

# Classification

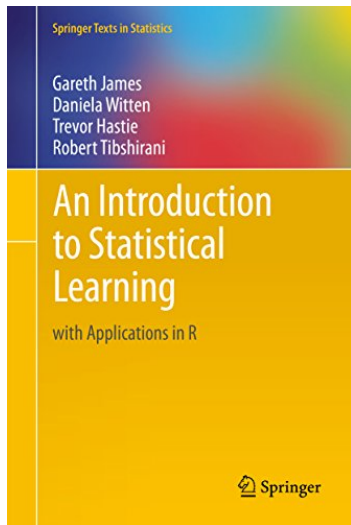
chapter 4 of *An Introduction to Statistical Learning* (ISL)

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# What we read (long description)



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Now in a shorter way

## What we read (short description)

At chapter 4 are discussed three of the most widely-used classifiers.

- » Logistic Regression
- » Linear Discriminant Analysis (LDA)
- » Quadratic Discriminant Analysis (QDA)

## What we didn't read

More computer-intensive methods are discussed in later chapters, such as

- » Generalized Additive Models (GAM)
- » Trees
- » Random Forests
- » Boosting
- » Support Vector Machines (SVM)

# On the Agenda

## 1 Why Not Linear Regression?

### 2 A typical dataset

### 3 Logistic Regression

- The model framework
- Estimating the Regression Coefficients

### 4 Linear Discriminant Analysis (LDA)

- To start... why do we need something different?

- LDA in a nutshell

- Living in a simple and *normal* world

- Now, with more than one predictor

- Some important details

### 5 Quadratic Discriminant Analysis (QDA)

### 6 Main remarks

We could consider encoding the response,  $Y$ , as a quantitative variable, e.g.,

Predict the medical condition of a patient on the basis of her symptoms.

$$Y = \begin{cases} 1 & \text{if stroke;} \\ 2 & \text{if drug overdose;} \\ 3 & \text{if epileptic seizure.} \end{cases}$$

We could consider encoding the response,  $Y$ , as a quantitative variable, e.g.,

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Unfortunately, this coding implies an ordering on the outcomes.

Each possible coding would produce a fundamentally different linear model that would ultimately lead to different sets of predictions.

## This leads us to other questions,

- » What if the response variable values did take on a **natural ordering**, such as **mild**, **moderate**, and **severe**?
- » For a **binary** (two level) qualitative response, the situation is **better**.
  - » **However**, if we use linear regression, some of our estimates might be **outside** the **[0, 1] interval**.
  - » **However**, the **dummy variable approach** cannot be easily extended to accommodate qualitative responses with more than two levels.



## This leads us to other questions,

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- » For a **binary** (two level) qualitative response, the situation is **better**.
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  - » **However**, the **dummy variable approach** cannot be easily extended to accommodate qualitative responses with more than two levels.

For these reasons, it is preferable to use a classification method that is truly suited for qualitative response values, such as the ones presented next.

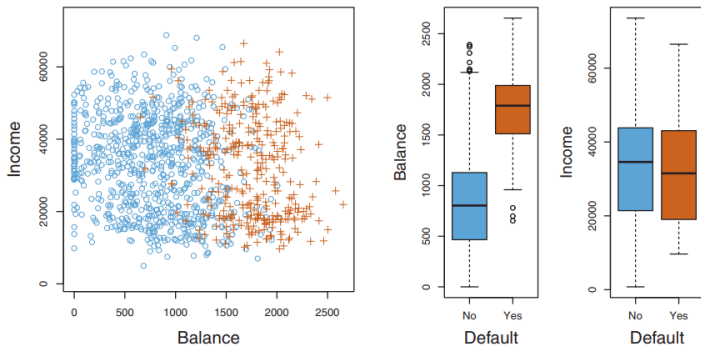
Curiously,

it turns out that the classifications that we get if we use **linear regression** to predict a binary response will be **the same** as for the linear discriminant analysis (**LDA**) procedure we discuss later.

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## A classic 'book example dataset relationship'



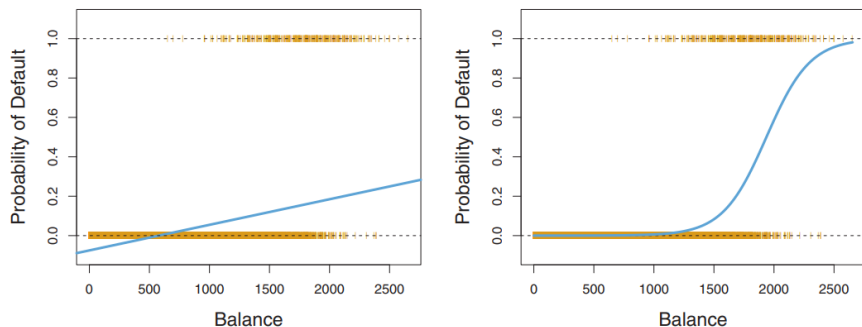
**FIGURE 4.1.** *The Default data set. Left: The annual incomes and monthly credit card balances of a number of individuals. The individuals who defaulted on their credit card payments are shown in orange, and those who did not are shown in blue. Center: Boxplots of balance as a function of default status. Right: Boxplots of income as a function of default status.*

... a very pronounced relationship between **balance** and **default**.

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# To start, a comparison with Linear Regression



**FIGURE 4.2.** Classification using the `Default` data. Left: Estimated probability of `default` using linear regression. Some estimated probabilities are negative! The orange ticks indicate the 0/1 values coded for `default` (No or Yes). Right: Predicted probabilities of `default` using logistic regression. All probabilities lie between 0 and 1.

*Logistic regression in two slides*

# Some math, but with just one predictor

## The model and its relations

$$p(X) = \underbrace{\frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}}_{\substack{\text{logistic} \\ \text{function} \\ \text{(S-shaped)}}} \Rightarrow \underbrace{\frac{p(X)}{1 - p(X)}}_{\text{odds} \in (0, \infty)} = e^{\beta_0 + \beta_1 X} \Rightarrow \underbrace{\log \frac{p(X)}{1 - p(X)}}_{\substack{\text{log-odds} \\ \text{or} \\ \text{logit}}} = \beta_0 + \beta_1 X$$

For example,

$$p(X) = 0.2 \Rightarrow \frac{0.2}{1 - 0.2} = \frac{1}{4} \quad \text{and} \quad p(X) = 0.9 \Rightarrow \frac{0.9}{1 - 0.9} = 9.$$

## Maximum likelihood

The estimates  $\hat{\beta}_0$  and  $\hat{\beta}_1$  are chosen to **maximize** a math equation called a

*likelihood function*

$$l(\beta_0, \beta_1) = \prod_{i:y_i=1} p(x_i) \prod_{i':y_{i'}=0} (1 - p(x_{i'})).$$

The coefficients  $\hat{\beta}_0$  and  $\hat{\beta}_1$  are unknown, and must be estimated. The general method of **maximum likelihood** is preferred, since it has better statistical properties.

Maximum likelihood is a very general approach that is used to fit many of the non-linear models examined throughout the book. In the linear regression setting, the least squares approach is in fact a special case of maximum likelihood.



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Different ideas, sometimes the same results

Different ideas,

Logistic REGRESSION :  $\mathbb{P}[Y = k | X = x]$  vs. LINEAR DISCRIMINANT ANALYSIS :  $\mathbb{P}[X = x | Y = k]$   
 via, logistic function via BAYES' THEOREM

With **LDA** we model the distribution of the predictors  $X$  separately in each of the response classes (i.e. given  $Y$ ), and then use Bayes' theorem to flip these around into estimates for  $\mathbb{P}[Y = k | X = x]$ .

## Different ideas,

Handwritten text comparing Logistic Regression and Linear Discriminant Analysis. On the left, 'LOGISTIC REGRESSION' is written in blue, followed by a red bracket under the expression  $\mathbb{P}[Y = k | X = x]$ . Below this bracket, it says 'VIA, logistic function'. In the center, 'vs.' is written in red. On the right, 'LINEAR DISCRIMINANT ANALYSIS' is written in blue, followed by a red bracket under the expression  $\mathbb{P}[X = x | Y = k]$ . Below this bracket, it says 'VIA BAYES' THEOREM'.

With **LDA** we model the distribution of the predictors  $X$  separately in each of the response classes (i.e. given  $Y$ ), and then use Bayes' theorem to flip these around into estimates for  $\mathbb{P}[Y = k | X = x]$ .

## Sometimes the same results

When these distributions are **assumed** to be **normal**, it turns out that the model is very similar in form to **logistic regression**.

But, ok... why not continue with logistic regression?

## But, ok... why not continue with logistic regression?

Simple, **LDA** is popular when we have more than two response classes.

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Now, a reason more serious: **stability**

- » When the classes are well-separated, the parameter estimates for the **logistic regression** model are surprisingly unstable. **LDA** does not suffer from this problem.
- » If  $n$  is small and the distribution of the predictors  $X$  is approximately **normal** in each of the classes, the **linear discriminant** model is again more stable than the **logistic regression** model.

# Model framework

$$\underbrace{P_k(X)}_{\text{POSTERIOR}} = \mathbb{P}[Y=k | X=x] = \frac{\overbrace{\pi_k}^{\text{PRIOR DENSITY}} \overbrace{f_k(x)}^{\text{FN}}}{\sum_{L=1}^K \pi_L f_L(x)}, \text{ with } f_k(x) = \mathbb{P}[X=x | Y=k]$$

- »  $\pi_k$  is the overall or **prior** prob. that a chosen obs. comes from  $k$ .
- » In general, estimating  $\pi_k$  is easy if we have a sample of  $Y$ s: we simply compute the fraction of observations that belong to the  $k$ th class. However, estimating  $f_k(x)$  tends to be more challenging, unless we assume some simple forms for these densities.

**Remember from Chap. 2** that the **Bayes classifier** has the lowest possible error rate out of all classifiers.

## Dealing with just one predictor

**Assumptions:**  $f_k(x)$  is normal with equal variance for the  $k$ th classes.

BAYES CLASSIFIER

$$p_k(x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^K \pi_l f_l(x)}$$

$\sim \mathcal{N}(\mu_k, \sigma_k^2)$

$\Rightarrow \delta_k(x) = x \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log \pi_k$

with SOME SIMPLE STEPS

$\sim \mathcal{N}(\mu_l, \sigma_l^2)$

$\sigma_k^2 = \sigma_l^2$

if  $k=2 \wedge \pi_1 = \pi_2$

BAYES DECISION

boundary:  $x = \frac{\mu_1 + \mu_2}{2}$

Putting a **hat** (simple average and a weighted average of the sample variances for each class) in everything, the **LDA approx.** this **Bayes classifier.**



Ok, nice! But... why the name **linear discriminant analysis**?

The word **linear** stems from the fact that the **discriminant functions**  $\hat{\delta}_k(x)$  are linear functions of  $x$ .

That is, the **LDA** decision rule depends on  $x$  only through a **linear combination** of its elements.

---

Ok, nice! But... why the name **linear discriminant analysis**?

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That is, the **LDA** decision rule depends on  $x$  only through a **linear combination** of its elements.

---

**LDA** is trying to **approximate** the **Bayes classifier**, which has the **lowest** total **error rate** out of all classifiers (if the Gaussian model is correct).

## Getting bigger

More than one predictor  $\Rightarrow$  Multivariate normal distribution,  
with a class-specific mean vector  
and a common covariance matrix

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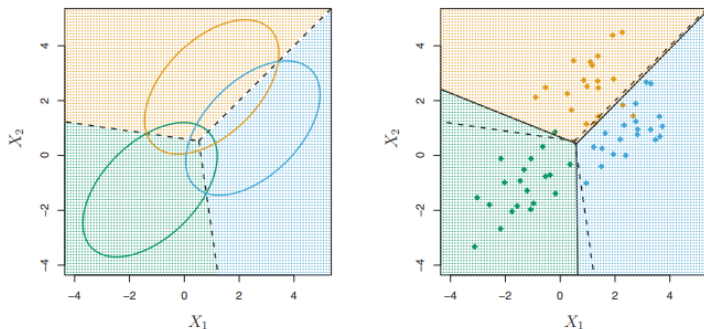
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$$f(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_k)^\top \Sigma^{-1} (x - \mu_k) \right\}$$



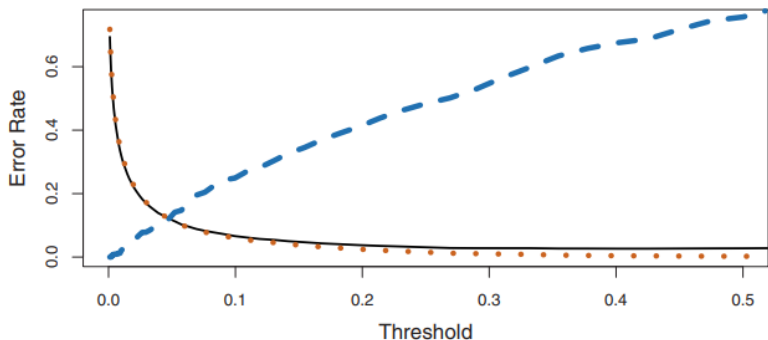
$$\hat{\delta}_k(x) = x^\top \hat{\Sigma}^{-1} \hat{\mu}_k - \frac{1}{2} \hat{\mu}_k^\top \hat{\Sigma}^{-1} \hat{\mu}_k + \log \hat{\pi}_k$$

## An example



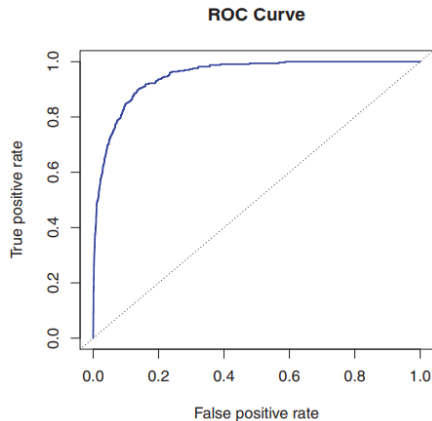
**FIGURE 4.6.** An example with three classes. The observations from each class are drawn from a multivariate Gaussian distribution with  $p = 2$ , with a class-specific mean vector and a common covariance matrix. Left: Ellipses that contain 95 % of the probability for each of the three classes are shown. The dashed lines are the Bayes decision boundaries. Right: 20 observations were generated from each class, and the corresponding LDA decision boundaries are indicated using solid black lines. The Bayes decision boundaries are once again shown as dashed lines.

Ok, and about what else do we need to talk? (1/2)



**FIGURE 4.7.** For the **Default** data set, error rates are shown as a function of the threshold value for the posterior probability that is used to perform the assignment. The black solid line displays the overall error rate. The blue dashed line represents the fraction of defaulting customers that are incorrectly classified, and the orange dotted line indicates the fraction of errors among the non-defaulting customers.

## Ok, and about what else do we need to talk? (2/2)



**FIGURE 4.8.** A ROC curve for the LDA classifier on the `Default` data. It traces out two types of error as we vary the threshold value for the posterior probability of default. The actual thresholds are not shown. The true positive rate is the sensitivity: the fraction of defaulters that are correctly identified, using a given threshold value. The false positive rate is  $1 - \text{specificity}$ : the fraction of non-defaulters that we classify incorrectly as defaulters, using that same threshold

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Unlike LDA, QDA assumes that each class has its own covariance matrix. Under this assumption, the approximation of the Bayes classifier becomes

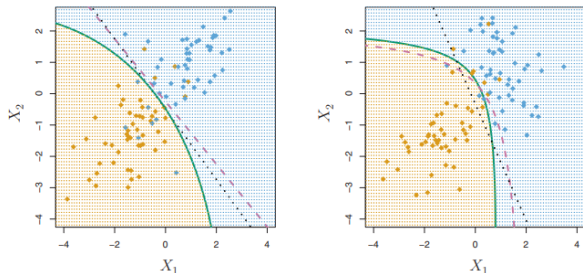
$$\text{QLA: } \hat{\delta}_k(x) = -\frac{1}{2}(x - \hat{\mu}_k)^\top \hat{\Sigma}_k^{-1}(x - \hat{\mu}_k) - \frac{1}{2} \log |\hat{\Sigma}_k| + \log \hat{\pi}_k.$$

$x$  appears as a quadratic function, this is where QDA gets its name.

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$x$  appears as a quadratic function, this is where QDA gets its name.



**FIGURE 4.9.** Left: The Bayes (purple dashed), LDA (black dotted), and QDA (green solid) decision boundaries for a two-class problem with  $\Sigma_1 = \Sigma_2$ . The shading indicates the QDA decision rule. Since the Bayes decision boundary is linear, it is more accurately approximated by LDA than by QDA. Right: Details are as given in the left-hand panel, except that  $\Sigma_1 \neq \Sigma_2$ . Since the Bayes decision boundary is non-linear, it is more accurately approximated by QDA than by LDA.

## Ok, but... in practice, what's the difference?

Why does it matter whether or not we assume that the  $K$  classes share a common covariance matrix?

The answer lies in the bias-variance trade-off.

When there ARE  $P$  predictors

$\rightarrow$  LDA:  $KP$

$\rightarrow$  QDA:  $K \frac{P(P+1)}{2}$

} PARAMETERS to estimate

$\Rightarrow$  LDA IS MUCH LESS FLEXIBLE THAN QDA

- LDA LOWER VARIANCE
- QDA LOWER BIAS

} NO FREE LUNCH.

## Concluding...

LDA tends to be a better bet than QDA if there are relatively few observations and so reducing variance is crucial.

In contrast, QDA is recommended if the data set is very large, so that the variance of the classifier is not a major concern, or if the assumption of a common covariance matrix for the  $K$  classes is clearly untenable.

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- » The **logistic regression** and **LDA** methods are **closely connected**, since both produce **linear decision boundaries**.

To make a nicer comparison, we may mention the **KNN**.

- » **KNN** is a completely **non-parametric** approach: no assumptions are made about the shape of the decision boundary. Nevertheless, **KNN** does not tell us which predictors are important.
- 

- » When the true **decision boundaries** are **linear**, the **LDA** and **logistic regression** approaches will tend to perform well. When the boundaries are **moderately non-linear**, **QDA** may give better results. Finally, for much more **complicated decision boundaries**, a non-parametric approach such as **KNN** can be superior. But the level of smoothness for a non-parametric approach must be chosen carefully.

and...



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