Extentions 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

Nate Wells (Math 243: Stat Learning)

LDA

Suppose Y is a categorical variable with ℓ levels, and for each level A_j , that

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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 μ_i and σ from the sample data:

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

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We estimate the values of μ_i and σ from the sample data:

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

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

Handmade LDA model	
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Simulated Data

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



Handmade LDA model	
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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 μ<sub>j</sub> and π<sub>j</sub>

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

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```
Estimates for \mu_i and \pi_i
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data.frame(mu0, mu1)
## m110
               m111
## 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
```

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

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c<- (2*sigma2*log(.75/.25) + mu1² - mu0²)/(2*(mu1 - mu0))
c

[1] 3.406004

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

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Write a function to create discriminant functions:

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

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

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}
```

Create discriminant function for each class:

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

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 $X = (X_1, X_2, ..., X_p)$ is said to have multivariate gaussian distribution if all linear combinations of coordinates $a1X_1 + a_2X_2 + \cdots + a_pX_p$ have a Normal distribution.

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

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

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

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

Multivariate Scatterplot



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

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As before, we consider the log-likelihood ratio:

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

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

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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

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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</pre>
```

##				
##		setosa	versicolor	virginica
##	setosa	49	0	0
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```
Overall error rate
(sum(conf_mlda) - sum(diag(conf_mlda)))/sum(conf_mlda)
```

[1] 0.2

Iris Decision Boundaries



Section 3

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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 $p \ge 2$).

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?

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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 $p \ge 2$).

Lifting this restriction leads to Quadratic Discriminant Analysis (QDA)

QDA

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As with LDA, we consider the log likelihood ratios

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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 $\delta_j(x)$:

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

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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</pre>
```

setosa versicolor virginica ## ## setosa 49 0 0 versicolor 37 16 ## 1 ## virginica 0 13 34

In R

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```
library(MASS)
mqda <- qda(Species ~ Sepal.Length + Sepal.Width,data = iris)
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```

##				
##		setosa	versicolor	virginica
##	setosa	49	0	0
##	versicolor	1	37	16
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How did we do?

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

[1] 0.2

QDA 0000●0

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)