Statistical Machine Learning

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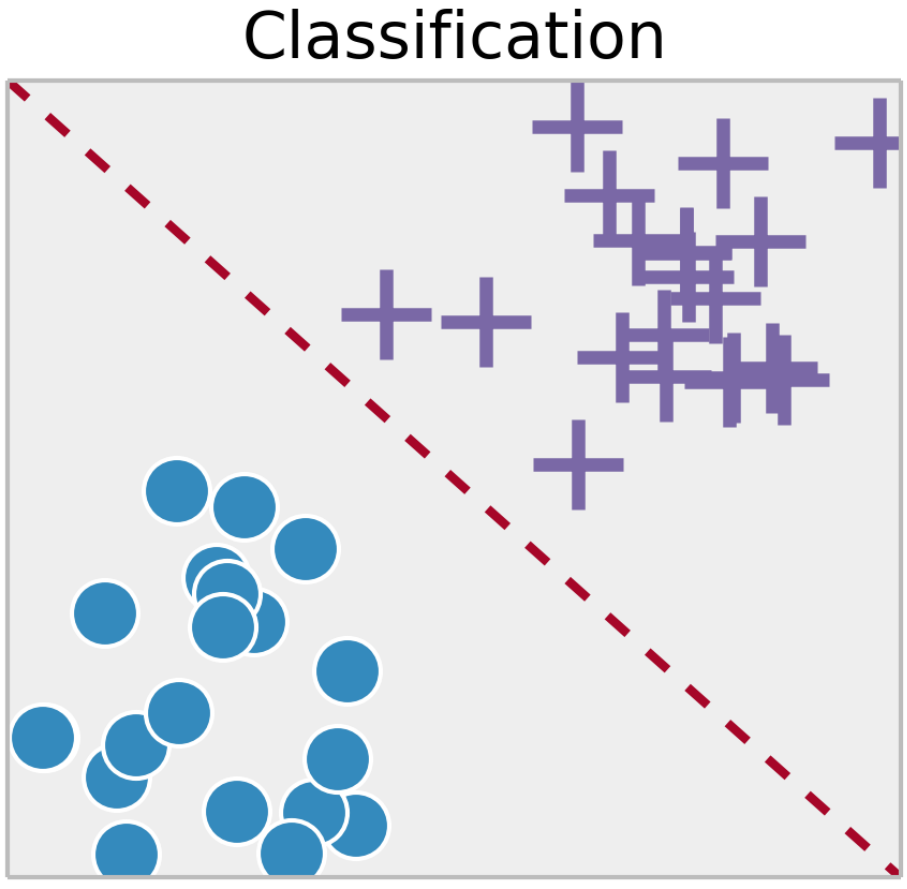
Slide credits and other course material can be found at:
http://www.stats.ox.ac.uk/~palamara/SML19_BDI.html

Classification



Recall: Loss function

- Suppose we made a prediction $\widehat{Y} = f(X) \in \mathcal{Y}$ based on observation of X.
- How good is the prediction? We can use a **loss function** $L : \mathcal{Y} \times \mathcal{Y} \mapsto \mathbb{R}^+$ to formalize the quality of the prediction.
- Typical loss functions:
  - **Squared loss** for regression
  $$L(Y, f(X)) = (f(X) - Y)^2 .$$
  - **Absolute loss** for regression
  $$L(Y, f(X)) = |f(X) - Y| .$$
  - **Misclassification loss** (or **0-1 loss**) for classification
  $$L(Y, f(X)) = \begin{cases} 0 & f(X) = Y \\ 1 & f(X) \neq Y \end{cases} .$$

  Many other choices are possible, e.g., **weighted misclassification loss**.
- In classification, if estimated probabilities $\widehat{p}(k)$ for each class $k \in \mathcal{Y}$ are returned, **log-likelihood loss** (or **log loss**) $L(Y, \widehat{p}) = -\log \widehat{p}(Y)$ is often used.

The Bayes Classifier

- What is the optimal classifier if the joint distribution (X, Y) were known?
- The density g of X can be written as a mixture of K components (corresponding to each of the classes):

$$g(x) = \sum_{k=1}^{K} \pi_k g_k(x),$$

where, for $k = 1, \ldots, K$,

  - $\mathbb{P}(Y = k) = \pi_k$ are the class probabilities,
  - $g_k(x)$ is the conditional density of X, given $Y = k$.

- The **Bayes classifier** $f_{\text{Bayes}} : x \mapsto \{1, \ldots, K\}$ is the one with minimum risk:

$$\begin{aligned} R(f) =& \mathbb{E}\left[L(Y, f(X))\right] = \mathbb{E}_X\left[\mathbb{E}_{Y|X}[L(Y, f(X))|X]\right] \\ =& \int_{\mathcal{X}} \mathbb{E}\left[L(Y, f(X))|X = x\right] g(x) dx \end{aligned}$$

- The minimum risk attained by the Bayes classifier is called **Bayes risk**.
- Minimizing $\mathbb{E}[L(Y, f(X))|X = x]$ separately for each x suffices.

The Bayes Classifier

- Consider the 0-1 loss.
- The risk simplifies to:

$$\begin{aligned}\mathbb{E}\Big[L(Y, f(X))\Big|X = x\Big] &= \sum_{k=1}^{K} L(k, f(x))\mathbb{P}(Y = k|X = x) \\ &= 1 - \mathbb{P}(Y = f(x)|X = x)\end{aligned}$$

- The risk is minimized by choosing the class with the greatest probability given the observation:

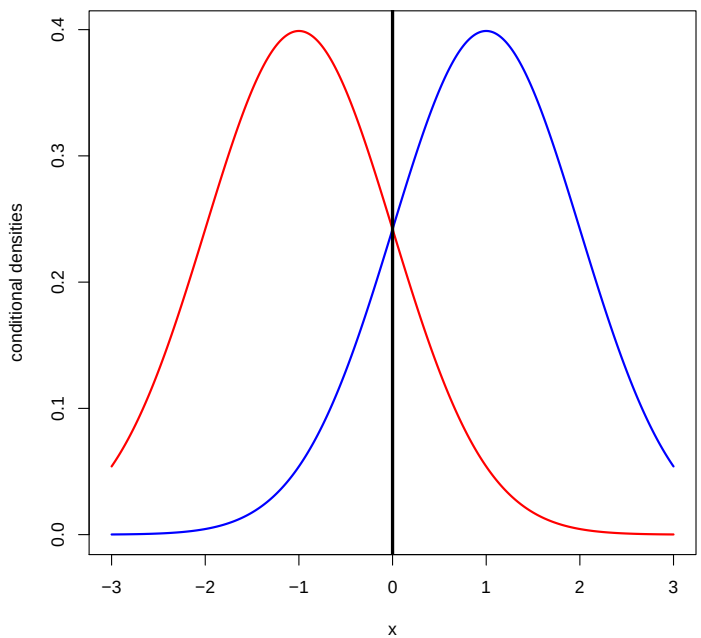
$$\begin{aligned}f_{\text{Bayes}}(x) &= \underset{k=1,\ldots,K}{\arg\max}\, \mathbb{P}(Y = k|X = x) \\ &= \underset{k=1,\ldots,K}{\arg\max}\, \frac{\pi_k g_k(x)}{\sum_{j=1}^{K} \pi_j g_j(x)} = \underset{k=1,\ldots,K}{\arg\max}\, \pi_k g_k(x).\end{aligned}$$

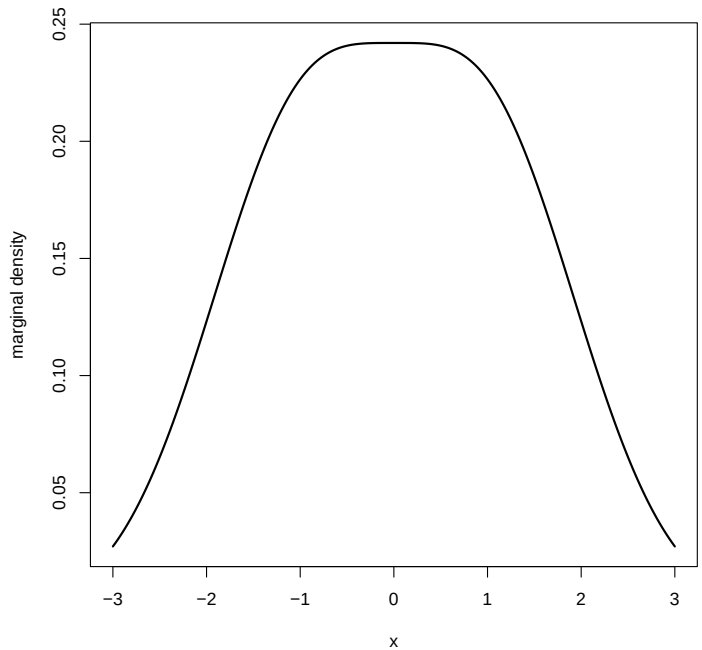
- The functions $x \mapsto \pi_k g_k(x)$ are called **discriminant functions**. The discriminant function with maximum value determines the predicted class of x.

The Bayes Classifier: Example

A simple two Gaussians example: Suppose $X \sim \mathcal{N}(\mu_Y, 1)$, where $\mu_1 = -1$ and $\mu_2 = 1$ and assume equal class probabilities $\pi_1 = \pi_2 = 1/2$.

$$g_1(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x+1)^2}{2}\right) \quad \text{and} \quad g_2(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x-1)^2}{2}\right).$$

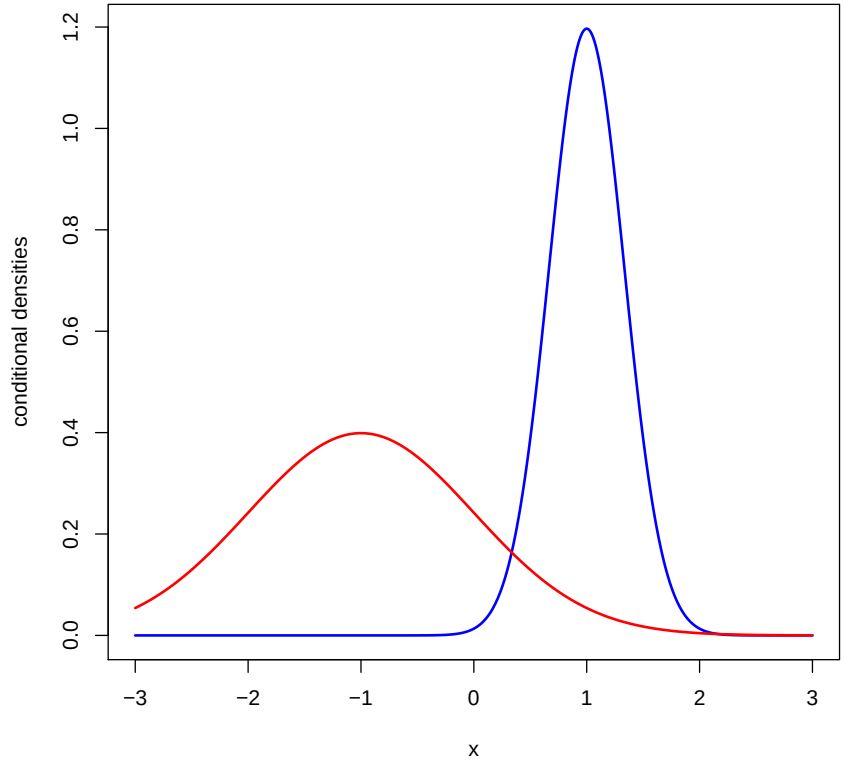


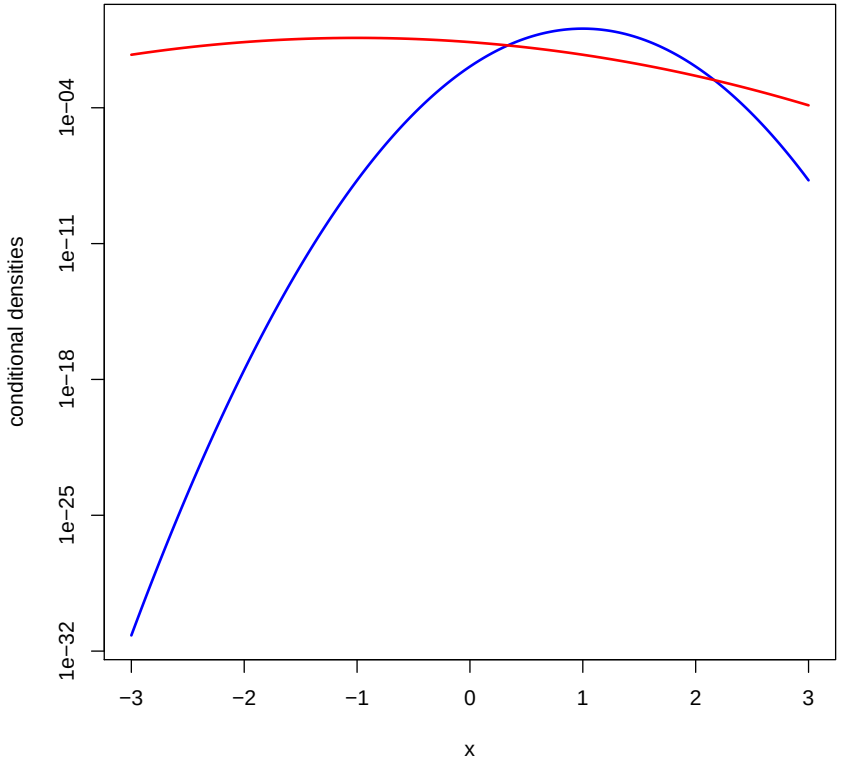


Optimal classification is $f_{\text{Bayes}}(x) = \underset{k=1,\ldots,K}{\arg\max}\ \pi_k g_k(x) = \begin{cases} 1 & \text{if } x < 0, \\ 2 & \text{if } x \geq 0. \end{cases}$

The Bayes Classifier: Example

How do you classify a new observation x if now the standard deviation is still 1 for class 1 but $1/3$ for class 2?





Looking at density in a log-scale, optimal classification is to select class 2 if and only if $x \in [0.34, 2.16]$.

Plug-in Classification

- The Bayes Classifier:

$$f_{\text{Bayes}}(x) = \underset{k=1,\ldots,K}{\arg\max}\, \pi_k g_k(x).$$

- We know neither the conditional densities g_k nor the class probabilities π_k!
- The **plug-in classifier** chooses the class

$$f(x) = \underset{k=1,\ldots,K}{\arg\max}\, \widehat{\pi}_k \widehat{g}_k(x),$$

- where we plugged in
  - estimates $\widehat{\pi}_k$ of π_k and $k = 1, \ldots, K$ and
  - estimates $\widehat{g}_k(x)$ of conditional densities,
- **Linear Discriminant Analysis** is an example of plug-in classification.

Linear Discriminant Analysis

- **LDA** is the most well-known and simplest example of plug-in classification.
- Assume multivariate normal conditional density $g_k(x)$ for each class k:

$$X|Y = k \sim \mathcal{N}(\mu_k, \Sigma),$$

$$g_k(x) = (2\pi)^{-p/2}|\Sigma|^{-1/2} \exp\left(-\frac{1}{2}(x-\mu_k)^\top \Sigma^{-1}(x-\mu_k)\right),$$

  - each class can have a **different mean** μ_k,
  - all classes share the **same covariance** Σ.
- For an observation x, the k-th log-discriminant function is

$$\log \pi_k g_k(x) = c + \log \pi_k - \frac{1}{2}(x-\mu_k)^\top \Sigma^{-1}(x-\mu_k)$$

  The quantity $(x-\mu_k)^\top \Sigma^{-1}(x-\mu_k)$ is the squared **Mahalanobis distance** between x and μ_k.
- If $\Sigma = I_p$ and $\pi_k = \frac{1}{K}$, LDA simply chooses the class k with the nearest (in the Euclidean sense) class mean.

Linear Discriminant Analysis

- Expanding the term $(x-\mu_k)^\top \Sigma^{-1}(x-\mu_k)$,

$$\log \pi_k g_k(x) = c + \log \pi_k - \frac{1}{2}\left(\mu_k^\top \Sigma^{-1}\mu_k - 2\mu_k^\top \Sigma^{-1}x + x^\top \Sigma^{-1}x\right)$$
$$= c' + \log \pi_k - \frac{1}{2}\mu_k^\top \Sigma^{-1}\mu_k + \mu_k^\top \Sigma^{-1}x$$

- Setting $a_k = \log(\pi_k) - \frac{1}{2}\mu_k^\top \Sigma^{-1}\mu_k$ and $b_k = \Sigma^{-1}\mu_k$, we obtain

$$\log \pi_k g_k(x) = c' + a_k + b_k^\top x$$

  i.e. a **linear** discriminant function in x.
- Consider choosing class k over k':

$$a_k + b_k^\top x > a_{k'} + b_{k'}^\top x \qquad \Leftrightarrow \qquad a_\star + b_\star^\top x > 0$$

  where $a_\star = a_k - a_{k'}$ and $b_\star = b_k - b_{k'}$.
- The Bayes classifier thus partitions $\mathcal{X}$ into regions with the same class predictions via **separating hyperplanes**.
- The Bayes classifier under these assumptions is more commonly known as the **LDA classifier**.

Parameter Estimation

- How to estimate the parameters of the LDA model?
- We can achieve this by maximum likelihood (EM algorithm is not needed here since the class variables y_i are observed!).
- Let $n_k = \#\{j : y_j = k\}$ be the number of observations in class k.

$$\ell(\pi, (\mu_k)_{k=1}^K, \Sigma) = \log p\left((x_i, y_i)_{i=1}^n \,|\pi, (\mu_k)_{k=1}^K, \Sigma\right) = \sum_{i=1}^n \log \pi_{y_i} g_{y_i}(x_i)$$

$$= c + \sum_{k=1}^K \sum_{j:y_j=k} \log \pi_k - \frac{1}{2}\left(\log|\Sigma| + (x_j - \mu_k)^\top \Sigma^{-1}(x_j - \mu_k)\right)$$

ML estimates:

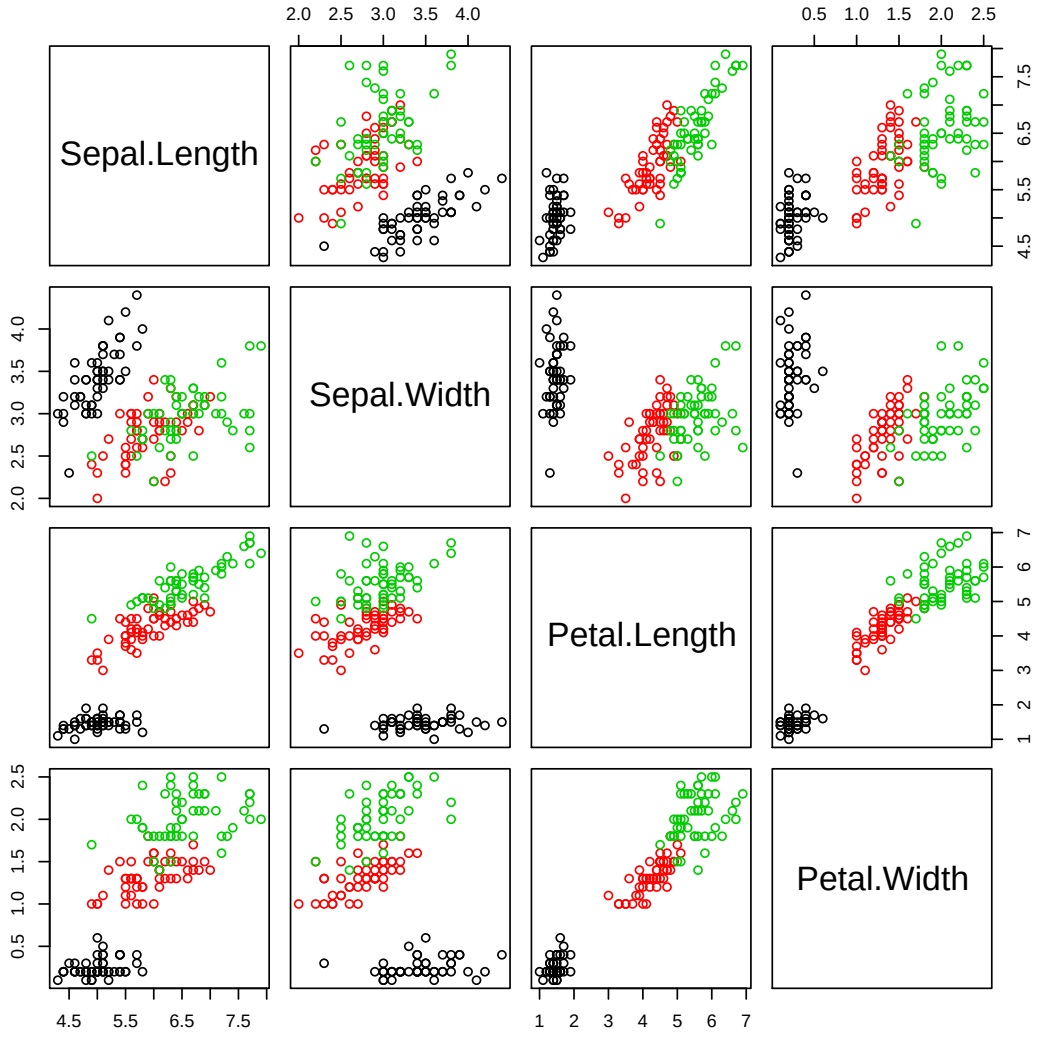
$$\widehat{\pi}_k = \frac{n_k}{n} \qquad \widehat{\mu}_k = \frac{1}{n_k} \sum_{j:y_j=k} x_j$$

$$\widehat{\Sigma} = \frac{1}{n} \sum_{k=1}^K \sum_{j:y_j=k} (x_j - \widehat{\mu}_k)(x_j - \widehat{\mu}_k)^\top$$

- Note: the ML estimate of Σ is biased. For an unbiased estimate we need to divide by $n - K$.

Iris Dataset

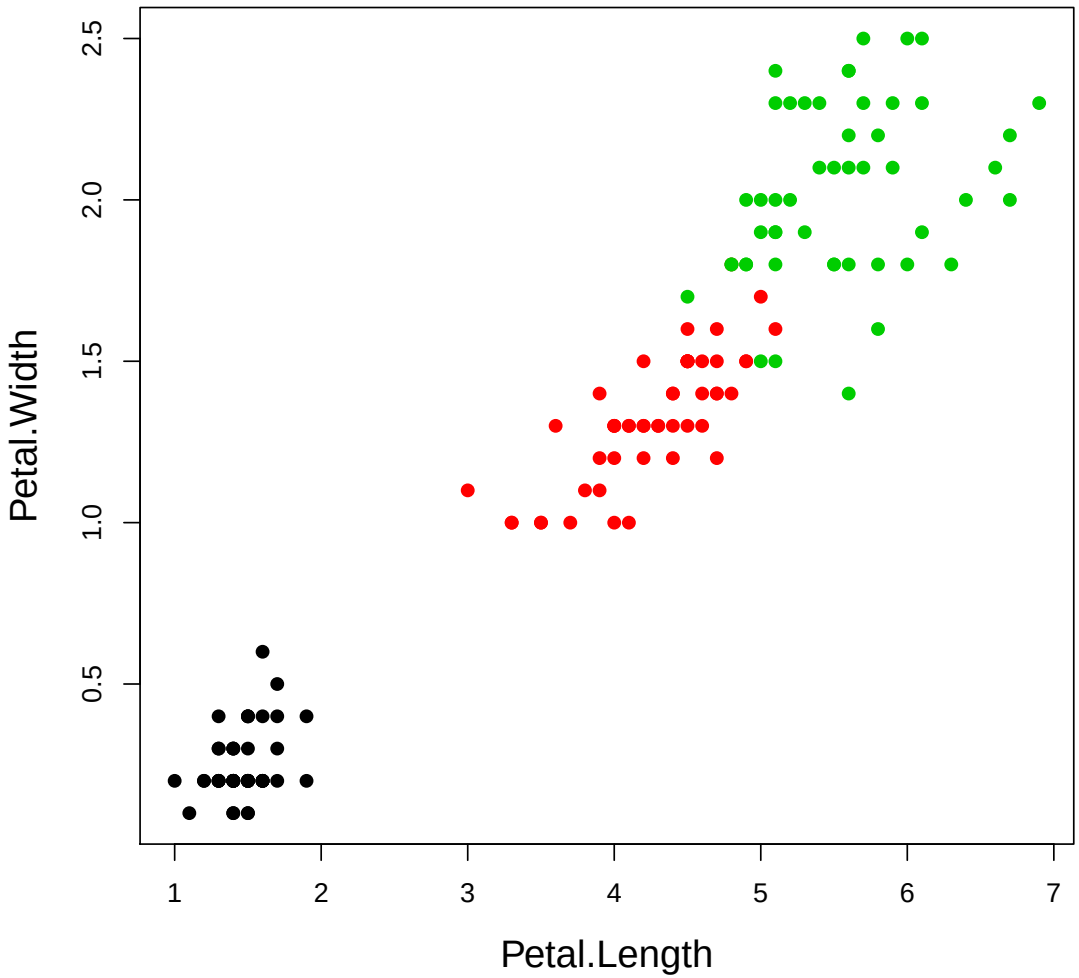
```
library(MASS)
data(iris)
##save class labels
ct <- unclass(iris$Species)
##pairwise plot
pairs(iris[,1:4],col=ct)
```



Iris Dataset

Just focus on two predictor variables.

```
iris.data <- iris[,3:4]
plot(iris.data,col=ct,pch=20,cex=1.5,cex.lab=1.4)
```

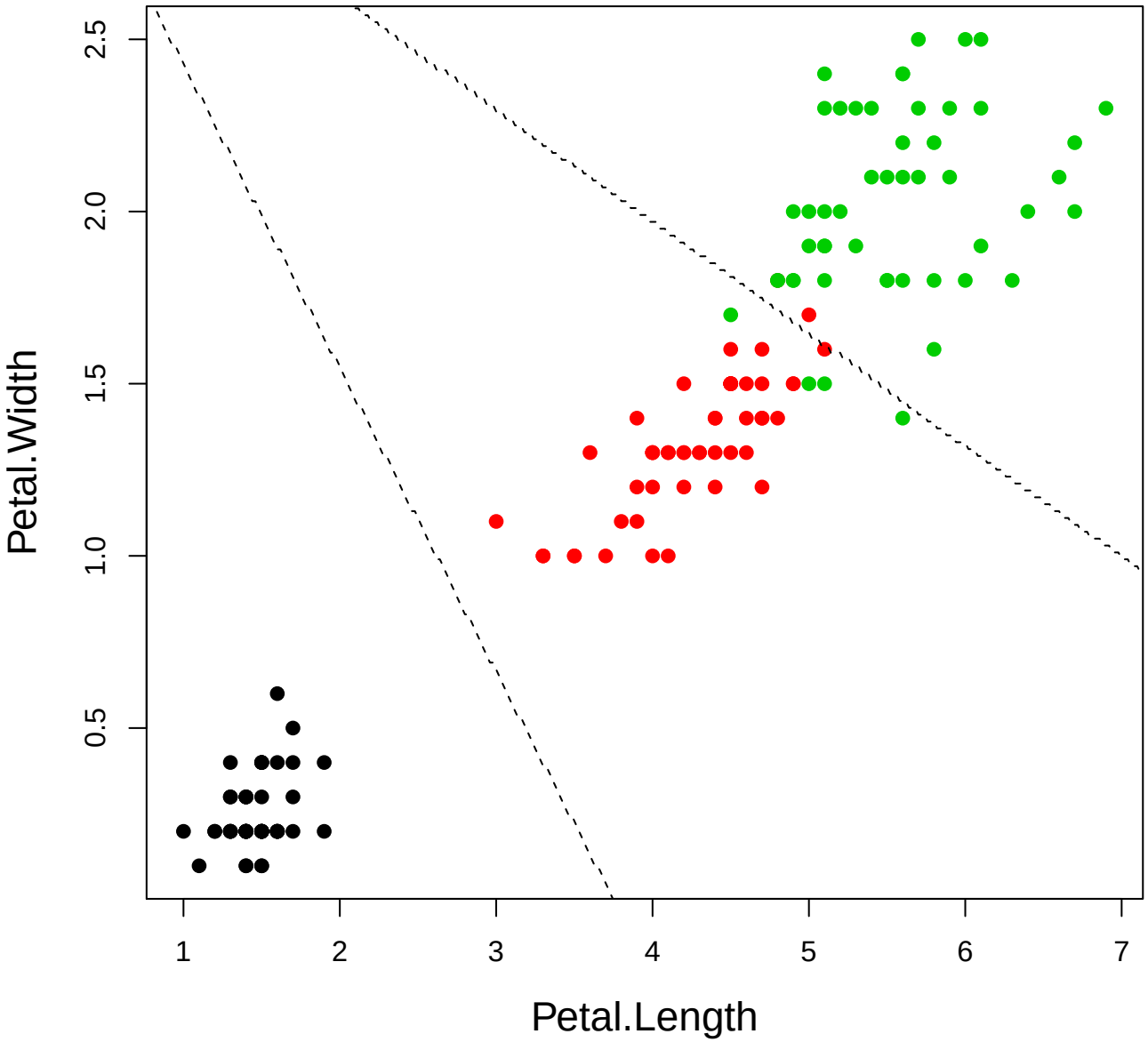


Iris Dataset

Computing and plotting the LDA boundaries.

```
##fit LDA
iris.lda <- lda(x=iris.data,grouping=ct)

##create a grid for our plotting surface
x <- seq(0,8,0.02)
y <- seq(0,3,0.02)
m <- length(x)
n <- length(y)
z <- as.matrix(expand.grid(x,y),0)
colnames(z) = colnames(iris.data)

##classes are 1,2 and 3, so set contours at 1.5 and 2.5
iris.ldp <- predict(iris.lda,z)$class
contour(x,y,matrix(iris.ldp,m,n),
        levels=c(1.5,2.5), add=TRUE, d=FALSE, lty=2)
```

Iris Dataset



Summary: **Linear Discriminant Analysis**

- **LDA**: a plug-in classifier assuming multivariate normal conditional density $g_k(x) = g_k(x|\mu_k, \Sigma)$ for each class k sharing the **same covariance** Σ:

$$X|Y = k \sim \mathcal{N}(\mu_k, \Sigma),$$

$$g_k(x|\mu_k, \Sigma) = (2\pi)^{-p/2}|\Sigma|^{-1/2} \exp\left(-\frac{1}{2}(x-\mu_k)^\top \Sigma^{-1}(x-\mu_k)\right).$$

- LDA minimizes the squared **Mahalanobis distance** between x and $\widehat{\mu}_k$, offset by a term depending on the estimated class proportion $\widehat{\pi}_k$:

$$\begin{aligned} f_{\text{LDA}}(x) &= \underset{k\in\{1,\ldots,K\}}{\operatorname{argmax}} \log \widehat{\pi}_k g_k(x|\widehat{\mu}_k, \widehat{\Sigma}) \\ &= \underset{k\in\{1,\ldots,K\}}{\operatorname{argmax}} \underbrace{\left(\log \widehat{\pi}_k - \frac{1}{2}\widehat{\mu}_k^\top \widehat{\Sigma}^{-1}\widehat{\mu}_k\right) + \left(\widehat{\Sigma}^{-1}\widehat{\mu}_k\right)^\top x}_{\text{terms depending on } k \text{ linear in } x} \\ &= \underset{k\in\{1,\ldots,K\}}{\operatorname{argmin}} \frac{1}{2}\underbrace{(x-\widehat{\mu}_k)^\top \widehat{\Sigma}^{-1}(x-\widehat{\mu}_k)}_{\text{squared Mahalanobis distance}} - \log \widehat{\pi}_k. \end{aligned}$$

Computations for LDA

- LDA minimizes the squared **Mahalanobis distance** between x and $\widehat{\mu}_k$, offset by a term depending on the estimated class proportion $\widehat{\pi}_k$:

$$f_{\text{LDA}}(x) \quad = \quad \underset{k \in \{1,\ldots,K\}}{\operatorname{argmin}} \; \frac{1}{2} \underbrace{(x - \widehat{\mu}_k)^\top \widehat{\Sigma}^{-1} (x - \widehat{\mu}_k)}_{\text{squared Mahalanobis distance}} - \log \widehat{\pi}_k.$$

- Thus, LDA classification can be implemented as the following two steps:

  (1) **Sphere** the data with respect to **the common covariance estimate** $\widehat{\Sigma} = \frac{1}{n} \sum_{k=1}^{K} \sum_{j:y_j=k} (x_j - \widehat{\mu}_k)(x_j - \widehat{\mu}_k)^\top$:

$$x^\bullet \leftarrow D^{-\frac{1}{2}} U^\top x, \quad \text{where} \quad \widehat{\Sigma} = U D U^\top.$$

  (2) Classify to the closest class mean $\widehat{\mu}_k^\bullet$ in the transformed space, modulo the effect of the estimated class proportions $\widehat{\pi}_k$.

Fisher's Reduced-Rank Linear Discriminant Analysis

- In LDA, data vectors are classified based on Mahalanobis distance to class means.
- There is K class means and they lie on a $(K-1)$-dimensional affine subspace of ambient space $\mathbb{R}^p$: Decision function is unaffected by the directions orthogonal to this subspace.
- Projecting data vectors onto the subspace can be viewed as a dimensionality reduction technique that preserves discriminative information about the labels $\{y_i\}_{i=1}^n$: going from $\mathbb{R}^p$ to $\mathbb{R}^{K-1}$ and potentially $K-1 \ll p$.
- Just like in PCA, we can visualise the structure in the data by choosing an appropriate basis for the subspace and projecting data onto it - immediate visualisation fully describing LDA for $K=3$.
- For $K>3$, Fisher proposed to look for the change of basis that finds **directions that best separate the classes** - the largest possible spread of the centroids after sphering.

LDA projections

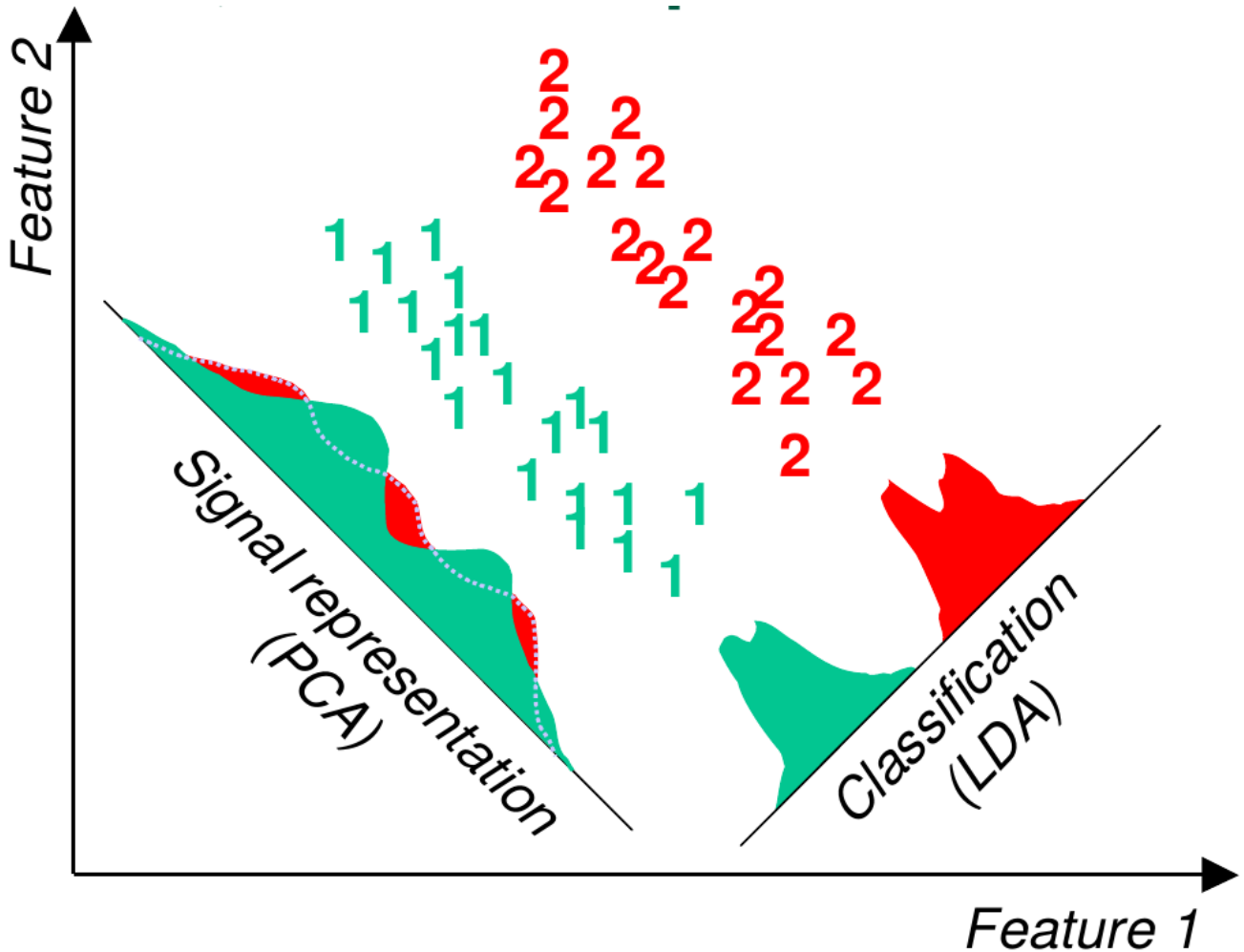


Figure by R. Gutierrez-Osuna

Discriminant Coordinates: 2-classes

- Centroids are $\widehat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i$.
- Centroids projected on a vector v are given by $m_k = v^\top \widehat{\mu}_k$.
- Variance of projected data on v given by $s_k^2 = \sum_{i:y_i=k} (v^\top x_i - m_k)^2$.
- Goal: find v such that the distance between centroids is maximized, while projected clusters are "tight":

$$\frac{(m_1 - m_2)^2}{s_1^2 + s_2^2}$$

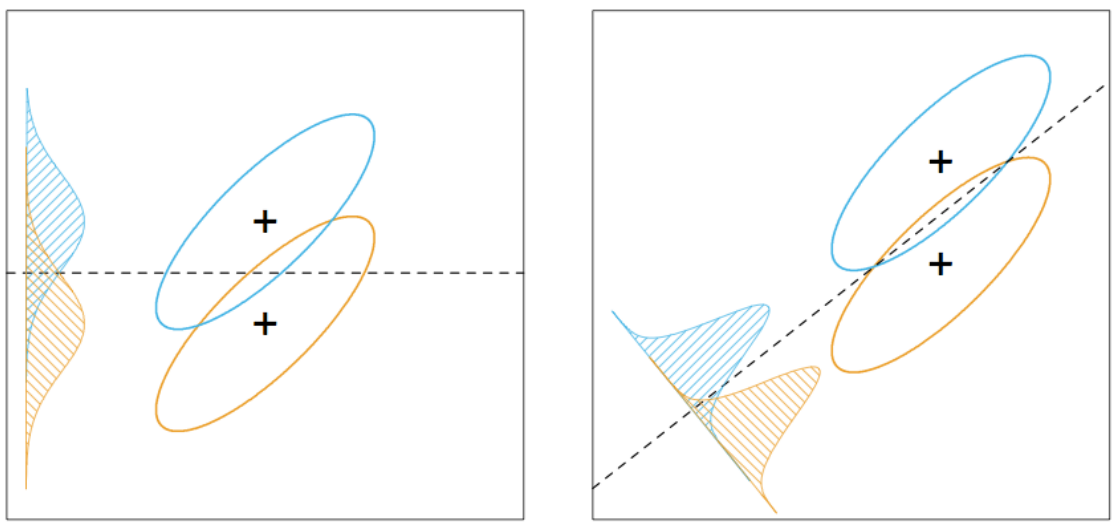


Figure from Hastie, Tibshirani and Friedman, Section 4.3.3

Discriminant Coordinates: 2-classes

- Centroids are $\widehat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i$.
- Centroids projected on a vector v are given by $m_k = v^\top \widehat{\mu}_k$.
- Variance of projected data on v given by $s_k^2 = \sum_{i:y_i=k} (v^\top x_i - m_k)^2$.
- Goal: find v such that the distance between centroids is maximized, while projected clusters are "tight":

$$\frac{(m_1 - m_2)^2}{s_1^2 + s_2^2} = \frac{v^\top B v}{v^\top \widehat{\Sigma} v}$$

where

$$B = (\widehat{\mu}_2 - \widehat{\mu}_1)(\widehat{\mu}_2 - \widehat{\mu}_1)^\top \qquad \text{(between-class covariance)}$$

$$\widehat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \widehat{\mu}_{y_i})(x_i - \widehat{\mu}_{y_i})^\top \qquad \text{(within-class covariance)}$$

(verify above calculations).

Discriminant Coordinates

- More generally:

$$\frac{v^\top B v}{v^\top \widehat{\Sigma} v}$$

where

$$B = \frac{1}{n}\sum_{k=1}^{K} n_k(\widehat{\mu}_k - \bar{x})(\widehat{\mu}_k - \bar{x})^\top \qquad \text{(between-class covariance)}$$

$$\widehat{\Sigma} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \widehat{\mu}_{y_i})(x_i - \widehat{\mu}_{y_i})^\top \qquad \text{(within-class covariance)}$$

and B has rank at most $K - 1$.

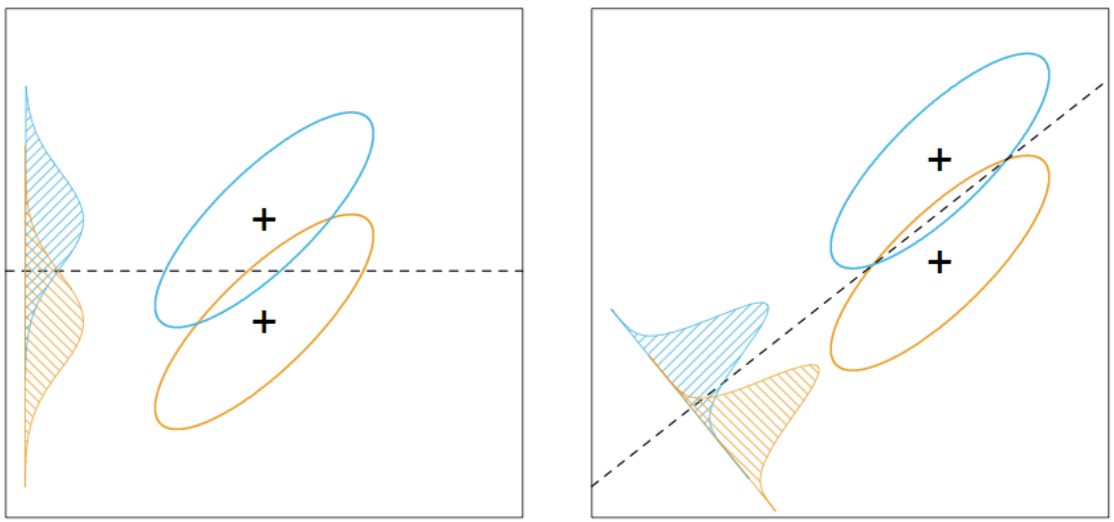


Figure from Hastie, Tibshirani and Friedman, Section 4.3.3

Discriminant Coordinates

- To solve for the optimal v, we first reparameterize it as $u = \widehat{\Sigma}^{\frac{1}{2}} v$.

$$\frac{v^\top B v}{v^\top \widehat{\Sigma} v} = \frac{u^\top (\widehat{\Sigma}^{-\frac{1}{2}})^\top B \widehat{\Sigma}^{-\frac{1}{2}} u}{u^\top u} = \frac{u^\top B^\bullet u}{u^\top u}$$

  where $B^\bullet = (\widehat{\Sigma}^{-\frac{1}{2}})^\top B \widehat{\Sigma}^{-\frac{1}{2}}$.
- We have solved something similar before. The maximization over u is achieved by the first eigenvector u_1 of $B^\bullet$.
- We also look at the remaining eigenvectors u_l associated to the non-zero eigenvalues and define the **discriminant coordinates** as $v_l = \widehat{\Sigma}^{-\frac{1}{2}} u_l$.
- The v_l's span exactly the affine subspace spanned by $(\widehat{\Sigma}^{-1}\widehat{\mu}_k)_{k=1}^K$ (these vectors are given as the "linear discriminants" in the R-function `lda`).

Crabs Dataset

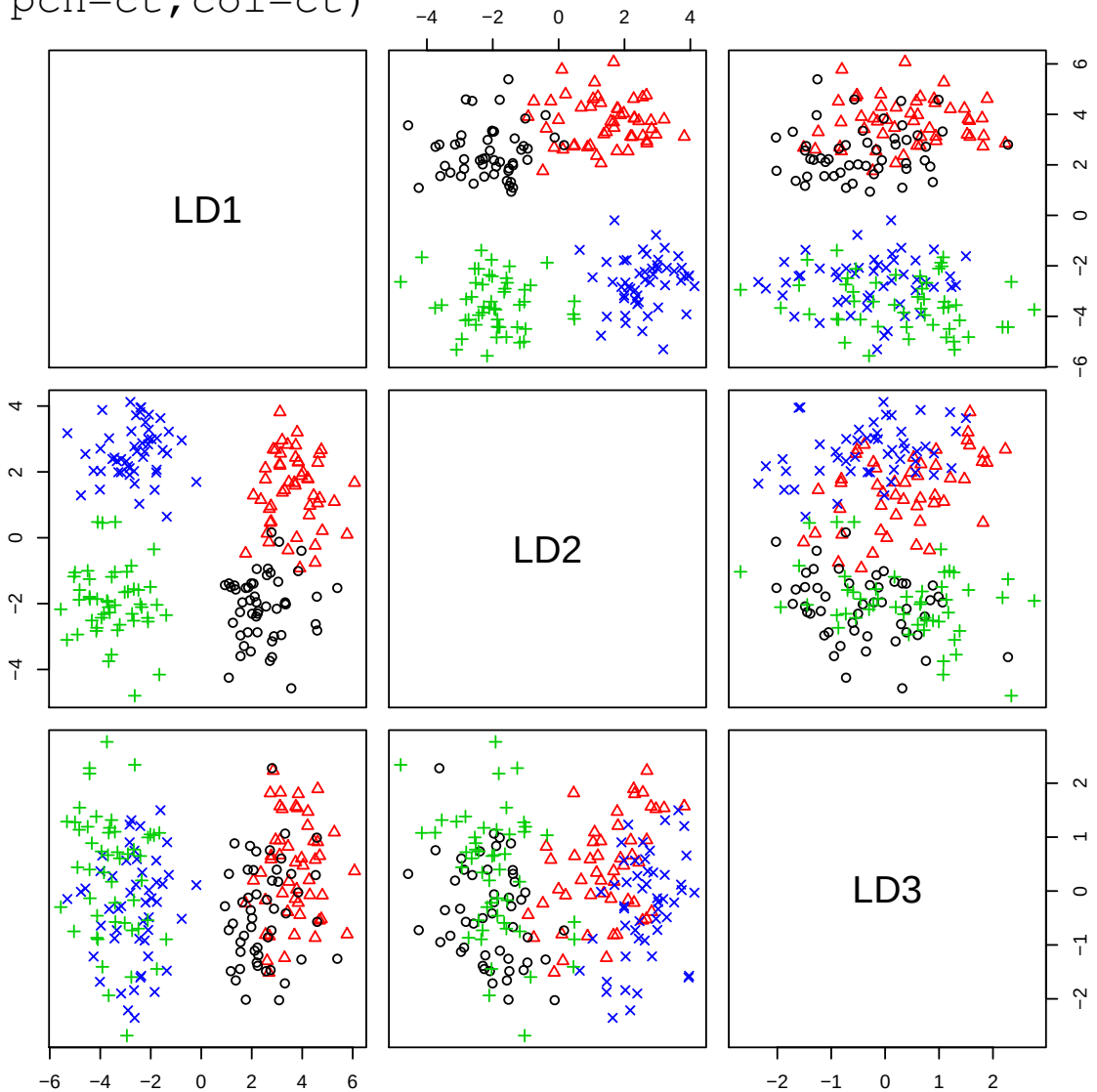
```
library(MASS)
data(crabs)

## create class labels (species+sex)
crabs$spsex=factor(paste(crabs$sp,crabs$sex,sep=""))
ct <- unclass(crabs$spsex)

## LDA on crabs in log-domain
cb.lda <- lda(log(crabs[,4:8]),ct)
```

Crabs Dataset

```
> cb.lda
Call:
lda(log(crabs[, 4:8]), ct)

Prior probabilities of groups:
   1    2    3    4
0.25 0.25 0.25 0.25

Group means:
        FL       RW       CL       CW       BD
1 2.564985 2.475174 3.312685 3.462327 2.441351
2 2.672724 2.443774 3.437968 3.578077 2.560806
3 2.852455 2.683831 3.529370 3.649555 2.733273
4 2.787885 2.489921 3.490431 3.589426 2.701580

Coefficients of linear discriminants:
          LD1        LD2        LD3
FL -31.217207  -2.851488  25.719750
RW  -9.485303 -24.652581  -6.067361
CL  -9.822169  38.578804 -31.679288
CW  65.950295 -21.375951  30.600428
BD -17.998493   6.002432 -14.541487

Proportion of trace:
   LD1    LD2    LD3
0.6891 0.3018 0.0091
```

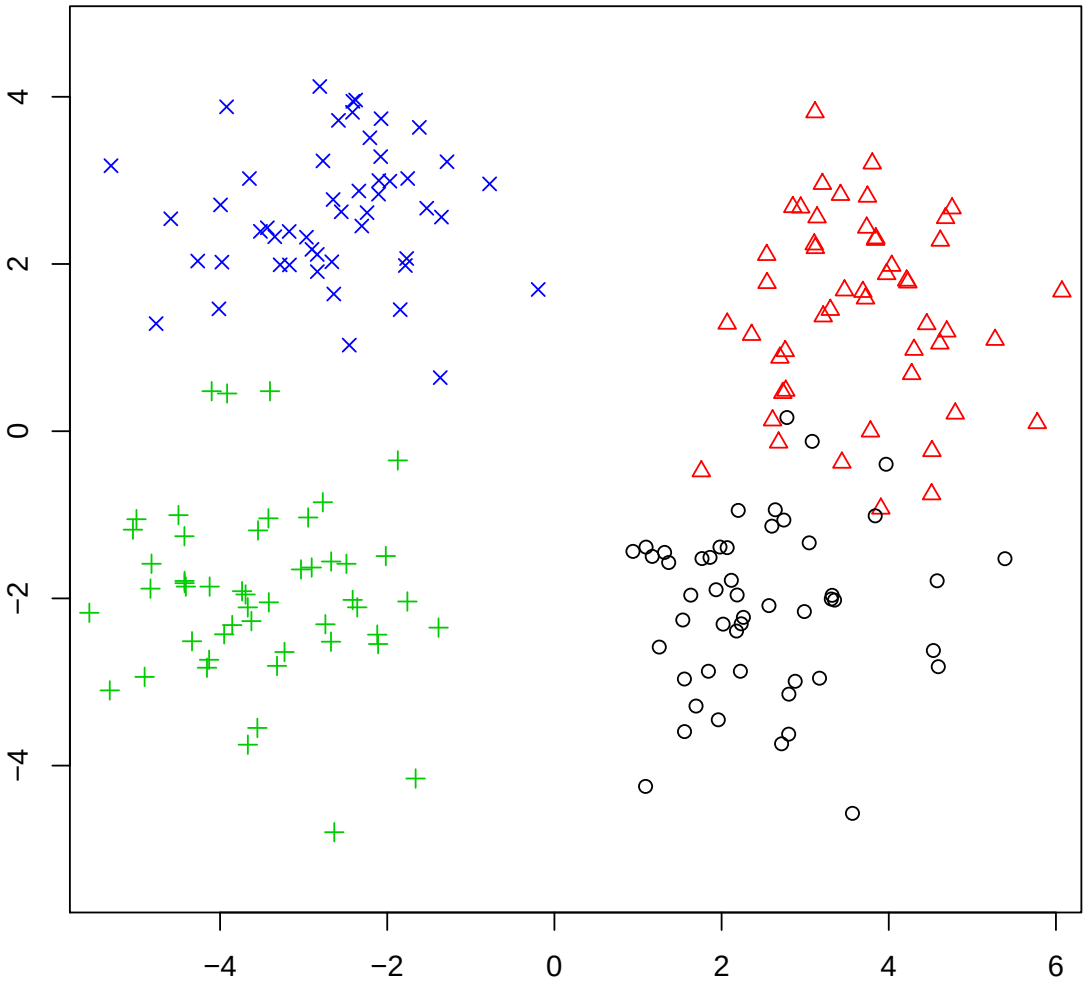
Crabs Dataset

```
cb.ldp <- predict(cb.lda)
pairs(cb.ldp$x,pch=ct,col=ct)
```



Crabs Dataset

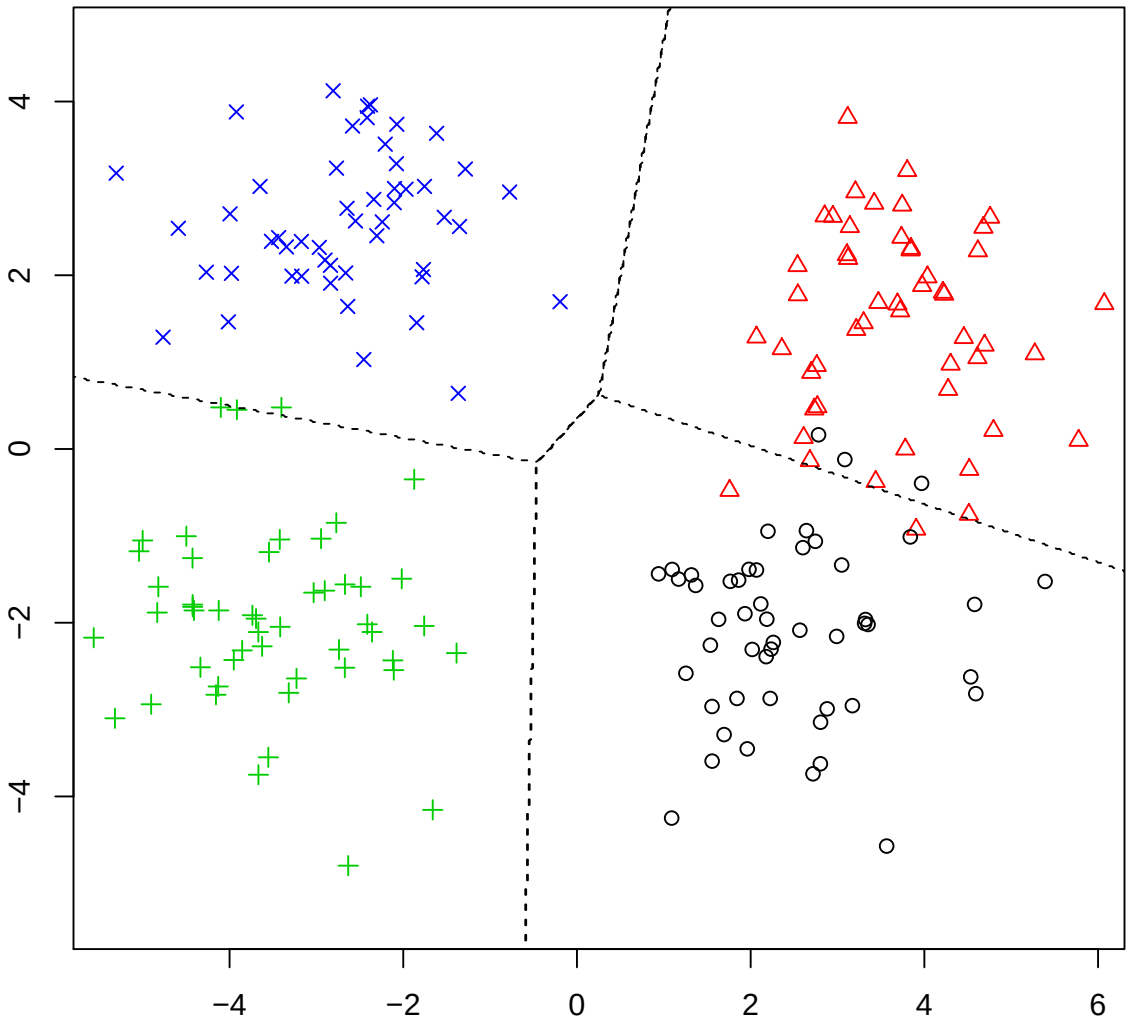
```
cb.ldp12 <- cb.ldp$x[,1:2]
eqscplot(cb.ldp12,pch=ct,col=ct)
```



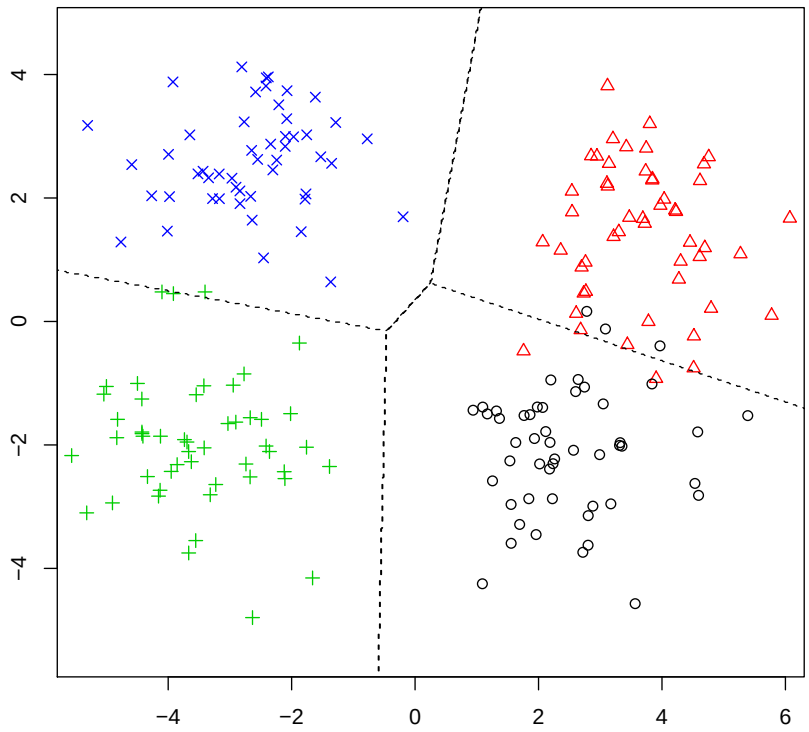
Crabs Dataset

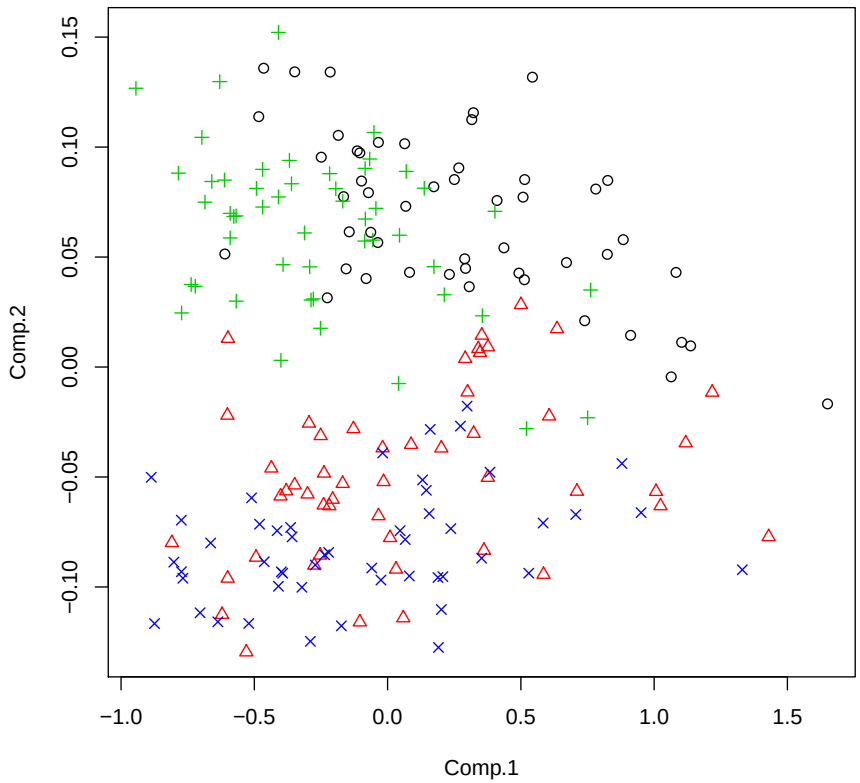
```
## display the decision boundaries
## take a lattice of points in LD-space
x <- seq(-6,7,0.02)
y <- seq(-6,7,0.02)
z <- as.matrix(expand.grid(x,y))
m <- length(x)
n <- length(y)

## perform LDA on first two discriminant directions
cb.lda_new <- lda(cb.ldp12,ct)
## predict onto the grid
cb.ldpp <- predict(cb.lda_new,z)$class

## classes are 1,2,3 and 4 so set contours
## at 1.5,2.5 and 3.5
contour(x,y,matrix(cb.ldpp,m,n),
        levels=c(1.5,2.5,3.5),
        add=TRUE,d=FALSE,lty=2)
```

Crabs Dataset



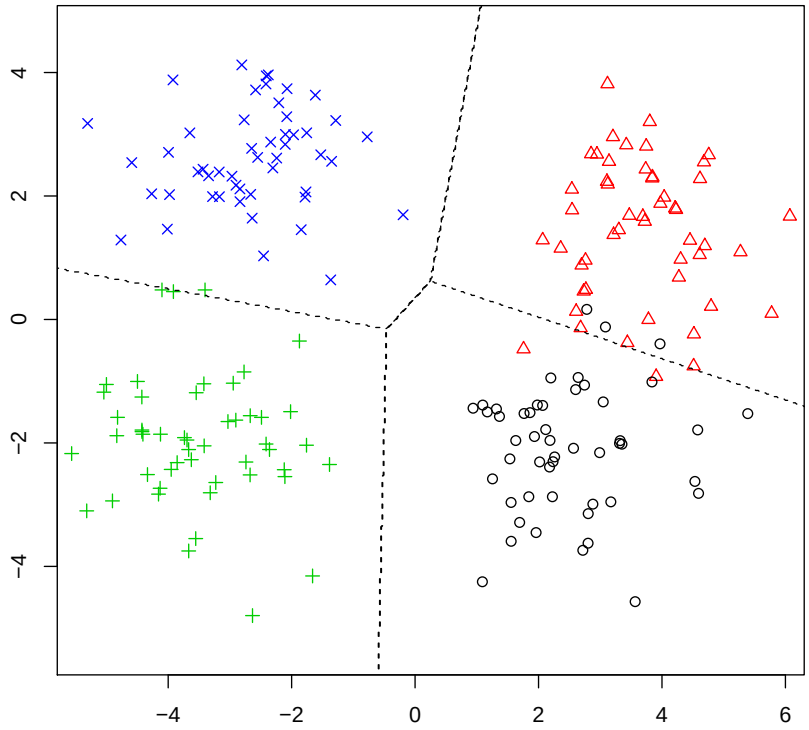
LDA vs PCA projections

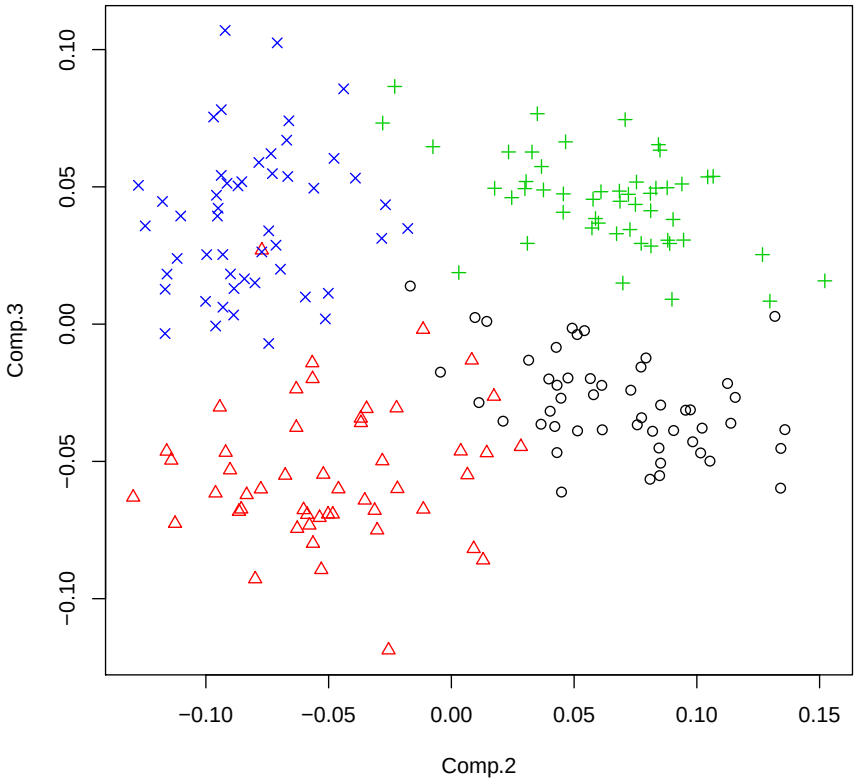




LDA separates the groups better.

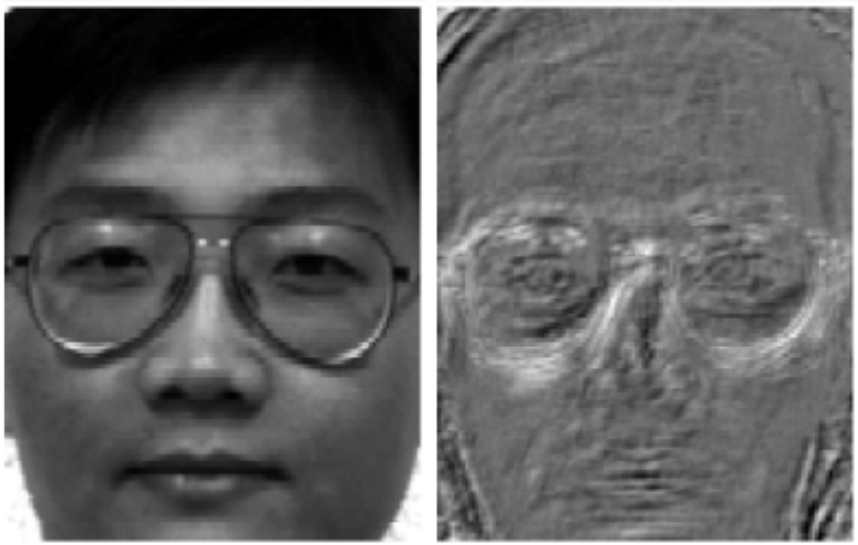
LDA vs PCA projections





LDA separates the groups better.

Fisherfaces



Eigenfaces vs. Fisherfaces, Belhumeur et al. 1997

http://ieeexplore.ieee.org/document/598228/