Lecture 12

Classification

Readings: Zelterman, 2015, Chapter 10.1-10.4; Izenman, 2008 Chapter 8.1-8.4; ISLR, 2021 Chapter 9; Johnson & Wichern 2007, Chapter 11

DSA 8070 Multivariate Analysis

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Agenda

1. **Background**

2. **Binary Linear Classification**

3. **Support Vector Machines**

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

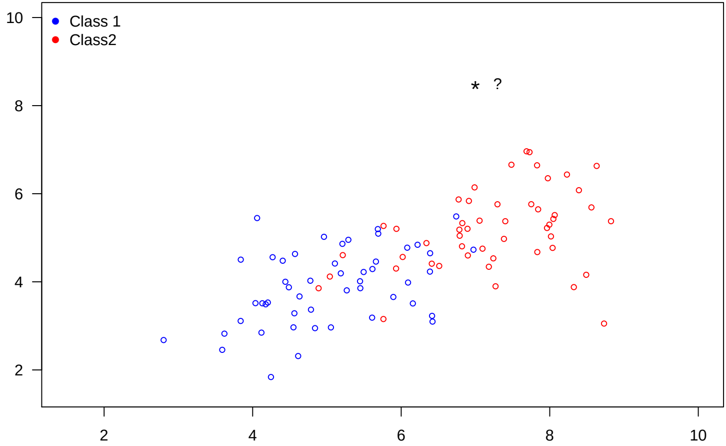
- Classification aims to classify a new observation (or several new observations) into one of those classes

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

- In this lecture we will focus on binary linear classification

Toy Example

Wish to classify a new observation $\boldsymbol{x}_i = (x_{1i}, x_{2i})$, denoted by $(*)$, into one of the two groups (class 1 or class 2)

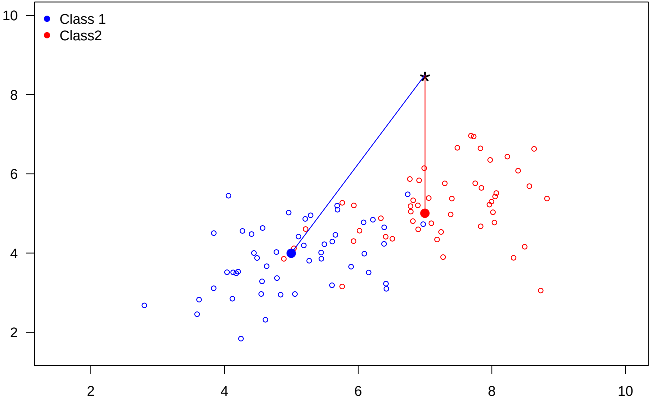


Toy Example Cont'd

We can compute the distances from this new observation $\boldsymbol{x} = (x_1, x_2)$ to the groups, for example,

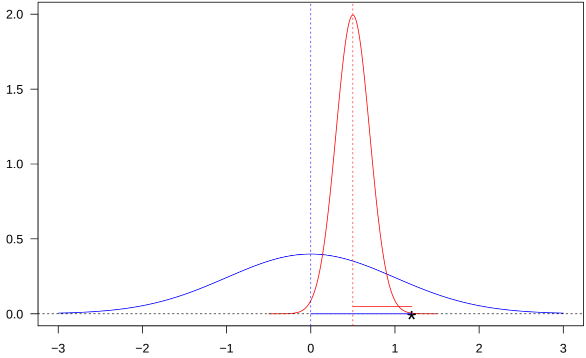
$$d_1 = \sqrt{(x_1 - \mu_{11})^2 + (x_2 - \mu_{12})^2},$$
$$d_2 = \sqrt{(x_1 - \mu_{21})^2 + (x_2 - \mu_{22})^2}.$$

We can assign $\boldsymbol{x}$ to the group with the smallest distance



Variance Corrected Distance

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



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

General Covariance Adjusted Distance: Mahalanobis Distance

The Mahalanobis distance [Mahalanobis, 1936] is a measure of the distance between a point x and a multivariate distribution of $\boldsymbol{X}$:

$$D_M(\boldsymbol{x}) = \sqrt{(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu})},$$

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

One can use the Mahalanobis distance, by computing the Mahalanobis distance between an observations $\boldsymbol{x}_i$ and the "center" of the k_{th} population $\boldsymbol{\mu}_k$, to carry out classification

Binary Classification with Multivariate Normal Populations

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

- Maximum Likelihood of group membership:

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

- Linear Discriminant Function:

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

- Minimize Mahalanobis distance:

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

All the criteria above are equivalent in terms of classification

Priors and Misclassification Costs

In addition to the observed characteristics of units $\{\boldsymbol{x}_i\}_{i=1}^n$, other considerations of classification rules are:

- Prior probability:

  If one population is more prevalent than the other, chances are higher that a new unit came from the larger population. Stronger evidence would be needed to allocate the unit to the population with the smaller prior probability.

- Costs of misclassification:

  It may be more costly to misclassify a seriously ill subject as healthy than to misclassify a healthy subject as being ill.

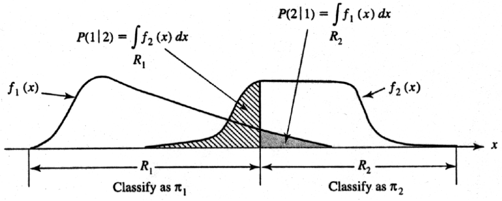
Classification Regions and Misclassifications

- The probability of misclassifying an object into π_2 when it belongs in π_1 is

$$P(2|1) = \mathbb{P}(\boldsymbol{X} \in \mathcal{R}_2|\pi_1)$$

- The probability of misclassifying an object into π_1 when it belongs in π_2 is

$$P(1|2) = \mathbb{P}(\boldsymbol{X} \in \mathcal{R}_1|\pi_2)$$



Source: Figure 11.3 from Applied Multivariate Statistical Analysis, 6th Ed (Johnson & Wichern). Visualization is for $p = 1$ variable.

Probability and Expected Cost of Misclassification

Let p_1 and p_2 denote the prior probabilities of π_1, π_2, and $c(1|2), c(2|1)$ be the costs of misclassification:

- Then probabilities of the four possible outcomes are:

$$\begin{aligned}
\mathbb{P}(\text{correctly classified as } \pi_1) &= \mathbb{P}(\boldsymbol{X} \in \mathcal{R}_1|\pi_1)\mathbb{P}(\pi_1) = P(1|1)p_1 \\
\mathbb{P}(\text{incorrectly classified as } \pi_1) &= \mathbb{P}(\boldsymbol{X} \in \mathcal{R}_1|\pi_2)\mathbb{P}(\pi_2) = P(1|2)p_2 \\
\mathbb{P}(\text{correctly classified as } \pi_2) &= \mathbb{P}(\boldsymbol{X} \in \mathcal{R}_2|\pi_2)\mathbb{P}(\pi_2) = P(2|2)p_2 \\
\mathbb{P}(\text{incorrectly classified as } \pi_2) &= \mathbb{P}(\boldsymbol{X} \in \mathcal{R}_2|\pi_1)\mathbb{P}(\pi_1) = P(2|1)p_1
\end{aligned}$$

- Classification rules are often evaluated in terms of the expected cost of misclassification (ECM):

$$\mathrm{ECM} = c(2|1)P(2|1)p_1 + c(1|2)P(1|2)p_2,$$

and we seek rules that minimize the ECM

Classification Rule and Special Cases of Minimum ECM Regions

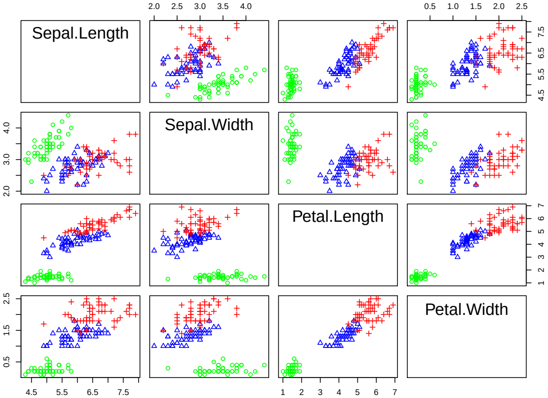
The regions $\mathcal{R}_1$, $\mathcal{R}_2$ that minimize the ECM are defined by the values of $\boldsymbol{x}$ for which

$$\mathcal{R}_1 : \frac{f_1(\boldsymbol{x})}{f_2(\boldsymbol{x})} > \left(\frac{c(1|2)}{c(2|1)}\right)\left(\frac{p_2}{p_1}\right)$$
$$\mathcal{R}_2 : \frac{f_1(\boldsymbol{x})}{f_2(\boldsymbol{x})} < \left(\frac{c(1|2)}{c(2|1)}\right)\left(\frac{p_2}{p_1}\right)$$

- if $p_1 = p_2 : \frac{f_1(\boldsymbol{x})}{f_2(\boldsymbol{x})} > \frac{c(1|2)}{c(2|1)} \Rightarrow \mathcal{R}_1$, otherwise $\mathcal{R}_2$
- if $c(1|2) = c(2|1) : \frac{f_1(\boldsymbol{x})}{f_2(\boldsymbol{x})} > \frac{p_2}{p_1} \Rightarrow \mathcal{R}_1$, otherwise $\mathcal{R}_2$
- if $c(1|2) = c(2|1)$ and $p_1 = p_2 : \frac{f_1(\boldsymbol{x})}{f_2(\boldsymbol{x})} > 1 \Rightarrow \mathcal{R}_1$, otherwise $\mathcal{R}_2$

Example: Fisher's Iris Data

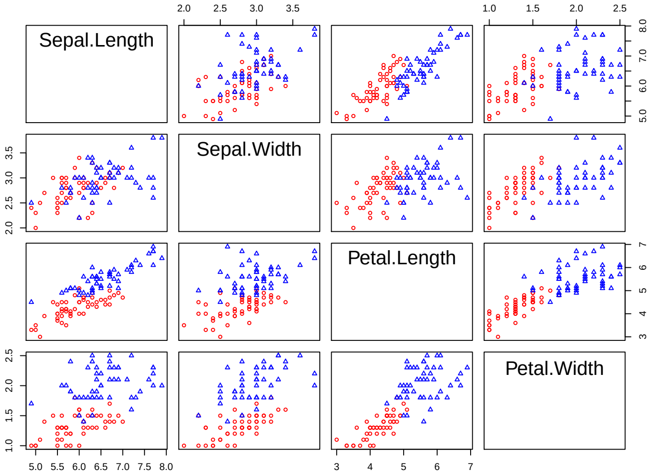
4 variables (sepal length and width and petal length and width), 3 species (setosa, versicolor, and virginica)



> **Task:** Classify flowers into different species based on lengths and widths of sepal and petal

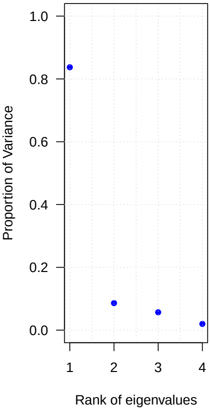
Fisher's Iris Data Cont'd

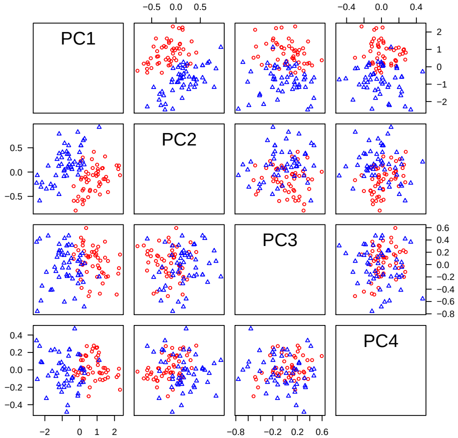
Let's focus on the latter two classes (versicolor, and virginica)



Fisher's iris Data Cont'd

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



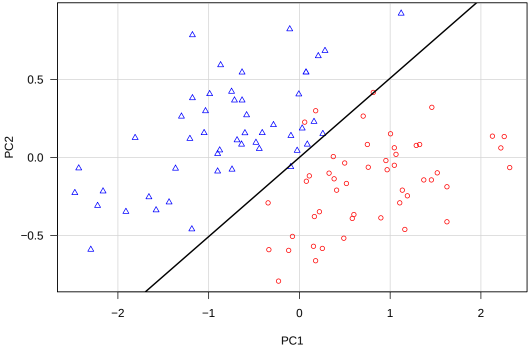


Linear Discriminant Analysis

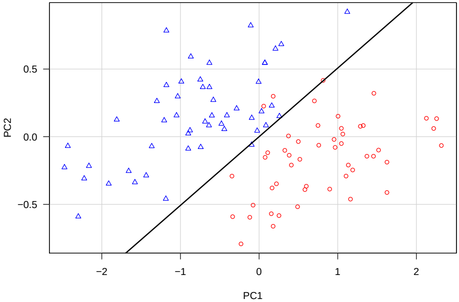
Main idea: Use Bayes rule to compute

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

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



Classification Performance Evaluation

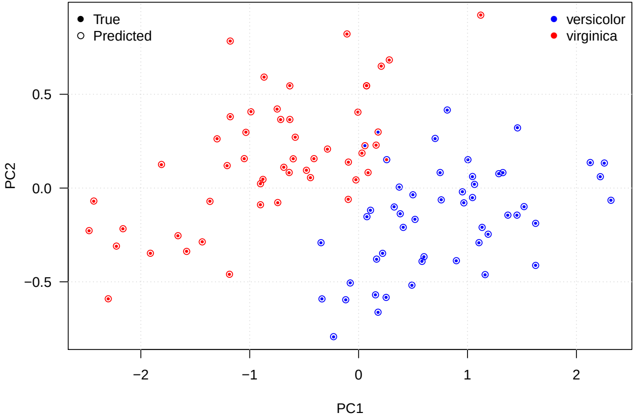



```
fit.LDA
           versicolor virginica
versicolor         47         3
virginica           1        49
```

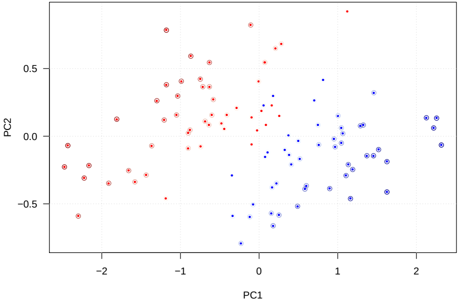
Misclassification rate: $\frac{3+1}{47+3+1+49} = 0.04$

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 (PC1 and PC2 in this case)



Logistic Regression Classifier Cont'd




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

Misclassification rate: $\frac{2+1}{48+2+1+49} = 0.03$

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

Quadratic Discriminant Analysis

In linear discriminant analysis, we **assume** $\{f_k(x)\}_{k=1}^{K}$ are normal densities and $\mathbf{\Sigma_1} = \mathbf{\Sigma_2}$, therefore we obtain a linear classifier.

What if $\mathbf{\Sigma}_1 \neq \mathbf{\Sigma}_2$? $\Rightarrow$ we get quadratic discriminant analysis

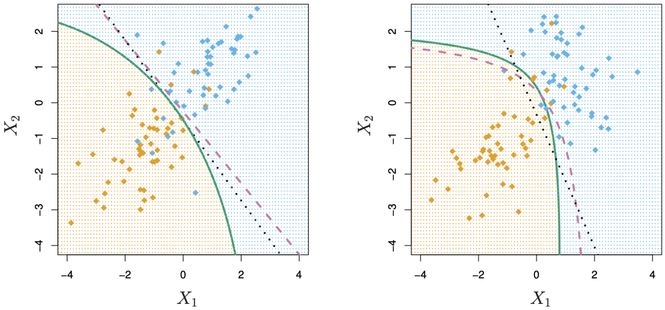
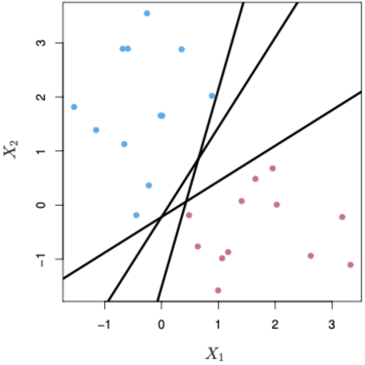


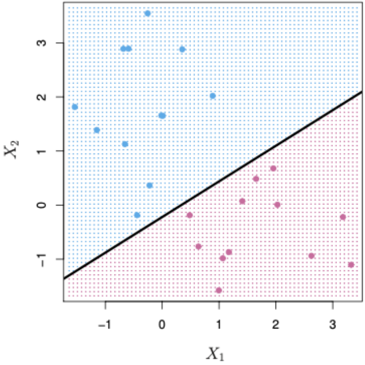
Figure courtesy of An Introduction of Statistical Learning by G. James et al. pp. 154

An Algorithmic Approach to Classification

Find a hyperplane that "best" separates the classes in feature space

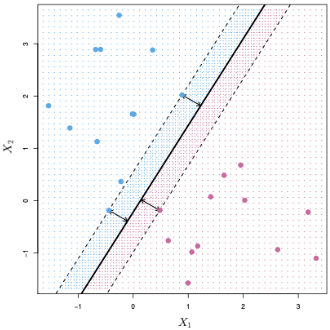
- what we mean by "separateness"?
- what is the feature space?





Maximal Margin Classifier

Main idea: among all separating hyperplanes, find the one that creates the biggest gap ("margin") between the two classes



doing so leads to the following optimization problem:

$$\text{maximzie}_{\beta_0,\beta_1,\beta_2} \mathrm{M}$$

$$\text{subject to } \sum_{j=1}^{2} \beta_j^2 = 1,$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2}) \geq M,$$

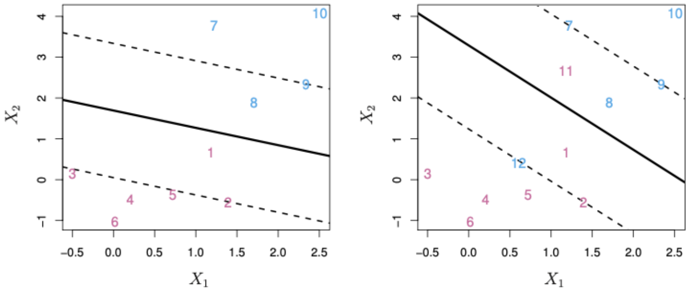
$$i = 1, \cdots, n$$

This problem can be solved efficiently using techniques from quadratic programming

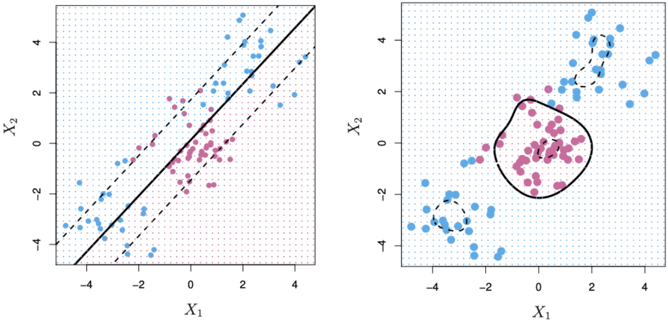
Supper Vector Classifier

- Sometimes the data can not be separated by a line
- data can be noisy which leads to unstable maximal-margin classifier

The support vector classifier maximizes a “soft” margin



Beyond Linear Classifier



- A linear boundary can fail to separate classes
- Can expand the feature space by including transformations, e.g., $X_1^2, X_2^2, X_1 X_2, \cdots \Rightarrow$ gives non-linear decision boundaries in the original feature space
- However, polynomials basis can be unstable, a more general way to introduce non-linearities is through the use of kernels, e.g., $f(\boldsymbol{x}) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i \exp(-\gamma \sum_{j=1}^{p} (x_j - x_{ij})^2)$

SVM Vesus Logistic Regression (LR) and LDA

- When classes are (nearly) separable, SVM does better than LR and LDA
- Use LR to estimate class probabilities as SVM is a non-probabilistic classifier
- For nonlinear boundaries, kernel SVMs are popular

Summary

In this lecture we learned about:

- Some classical classifiers for performing classification
- How to assess the efficacy of a classifier
- Support vector machines (SVMs)

`R` functions to know

- `lda/qda` from the `MASS` library
- `svm` from the `e1071` library

In the next lecture, we will learn about Cluster Analysis