# Extentions of Discriminant Analysis 

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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

Suppose $Y$ is a categorical variable with $\ell$ levels, and for each level $A_{j}$, that

$$
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## LDA

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The discriminant function

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\delta_{j}(x)=x \cdot \frac{\mu_{j}}{\sigma^{2}}-\frac{\mu_{j}^{2}}{2 \sigma^{2}}+\ln \pi_{j}
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can be used to classify an observation by choosing the level $A_{j}$ whose discriminant is largest at $x$.

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We estimate the values of $\mu_{j}$ and $\sigma$ from the sample data:

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\hat{\mu}_{j}=\frac{1}{n_{j}} \sum_{i: y_{i}=A_{k}} x_{i}
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We estimate the values of $\mu_{j}$ and $\sigma$ from the sample data:

$$
\begin{gathered}
\hat{\mu}_{j}=\frac{1}{n_{j}} \sum_{i: y_{i}=A_{k}} x_{i} \\
\hat{\sigma}^{2}=\frac{1}{n-\ell} \sum_{j=1}^{\ell} \sum_{i: y_{i}=A_{k}}\left(x_{i}-\hat{\mu_{j}}\right)^{2}
\end{gathered}
$$

## Simulated Data

Suppose $X \mid Y=0 \sim N(1,1)$ and $X \mid Y=1 \sim N(3,1)$, and that $\pi_{0}=.75$ and $\pi_{1}=.25$.


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Suppose $X \mid Y=0 \sim N(1,1)$ and $X \mid Y=1 \sim N(3,1)$, 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 \(\pi_{j}\)
pio <- 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
\#\# 11.428493 .168335
```


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data.frame(mu0, mu1)
## mu0 mu1
## 1 1.42849 3.168335
Estimates for }\sigma\mathrm{ .
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
```


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$$
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c=\frac{2 \sigma^{2} \ln \frac{\pi_{0}}{\pi_{1}}+\mu_{1}^{2}-\mu_{0}^{2}}{2\left(\mu_{1}-\mu_{0}\right)}
\end{gathered}
$$

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\begin{aligned}
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& \qquad c=\frac{2 \sigma^{2} \ln \frac{\pi_{0}}{\pi_{1}}+\mu_{1}^{2}-\mu_{0}^{2}}{2\left(\mu_{1}-\mu_{0}\right)} \\
& \begin{array}{l}
c<-\left(2 * \operatorname{sigma} 2 * \log (.75 / .25)+\operatorname{mu} 1^{\wedge} 2-m u 0^{\wedge} 2\right) /(2 *(m u 1-\operatorname{mu} 0)) \\
\text { \#\# [1] } 3.406004
\end{array} \\
& \text { \# }
\end{aligned}
$$

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Write a function to create discriminant functions:

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


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```

Create discriminant function for each class:

```
dO <- 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 $X=\left(X_{1}, X_{2}, \ldots, X_{p}\right)$ is said to have multivariate gaussian distribution if all linear combinations of coordinates $a 1 X_{1}+a_{2} X_{2}+\cdots+a_{p} X_{p}$ have a Normal distribution.

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A multivariate gaussian distribution is specified by mean vector $\mu=\left(\mu_{1}, \mu_{2}, \ldots, \mu_{p}\right)$ and covariance matrix

$$
\Sigma=\left(\begin{array}{cccc}
\operatorname{Var}\left(X_{1}\right) & \operatorname{Cov}\left(X_{1}, X_{2}\right) & \cdots & \operatorname{Cov}\left(X_{1}, X_{p}\right) \\
\operatorname{Cov}\left(X_{2}, X_{1}\right) & \operatorname{Var}\left(X_{2}\right) & \cdots & \operatorname{Cov}\left(X_{2}, X_{p}\right) \\
\vdots & & \ddots & \vdots \\
\operatorname{Cov}\left(X_{p}, X_{1}\right) & \operatorname{Cov}\left(X_{p}, X_{2}\right) & & \operatorname{Var}\left(X_{p}\right)
\end{array}\right)
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\vdots & & \ddots & \vdots \\
\operatorname{Cov}\left(X_{p}, X_{1}\right) & \operatorname{Cov}\left(X_{p}, X_{2}\right) & & \operatorname{Var}\left(X_{p}\right)
\end{array}\right)
$$

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

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

## Multivariate Scatterplot



## LDA with multiple predictors

Suppose that $Y$ is categorical with $\ell$ levels and that $X=\left(X_{1}, \ldots, X_{p}\right)$ are a vector of predictors. Assume that $X \mid Y=A_{j} \sim N\left(\mu_{j}, \Sigma\right)$ with conditional density $f_{j}$, where $\Sigma$ is common to all conditional densities.

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As before, we consider the log-likelihood ratio:

$$
\ln \frac{P\left(Y=A_{j} \mid X=x\right)}{P\left(Y=A_{k} \mid X=x\right)}=\ln \frac{f_{j}(x) \pi_{j}}{f_{k}(x) \pi_{k}}
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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}
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## Classification

Let's investigate the classic iris dataset:


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| \#\# | 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 discrimant 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 |
| :--- | :--- | ---: | ---: | ---: |
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It looks like LDA had a hard time distinguishing between vesicolor 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

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One underlying assumption for LDA was that all conditional distribution of predictors $P\left(X=x \mid Y=y_{j}\right)$ had the same variance (or covariance matrix, for $p \geq 2$ ).

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One underlying assumption for LDA was that all conditional distribution of predictors $P\left(X=x \mid Y=y_{j}\right)$ 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 $X=\left(X_{1}, \ldots, X_{p}\right)$ are a vector of predictors. Assume that $X \mid Y=A_{j} \sim N\left(\mu_{j}, \Sigma_{j}\right)$ with conditional density $f_{j}$.

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As with LDA, we consider the log likelihood ratios

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This leads to the QDA discriminant function $\delta_{j}(x)$ :

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\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 \operatorname{det} \Sigma_{j}+\ln \pi_{j}
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$$

Which simplifes 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

| \#\# |  |  |  |  |
| :--- | :--- | ---: | ---: | ---: |
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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)

