4.4.2 Linear Discriminant Analysis for $p > 1$

Dr. Lauren Perry

Multivariate Normal Distribution

We now assume the predictors $X = (X_1, X_2, \ldots, X_p)$ are drawn from a *multivariate normal distribution*.

$$X \sim N(\mu, \Sigma)$$

- Each individual predictor follows a one-dimensional normal distribution.
  - The vector μ contains all p means.
- Each pair of predictors is allowed to be correlated.
  - We represent this correlation with a $p \times p$ covariance matrix Σ that contains each variable's variance and all pairwise covariances.

LDA for $p > 1$

Assume the observations in the kth class are drawn from a multivariate normal distribution $N(\mu_k, \Sigma)$.

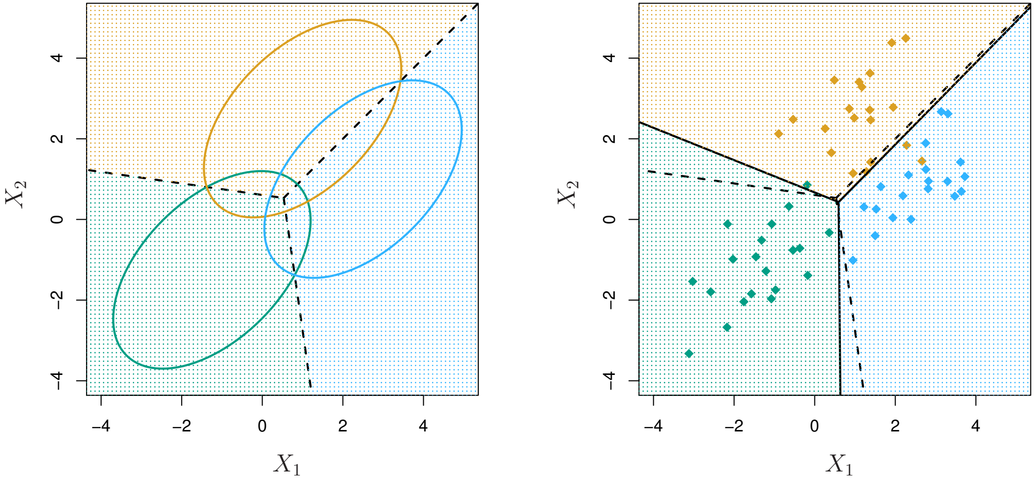
- μ_k is a class-specific vector of (p) means.
- Σ is the covariance matrix, assumed common to all K classes.

The Bayes classifier assigns an observation $X = x$ to the class for which

$$\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log \pi_k$$

where π_k is again $P(Y = k)$.

Example: Simulated Data with $p = 2$



LDA in Practice

We estimate the unknown parameters $\mu_1, \ldots, \mu_K$, $\pi_1, \ldots, \pi_K$, and Σ similar to how we estimated those used in the one-dimensional case.

The LDA then assigns an observation $X = x$ to the class for which

$$\hat{\delta}_k(x) = x^T \hat{\Sigma}^{-1} \hat{\mu}_k - \frac{1}{2} \hat{\mu}_k^T \hat{\Sigma}^{-1} \hat{\mu}_k + \log \hat{\pi}_k$$

is largest.

Example: Predicting Penguin Species

```r
data(penguins, package = "palmerpenguins")
mod1 <- lda(species ~ ., penguins)
predval <- predict(mod1)$class
species <- penguins$species[-unique(which(is.na(penguins), arr.ind=T)[,1])]
table(predval, species)
```

```
##            species
## predval     Adelie Chinstrap Gentoo
##   Adelie       145         0      0
##   Chinstrap      1        68      0
##   Gentoo         0         0    119
```

```r
mean(predval == species)
```

```
## [1] 0.996997
```

Example: Test and Training Data

- The error rate ($< 1\%$) seems very low, but we're only examining *training* error rate.

```r
data(penguins, package = "palmerpenguins")
set.seed(1)

# Remove missing data
pens <- penguins[-unique(which(is.na(penguins), arr.ind=T)[,1]),]
# Use 80% of the data as training data
train.ind <- sample(1:nrow(pens), floor(0.8*nrow(pens)), replace=F)
train.pen <- pens[train.ind, ]
# The rest us test data
test.pen <- pens[-train.ind, ]
```

Example: Test and Training Data

```r
mod2 <- lda(species ~ ., train.pen)
predval <- predict(mod2, test.pen)$class
species <- test.pen$species
table(predval, species)
```

```
##              species
## predval     Adelie Chinstrap Gentoo
##   Adelie        31         1      0
##   Chinstrap      0        10      0
##   Gentoo         0         0     25
```

```r
mean(predval == species)
```

```
## [1] 0.9850746
```

Example: Default Data

```
library(ISLR2)
data(Default)
set.seed(1)

train.ind <- sample(1:nrow(Default), floor(0.8*nrow(Default)), replace=F)
def.train <- Default[train.ind,]
def.test <- Default[-train.ind,]

mod3 <- lda(default ~ ., def.train)
predval <- predict(mod3, def.test)$class
actual <- def.test$default
mean(predval==actual)
```

```
## [1] 0.9705
```

Example: Default Data Confusion Matrix

```
table(predval, actual)
```

```
##         actual
## predval   No  Yes
##      No  1929   58
##      Yes    1   12
```

- Overall error is low (approx 3%).
- But, only 3/3% of those in the training data defaulted, so a model that predicted *no default* would have a very low overall error rate.
- Also, error rate is very high among people who actually defaulted!
    - The model correctly identified only 17% (12/70) of the people who defaulted.

Error Rates

Why does this happen? Consider the two-class case.

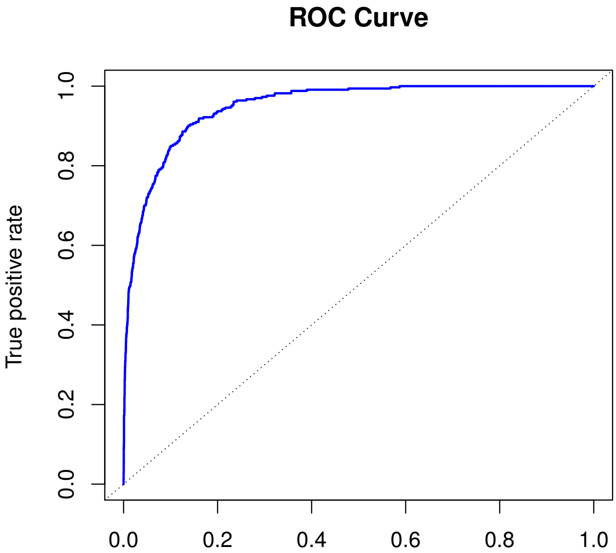
- Bayes classifier - which LDA approximates - has lowest *overall* error rate.
- The classifier assigns to the posterior probability which is greatest.
- It will assign to *default* if $P(\text{default} = \text{Yes}|X = x) > 0.5$.
  - But if only 3% of people default, this can be a pretty high threshold to reach!
- It is also possible to change these assignments, e.g., assign to *default* if $P(\text{default} = \text{Yes}|X = x) > 0.2$.
  - ... but this will come with a trade off in accuracy of assigning people to *not default*.

ROC Curves

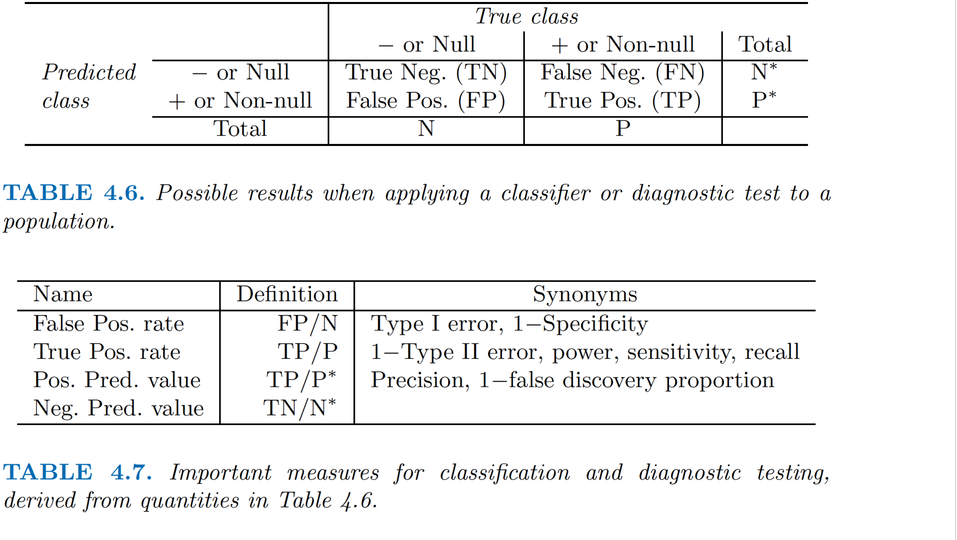
Receiver Operating Characteristics curves display the relationship between false positive rate and true positive rate, which vary with different probability thresholds.

- Classifier performance over all possible thresholds can be summarized by ROC area under the curve (AUC).
- Ideal ROC curves hug the top left corner.
- The true positive rate is referred to as *sensitivity*.
- The false positive rate is $1-$ *specificity*.
  - (I.e., specificity is the true negative rate.)

ROC Curves



Model Performance and Misclassification



		True class		
		− or Null	+ or Non-null	Total
Predicted class	− or Null	True Neg. (TN)	False Neg. (FN)	N*
	+ or Non-null	False Pos. (FP)	True Pos. (TP)	P*
	Total	N	P	

TABLE 4.6. *Possible results when applying a classifier or diagnostic test to a population.*

Name	Definition	Synonyms
False Pos. rate	FP/N	Type I error, 1−Specificity
True Pos. rate	TP/P	1−Type II error, power, sensitivity, recall
Pos. Pred. value	TP/P*	Precision, 1−false discovery proportion
Neg. Pred. value	TN/N*	

TABLE 4.7. *Important measures for classification and diagnostic testing, derived from quantities in Table 4.6.*