CLEMSON UNIVERSITY

Lecture 13

Classification and Cluster Analysis

Reading: JWHT Chapters 4 and 10

DSA 8020 Statistical Methods II
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Agenda

1. **Classification**
2. **Cluster Analysis**

Classification

- **Data:**

$$\{\boldsymbol{X}_i, Y_i\}_{i=1}^{n},$$

where Y_i is the class information for the i_{th} observation
$\Rightarrow Y$ is a qualitative variable

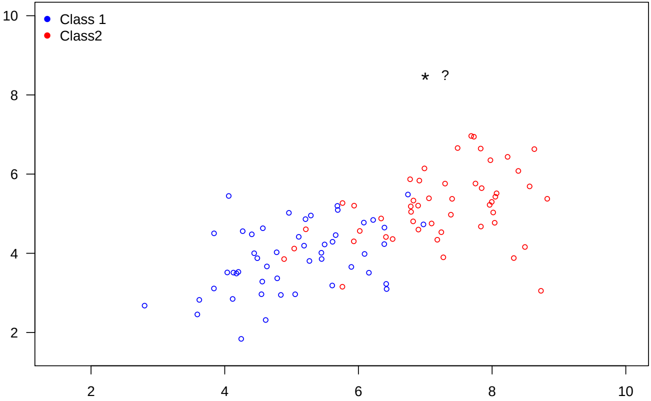
- Classification aims to classify a new observation (or several new observations) into one of those classes

Quantity of interest: $\mathrm{P}(Y = k_{th}$ category$|\boldsymbol{X} = \boldsymbol{x})$

- In this lecture we will focus on binary linear classification

Illustrating Example

Wish to classify a new observation $z(*)$ into one of the two groups (class 1 or class 2)



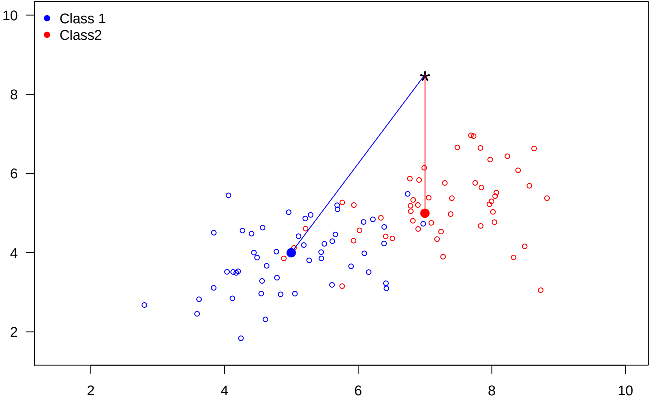
Illustrating Example Cont'd

We could compute the distances from this new observation $\boldsymbol{z} = (z_1, z_2)$ to the groups, for example,

$d_1 = \sqrt{(z_1 - \mu_{11})^2 + (z_2 - \mu_{12})^2}$,

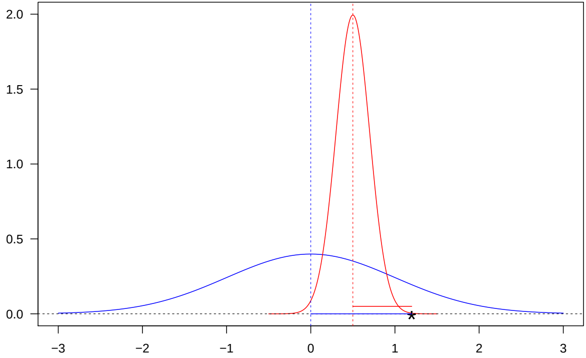
$d_2 = \sqrt{(z_1 - \mu_{21})^2 + (z_2 - \mu_{22})^2}$.

We could assign $\boldsymbol{z}$ to the group with the smallest distance



Variance Corrected Distance

In this one-dimensional example, $d_1 = |z - \mu_1| > |z - \mu_2|$. Does that mean z is "closer" to group 2 (red) than group 1 (blue)?



We should take the "spread" of each group into account.
$\tilde{d}_1 = |z - \mu_1|/\sigma_1 < \tilde{d}_2 = |z - \mu_2|/\sigma_2$

General Covariance Adjusted Distance: Mahalanobis Distance

The Mahalanobis distance is a measure of the distance between a point z and a multivariate distribution of $\boldsymbol{X}$:

$$D_M(\boldsymbol{z}) = \sqrt{(\boldsymbol{z}-\boldsymbol{\mu})^T \Sigma (\boldsymbol{z}-\boldsymbol{\mu})},$$

where $\boldsymbol{\mu}$ is the mean vector and Σ is the variance-covariance matrix of $\boldsymbol{X}$

Binary Classification

Assume $\boldsymbol{X}_1 \sim \mathrm{MVN}(\boldsymbol{\mu}_1, \Sigma)$, $\boldsymbol{X}_2 \sim \mathrm{MVN}(\boldsymbol{\mu}_2, \Sigma)$, that is, $\Sigma_1 = \Sigma_2 = \Sigma$

- Maximum Likelihood of group membership:

  Group 1 if $\ell(\boldsymbol{z}, \boldsymbol{\mu}_1, \Sigma) > \ell(\boldsymbol{z}, \boldsymbol{\mu}_2, \Sigma)$

- Linear Discriminant Function:

  Group 1 if $(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^T \Sigma^{-1} \boldsymbol{z} - \frac{1}{2}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^T \Sigma^{-1} (\boldsymbol{\mu}_1 + \boldsymbol{\mu}_2) > 0$

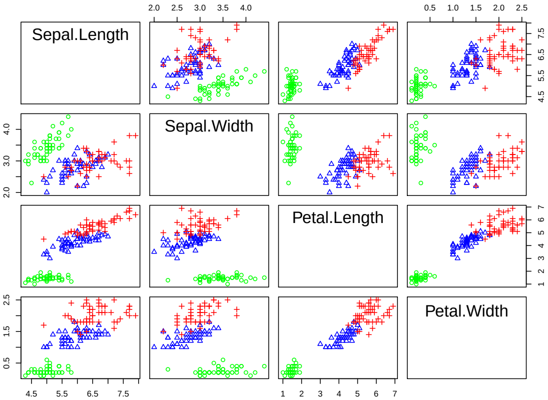
- Minimize Mahalanobis distance:

  Group 1 if $(\boldsymbol{z} - \boldsymbol{\mu}_1)^T \Sigma^{-1} (\boldsymbol{z} - \boldsymbol{\mu}_1) < (\boldsymbol{z} - \boldsymbol{\mu}_2)^T \Sigma^{-1} (\boldsymbol{z} - \boldsymbol{\mu}_2)$

All the classification methods above are equivalent

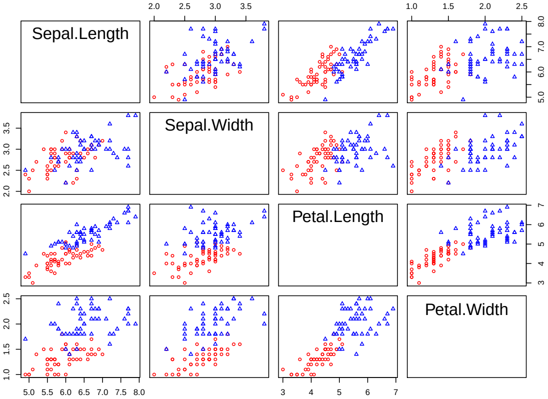
Example: Fisher's Iris Data

4 variables (sepal length and width and petal length and width), 3 species (setosa, versicolor, and virginica)



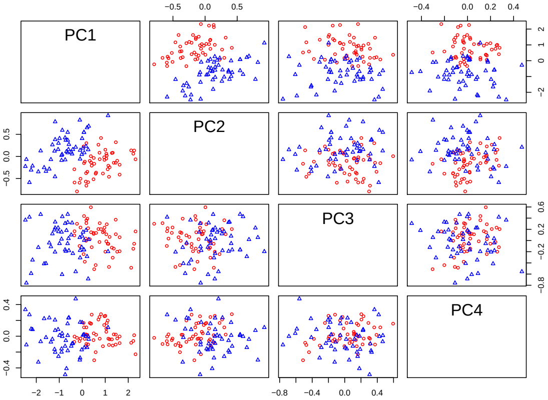
Fisher's Iris Data Cont'd

Let's focus on the latter two classes (versicolor, and virginica)

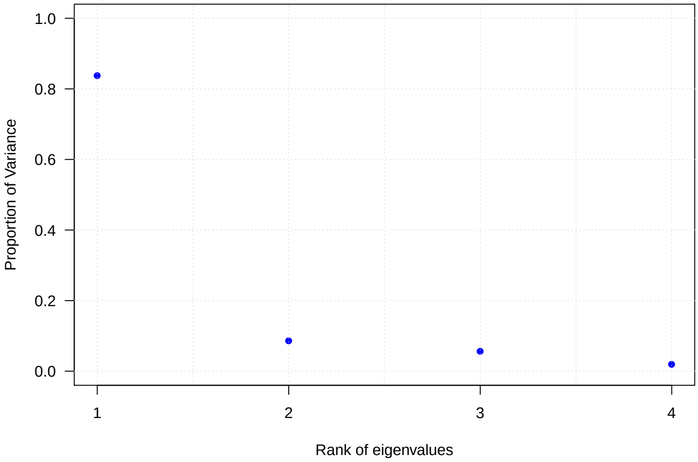


Fisher's iris Data Cont'd

To further simplify the matter, let's focus on the first two PCs of $\boldsymbol{X}$



Screen Plot

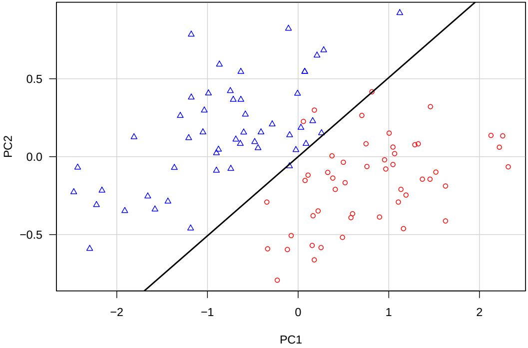

1.0
0.8
0.6
0.4
0.2
0.0
Proportion of Variance
1
2
3
4
Rank of eigenvalues

Linear Discriminant Analysis

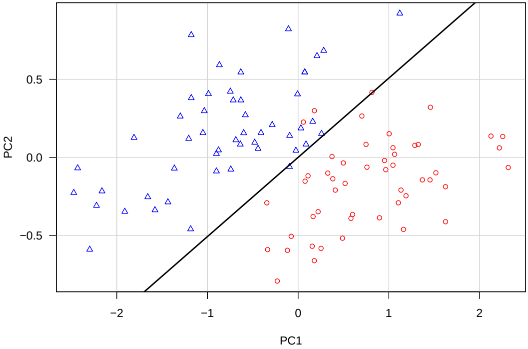
Main idea: Use Bayes rule to compute

$$P(Y = k|\boldsymbol{X} = \boldsymbol{x}) = \frac{P(Y = k)P(\boldsymbol{X} = \boldsymbol{x}|Y = k)}{P(\boldsymbol{X} = \boldsymbol{x})} = \frac{\pi_k f_k(\boldsymbol{x})}{\sum_{k=1}^{K} \pi_k f_k(\boldsymbol{x})}.$$

Assuming $f_k(\boldsymbol{x}) \sim \mathrm{MVN}(\boldsymbol{\mu}_k, \Sigma), \quad k = 1, \cdots, K$ and use $\hat{\pi}_k = \frac{n_k}{n} \Rightarrow$ it turns out the resulting classifier is linear in $\boldsymbol{X}$



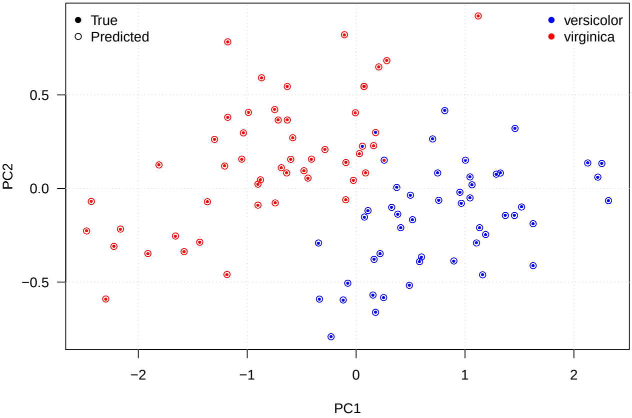
Classification Performance Evaluation



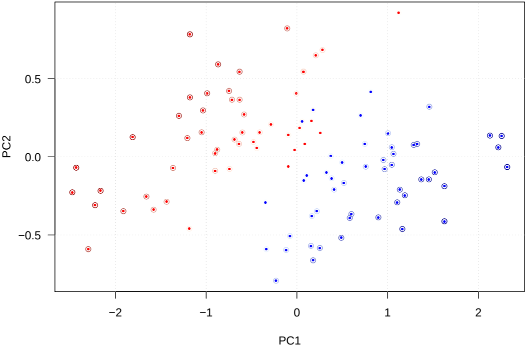

```
fit.LDA
           versicolor virginica
versicolor         47         3
virginica           1        49
```

Logistic Regression Classifier

Main idea: Model the logit $\log\left(\frac{P(Y=1)}{1-P(Y=1)}\right)$ as a linear function in x



Logistic Regression Classifier Cont'd



logisticPred

	versicolor	virginica
versicolor	48	2
virginica	1	49

Quadratic Discriminant Analysis

In Linear Discriminant Analysis, we **assume** $\{f_k(\boldsymbol{x})\}_{k=1}^{K}$ are normal densities and $\Sigma_1 = \Sigma_2$, therefore we obtain a linear classifier. What if $\Sigma_1 \neq \Sigma_2 \Rightarrow$ we get quadratic discriminant analysis

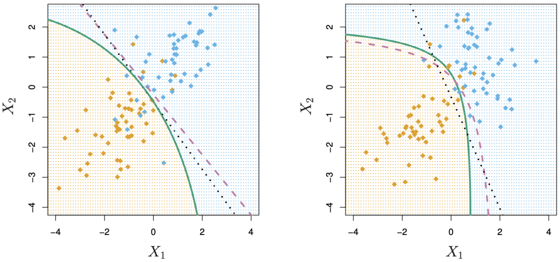


Figure: Figure courtesy of An Introduction of Statistical Learning by G. James et al. pp. 150

What is Cluster Analysis?

- Cluster: a collection of data objects
  - “Similar” to one another within the same cluster
  - “Dissimilar” to the objects in other clusters
- Cluster analysis: Grouping a set of data objects into clusters
- Clustering is unsupervised classification, unlike classification, there is no predefined classes, and the number of clusters is usually unknown

Major Clustering Approaches

- **Partitioning algorithm:** partition the observations into a pre-specified number of clusters, for example, k-means clustering
- **Hierarchy algorithm:** Construct a hierarchical decomposition of the observations to build a hierarchy of clusters, for example, hierarchical agglomerative clustering
- **Model-based Clustering:** A model is hypothesized for each of the clusters, for example, Gaussian mixture models

We will focus on **partitioning algorithm** and **Model-based Clustering**

Partitioning Algorithm

Let $C_1, \cdots, C_K$ denote sets containing the indices of the observations $\{\boldsymbol{x}_i\}_{i=1}^n$ in each cluster. These sets satisfy two properties:

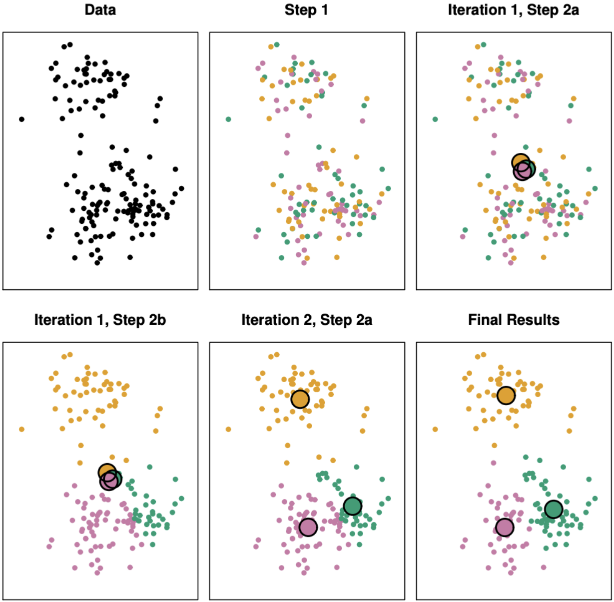
- $C_1 \cup C_2 \cup \cdots \cup C_K = \{1, \cdots, n\} \Rightarrow$ each observation belongs to at least one of the K clusters
- $C_k \cap C_{k'} = \varnothing \; \forall k \neq k' \Rightarrow$ no observation belongs to more than one cluster

For instance, if the i_{th} observation (i.e. $\boldsymbol{x}_i$) is in the k_{th} cluster, then $i \in C_k$

The k-Means Algorithm

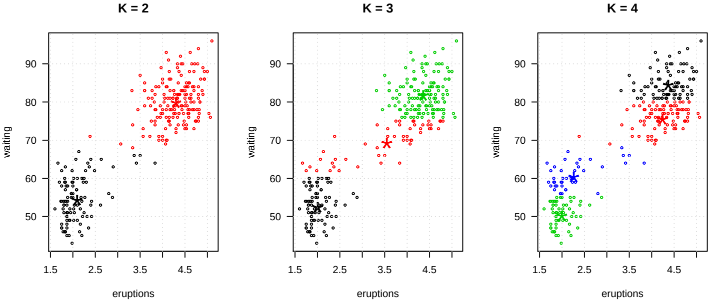
- **Step 0:** Choose the number of clusters K
- **Step 1:** Randomly assign a cluster (from 1 to K), to each of the observations. These serve as the initial cluster assignmemts
- **Step 2:** Iterate until the cluster assignment stop changing
  - For each of the K cluster, compute the cluster centroid. The k_{th} cluster centroid is the mean vector of the observations in the k_{th} cluster
  - Assign each observations to the cluster whose centroid is closest in terms of Euclidean distance

k-Means Clustering Illustration



K-Means Clustering in R


```
kmean3.faithful <- kmeans(x = faithful, centers = 3)
```



Model-based clustering

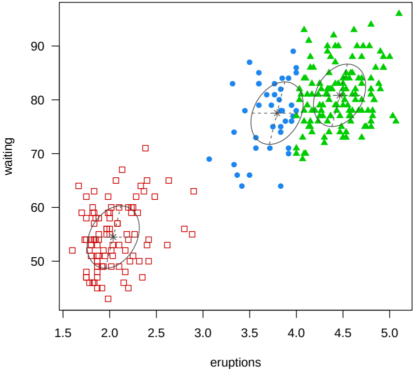
- One disadvantage of k-means is that they are largely heuristic and not based on formal statistical models. Formal inference is not possible
- Model-based clustering is an alternative:
  - Sample observations arise from a mixture distribution of two or more components
  - Each component (cluster) is described by a probability distribution and has an associated probability in the mixture.
  - In Gaussian mixture models, we assume each cluster follows a multivariate normal distribution
  - Therefore, in Gaussian mixture models, the model for clustering is a mixture of multivariate normal distributions

Fitting a Gaussian Mixture Model in R

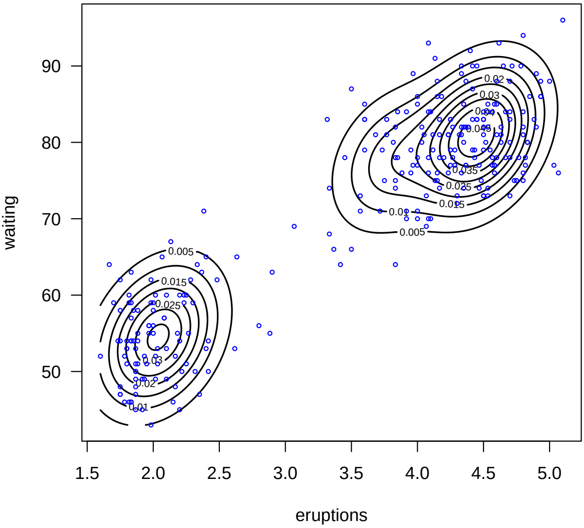
```
library(mclust)
```

```
## Package 'mclust' version 5.4.5
## Type 'citation("mclust")' for citing this R package in publications.
```

```
BIC <- mclustBIC(faithful)
model1 <- Mclust(faithful, x = BIC)
```



Fitting a Gaussian Mixture Model in R Cond't



Model-Based Clustering Analysis for Iris Data