

Classification

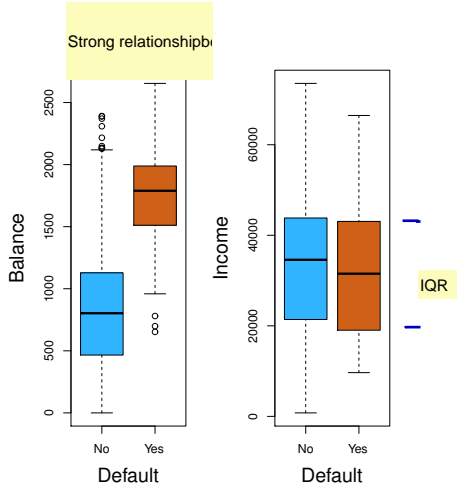
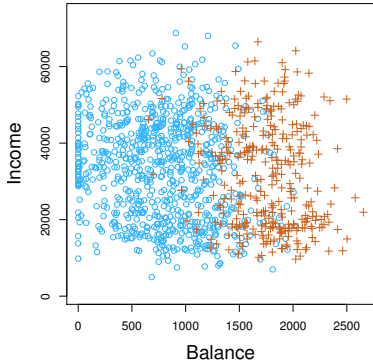
- Qualitative variables take values in an unordered set \mathcal{C} , such as:
 $\text{eye color} \in \{\text{brown}, \text{blue}, \text{green}\}$
 $\text{email} \in \{\text{spam}, \text{ham}\}.$
- Given a feature vector X and a qualitative response Y taking values in the set \mathcal{C} , the classification task is to build a function $C(X)$ that takes as input the feature vector X and predicts its value for Y ; i.e. $C(X) \in \mathcal{C}$.
- Often we are more interested in estimating the *probabilities* that X belongs to each category in \mathcal{C} .

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For example, it is more valuable to have an estimate of the probability that an insurance claim is fraudulent, than a classification fraudulent or not.

Example: Credit Card Default



- Question: Will person default on credit card payment, Y/N? - Plot

- Outliers (typically): - lower than $(Q1 - 1.5IQR)$ or - higher

Can we use Linear Regression?

Suppose for the **Default** classification task that we code

$$Y = \begin{cases} 0 & \text{if No} \\ 1 & \text{if Yes.} \end{cases}$$

Can we simply perform a linear regression of Y on X and classify as **Yes** if $\hat{Y} > 0.5$?

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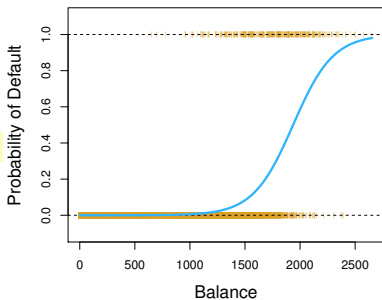
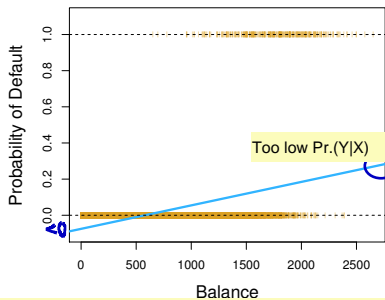
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- In this case of a binary outcome, linear regression does a good job as a classifier, and is equivalent to *linear discriminant analysis* which we discuss later.
- Since in the population $E(Y|X = x) = \Pr(Y = 1|X = x)$, we might **think** that regression is perfect for this task.
- However, *linear* regression might produce probabilities less than zero or bigger than one. *Logistic regression* is more appropriate.

Linear versus Logistic Regression



$\hat{Pr} < 0$ is not at good estimate of probability

The orange marks indicate the response Y , either 0 or 1. Linear regression does not estimate $\Pr(Y = 1|X)$ well. Logistic regression seems well suited to the task.

Linear Regression continued

Now suppose we have a response variable with three possible values. A patient presents at the emergency room, and we must classify them according to their symptoms.

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

This coding suggests an ordering, and in fact implies that the difference between **stroke** and **drug overdose** is the same as between **drug overdose** and **epileptic seizure**.

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Linear regression is not appropriate here. **either**
Multiclass Logistic Regression or *Discriminant Analysis* are more appropriate.

Logistic Regression

Let's write $p(X) = \Pr(Y = 1|X)$ for short and consider using **balance** to predict **default**. Logistic regression uses the form

$$p(X) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}.$$

Transformation of our linear model

($e \approx 2.71828$ is a mathematical constant [Euler's number].)

It is easy to see that no matter what values β_0 , β_1 or X take, $p(X)$ will have values between 0 and 1.

If you are not convinced, try it out.

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Still we have two model parameters, β_0 and β_1 .

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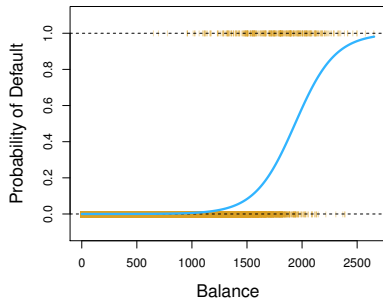
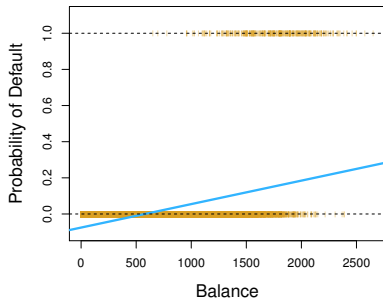
A bit of rearrangement gives

Name logistic comes from the transformation of the

$$\log \left(\frac{p(X)}{1 - p(X)} \right) = \beta_0 + \beta_1 X.$$

This monotone transformation is called the *log odds* or *logit* transformation of $p(X)$.

Linear versus Logistic Regression



Logistic regression ensures that our estimate for $p(X)$ lies between 0 and 1.

Maximum Likelihood

We use maximum likelihood to estimate the parameters.

$$\ell(\beta_0, \beta) = \prod_{i:y_i=1} p(x_i) \prod_{i:y_i=0} (1 - p(x_i)).$$

This *likelihood* gives the probability of the observed zeros and ones in the data. We pick β_0 and β_1 to maximize the likelihood of the observed data.

Remember: $p(x) = \text{pr}(y=1 \mid x)$ We try to find B_0 and B_1 such that plugging these es

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Most statistical packages can fit linear logistic regression models by maximum likelihood. In **R** we use the **glm** function.

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-10.6513	0.3612	-29.5	< 0.0001
balance	0.0055	0.0002	24.9	< 0.0001

Making Predictions

What is our estimated probability of **default** for someone with a balance of \$1000?

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 X}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 X}} = \frac{e^{-10.6513 + 0.0055 \times 1000}}{1 + e^{-10.6513 + 0.0055 \times 1000}} = 0.006$$

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With a balance of \$2000?

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 X}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 X}} = \frac{e^{-10.6513 + 0.0055 \times 2000}}{1 + e^{-10.6513 + 0.0055 \times 2000}} = 0.586$$

Lets do it again, using **student** as the predictor.

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-3.5041	0.0707	-49.55	< 0.0001
student[Yes]	0.4049	0.1150	3.52	0.0004

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$$\widehat{\Pr}(\text{default}=\text{Yes}|\text{student}=\text{Yes}) = \frac{e^{-3.5041+0.4049 \times 1}}{1 + e^{-3.5041+0.4049 \times 1}} = 0.0431,$$

$$\widehat{\Pr}(\text{default}=\text{Yes}|\text{student}=\text{No}) = \frac{e^{-3.5041+0.4049 \times 0}}{1 + e^{-3.5041+0.4049 \times 0}} = 0.0292.$$

Logistic regression with several variables

$$\log \left(\frac{p(X)}{1 - p(X)} \right) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$

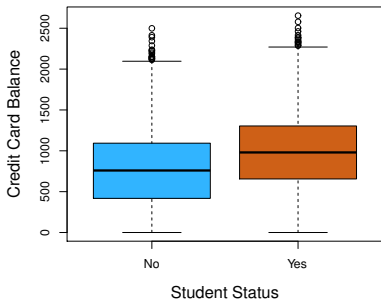
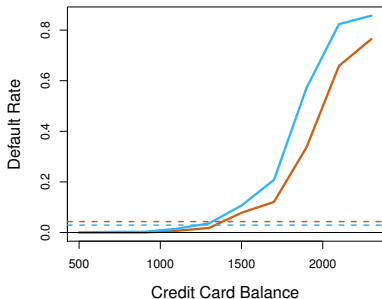
$$p(X) = \frac{e^{\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p}}{1 + e^{\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p}}$$

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-10.8690	0.4923	-22.08	< 0.0001
balance	0.0057	0.0002	24.74	< 0.0001
income	0.0030	0.0082	0.37	0.7115
student[Yes]	-0.6468	0.2362	-2.74	0.0062

Why is coefficient for **student** negative, while it was positive before?

Thus, even though an individual student with a given credit card balance will tend to have a lower probability of

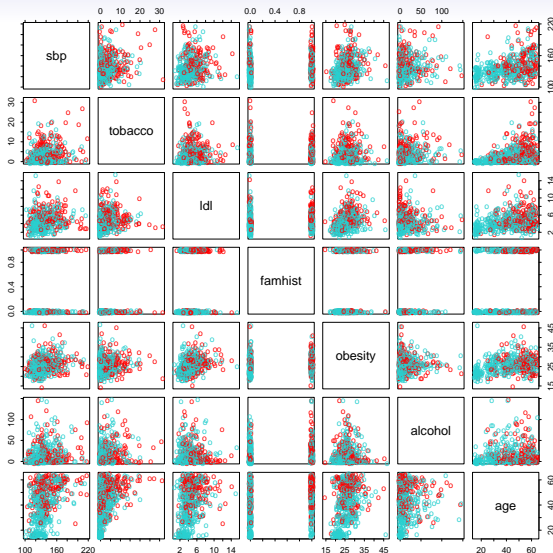
Confounding



- Students tend to have higher balances than non-students, so their marginal default rate is higher than for non-students.
- But for each level of balance, students default less than non-students.
- Multiple logistic regression can tease this out.

Example: South African Heart Disease

- 160 cases of MI (myocardial infarction) and 302 controls (all male in age range 15-64), from Western Cape, South Africa in early 80s.
- Overall prevalence very high in this region: 5.1%.
- Measurements on seven predictors (risk factors), shown in scatterplot matrix.
- Goal is to identify relative strengths and directions of risk factors.
- This was part of an intervention study aimed at educating the public on healthier diets.



Scatterplot matrix of the *South African Heart Disease* data. The response is color coded — The cases (MI) are red, the controls turquoise. **famhist** is a binary variable, with 1 indicating family history of MI.

```
> heartfit<-glm(chd~.,data=heart,family=binomial)
> summary(heartfit)
```

Call:

```
glm(formula = chd ~ ., family = binomial, data = heart)
```

Coefficients:

	Estimate	Std. Error	z value	Pr(> z)	
(Intercept)	-4.1295997	0.9641558	-4.283	1.84e-05	***
sbp	0.0057607	0.0056326	1.023	0.30643	
tobacco	0.0795256	0.0262150	3.034	0.00242	**
ldl	0.1847793	0.0574115	3.219	0.00129	**
famhistPresent	0.9391855	0.2248691	4.177	2.96e-05	***
obesity	-0.0345434	0.0291053	-1.187	0.23529	
alcohol	0.0006065	0.0044550	0.136	0.89171	
age	0.0425412	0.0101749	4.181	2.90e-05	***

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 596.11 on 461 degrees of freedom
Residual deviance: 483.17 on 454 degrees of freedom
AIC: 499.17

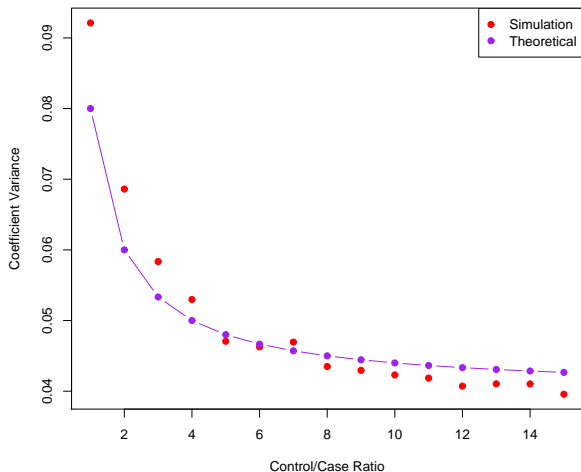
Case-control sampling and logistic regression

- In South African data, there are 160 cases, 302 controls — $\tilde{\pi} = 0.35$ are cases. Yet the prevalence of MI in this region is $\pi = 0.05$.
- With case-control samples, we can estimate the regression parameters β_j accurately (if our model is correct); the constant term β_0 is incorrect.
- We can correct the estimated intercept by a simple transformation

$$\hat{\beta}_0^* = \hat{\beta}_0 + \log \frac{\pi}{1 - \pi} - \log \frac{\tilde{\pi}}{1 - \tilde{\pi}}$$

- Often cases are rare and we take them all; up to five times that number of controls is sufficient. See next frame

Diminishing returns in unbalanced binary data



Sampling more controls than cases reduces the variance of the parameter estimates. But after a ratio of about 5 to 1 the variance reduction flattens out.

Logistic regression with more than two classes

So far we have discussed logistic regression with two classes. It is easily generalized to more than two classes. One version (used in the R package **glmnet**) has the symmetric form

$$\Pr(Y = k|X) = \frac{e^{\beta_{0k} + \beta_{1k}X_1 + \dots + \beta_{pk}X_p}}{\sum_{\ell=1}^K e^{\beta_{0\ell} + \beta_{1\ell}X_1 + \dots + \beta_{p\ell}X_p}}$$

Here there is a linear function for *each* class.

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Multiclass logistic regression is also referred to as *multinomial regression*.

Discriminant Analysis

Here the approach is to model the distribution of X in each of the classes separately, and then use *Bayes theorem* to flip things around and obtain $\Pr(Y|X)$.

When we use normal (Gaussian) distributions for each class, this leads to linear or quadratic discriminant analysis.

However, this approach is quite general, and other distributions can be used as well. We will focus on normal distributions.

Why LDA rather than logistic regression- When the classes are well-separated, the parameter estimates for the logistic regres

Bayes theorem for classification

Thomas Bayes was a famous mathematician whose name represents a big subfield of statistical and probabilistic modeling. Here we focus on a simple result, known as Bayes theorem:

$$\Pr(Y = k|X = x) = \frac{\Pr(X = x|Y = k) \cdot \Pr(Y = k)}{\Pr(X = x)}$$

Proof slide...

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One writes this slightly differently for discriminant analysis:

$$\Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^K \pi_l f_l(x)}, \quad \text{where}$$

If π_k and f_k are corre

$p_k(x) = \Pr(Y=k | X=x)$ is called the posterior probability that the observation belongs to the k 'th class given the predi

- $f_k(x) = \Pr(X = x|Y = k)$ is the *density* for X in class k .

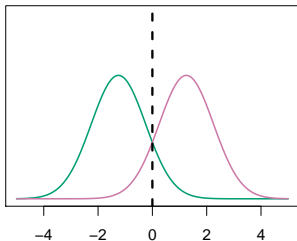
Here we will use normal densities for these, separately in each class. We model the distribution of the predictors X separately in each of the response classes (i.e. g

- $\pi_k = \Pr(Y = k)$ is the marginal or *prior* probability for class k .

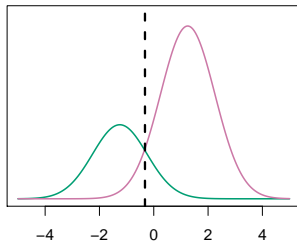
Prior probability that a randomly chosen observation comes from the k 'th class. Estimated by

Classify to the highest density

$$\pi_1=.5, \pi_2=.5$$

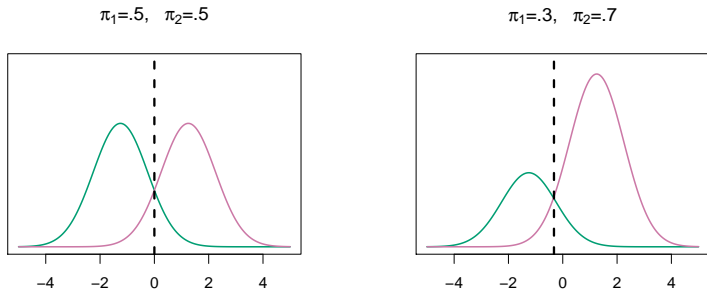


$$\pi_1=.3, \pi_2=.7$$



We classify a new point according to which density is highest.

Classify to the highest density



We classify a new point according to which density is highest.

When the priors are different, we take them into account as well, and compare $\pi_k f_k(x)$. On the right, we favor the pink class — the decision boundary has shifted to the left.

The class k that gives the largest numerator in Bayes Theorem yields the largest posterior probability that an observation be

Why discriminant analysis?

- When the classes are well-separated, the parameter estimates for the logistic regression model are surprisingly unstable. Linear discriminant analysis 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. We assume we can model the densities with Gaussians
- Linear discriminant analysis is popular when we have more than two response classes, because it also provides low-dimensional views of the data.

Linear Discriminant Analysis when $p = 1$

The Gaussian density has the form

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

Here μ_k is the mean, and σ_k^2 the variance (in class k). We will **assume** that all the $\sigma_k = \sigma$ are the same.

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Plugging this into Bayes formula, we get a rather complex expression for $p_k(x) = \Pr(Y = k|X = x)$:

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu_k}{\sigma}\right)^2}}{\sum_{l=1}^K \pi_l \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu_l}{\sigma}\right)^2}}$$

In Bayes classification the observa

Happily, **there are simplifications and cancellations.**

Discriminant functions

To classify at the value $X = x$, we need to see which of the $p_k(x)$ is largest. Taking logs, and discarding terms that do not depend on k , we see that this is equivalent to assigning x to the class with the largest *discriminant score*:

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

Note that $\delta_k(x)$ is a *linear* function of x .

As the discriminant score is a linear function of x , the method is called linear discriminant analysis

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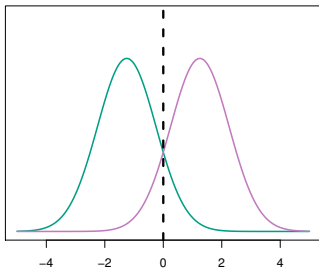
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If there are $K = 2$ classes and $\pi_1 = \pi_2 = 0.5$, then one can see that the *decision boundary* is at

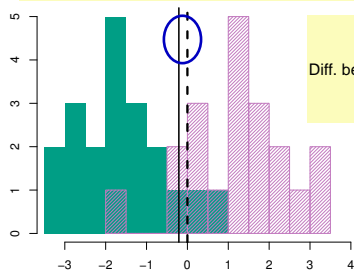
$$x = \frac{\mu_1 + \mu_2}{2}.$$

(See if you can show this)

Perfect theoretical case



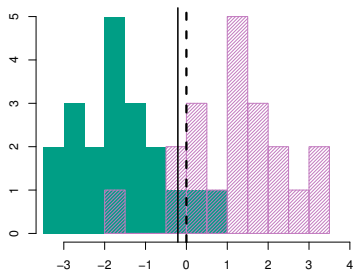
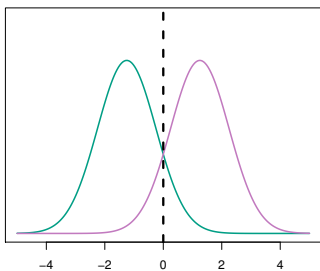
Imperfect practical case. In this case $n_1 = n_2 = 20$. Thus $\pi_1 = \pi_2 = 0.5$



Diff. between optim

Example with $\mu_1 = -1.5$, $\mu_2 = 1.5$, $\pi_1 = \pi_2 = 0.5$, and $\sigma^2 = 1$.

An observation is equally likely to come from either class



Example with $\mu_1 = -1.5$, $\mu_2 = 1.5$, $\pi_1 = \pi_2 = 0.5$, and $\sigma^2 = 1$.

Typically we don't know these parameters; we just have the training data. In that case we simply estimate the parameters and plug them into the rule.

Estimating the parameters

n : the total number of training observations
 n_k : the number of training observations in the k 'th class

$$\hat{\pi}_k = \frac{n_k}{n}$$

Prior probability that a randomly chosen observation comes from the k 'th class

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

The sample mean for each class

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

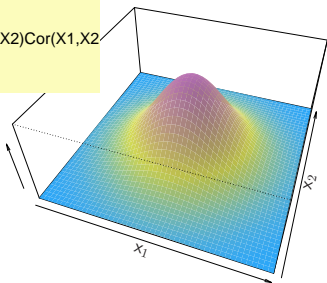
$$= \sum_{k=1}^K \frac{n_k - 1}{n - K} \cdot \hat{\sigma}_k^2$$

Weighted average of the sample variances for each class

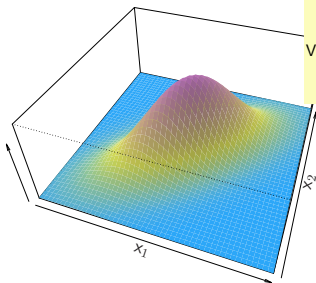
where $\hat{\sigma}_k^2 = \frac{1}{n_k - 1} \sum_{i: y_i=k} (x_i - \hat{\mu}_k)^2$ is the usual formula for the estimated variance in the k th class.

Linear Discriminant Analysis when $p > 1$

$\text{Var}(X_1) = \text{Var}(X_2)\text{Cor}(X_1, X_2)$



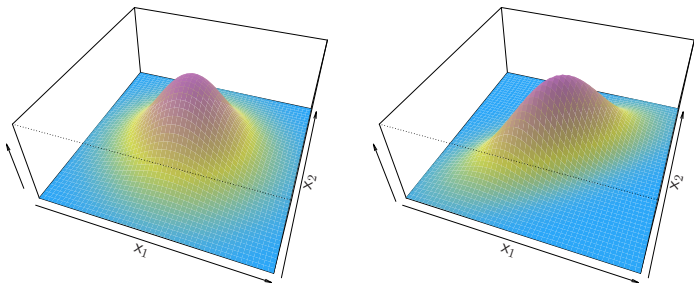
$\text{Var}(X_1) \neq \text{Var}(X_2)\text{Cor}(X_1, X_2)$



$$\text{Density: } f(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)}$$

In the PDF for the multivariate Gaussian, the variance is replaced by a covariance matrix Sigma. If a p-dimensional random

Linear Discriminant Analysis when $p > 1$

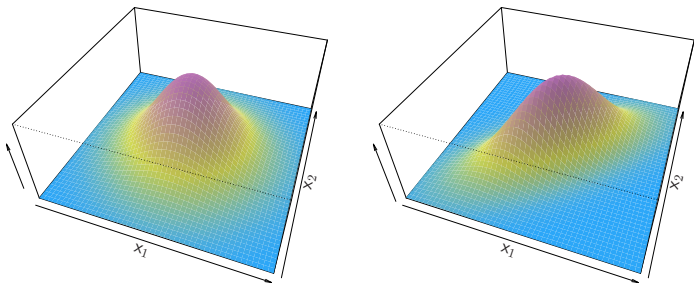


$$\text{Density: } f(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)}$$

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

The discriminant function is simply a vector/matrix version of the discriminant function we saw earlier

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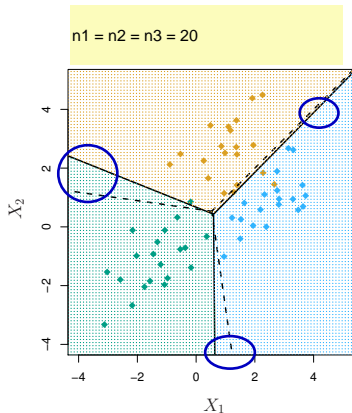
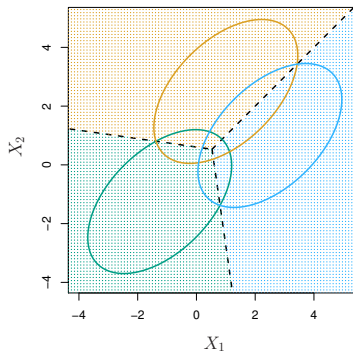
Discriminant function: $\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log \pi_k$

Despite its complex form,

Still linear discriminant analysis just in more dimensions

$\delta_k(x) = c_{k0} + c_{k1}x_1 + c_{k2}x_2 + \dots + c_{kp}x_p$ — a **linear function**.

Illustration: $p = 2$ and $K = 3$ classes



Discrepancies ill

Here $\pi_1 = \pi_2 = \pi_3 = 1/3$.

The dashed lines are known as the *Bayes decision boundaries*.

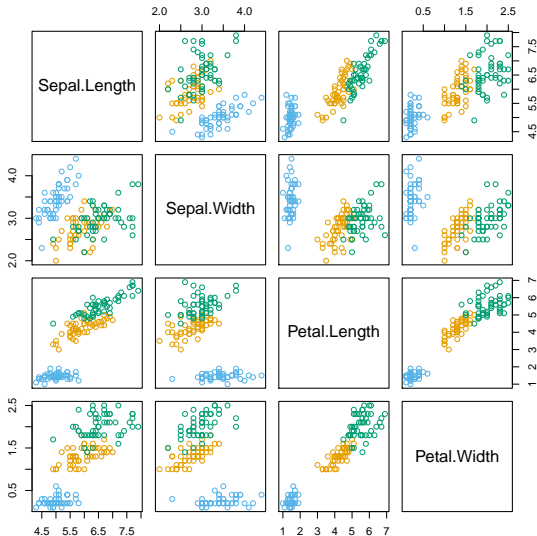
Were they known, they would yield the fewest misclassification errors, among all possible classifiers.

Fisher's Iris Data

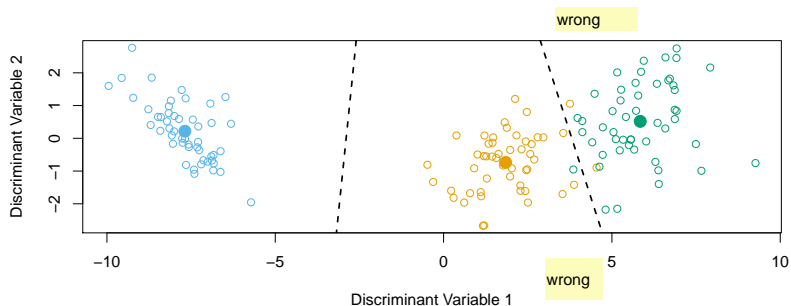
4 variables
3 species
50 samples/class

- Setosa
- Versicolor
- Virginica

LDA classifies all
but 3 of the 150
training samples
correctly.



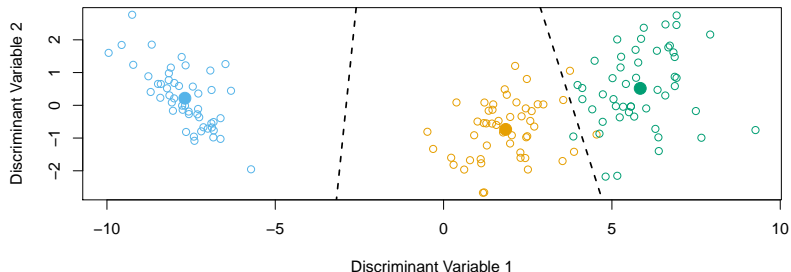
Fisher's Discriminant Plot



When there are K classes, linear discriminant analysis can be viewed exactly in a $K - 1$ dimensional plot.

Why?

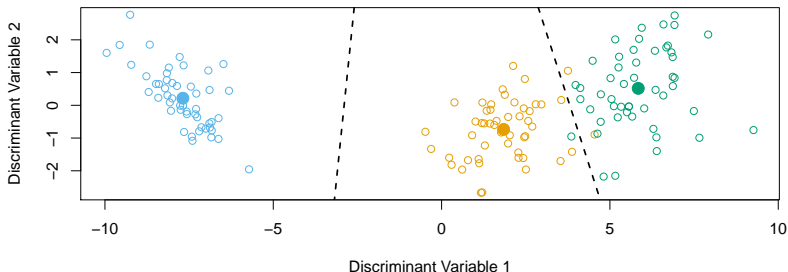
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Even when $K > 3$, we can find the “best” 2-dimensional plane for visualizing the discriminant rule.

From $\delta_k(x)$ to probabilities

Same principle as earlier for 1 dimensional case

Once we have estimates $\hat{\delta}_k(x)$, we can turn these into estimates for class probabilities:

$$\widehat{\Pr}(Y = k|X = x) = \frac{e^{\hat{\delta}_k(x)}}{\sum_{l=1}^K e^{\hat{\delta}_l(x)}}.$$

So classifying to the largest $\hat{\delta}_k(x)$ amounts to classifying to the class for which $\widehat{\Pr}(Y = k|X = x)$ is largest.

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When $K = 2$, we classify to class 2 if $\widehat{\Pr}(Y = 2|X = x) \geq 0.5$, else to class 1.

LDA on Credit Data

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

Confusion matrix.Pre

$(23 + 252)/10000$ errors — a 2.75% misclassification rate!

Some caveats:

Training error rate.Test error rate usually large

- This is *training* error, and we may be overfitting.

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Large ratios of p/n may yield larger overfitting problems

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- If we classified to the prior — always to class **No** in this case — we would make $333/10000$ errors, or only 3.33%.

A NULL classifier that simply says that NO ONE will default regardless of credit card balance will give an error rate of 333/

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- If we classified to the prior — always to class **No** in this case — we would make $333/10000$ errors, or only 3.33%.
- Of the true **No**'s, we make $23/9667 = 0.2\%$ errors; of the true **Yes**'s, we make $252/333 = 75.7\%$ errors!

Types of errors

False positive rate: The fraction of negative examples that are classified as positive — 0.2% in example.

False negative rate: The fraction of positive examples that are classified as negative — 75.7% in example.

We produced this table by classifying to class **Yes** if

$$\widehat{\Pr}(\text{Default} = \text{Yes} | \text{Balance}, \text{Student}) \geq 0.5$$

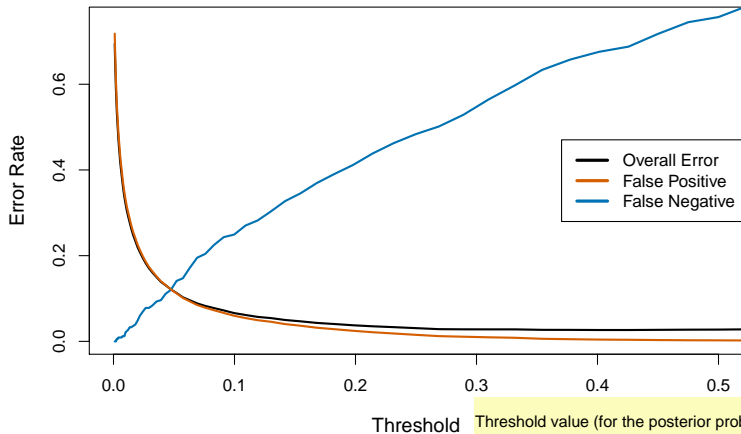
We can change the two error rates by changing the threshold from 0.5 to some other value in $[0, 1]$:

$$\widehat{\Pr}(\text{Default} = \text{Yes} | \text{Balance}, \text{Student}) \geq \textit{threshold},$$

and vary *threshold*.

A bank might particularly wish to AVOID incorrectly classifying an individual who WILL d

Varying the *threshold*

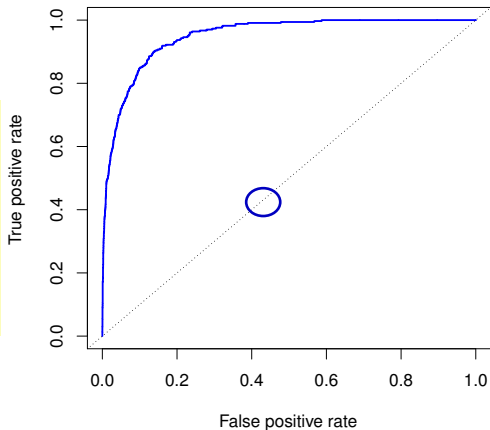


In order to reduce the **false negative** rate, we may want to reduce the threshold to 0.1 or less.

False neg: Predicting a person will NOT default, but in r

ROC Curve

ROC: Receiver Operating Characteristics



True positive rate = TP/F

"no information"-classifier, i.e. st

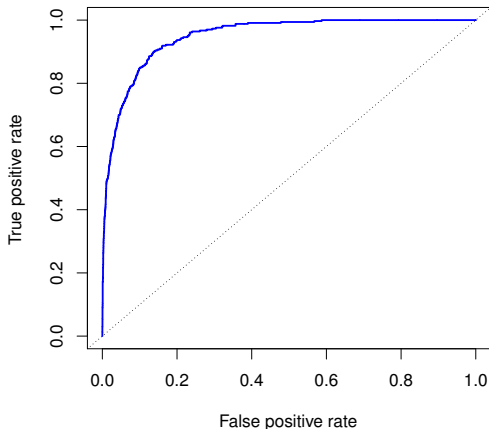
False positive rate = $FP/N = 1 -$

The *ROC plot* displays both simultaneously.

error rates

... for all possible threshold values in $[0;1]$ (for the p

ROC Curve



The *ROC plot* displays both simultaneously.

Sometimes we use the *AUC* or *area under the curve* to summarize the overall performance. **Higher AUC is good.**

Other forms of Discriminant Analysis

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

When $f_k(x)$ are Gaussian densities, with the same covariance matrix Σ in each class, this leads to linear discriminant analysis.

By altering the forms for $f_k(x)$, we get different classifiers.

- With Gaussians but different Σ_k in each class, we get *quadratic discriminant analysis*.

We assume that an observation from the k 'th class is \mathbf{x}

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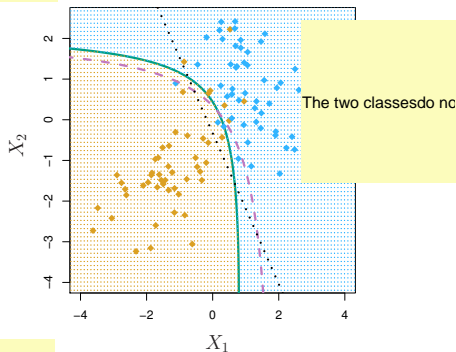
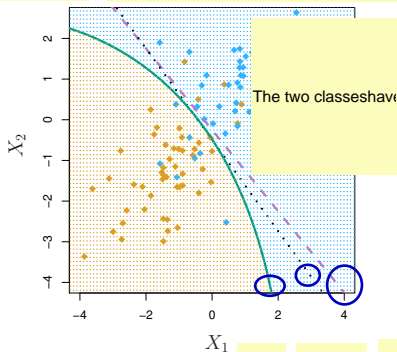
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- Many other forms, by proposing specific density models for $f_k(x)$, including nonparametric approaches.

Quadratic Discriminant Analysis

LDA is a much less flexible

LDA is recommended if: - Training set is small -

QDA is recommended if: - The training set is large -



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

Because the Σ_k are different, the quadratic terms matter.

Naive Bayes

Assumes features are independent in each class.

Useful when p is large, and so multivariate methods like QDA and even LDA break down.

- Gaussian naive Bayes assumes each Σ_k is diagonal:

$$\delta_k(x) \propto \log \left[\pi_k \prod_{j=1}^p f_{kj}(x_j) \right] = -\frac{1}{2} \sum_{j=1}^p \frac{(x_j - \mu_{kj})^2}{\sigma_{kj}^2} + \log \pi_k$$

- can use for *mixed* feature vectors (qualitative and quantitative). If X_j is qualitative, replace $f_{kj}(x_j)$ with probability mass function (histogram) over discrete categories.

Despite strong assumptions, naive Bayes often produces good classification results.

Logistic Regression versus LDA

For a two-class problem, one can show that for LDA

$$\log \left(\frac{p_1(x)}{1 - p_1(x)} \right) = \log \left(\frac{p_1(x)}{p_2(x)} \right) = c_0 + c_1 x_1 + \dots + c_p x_p$$

So it has the same form as logistic regression.

The difference is in how the parameters are estimated.

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Parameters $\text{beta}_0, \text{beta}_1, \dots, \text{beta}_n$ are estimated via maximum likelihood

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- Logistic regression uses the conditional likelihood based on $\Pr(Y|X)$ (known as *discriminative learning*).
- LDA uses the full likelihood based on $\Pr(X, Y)$ (known as *generative learning*).

Parameters c_0, c_1, \dots, c_n are estimated via mean and variance from a normal distribution

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- Despite these differences, in practice the results are often very similar.

parameter estimation techniques and for LDA assumptions: - common covari

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Footnote: logistic regression can also fit quadratic boundaries like QDA, by explicitly including quadratic terms in the model.

Summary

- Logistic regression is very popular for classification, especially when $K = 2$.
- LDA is useful when n is small, or the classes are well separated, and Gaussian assumptions are reasonable. Also when $K > 2$.
- Naive Bayes is useful when p is very large. i.e. we have many predictors
- See Section 4.5 for some comparisons of logistic regression, LDA and KNN.