Classification Methods
LDA & QDA

ISLR Chapter 4 – Part II

Linear Discriminant Analysis (LDA) &

Quadratic Discriminant Analysis (QDA)

Outline

- Overview of LDA
- Why not Logistic Regression?
- Estimating Bayes' Classifier
- LDA Example with One Predictor (p=1)
- LDA Example with more than One Predictor (P>1)
- LDA on Default Data
- Overview of QDA
- Comparison between LDA and QDA

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Linear Discriminant Analysis

LDA undertakes the same task as Logistic Regression.

It classifies data based on categorical variables

- Making profit or not
- Buy a product or not
- Satisfied customer or not
- Political party voting intention

Why Linear? Why Discriminant?

LDA involves the determination of linear equation

- **(just like linear regression)**
- **that will predict which group the case belongs to.**

$$D = v_1 X_1 + v_2 X_2 + \ldots + v_i X_i + a$$

- *D*: discriminant function
- [illegible] : discriminant coefficient or weight for the variable
- *X*: variable
- *a*: constant

Purpose of LDA

Choose the ⊏ ’s in a way

- **to maximize the distance between the means of different categories**

Good predictors tend to have large ⊏ ’s (weight)

We want to discriminate between the different categories

Think of food recipe.

Changing the proportions (weights) of the ingredients

- **will change the characteristics of the finished cakes.**
- **Hopefully that will produce different types of cake!**

Assumptions of LDA

The observations are a random sample

Each predictor variable is normally distributed

Why not Logistic Regression?

Logistic regression is unstable

- **when the classes are well separated**

In the case where n is small,

- **and the distribution of predictors X is approximately normal,**
- **then LDA is more stable than Logistic Regression**

LDA is more popular

- **when we have more than two response classes**

Bayes' Classifier

Bayes' Classifier is the golden standard.

- **Unfortunately, it is unattainable.**

So far, we have estimated it with two methods:

- KNN classifier
- Logistic Regression

Naïve Bayes' Classifier

Naive Bayes is a simple technique for constructing classifiers:

- models that assign class labels to problem instances,
- represented as vectors of feature values,
- where the class labels are drawn from some finite set.

There is not a single algorithm for training such classifiers, but a family of algorithms based on a common principle:

- all naive Bayes classifiers assume that the value of a particular feature
- is independent of the value of any other feature, given the class variable.

For example, a fruit may be considered to be an apple if it is red, round, and about 10 cm in diameter.

A naive Bayes classifier considers each of these features to contribute independently to the probability that this fruit is an apple, regardless of any possible correlations between the color, roundness, and diameter features.

For some types of probability models, naive Bayes classifiers can be trained very efficiently in a supervised learning setting. In many practical applications, parameter estimation for naive Bayes models uses the method of maximum likelihood; in other words, one can work with the naive Bayes model without accepting Bayesian probability or using any Bayesian methods.

Despite their naive design and apparently oversimplified assumptions, naive Bayes classifiers have worked quite well in many complex real-world situations.

In 2004, an analysis of the Bayesian classification problem showed that there are sound theoretical reasons for the apparently implausible efficacy of naive Bayes classifiers. Still, a comprehensive comparison with other classification algorithms in 2006 showed that Bayes classification is outperformed by other approaches, such as boosted trees or random forests.

An advantage of naive Bayes is that it only requires a small number of training data to estimate the parameters necessary for classification

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Estimating Bayes' Classifier

With Logistic Regression

- **we modeled the probability of Y being from the kth class as**

$$p(X) = \Pr(Y = k|X = x) = \frac{e^{\beta_0+\beta_1 X}}{1 + e^{\beta_0+\beta_1 X}}.$$

- However, Bayes' Theorem states

$$p(X) = \Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}.$$

π_k : Probability of coming from class k (prior probability)

$f_k(x)$: Density function for X given that X is an observation from class k

Estimate π_k and $f_k(x)$

- We can estimate π_k and $f_k(x)$ to compute $p(X)$
- The most common model for $f_k(x)$ is the Normal Density

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}(x-\mu_k)^2\right)$$

- Using the density, we only need to estimate three quantities to compute $p(X)$

$$\mu_k \qquad \sigma_k^2 \qquad \pi_k$$

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Use Training Data set for Estimation

- The mean μ_k could be estimated by the average of all training observations from the kth class.
- The variance σ_k^2 could be estimated as the weighted average of variances of all k classes.
- And, π_k is estimated as the proportion of the training observations that belong to the kth class.

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i$$

$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2$$

$$\hat{\pi}_k = n_k/n.$$

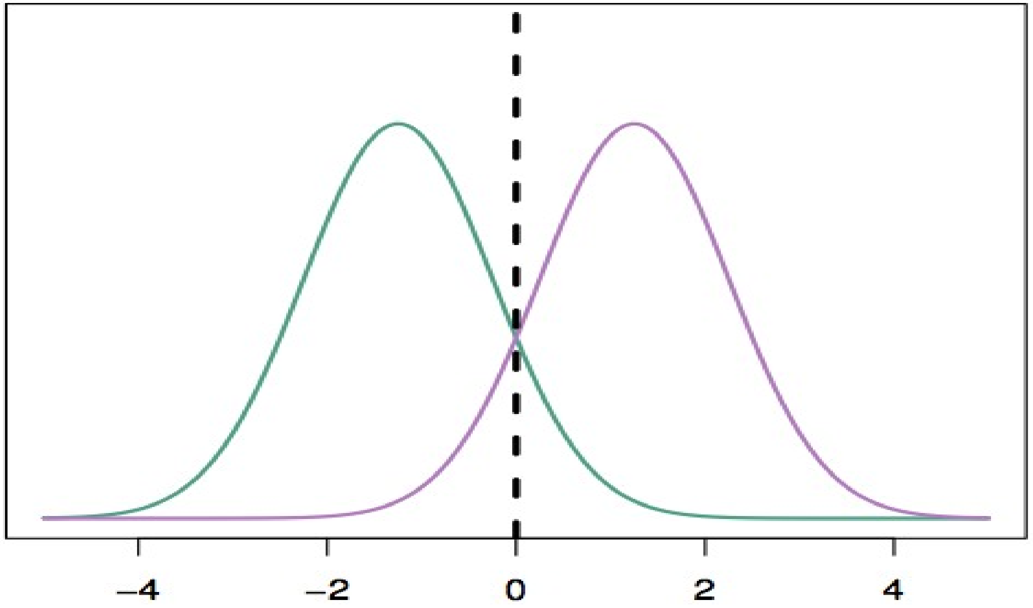
A Simple Example with One Predictor (*p* =1)

Suppose we have only one predictor (*p* = 1)

Two normal density function $f_1(x)$ and $f_2(x)$, represent two distinct classes

The two density functions overlap, so there is some uncertainty about the class to which an observation with an unknown class belongs

The dashed vertical line represents Bayes' decision boundary



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Apply LDA

LDA starts by assuming that each class

- has a normal distribution with a common variance

The mean and the variance are estimated

Finally, Bayes' theorem is used to compute p_k

- and the observation is assigned to the class
- with the maximum probability
- among all k probabilities

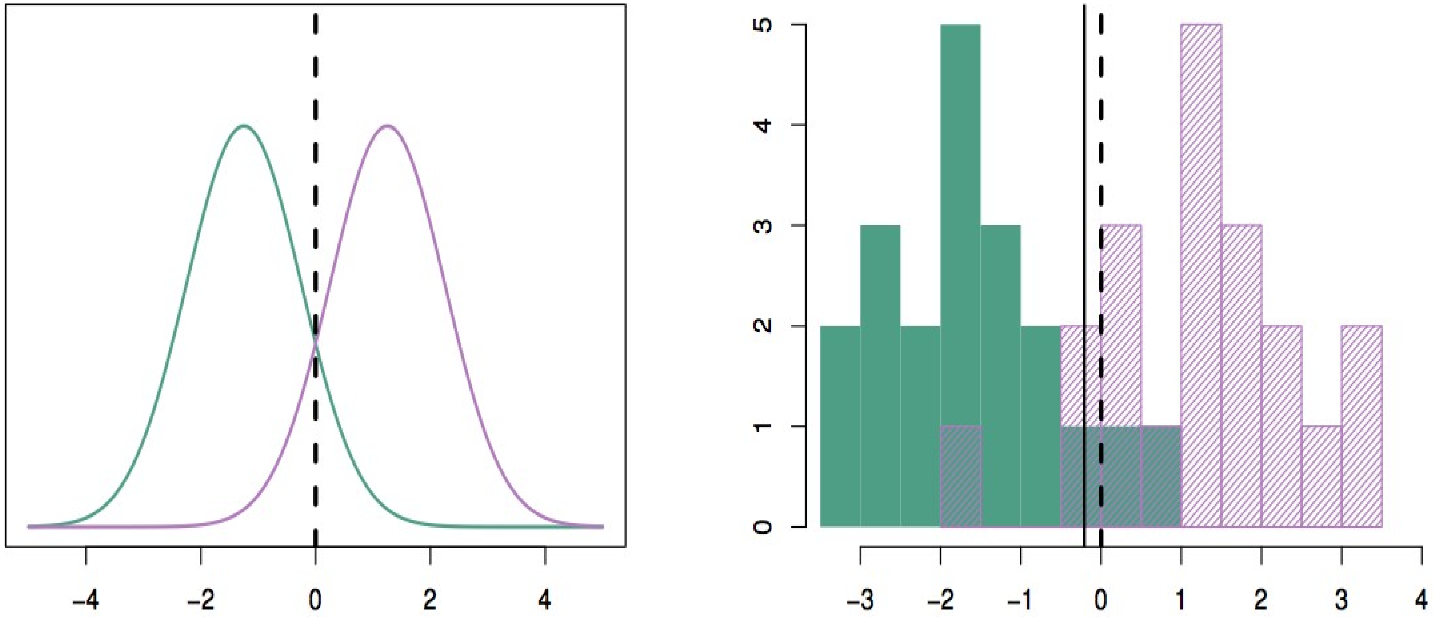
20 observations were drawn from each of the two classes

The dashed vertical line is the Bayes’ decision boundary

The solid vertical line is the LDA decision boundary

- Bayes’ error rate: 10.6%
- LDA error rate: 11.1%

Thus, LDA is performing pretty well!



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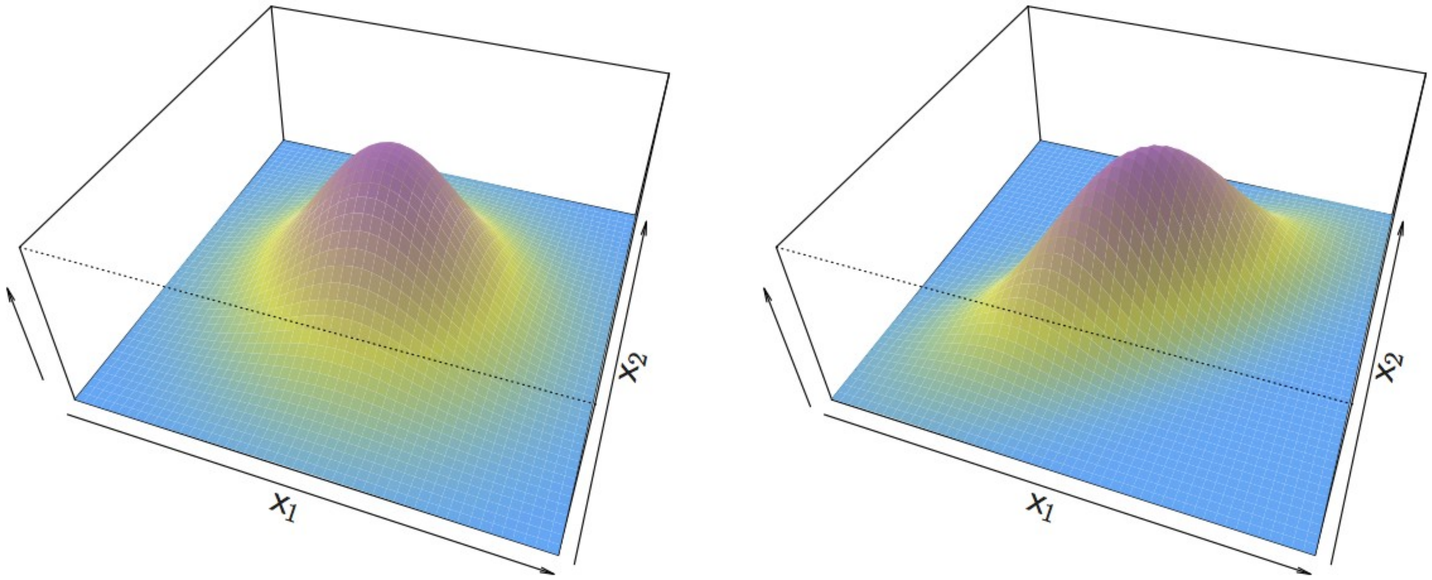
An Example When *p* > 1

If *X* is multidimensional (*p* > 1),

- **we use exactly the same approach**
- **except the density function *f(x)* is modeled**
  - using the multivariate normal density



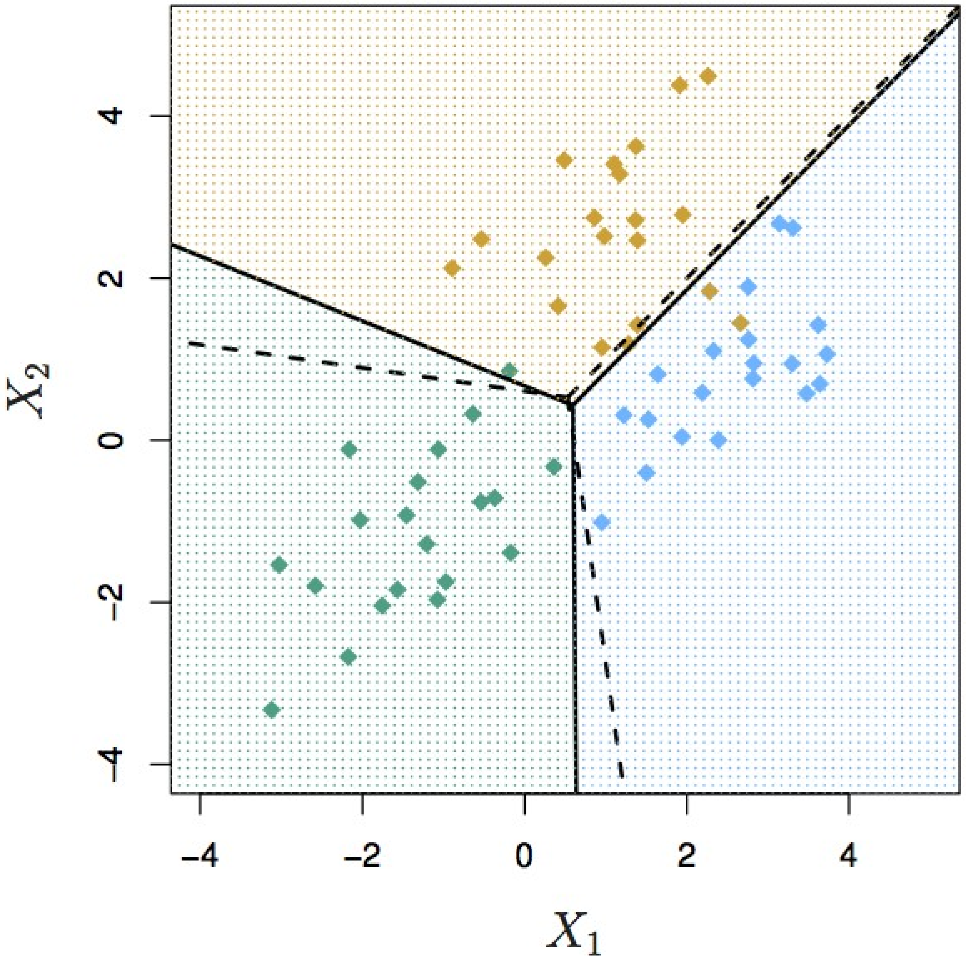
We have two predictors (*p* = 2)

Three classes

20 observations were generated from each class

The solid lines are Bayes' boundaries

The dashed lines are LDA boundaries



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Running LDA on Default Data

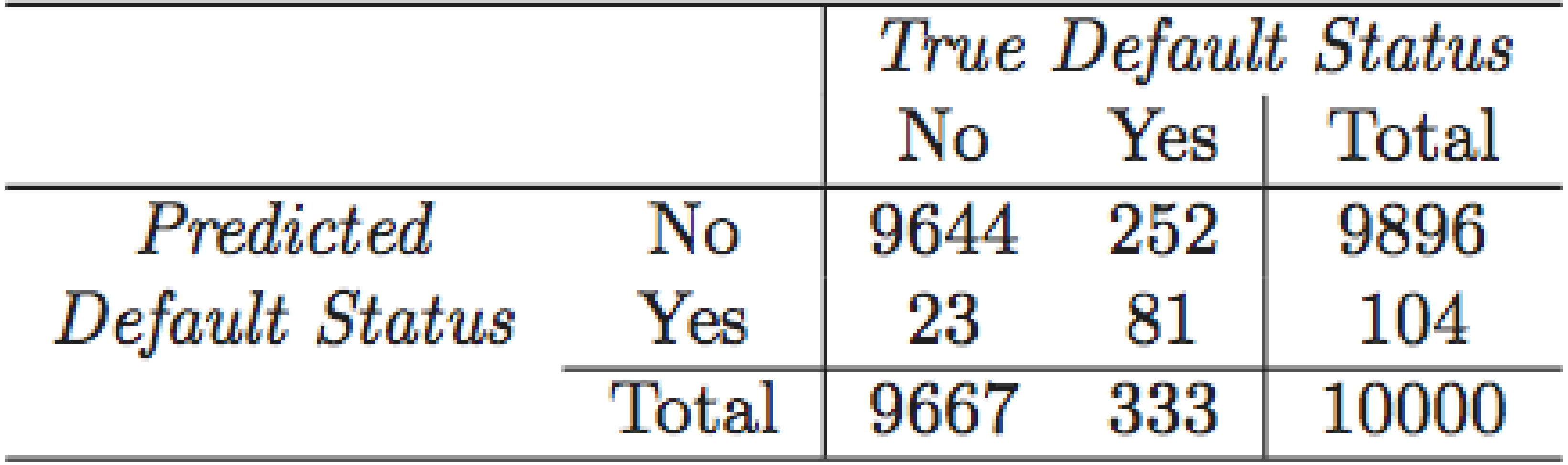
LDA makes 252+ 23 mistakes on 10000 predictions

- **(2.75% misclassification error rate)**

But LDA miss-predicts 252/333 = 75.5% of defaulters!

Perhaps, we shouldn’t use 0.5

- **as threshold for predicting default?**



		True Default Status		
		No	Yes	Total
Predicted	No	9644	252	9896
Default Status	Yes	23	81	104
	Total	9667	333	10000

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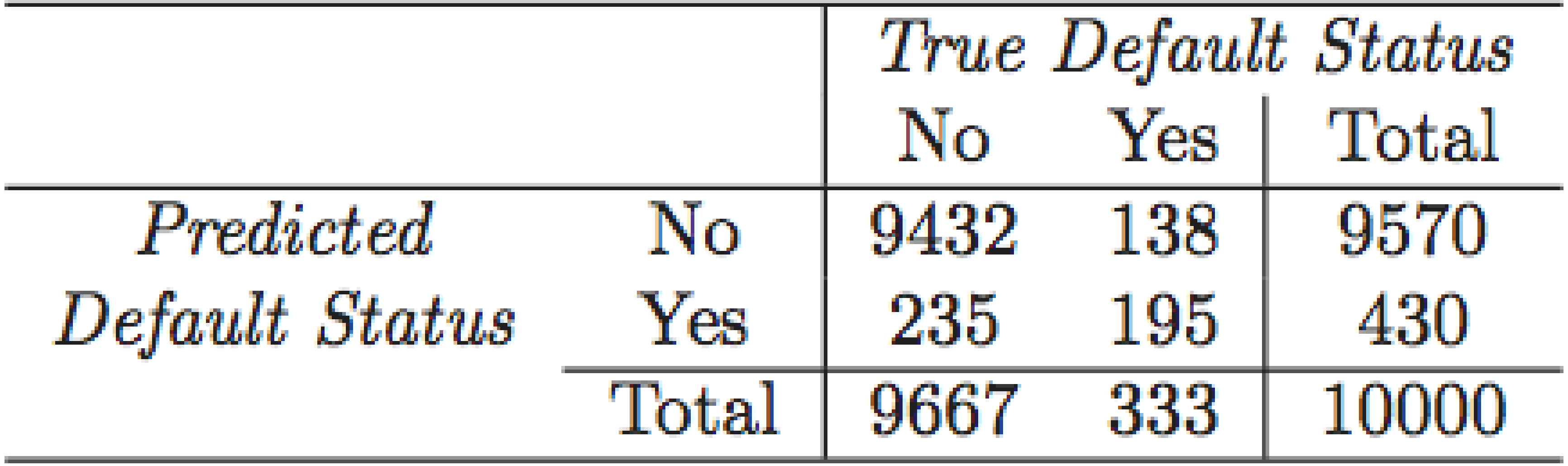
Use 0.2 as Threshold for Default

Now the total number of mistakes is 235+138 = 373

- (3.73% misclassification error rate)

But we only miss-predicted 138/333 = 41.4% of defaulters

We can examine the error rate with other thresholds



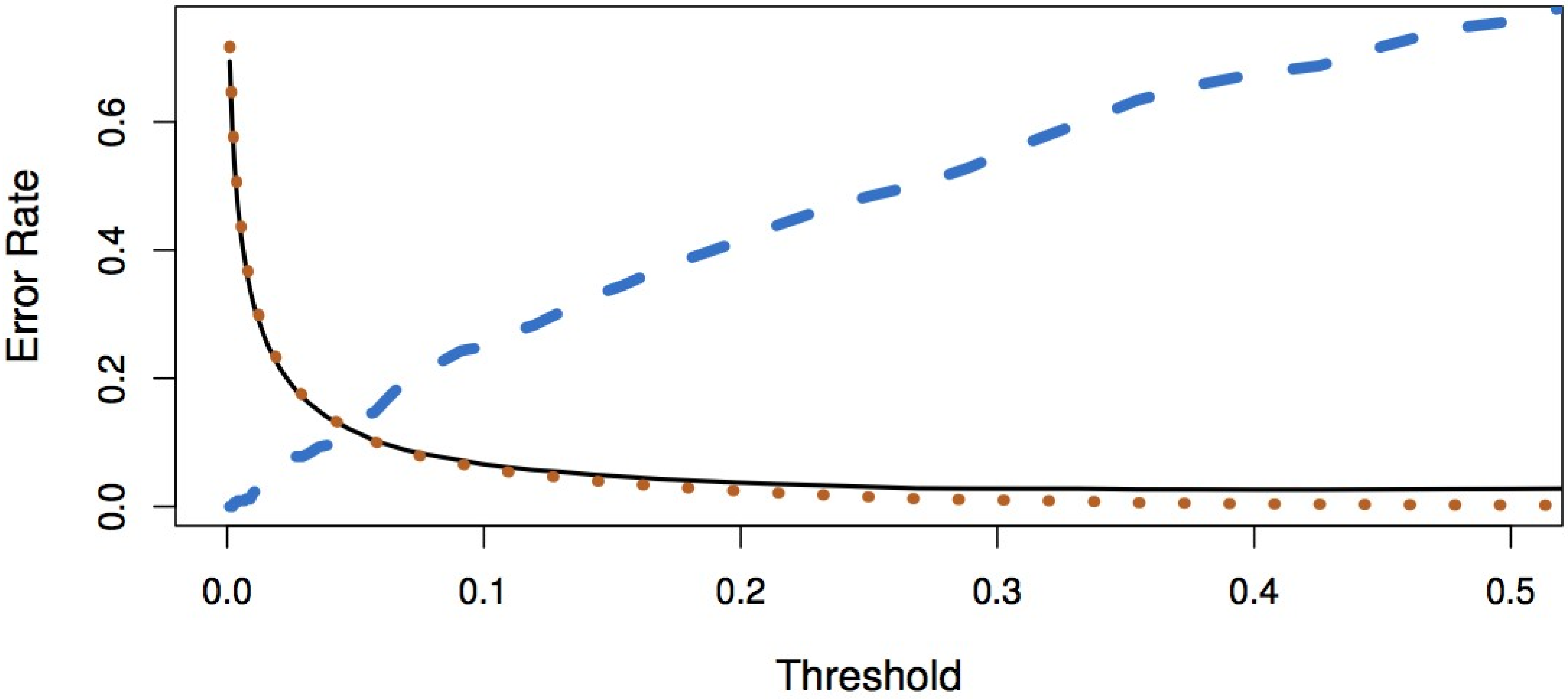
		True Default Status		
		No	Yes	Total
Predicted Default Status	No	9432	138	9570
	Yes	235	195	430
	Total	9667	333	10000

Default Threshold Values vs. Error Rates

Black solid: overall error rate

Blue dashed: Fraction of defaulters missed

Orange dotted: non defaulters incorrectly classified



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Quadratic Discriminant Analysis (QDA)

LDA assumed

- that every class has the same variance/ covariance

However, LDA may perform poorly

- if this assumption is far from true

QDA works identically as LDA

- except that it estimates separate variances/ covariance for each class

Which is better? LDA or QDA?

Since QDA allows for different variances among classes,

- **the resulting boundaries become quadratic**

Which approach is better: LDA or QDA?

- QDA will work best

  when the variances are very different between classes

  and we have enough observations to accurately estimate the variances

- LDA will work best

  when the variances are similar among classes

  or we don’t have enough data to accurately estimate the variances

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Comparing LDA to QDA

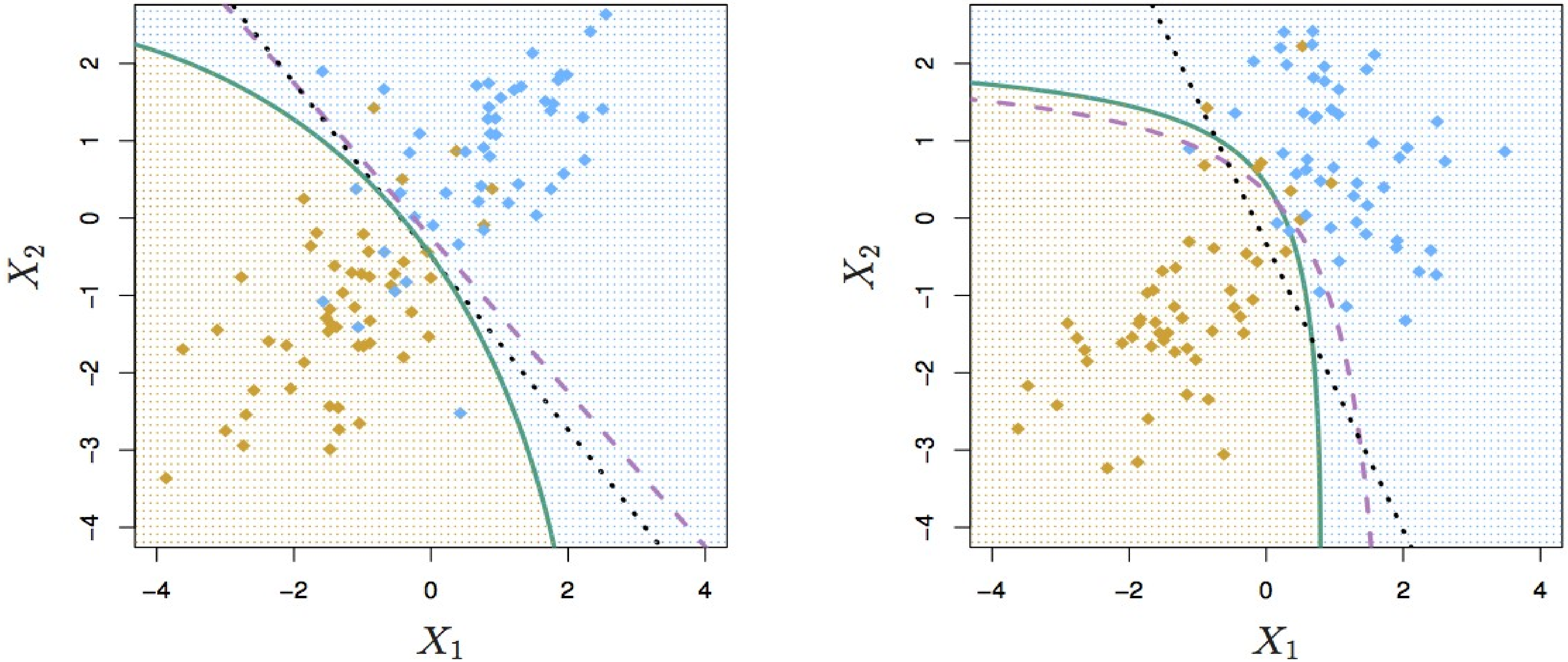
Black dotted: LDA boundary

Purple dashed: Bayes' boundary

Green solid: QDA boundary

Left: variances of the classes are equal (LDA is better fit)

Right: variances of the classes are not equal (QDA is better fit)



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Comparison of Classification Methods

KNN (Chapter 2)

Logistic Regression (Chapter 4)

LDA (Chapter 4)

QDA (Chapter 4)

Logistic Regression vs. LDA

Similarity:

- **Both Logistic Regression and LDA produce linear boundaries**

Difference:

- **LDA assumes that the observations are drawn from the normal distribution**
  - with common variance in each class,
  - while logistic regression does not have this assumption.
- **LDA would do better than Logistic Regression**
  - if the assumption of normality hold,
  - otherwise logistic regression can outperform LDA

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KNN vs. (LDA and Logistic Regression)

KNN takes a completely different approach

KNN is completely non-parametric:

- **No assumptions are made about the shape of the decision boundary!**

Advantage of KNN: We can expect KNN to dominate both LDA and Logistic Regression

- **when the decision boundary is highly non-linear**

Disadvantage of KNN: KNN does not tell us

- **which predictors are important (no table of coefficients)**

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QDA vs. (LDA, Logistic Regression, and KNN)

QDA is a compromise

- **between non-parametric KNN method**
- **and the linear LDA and logistic regression**

If the true decision boundary is:

- Linear: LDA and Logistic outperforms
- Moderately Non-linear: QDA outperforms
- More complicated: KNN is superior

LDA and QDA

Classification

Info from Wikipedia

https://en.wikipedia.org/wiki/Linear_discriminant_analysis

Discriminant Analysis, in comparison with other approaches

Linear discriminant analysis (LDA), is a generalization of Fisher's linear discriminant,

- a method used to find a linear combination of features that characterizes or separates two or more classes of objects or events.
- The resulting combination may be used as a linear classifier,
    - or, more commonly, for dimensionality reduction before later classification.

LDA is closely related to analysis of variance (ANOVA) and regression analysis, which also attempt to express one dependent variable as a linear combination of other features or measurements.

- However, ANOVA uses categorical independent variables and a continuous dependent variable,
- Whereas discriminant analysis has continuous independent variables and a categorical dependent variable (i.e. the class label).
- Logistic regression are more similar to LDA than ANOVA is,
    - as they also explain a categorical variable by the values of continuous independent variables.

These other methods are preferable in applications

- where it is not reasonable to assume that the independent variables are normally distributed,
- which is a fundamental assumption of the LDA method.

LDA is also closely related to principal component analysis (PCA) and factor analysis

- in that they both look for linear combinations of variables which best explain the data.
- LDA explicitly attempts to model the difference between the classes of data.
- PCA, in contrast, does not take into account any difference in class, and
- Factor analysis builds the feature combinations based on differences rather than similarities.

Discriminant analysis is also different from factor analysis in that it is not an interdependence technique:

- a distinction between independent variables and dependent variables (also called criterion variables) must be made.

LDA works when the measurements made on independent variables for each observation are continuous quantities.

Discriminant analysis is used when groups are known a priori (unlike in cluster analysis).

- Each case must have a score on one or more quantitative predictor measures, and a score on a group measure.[7]
- In simple terms, discriminant function analysis is classification
    - the act of distributing things into groups, classes or categories of the same type.

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