An Overview of Multivariate Analysis
Classification Problems
Linear Discriminant Analysis & Logistic Regression

Lecture 38

Statistical Classification

STAT 8020 Statistical Methods II
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Agenda

1. An Overview of Multivariate Analysis
2. Classification Problems
3. Linear Discriminant Analysis & Logistic Regression

An Overview of Multivariate Analysis

Classification Problems

Linear Discriminant Analysis & Logistic Regression

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An Overview of Multivariate Analysis

- In many studies, observations are collected on several variables on each experimental/observational unit
- Multivariate analysis is a collection of statistical methods for analyzing these multivariate data sets
- **Common Objectives**
  - Dimensionality reduction
  - Classification
  - Grouping (Clustering)

Multivariate Data

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We display a multivariate data that contains n units on p variables using a matrix

$$\boldsymbol{X} = \begin{pmatrix} X_{1,1} & X_{2,1} & \cdots & X_{p,1} \\ X_{1,2} & X_{2,2} & \cdots & X_{p,2} \\ \vdots & \cdots & \ddots & \vdots \\ X_{1,n} & X_{2,n} & \cdots & X_{p,n} \end{pmatrix}$$

Summary Statistics

- Mean Vector: $\bar{\boldsymbol{X}} = (\bar{X}_1, \bar{X}_2, \cdots, \bar{X}_p)^T$
- Variance-Covariance Matrix: $\Sigma = \{\sigma_{ij}\}_{i,j=1}^{p}$, where $\sigma_{ii} = \mathrm{Var}(X_i), \quad i = 1, \cdots, p$ and $\sigma_{ij} = \mathrm{Cov}(X_i, X_j), i \neq j$

Classification and Discriminant Analysis

- **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: $\mathrm{P}(Y = k_{th}\text{ category}|\boldsymbol{X} = \boldsymbol{x})$

- In this lecture we will focus on binary linear classification

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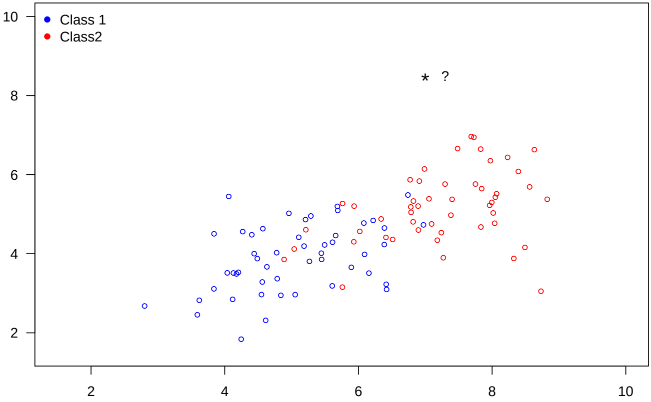
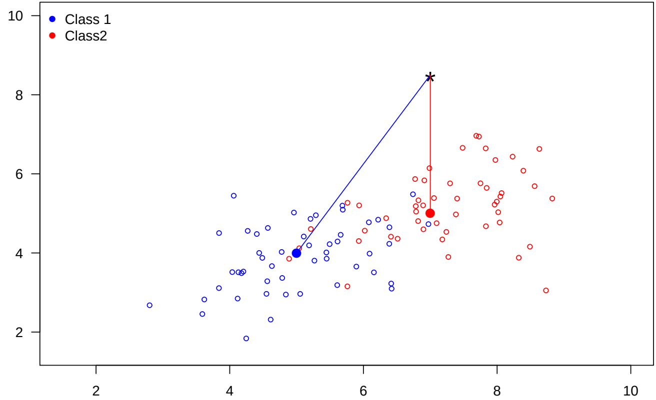
Illustrating Example

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



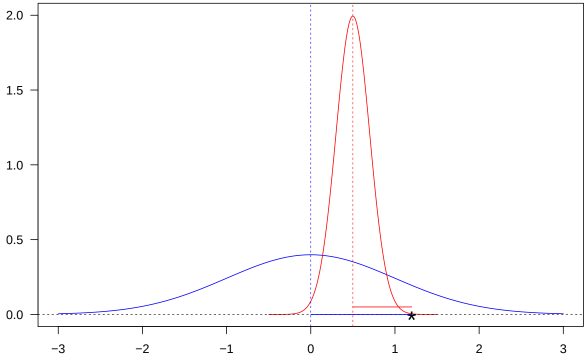
Illustrating Example Cont'd

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 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 distribution F:

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

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

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

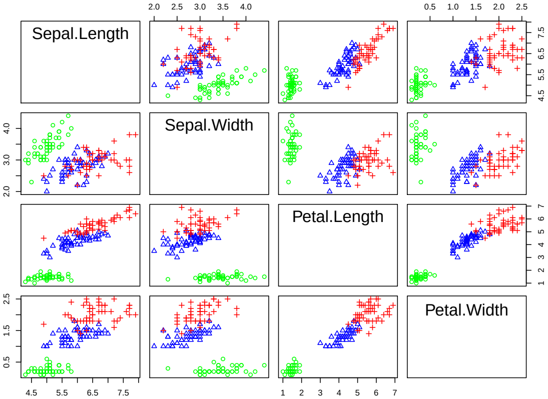
- Minimize Mahalanobis distance:

  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

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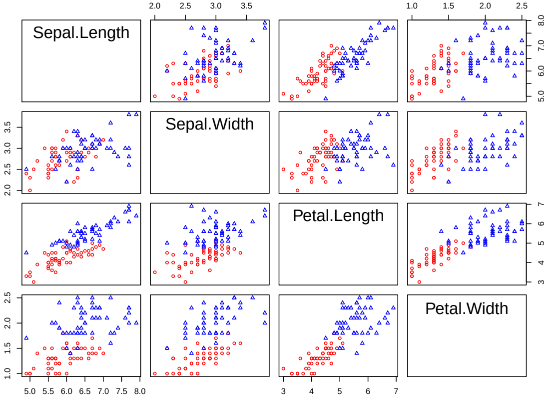
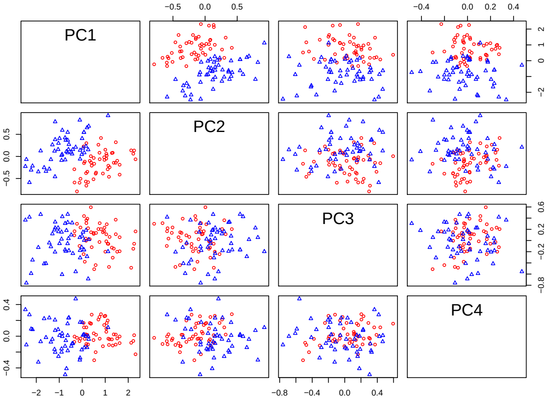
Let's focus on the latter two classes (versicolor, and virginica)

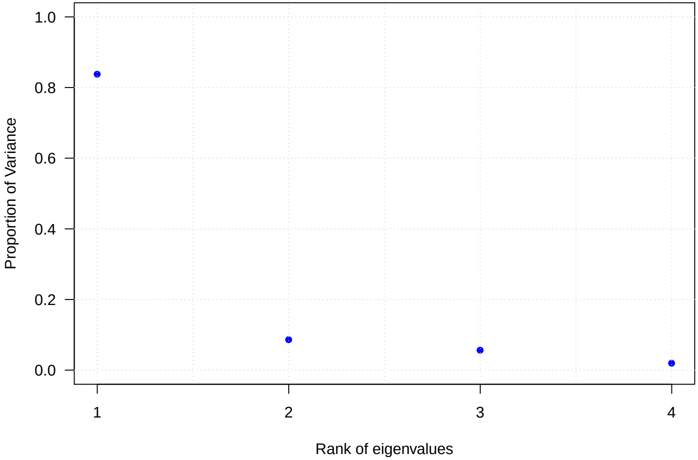


Fisher's iris Data Cont'd

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



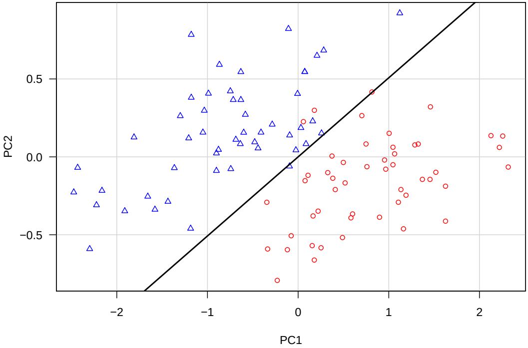
Screen Plot



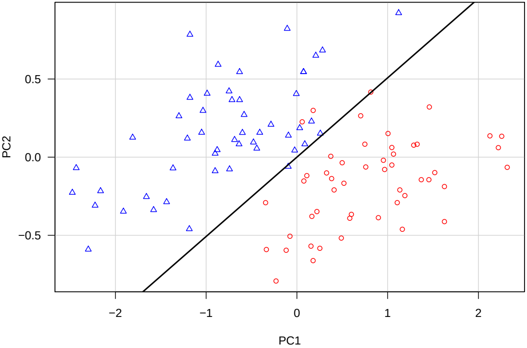
1.0
0.8
0.6
0.4
0.2
0.0
Proportion of Variance
1
2
3
4
Rank of eigenvalues

Linear Discriminant Analysis

Main idea: Use Bayes rule to compute $\mathrm{P}(Y=k|\boldsymbol{X}=\boldsymbol{x}) = \frac{\mathrm{P}(Y=k)\mathrm{P}(\boldsymbol{X}=\boldsymbol{x}|Y=k)}{\mathrm{P}(\boldsymbol{X}=\boldsymbol{x})} = \frac{\pi_k f_k(\boldsymbol{x})}{\sum_{k=1}^{K}\pi_k f_k(\boldsymbol{x})}$. Assuming $f_k(\boldsymbol{x}) \sim \mathrm{MVN}(\boldsymbol{\mu}_k, \Sigma), \quad k=1,\cdots,K$. Use $\hat{\pi}_k = \frac{n_k}{n} \Rightarrow$ it turns out the resulting classifier is linear in $\boldsymbol{X}$



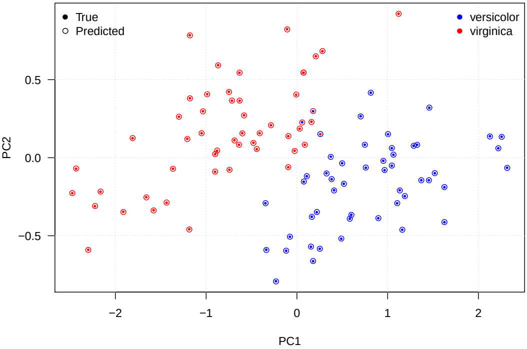
Classification Performance Evaluation



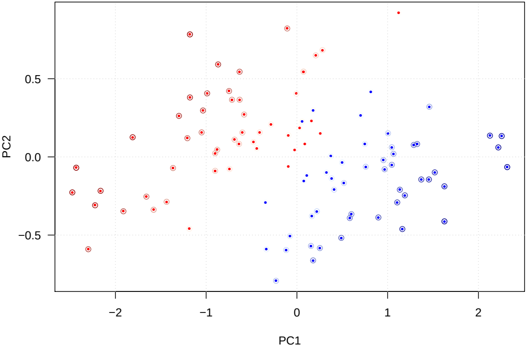

```
fit.LDA
           versicolor virginica
versicolor         47         3
virginica           1        49
```

Logistic Regression Classifier

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



Logistic Regression Classifier Cont'd




```
                logisticPred
                 versicolor virginica
versicolor               48         2
virginica                 1        49
```

Quadratic Discriminant Analysis

In Linear Discriminant Analysis, we **assume** $\{f_k(x)\}_{k=1}^{K}$ 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

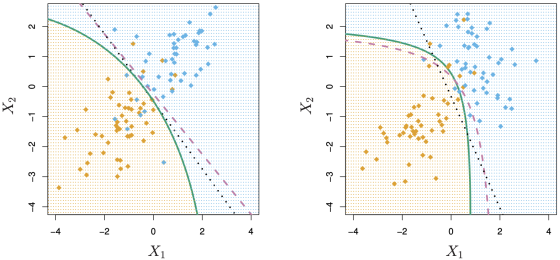


Figure: Figure courtesy of An Introduction of Statistical Learning by G. James et al. pp. 150

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Linear Discriminant Analysis Versus Logistic Regression

For a binary classification problem, one can show that both Linear Discriminant Analysis (LDA) and Logistic Regression are linear classifiers. The difference is in how the parameters are estimated:

- Logistic regression uses the conditional likelihood based on $\mathrm{P}(Y|\boldsymbol{X} = \boldsymbol{x})$
- LDA uses the full likelihood based on multivariate normal assumption on $\boldsymbol{X}$
- Despite these differences, in practice the results are often very similar