

# Extensions of Discriminant Analysis

Nate Wells

Math 243: Stat Learning

October 9th, 2020

# Outline

In today's class, we will. . .

- Create a handmade LDA model
- Discuss LDA with two or more predictors
- Implement LDA in R
- Define QDA and compare to LDA

## Section 1

### Handmade LDA model

# LDA

Suppose  $Y$  is a categorical variable with  $\ell$  levels, and for each level  $A_j$ , that

$$X|Y = A_j \sim N(\mu_j, \sigma).$$

# LDA

Suppose  $Y$  is a categorical variable with  $\ell$  levels, and for each level  $A_j$ , that

$$X|Y = A_j \sim N(\mu_j, \sigma).$$

The discriminant function

$$\delta_j(x) = x \cdot \frac{\mu_j}{\sigma^2} - \frac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

can be used to classify an observation by choosing the level  $A_j$  whose discriminant is largest at  $x$ .

# LDA

Suppose  $Y$  is a categorical variable with  $\ell$  levels, and for each level  $A_j$ , that

$$X|Y = A_j \sim N(\mu_j, \sigma).$$

The discriminant function

$$\delta_j(x) = x \cdot \frac{\mu_j}{\sigma^2} - \frac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

can be used to classify an observation by choosing the level  $A_j$  whose discriminant is largest at  $x$ .

We estimate the values of  $\mu_j$  and  $\sigma$  from the sample data:

$$\hat{\mu}_j = \frac{1}{n_j} \sum_{i: y_i = A_j} x_i$$

# LDA

Suppose  $Y$  is a categorical variable with  $\ell$  levels, and for each level  $A_j$ , that

$$X|Y = A_j \sim N(\mu_j, \sigma).$$

The discriminant function

$$\delta_j(x) = x \cdot \frac{\mu_j}{\sigma^2} - \frac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

can be used to classify an observation by choosing the level  $A_j$  whose discriminant is largest at  $x$ .

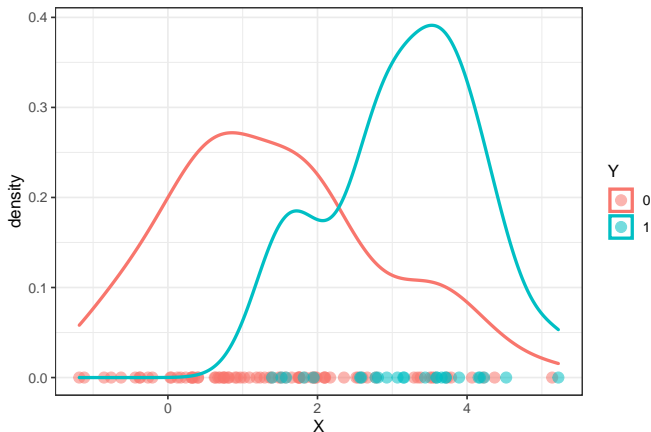
We estimate the values of  $\mu_j$  and  $\sigma$  from the sample data:

$$\hat{\mu}_j = \frac{1}{n_j} \sum_{i: y_i = A_j} x_i$$

$$\hat{\sigma}^2 = \frac{1}{n - \ell} \sum_{j=1}^{\ell} \sum_{i: y_i = A_j} (x_i - \hat{\mu}_j)^2$$

# Simulated Data

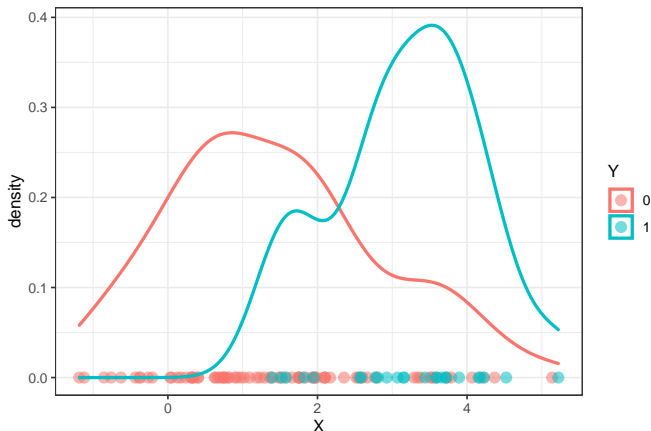
Suppose  $X|Y = 0 \sim N(1, 1)$  and  $X|Y = 1 \sim N(3, 1)$ , and that  $\pi_0 = .75$  and  $\pi_1 = .25$ .





# Simulated Data

Suppose  $X|Y = 0 \sim N(1, 1)$  and  $X|Y = 1 \sim N(3, 1)$ , and that  $\pi_0 = .75$  and  $\pi_1 = .25$ .



What feature of the graph shows that  $\pi_0 = .75$  and  $\pi_1 = .25$ ?

## Find Estimates

Estimates for  $\mu_j$  and  $\pi_j$

```
pi0 <- 3/4  
pi1 <- 1/4  
mu0<-d %>% filter(Y == 0) %>% summarise(mu = mean(X) ) %>% pull()  
mu1<-d %>% filter(Y == 1) %>% summarise(mu = mean(X) ) %>% pull()  
data.frame(mu0, mu1)
```

```
##          mu0          mu1  
## 1  1.42849  3.168335
```

# Find Estimates

Estimates for  $\mu_j$  and  $\pi_j$

```
pi0 <- 3/4
pi1 <- 1/4
mu0<-d %>% filter(Y == 0) %>% summarise(mu = mean(X) ) %>% pull()
mu1<-d %>% filter(Y == 1) %>% summarise(mu = mean(X) ) %>% pull()
data.frame(mu0, mu1)
```

```
##          mu0          mu1
## 1 1.42849 3.168335
```

Estimates for  $\sigma$ .

```
ssx <- d %>% group_by(Y) %>% summarize(ssx = var(X) * (n() - 1), n()) %>% pull(2,)
ssx
```

```
## [1] 148.19201 23.70648
```

```
sigma2 <- sum(ssx)/(n - 2)
sigma2
```

```
## [1] 1.754066
```

## The discriminant function

Solve for intersection of discriminant functions:

## The discriminant function

Solve for intersection of discriminant functions:

$$c \frac{\mu_1}{\sigma^2} - \frac{\mu_1^2}{2\sigma^2} + \ln \pi_1 = c \frac{\mu_0}{\sigma^2} - \frac{\mu_0^2}{2\sigma^2} + \ln \pi_0$$

## The discriminant function

Solve for intersection of discriminant functions:

$$c \frac{\mu_1}{\sigma^2} - \frac{\mu_1^2}{2\sigma^2} + \ln \pi_1 = c \frac{\mu_0}{\sigma^2} - \frac{\mu_0^2}{2\sigma^2} + \ln \pi_0$$

$$c = \frac{2\sigma^2 \ln \frac{\pi_0}{\pi_1} + \mu_1^2 - \mu_0^2}{2(\mu_1 - \mu_0)}$$

## The discriminant function

Solve for intersection of discriminant functions:

$$c \frac{\mu_1}{\sigma^2} - \frac{\mu_1^2}{2\sigma^2} + \ln \pi_1 = c \frac{\mu_0}{\sigma^2} - \frac{\mu_0^2}{2\sigma^2} + \ln \pi_0$$

$$c = \frac{2\sigma^2 \ln \frac{\pi_0}{\pi_1} + \mu_1^2 - \mu_0^2}{2(\mu_1 - \mu_0)}$$

```
c<- (2*sigma2*log(.75/.25) + mu1^2 - mu0^2)/(2*(mu1 - mu0))  
c
```

```
## [1] 3.406004
```

## The discriminant function

Solve for intersection of discriminant functions:

$$c \frac{\mu_1}{\sigma^2} - \frac{\mu_1^2}{2\sigma^2} + \ln \pi_1 = c \frac{\mu_0}{\sigma^2} - \frac{\mu_0^2}{2\sigma^2} + \ln \pi_0$$

$$c = \frac{2\sigma^2 \ln \frac{\pi_0}{\pi_1} + \mu_1^2 - \mu_0^2}{2(\mu_1 - \mu_0)}$$

```
c<- (2*sigma2*log(.75/.25) + mu1^2 - mu0^2)/(2*(mu1 - mu0))  
c
```

```
## [1] 3.406004
```

Write a function to create discriminant functions:

```
my_lda <- function(x, pi, mu, sigma2) {  
  x * (mu/sigma2) - (mu^2)/(2 * sigma2) + log(pi)  
}
```



## The discriminant function

Solve for intersection of discriminant functions:

$$c \frac{\mu_1}{\sigma^2} - \frac{\mu_1^2}{2\sigma^2} + \ln \pi_1 = c \frac{\mu_0}{\sigma^2} - \frac{\mu_0^2}{2\sigma^2} + \ln \pi_0$$

$$c = \frac{2\sigma^2 \ln \frac{\pi_0}{\pi_1} + \mu_1^2 - \mu_0^2}{2(\mu_1 - \mu_0)}$$

```
c<- (2*sigma2*log(.75/.25) + mu1^2 - mu0^2)/(2*(mu1 - mu0))  
c
```

```
## [1] 3.406004
```

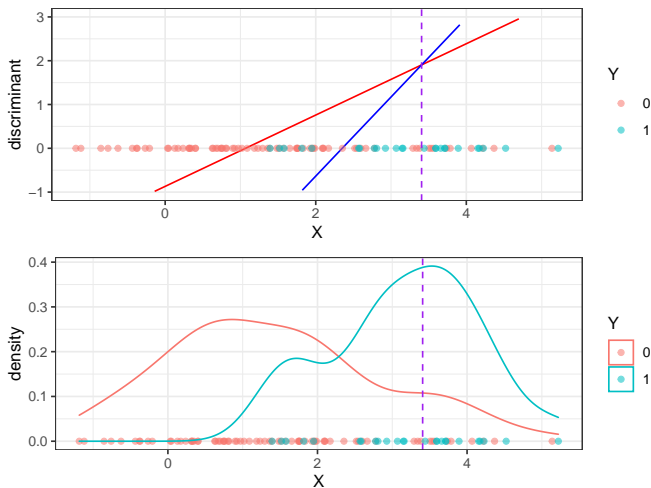
Write a function to create discriminant functions:

```
my_lda <- function(x, pi, mu, sigma2) {  
  x * (mu/sigma2) - (mu^2)/(2 * sigma2) + log(pi)  
}
```

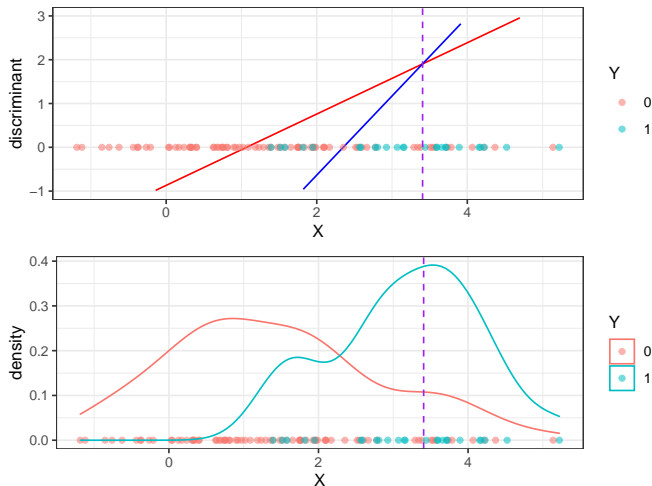
Create discriminant function for each class:

```
d0 <- my_lda(d$X, pi0, mu0, sigma2)  
d1 <- my_lda(d$X, pi1, mu1, sigma2)
```

## Plots



# Plots



Why don't the discriminant functions intersect at the same point as the density curves?

## Section 2

### LDA with multiple predictors

## Multivariate Gaussian Distributions

A vector  $X = (X_1, X_2, \dots, X_p)$  is said to have multivariate gaussian distribution if all linear combinations of coordinates  $a_1X_1 + a_2X_2 + \dots + a_pX_p$  have a Normal distribution.

## Multivariate Gaussian Distributions

A vector  $X = (X_1, X_2, \dots, X_p)$  is said to have multivariate gaussian distribution if all linear combinations of coordinates  $a_1X_1 + a_2X_2 + \dots + a_pX_p$  have a Normal distribution.

A multivariate gaussian distribution is specified by mean vector  $\mu = (\mu_1, \mu_2, \dots, \mu_p)$  and covariance matrix

$$\Sigma = \begin{pmatrix} \text{Var}(X_1) & \text{Cov}(X_1, X_2) & \cdots & \text{Cov}(X_1, X_p) \\ \text{Cov}(X_2, X_1) & \text{Var}(X_2) & \cdots & \text{Cov}(X_2, X_p) \\ \vdots & & \ddots & \vdots \\ \text{Cov}(X_p, X_1) & \text{Cov}(X_p, X_2) & & \text{Var}(X_p) \end{pmatrix}$$

## Multivariate Gaussian Distributions

A vector  $X = (X_1, X_2, \dots, X_p)$  is said to have multivariate gaussian distribution if all linear combinations of coordinates  $a_1X_1 + a_2X_2 + \dots + a_pX_p$  have a Normal distribution.

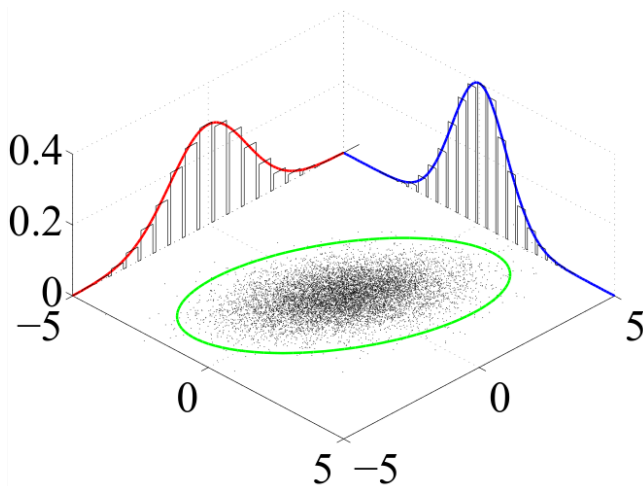
A multivariate gaussian distribution is specified by mean vector  $\mu = (\mu_1, \mu_2, \dots, \mu_p)$  and covariance matrix

$$\Sigma = \begin{pmatrix} \text{Var}(X_1) & \text{Cov}(X_1, X_2) & \dots & \text{Cov}(X_1, X_p) \\ \text{Cov}(X_2, X_1) & \text{Var}(X_2) & \dots & \text{Cov}(X_2, X_p) \\ \vdots & & \ddots & \vdots \\ \text{Cov}(X_p, X_1) & \text{Cov}(X_p, X_2) & & \text{Var}(X_p) \end{pmatrix}$$

The multivariate Gaussian density  $f$  on  $x \in \mathbb{R}^p$  is

$$f(x) = \frac{1}{(2\pi)^{p/2}(|\det \Sigma|)^{1/2}} \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)\right)$$

# Multivariate Scatterplot





## LDA with multiple predictors

Suppose that  $Y$  is categorical with  $\ell$  levels and that  $X = (X_1, \dots, X_p)$  are a vector of predictors. Assume that  $X|Y = A_j \sim N(\mu_j, \Sigma)$  with conditional density  $f_j$ , where  $\Sigma$  is common to all conditional densities.

## LDA with multiple predictors

Suppose that  $Y$  is categorical with  $\ell$  levels and that  $X = (X_1, \dots, X_p)$  are a vector of predictors. Assume that  $X|Y = A_j \sim N(\mu_j, \Sigma)$  with conditional density  $f_j$ , where  $\Sigma$  is common to all conditional densities.

As before, we consider the log-likelihood ratio:

$$\ln \frac{P(X = x | Y = A_j)}{P(X = x | Y = A_k)} = \ln \frac{f_j(x)\pi_j}{f_k(x)\pi_k}$$

## LDA with multiple predictors

Suppose that  $Y$  is categorical with  $\ell$  levels and that  $X = (X_1, \dots, X_p)$  are a vector of predictors. Assume that  $X|Y = A_j \sim N(\mu_j, \Sigma)$  with conditional density  $f_j$ , where  $\Sigma$  is common to all conditional densities.

As before, we consider the log-likelihood ratio:

$$\ln \frac{P(X = x | Y = A_j)}{P(X = x | Y = A_k)} = \ln \frac{f_j(x)\pi_j}{f_k(x)\pi_k}$$

The discriminant function  $\delta_j(x)$  for  $x \in \mathbb{R}^p$  is

$$\delta_j(x) = x^T \Sigma^{-1} \mu_j - \frac{1}{2} \mu_j^T \Sigma^{-1} \mu_j + \ln \pi_j$$

## LDA with multiple predictors

Suppose that  $Y$  is categorical with  $\ell$  levels and that  $X = (X_1, \dots, X_p)$  are a vector of predictors. Assume that  $X|Y = A_j \sim N(\mu_j, \Sigma)$  with conditional density  $f_j$ , where  $\Sigma$  is common to all conditional densities.

As before, we consider the log-likelihood ratio:

$$\ln \frac{P(X = x | Y = A_j)}{P(X = x | Y = A_k)} = \ln \frac{f_j(x)\pi_j}{f_k(x)\pi_k}$$

The discriminant function  $\delta_j(x)$  for  $x \in \mathbb{R}^p$  is

$$\delta_j(x) = x^T \Sigma^{-1} \mu_j - \frac{1}{2} \mu_j^T \Sigma^{-1} \mu_j + \ln \pi_j$$

We classify a point  $x$  by assigning it to the level with largest discriminant function at  $x$ .

## LDA with multiple predictors

Suppose that  $Y$  is categorical with  $\ell$  levels and that  $X = (X_1, \dots, X_p)$  are a vector of predictors. Assume that  $X|Y = A_j \sim N(\mu_j, \Sigma)$  with conditional density  $f_j$ , where  $\Sigma$  is common to all conditional densities.

As before, we consider the log-likelihood ratio:

$$\ln \frac{P(X = x | Y = A_j)}{P(X = x | Y = A_k)} = \ln \frac{f_j(x)\pi_j}{f_k(x)\pi_k}$$

The discriminant function  $\delta_j(x)$  for  $x \in \mathbb{R}^p$  is

$$\delta_j(x) = x^T \Sigma^{-1} \mu_j - \frac{1}{2} \mu_j^T \Sigma^{-1} \mu_j + \ln \pi_j$$

We classify a point  $x$  by assigning it to the level with largest discriminant function at  $x$ .

Decision boundaries are given by solving for intersections of the  $\binom{p}{2}$  pairs of discriminant functions:

$$x^T \Sigma^{-1} \mu_j - \frac{1}{2} \mu_j^T \Sigma^{-1} \mu_j + \ln \pi_j = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \ln \pi_k$$

# Classification

Let's investigate the classic iris dataset:



# Classification

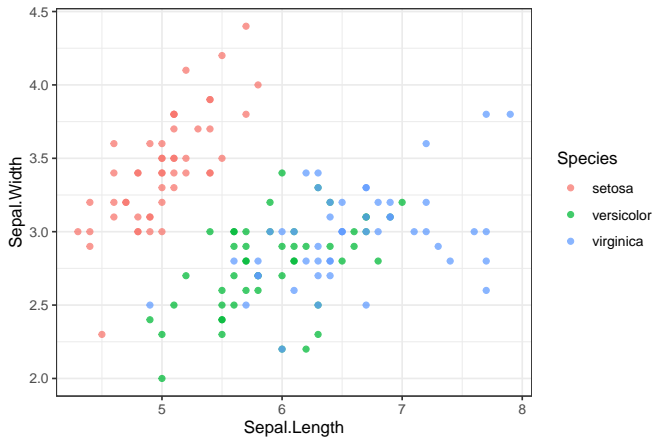
Let's investigate the classic iris dataset:



##	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
## 1	4.8	3.4	1.6	0.2	setosa
## 2	6.1	2.9	4.7	1.4	versicolor
## 3	5.7	2.8	4.1	1.3	versicolor
## 4	6.8	3.2	5.9	2.3	virginica
## 5	6.7	2.5	5.8	1.8	virginica

Can we classify Species based on Sepal.Length and Sepal.Width?

# Iris Plot



Where should we place our **linear** decision boundaries?



## LDA in R

It would be tedious to compute LDA discriminant functions by hand. So we use the `lda` function in the `mass` package.

```
library(MASS)
mlda <- lda(Species ~ Sepal.Length + Sepal.Width, data = iris)
mlda_pred <- predict(mlda)
conf_mlda <- table(mlda_pred$class, iris$Species)
conf_mlda
```

```
##
##           setosa versicolor virginica
## setosa           49             0         0
## versicolor        1            36        15
## virginica         0            14        35
```

## LDA in R

It would be tedious to compute LDA discriminant functions by hand. So we use the `lda` function in the `mass` package.

```
library(MASS)
mlda <- lda(Species ~ Sepal.Length + Sepal.Width, data = iris)
mlda_pred <- predict(mlda)
conf_mlda <- table(mlda_pred$class, iris$Species)
conf_mlda
```

```
##
##           setosa versicolor virginica
## setosa           49             0         0
## versicolor        1            36        15
## virginica         0            14        35
```

It looks like LDA had a hard time distinguishing between vesicolor and virginica.

## LDA in R

It would be tedious to compute LDA discriminant functions by hand. So we use the `lda` function in the `mass` package.

```
library(MASS)
mlda <- lda(Species ~ Sepal.Length + Sepal.Width, data = iris)
mlda_pred <- predict(mlda)
conf_mlda <- table(mlda_pred$class, iris$Species)
conf_mlda
```

```
##
##           setosa versicolor virginica
## setosa           49           0           0
## versicolor        1          36          15
## virginica         0          14          35
```

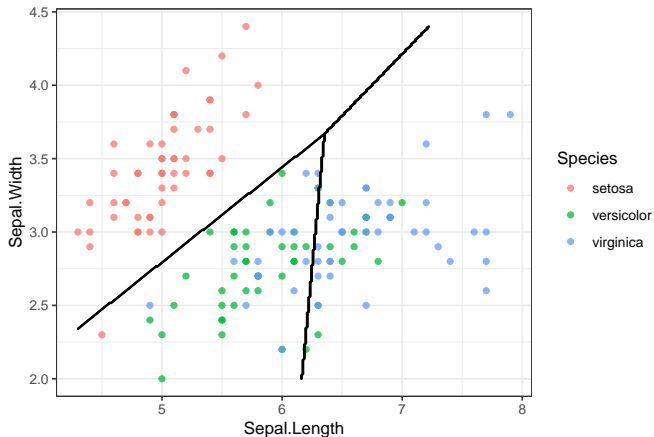
It looks like LDA had a hard time distinguishing between versicolor and virginica.

Overall error rate

```
(sum(conf_mlda) - sum(diag(conf_mlda)))/sum(conf_mlda)
```

```
## [1] 0.2
```

# Iris Decision Boundaries



## Section 3

### QDA

## Generalized Model

For a data set with 15 predictors and 1000 observations, would you be more worried about bias (Y) or variance (N) for an LDA model?

## Generalized Model

For a data set with 15 predictors and 1000 observations, would you be more worried about bias (Y) or variance (N) for an LDA model?

- With lots of data, variance is likely low. But the modeling restrictions of LDA might make bias problematic.

## Generalized Model

For a data set with 15 predictors and 1000 observations, would you be more worried about bias (Y) or variance (N) for an LDA model?

- With lots of data, variance is likely low. But the modeling restrictions of LDA might make bias problematic.
- We might be able to improve MSE by considering a more **complex** model.



## Generalized Model

For a data set with 15 predictors and 1000 observations, would you be more worried about bias (Y) or variance (N) for an LDA model?

- With lots of data, variance is likely low. But the modeling restrictions of LDA might make bias problematic.
- We might be able to improve MSE by considering a more **complex** model.

One underlying assumption for LDA was that all conditional distribution of predictors  $P(X = x | Y = y_j)$  had the same variance (or covariance matrix, for  $p \geq 2$ ).

## Generalized Model

For a data set with 15 predictors and 1000 observations, would you be more worried about bias (Y) or variance (N) for an LDA model?

- With lots of data, variance is likely low. But the modeling restrictions of LDA might make bias problematic.
- We might be able to improve MSE by considering a more **complex** model.

One underlying assumption for LDA was that all conditional distribution of predictors  $P(X = x | Y = y_j)$  had the same variance (or covariance matrix, for  $p \geq 2$ ).

Lifting this restriction leads to **Quadratic Discriminant Analysis (QDA)**

# QDA

Suppose that  $Y$  is categorical with  $\ell$  levels and that  $X = (X_1, \dots, X_p)$  are a vector of predictors. Assume that  $X|Y = A_j \sim N(\mu_j, \Sigma_j)$  with conditional density  $f_j$ .

# QDA

Suppose that  $Y$  is categorical with  $\ell$  levels and that  $X = (X_1, \dots, X_p)$  are a vector of predictors. Assume that  $X|Y = A_j \sim N(\mu_j, \Sigma_j)$  with conditional density  $f_j$ .

As with LDA, we consider the log likelihood ratios

$$\ln \frac{P(X = x | Y = A_j)}{P(X = x | Y = A_k)} = \ln \frac{f_j(x)\pi_j}{f_k(x)\pi_k}$$

# QDA

Suppose that  $Y$  is categorical with  $\ell$  levels and that  $X = (X_1, \dots, X_p)$  are a vector of predictors. Assume that  $X|Y = A_j \sim N(\mu_j, \Sigma_j)$  with conditional density  $f_j$ .

As with LDA, we consider the log likelihood ratios

$$\ln \frac{P(X = x | Y = A_j)}{P(X = x | Y = A_k)} = \ln \frac{f_j(x)\pi_j}{f_k(x)\pi_k}$$

But now when we substitute the formula for multivariate densities  $f_i$ , the variance (or covariance) terms in numerator and denominator do **not** cancel.

## QDA

Suppose that  $Y$  is categorical with  $\ell$  levels and that  $X = (X_1, \dots, X_p)$  are a vector of predictors. Assume that  $X|Y = A_j \sim N(\mu_j, \Sigma_j)$  with conditional density  $f_j$ .

As with LDA, we consider the log likelihood ratios

$$\ln \frac{P(X = x | Y = A_j)}{P(X = x | Y = A_k)} = \ln \frac{f_j(x)\pi_j}{f_k(x)\pi_k}$$

But now when we substitute the formula for multivariate densities  $f_i$ , the variance (or covariance) terms in numerator and denominator do **not** cancel.

This leads to the QDA discriminant function  $\delta_j(x)$ :

$$\delta_j(x) = -\frac{1}{2}x^T \Sigma_j^{-1}x + x^T \Sigma_j^{-1}\mu_j - \frac{1}{2}\mu_j^T \Sigma_j^{-1}\mu_j - \frac{1}{2} \ln \det \Sigma_j + \ln \pi_j$$

## QDA

Suppose that  $Y$  is categorical with  $\ell$  levels and that  $X = (X_1, \dots, X_p)$  are a vector of predictors. Assume that  $X|Y = A_j \sim N(\mu_j, \Sigma_j)$  with conditional density  $f_j$ .

As with LDA, we consider the log likelihood ratios

$$\ln \frac{P(X = x | Y = A_j)}{P(X = x | Y = A_k)} = \ln \frac{f_j(x)\pi_j}{f_k(x)\pi_k}$$

But now when we substitute the formula for multivariate densities  $f_i$ , the variance (or covariance) terms in numerator and denominator do **not** cancel.

This leads to the QDA discriminant function  $\delta_j(x)$ :

$$\delta_j(x) = -\frac{1}{2}x^T \Sigma_j^{-1}x + x^T \Sigma_j^{-1}\mu_j - \frac{1}{2}\mu_j^T \Sigma_j^{-1}\mu_j - \frac{1}{2} \ln \det \Sigma_j + \ln \pi_j$$

Which simplifies to the following when  $p = 1$ :

$$\delta_j(x) = -x^2 \frac{1}{2\sigma_j} + x \frac{\mu_j}{\sigma_j} - \frac{\mu_j^2}{2\sigma_j} - \frac{1}{2} \ln \sigma_j + \ln \pi_j$$

# In R

We use the `qda` function in the `mass` package.

```
library(MASS)
mqda <- qda(Species ~ Sepal.Length + Sepal.Width, data = iris)
mqda_pred <- predict(mqda)
conf_mqda <- table(mqda_pred$class, iris$Species)
conf_mqda
```

```
##
##           setosa versicolor virginica
## setosa      49           0           0
## versicolor   1          36          15
## virginica    0          14          35
```



# In R

We use the `qda` function in the `mass` package.

```
library(MASS)
mqda <- qda(Species ~ Sepal.Length + Sepal.Width, data = iris)
mqda_pred <- predict(mqda)
conf_mqda <- table(mqda_pred$class, iris$Species)
conf_mqda
```

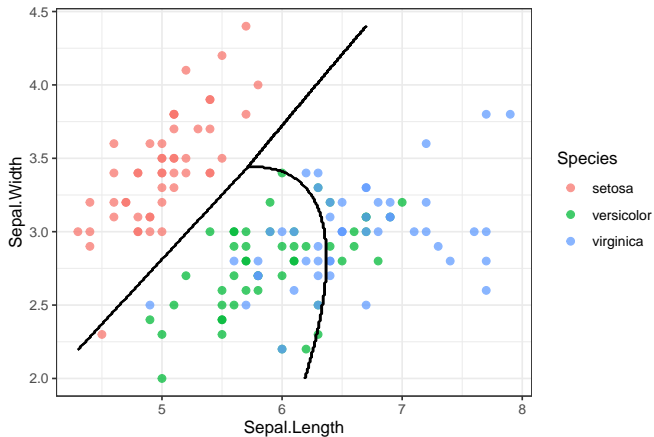
```
##
##           setosa versicolor virginica
## setosa           49             0         0
## versicolor        1            36        15
## virginica         0            14        35
```

How did we do?

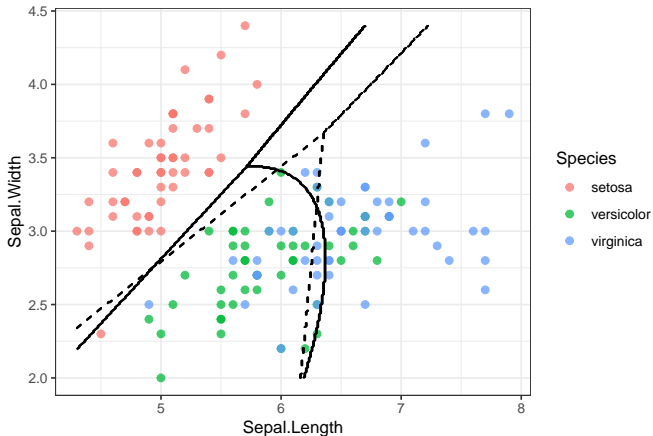
```
(sum(conf_mqda) - sum(diag(conf_mqda))) / sum(conf_mqda)
```

```
## [1] 0.2
```

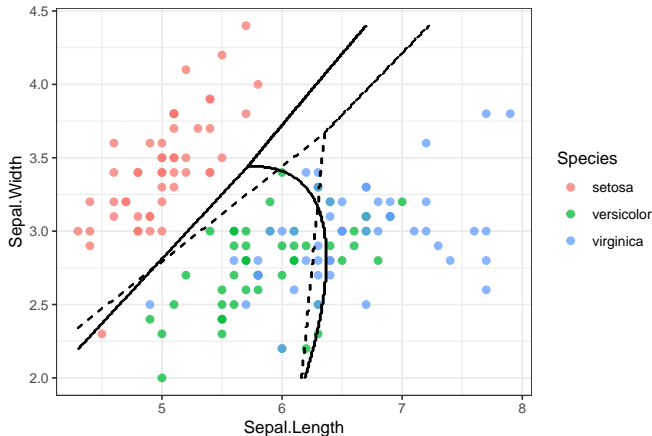
# QDA Decision Boundaries



# LDA - QDA Comparison



## LDA - QDA Comparison



Which model do you think would perform better on test data? LDA(Y) or QDA (N)