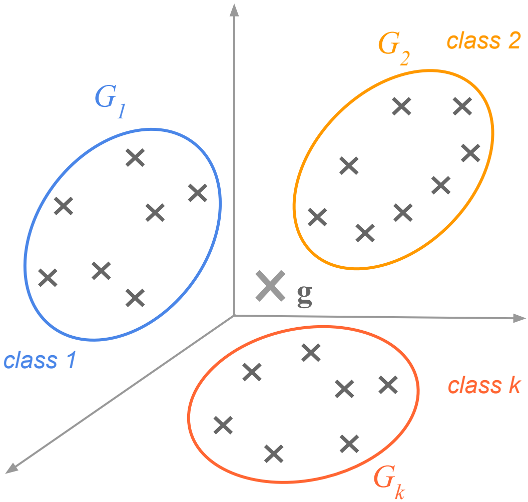
Assuming centered variables, a matrix of total dispersion is given by the *Total Sums of Squares* (TSS):

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

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

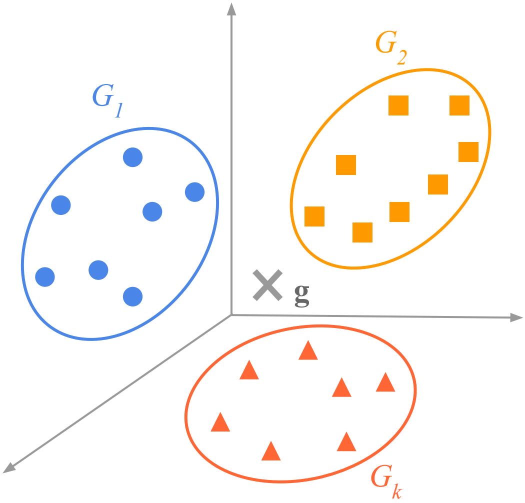
$$\mathbf{V} = \frac{1}{n-1}\mathbf{X}^\mathsf{T}\mathbf{X}$$

Class (group) structure



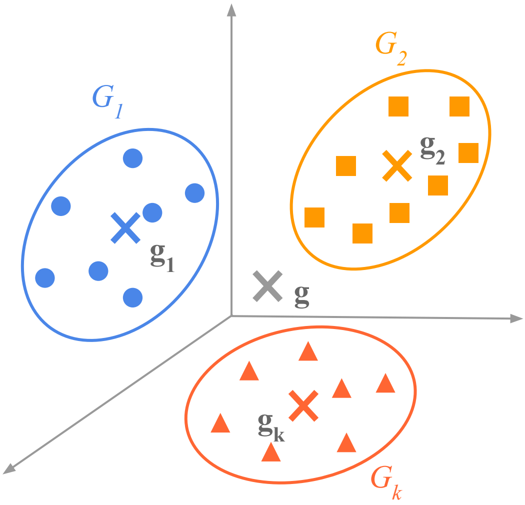
The objects are divided into classes or groups

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 $\mathbf{g_k}$

Group Centroids

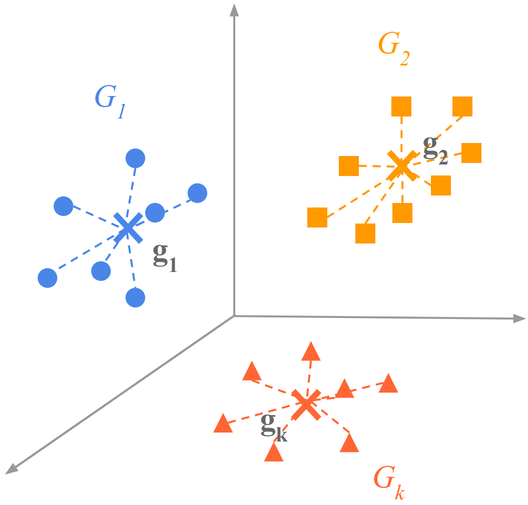
The group centroid $\mathbf{g_k}$ is the point of averages for those observations in group k:

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

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):

$$\mathsf{GSS}_k = \mathbf{X_k^\mathsf{T} X_k}$$

Equivalently, there is an associated variance matrix $\mathbf{W_k}$ for each group

$$\mathbf{W_k} = \frac{1}{n_k - 1} \mathbf{X_k^\mathsf{T} X_k}$$

where $\mathbf{X_k}$ is the data matrix of the k-th group

Within-groups dispersion

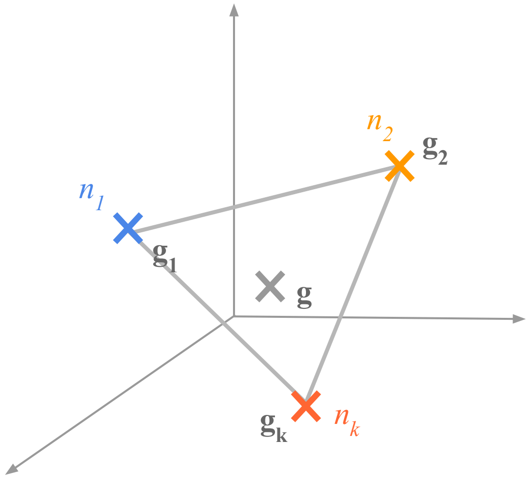
We can combine the groups dispersion to obtain a Within-groups Sums of Squares (WSS) matrix:

$$\text{WSS} = \sum_{k=1}^{K} \mathbf{X_k}^\mathsf{T} \mathbf{X_k}$$

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?

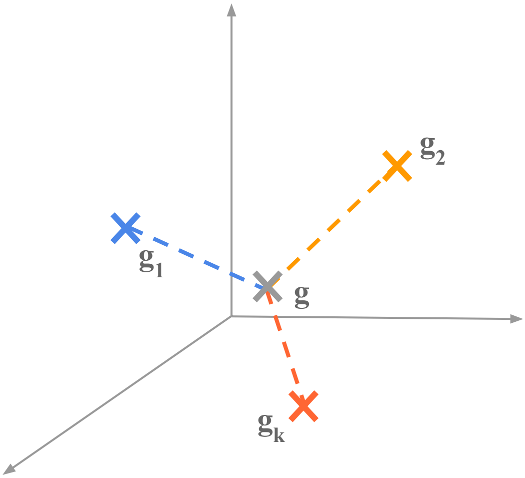
Global and Group Centroids

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):

$$\text{BSS} = \sum_{k=1}^{K} n_k (\mathbf{g_k} - \mathbf{g})(\mathbf{g_k} - \mathbf{g})^\mathsf{T}$$

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

$$\mathbf{B} = \sum_{k=1}^{K} \frac{n_k}{n-1} (\mathbf{g_k} - \mathbf{g})(\mathbf{g_k} - \mathbf{g})^\mathsf{T}$$

Three types of Dispersions

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

- TSS: Total Sums fo Squares
- WSS: Within-groups Sums fo Squares
- BSS: Between-groups Sums fo Squares

Alternatively, we also have three types of variance matrices:

- $\mathbf{V}$: Total variance
- $\mathbf{W}$: Within-groups variance
- $\mathbf{B}$: Between-groups variance

Dispersion Decomposition

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

- TSS = BSS + WSS
- $\mathbf{V} = \mathbf{B} + \mathbf{W}$

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

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

References

- **Principles of Multivariate Analysis: A User's Perspective** by W.J. Krzanowski (1988). *Chapter 11: Incorporating group structure: descriptive methods*. Wiley.
- **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*.

References (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.