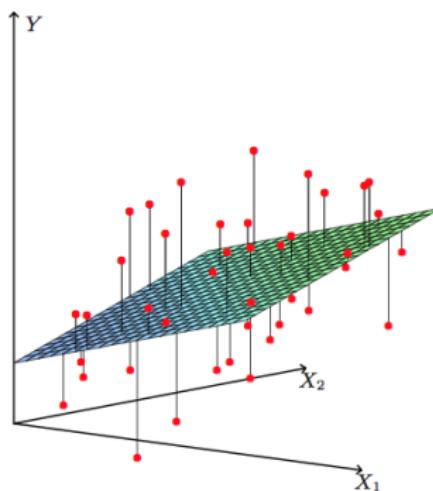


# Statistical Methods for Data Mining

Kuangnan Fang

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# Classification

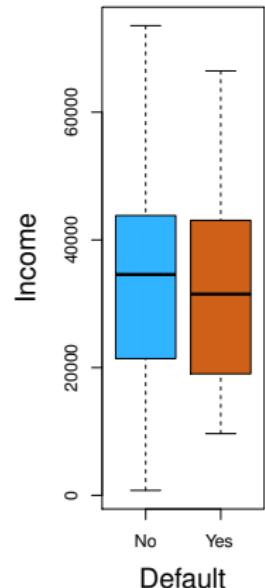
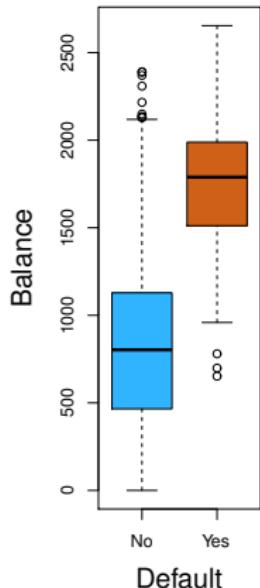
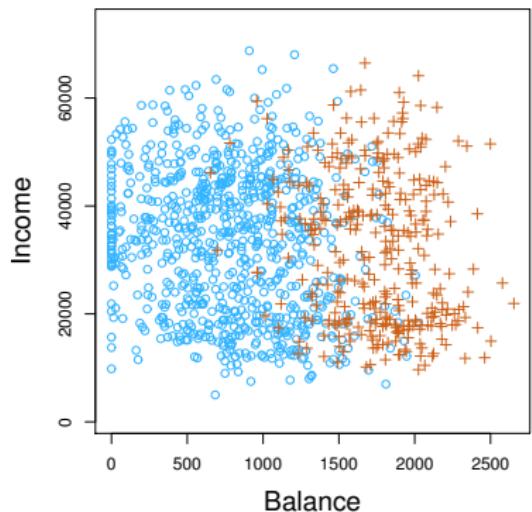
- Qualitative variables take values in an unordered set  $\mathcal{C}$ , such as:  
 $\text{eye color} \in \{\text{brown, blue, green}\}$   
 $\text{email} \in \{\text{spam, ham}\}.$
- Given a feature vector  $X$  and a qualitative response  $Y$  taking values in the set  $\mathcal{C}$ , the classification 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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- Often we are more interested in estimating the *probabilities* that  $X$  belongs to each category in  $\mathcal{C}$ .

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 Defualt



## Can we use Linear Regression?

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

Two problems:  
coding & [0,1]

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

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

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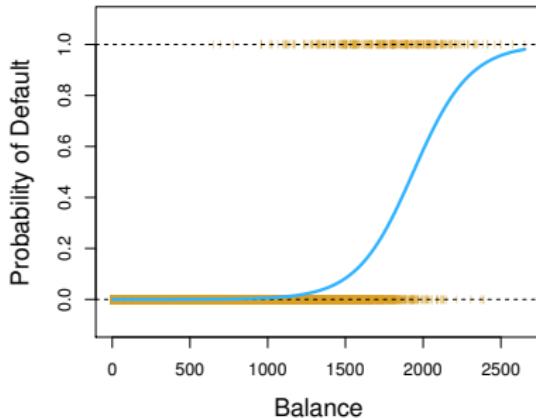
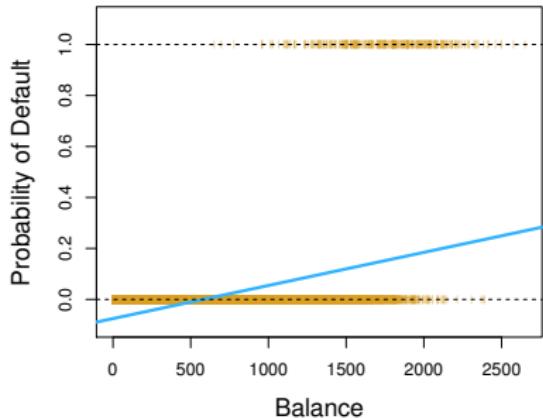
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- Since in the population  $E(Y|X = x) = \Pr(Y = 1|X = x)$ , we might think that regression is perfect for this task.
- However, ~~linear regression might produce probabilities less than zero or bigger than one.~~ *Logistic regression* is more appropriate.

# Linear versus Logistic Regression



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.

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

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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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**.

Linear regression is not appropriate here.

*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

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

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

It is easy to see that no matter what values  $\beta_0$ ,  $\beta_1$  or  $X$  take,  $p(X)$  will have values between 0 and 1.

Probit:

$$\begin{aligned} Y &= X\beta + \varepsilon \in (-\infty, +\infty) \\ \downarrow &\quad \rightarrow \text{CDF} \\ Y &= \Phi(X\beta + \varepsilon) \in (0, 1) \\ \downarrow & \\ Y' &= \Phi^{-1}(Y) = X\beta + \varepsilon \end{aligned}$$

probit

logistic

$$\begin{aligned} Y &= X\beta + \varepsilon \in (-\infty, +\infty) \\ \downarrow & \\ p(X) &= \Pr(Y=1|X) = \frac{e^{X\beta}}{1+e^{X\beta}} \\ \downarrow & \\ \log \frac{p(X)}{1-p(X)} &= X\beta \end{aligned}$$

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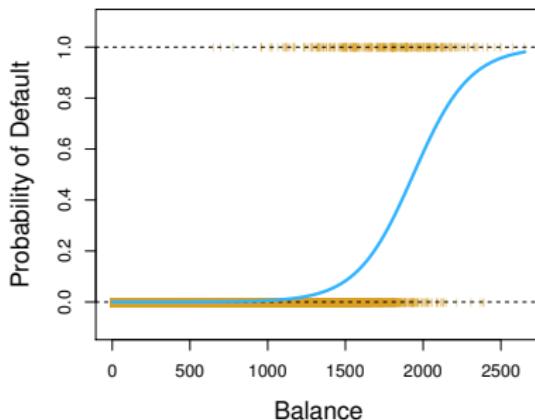
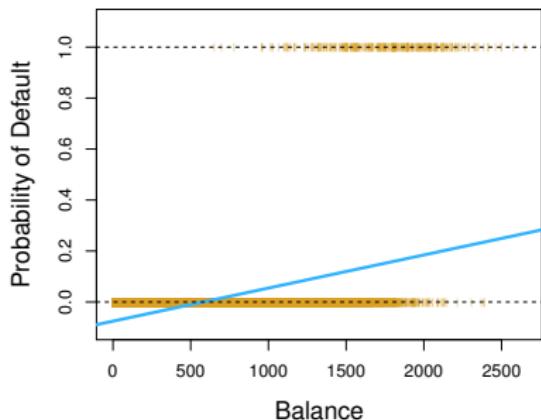
A bit of rearrangement gives

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

How to interpret?

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.

How to estimate?

## 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  $\beta_0$  and  $\beta_1$  to maximize the likelihood of the observed data.

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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
<b>Intercept</b>	-3.5041	0.0707	-49.55	< 0.0001
<b>student [Yes]</b>	0.4049	0.1150	3.52	0.0004

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Intercept	-3.5041	0.0707	-49.55	< 0.0001
student [Yes]	0.4049	0.1150	3.52	0.0004

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

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

平均  
违约率  
student [Yes]

均表示  
违约

## Logistic regression with several variables

对数比 (logit)

對數比 odds ratio (log)  
比率

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

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

	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

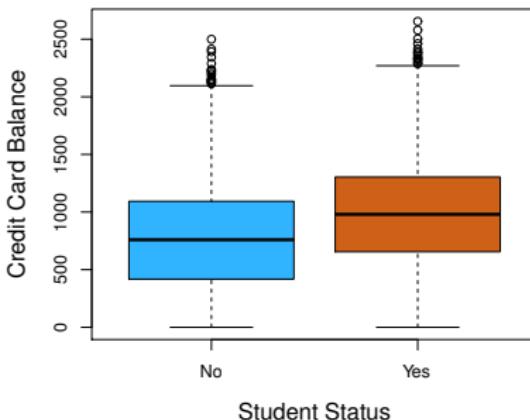
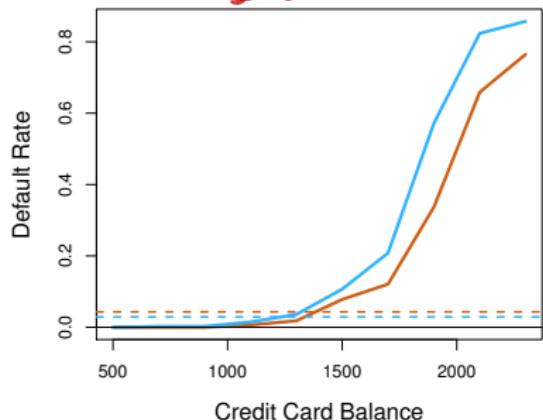
Why is coefficient for student negative, while it was positive before?

student 不归行

一般单变量线性回归  
引入控制变量

## Confounding

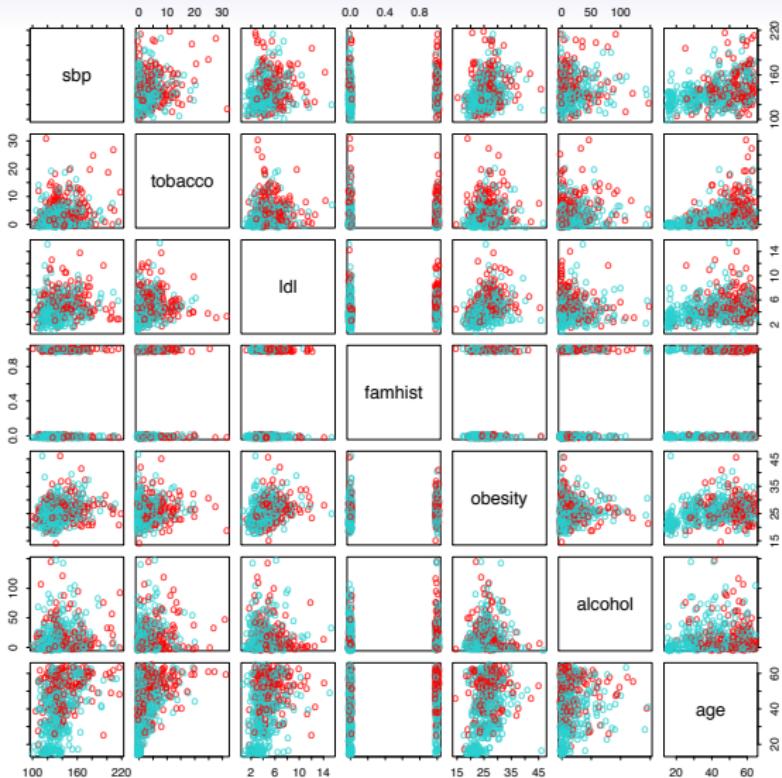
遗漏变量会使  
估计量不一致



- 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
```

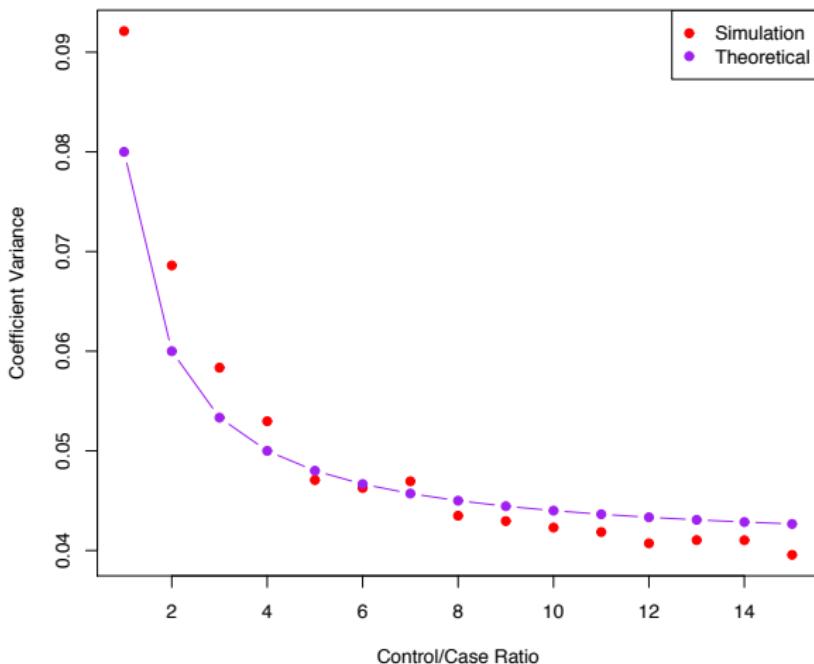
## Case-control sampling and logistic regression

- 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  $\beta_j$  accurately (if our model is correct); the constant term  $\beta_0$  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.

## 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:

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

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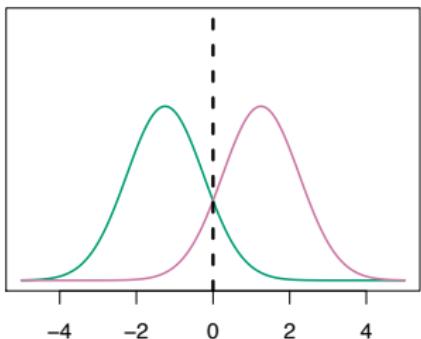
One writes this slightly differently for discriminant analysis:

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

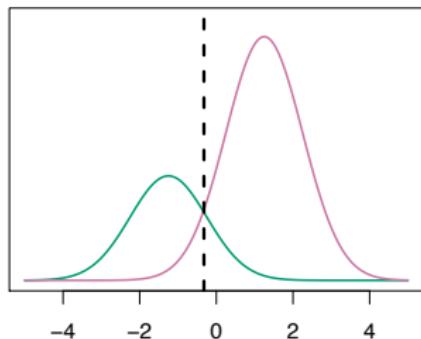
- $f_k(x) = \Pr(X = x|Y = k)$  is the *density* for  $X$  in class  $k$ .  
Here we will use normal densities for these, separately in each class.
- $\pi_k = \Pr(Y = k)$  is the marginal or *prior* probability for class  $k$ .

## Classify to the highest density

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



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

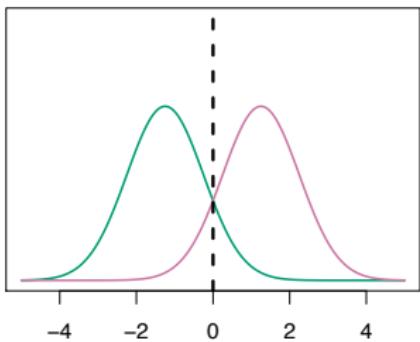


分类点在二者的密度相等的点

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

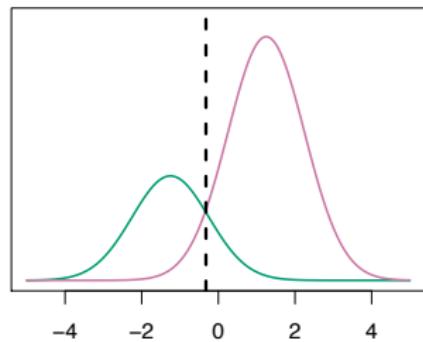
## Classify to the highest density

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



两类先验概率相同(均分)

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



两类先验概率不同(偏向右侧)

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.

## Why discriminant analysis?

用判别分析而不用 logistic 因为：  
①当两类是 well-separated (类别的区分) /  $\rightarrow N$  比较小  
且  $X \rightarrow$  Normal / ③ 易分类  
② 可靠

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

## Linear Discriminant Analysis when $p = 1$

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高斯判别分析

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

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

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

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

Happily, there are simplifications and cancellations.

↓ 化简

## 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*:

$$p(x) \rightarrow \log(p(x)) \rightarrow \text{去常数项} \rightarrow \delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k) = ax + b$$

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

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

→ 判斷判別分析五步曲。  
(并不知道各考慮)

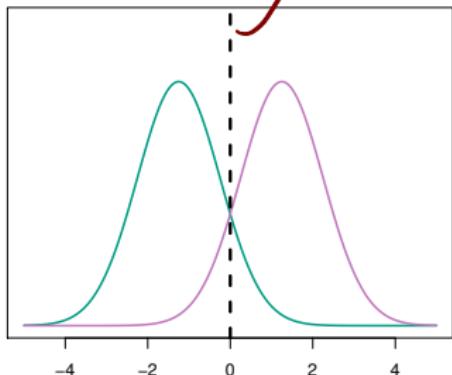
Note that  $\delta_k(x)$  is a *linear* function of  $x$ .

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

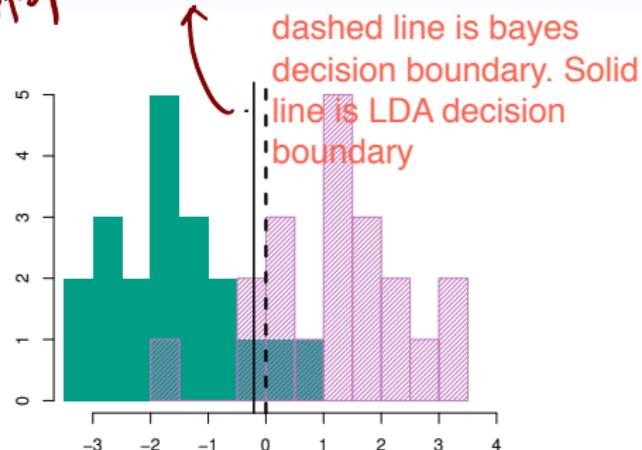
$$x = \frac{\mu_1 + \mu_2}{2}. \quad (K=2, \pi_1 = \pi_2 = 0.5)$$

(See if you can show this)

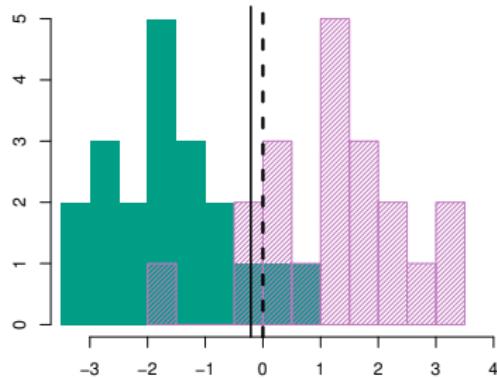
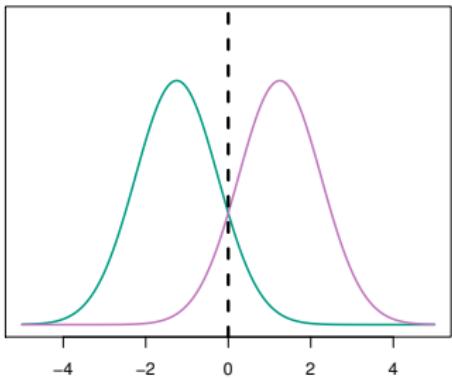
$$x=(\mu_1+\mu_2)/2$$



样本的线性判别分析.



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



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

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

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

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

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

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.

LDA 假设： $k$ 类同方差且同为 Normal .

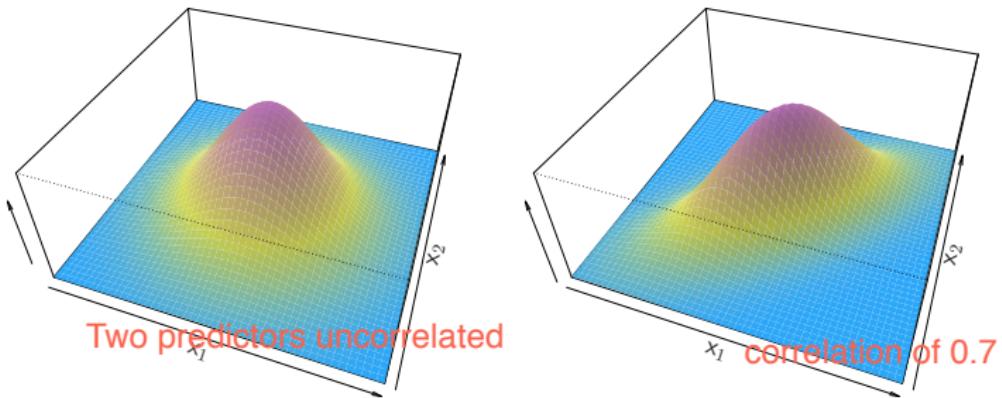
- The LDA classifier plugs the estimates given in (4.15) and (4.16) into (4.13), and assigns an observation  $X = x$  to the class for which

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

→ 线性判别函数  
(用 sample 来估计参数)

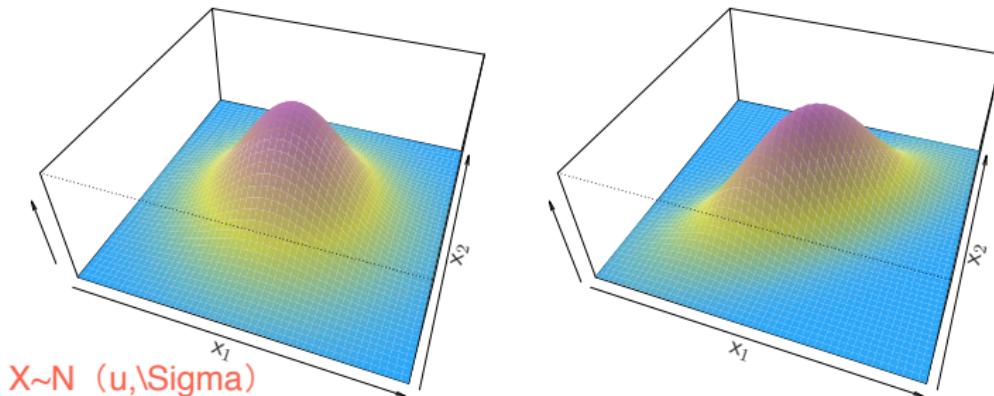
is largest. The word linear in the classifiers name stems from the fact that the discriminant functions  $\hat{\delta}_k(x)$  in (4.17) are linear functions of  $x$  (as opposed to a more complex function of  $x$ ).

## Linear Discriminant Analysis when $p > 1$



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

## Linear Discriminant Analysis when $p > 1$



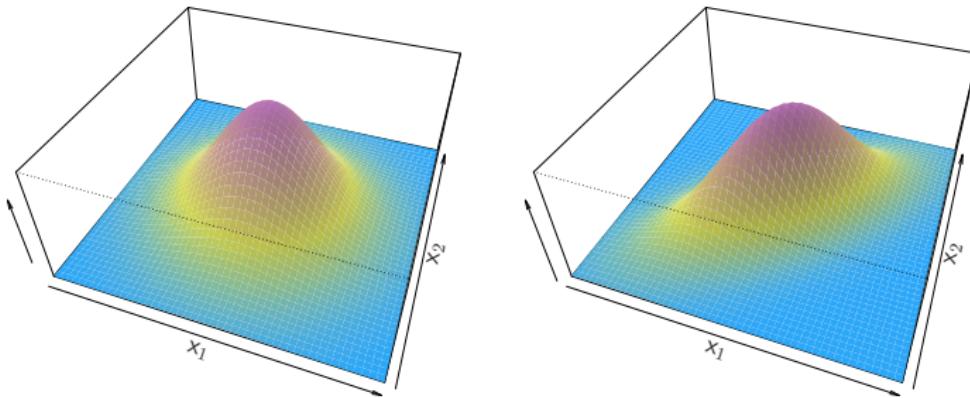
$$\text{Density: } f(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)}$$

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

## Linear Discriminant Analysis when $p > 1$

二維

每基都是  
二維.



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

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

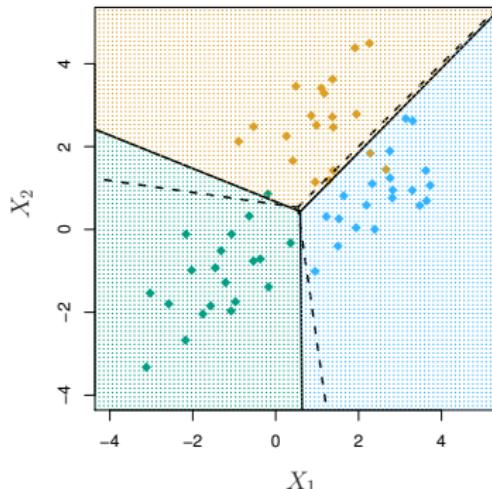
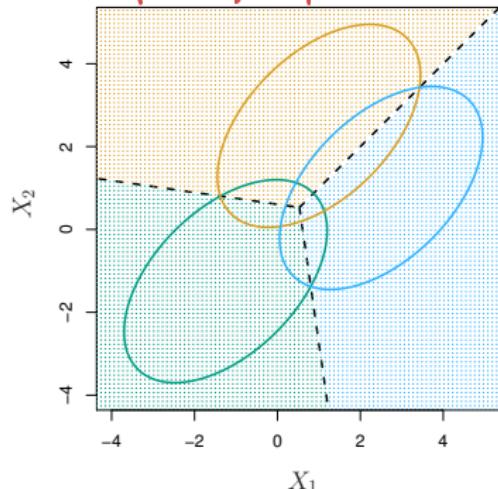
Despite its complex form,

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

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

已知分布和参数时的贝叶斯分类。  
↓ 也是(LDA)

二组三类。未知分布及参数时的  
LDA 分类边界(实线)



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

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

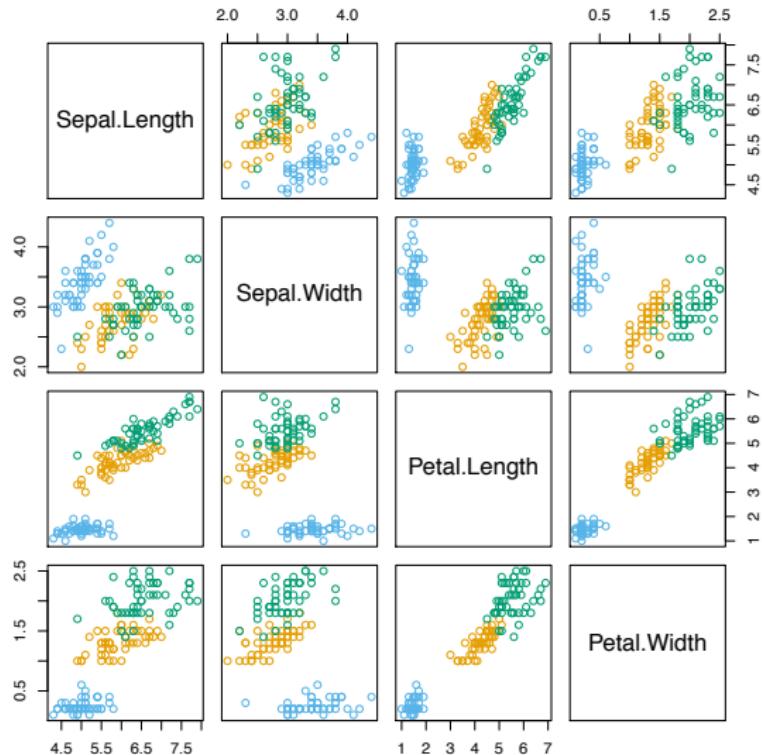
Were they known, they would yield the fewest misclassification errors, among all possible classifiers.

# Fisher's Iris Data

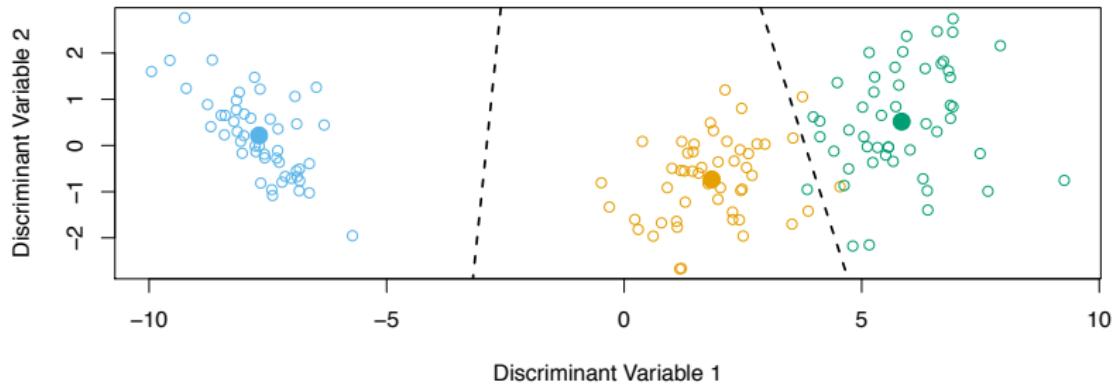
4 variables  
3 species  
50 samples/class

- Setosa
- Versicolor
- Virginica

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



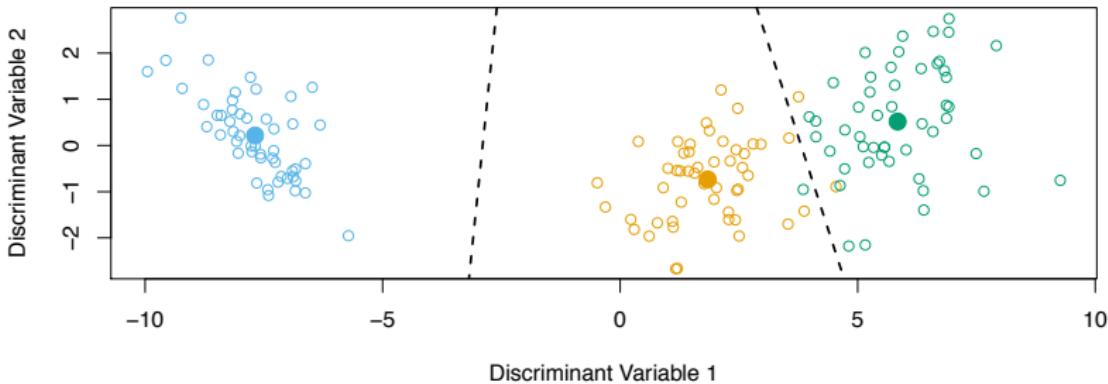
# Fisher's Discriminant Plot



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

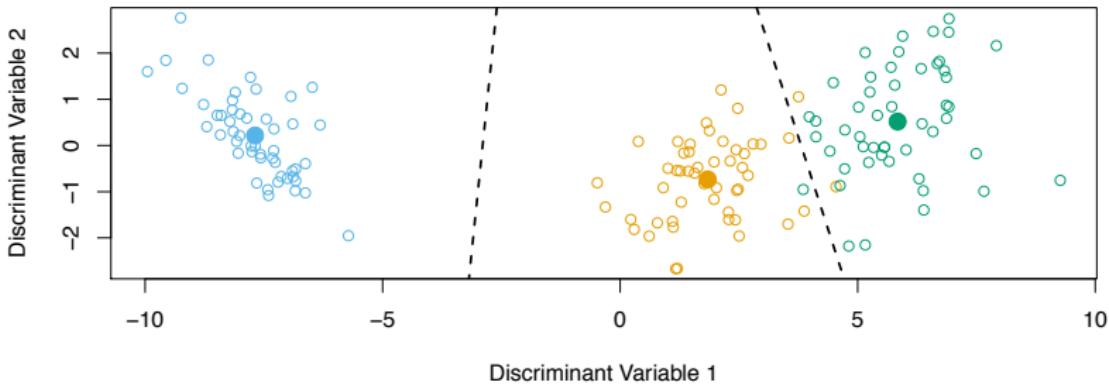
Why?

## Fisher's Discriminant Plot



When there are  $K$  classes, linear discriminant analysis can be viewed exactly in a  $K - 1$  dimensional plot.  
Why? Because it essentially classifies to the closest centroid, and they span a  $K - 1$  dimensional plane.

## Fisher's Discriminant Plot



When there are  $K$  classes, linear discriminant analysis can be viewed exactly in a  $K - 1$  dimensional plot. 对 k 类问题, LDA( $\rightarrow$ )  $K - 1$  维 + 边界  
Why? Because it essentially classifies to the closest centroid, and they span a  $K - 1$  dimensional plane.  
Even when  $K > 3$ , we can find the “best” 2-dimensional plane for visualizing the discriminant rule.

## From $\delta_k(x)$ to probabilities

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

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

用激励函数来  
估计属于某类概率.

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.

## From $\delta_k(x)$ to probabilities

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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.

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

		confusion matrix		
		True Default Status		Total <small>(cont'd)</small>
Predicted Default Status	No	No	Yes	
	Yes	23	81	104
Total	9667	333		10000

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

Some caveats:

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

## LDA on Credit Data

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

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

Some caveats:

- This is *training* error, and we may be overfitting. Not a big concern here since  $n = 10000$  and  $p = 4$ !

## LDA on Credit Data

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		No	Yes	Total
Predicted Default Status	No	9644	252	9896
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$(23 + 252)/10000$  errors — a 2.75% misclassification rate!

Some caveats:

- This is *training* error, and we may be overfitting. Not a big concern here since  $n = 10000$  and  $p = 4$ !
- If we classified to the prior — always to class **No** in this case — we would make  $333/10000$  errors, or only 3.33%.

	<i>N</i>	<i>P</i>
<i>p</i>	<i>TN</i>	<i>FN</i>
<i>N</i>	<i>FP</i>	<i>TP</i>

真正率:  $\frac{TP}{TP+FN} = \frac{81}{81+252}$  (sensitivity, recall)

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

假阴率:  $\frac{FP}{TN+FP} = 1 - \text{specificity}$

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

Some caveats: 总体错判率

- This is *training* error, and we may be overfitting. Not a big concern here since  $n = 10000$  and  $p = 4$ !
- 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!  $FP/(FP+TN)$

sensitivity:  $TP/(TP+FN) = 24.3\%$ ; specificity:  $TN/(TN+FP) = 99.8\%$

敏感性(真正率)

特异牲(1-假阴率)

## Types of errors

$$\text{假正率} = 1 - \text{特异度} = \frac{FP}{TN + FP}$$

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  $[0, 1]$ :

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

and vary *threshold*.

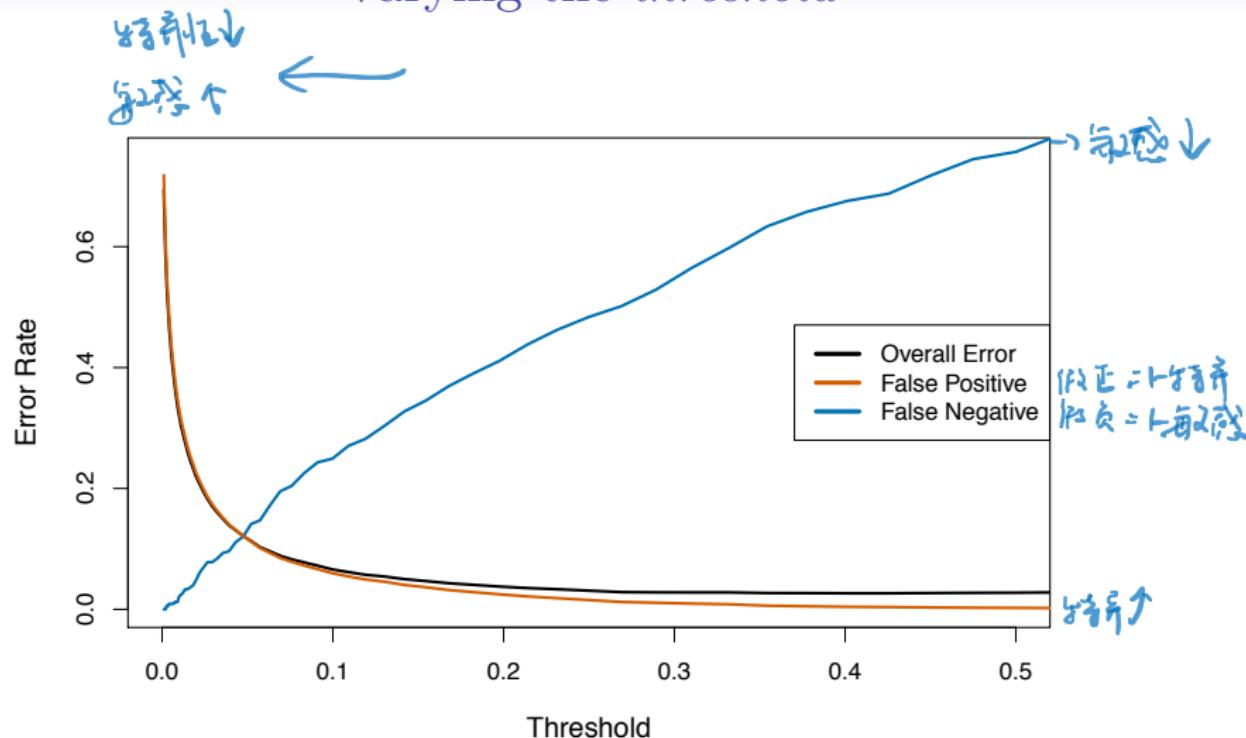
# LDA

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

**TABLE 4.5.** A confusion matrix compares the LDA predictions to the true default statuses for the 10,000 training observations in the **Default** data set, using a modified threshold value that predicts default for any individuals whose posterior default probability exceeds 20%.

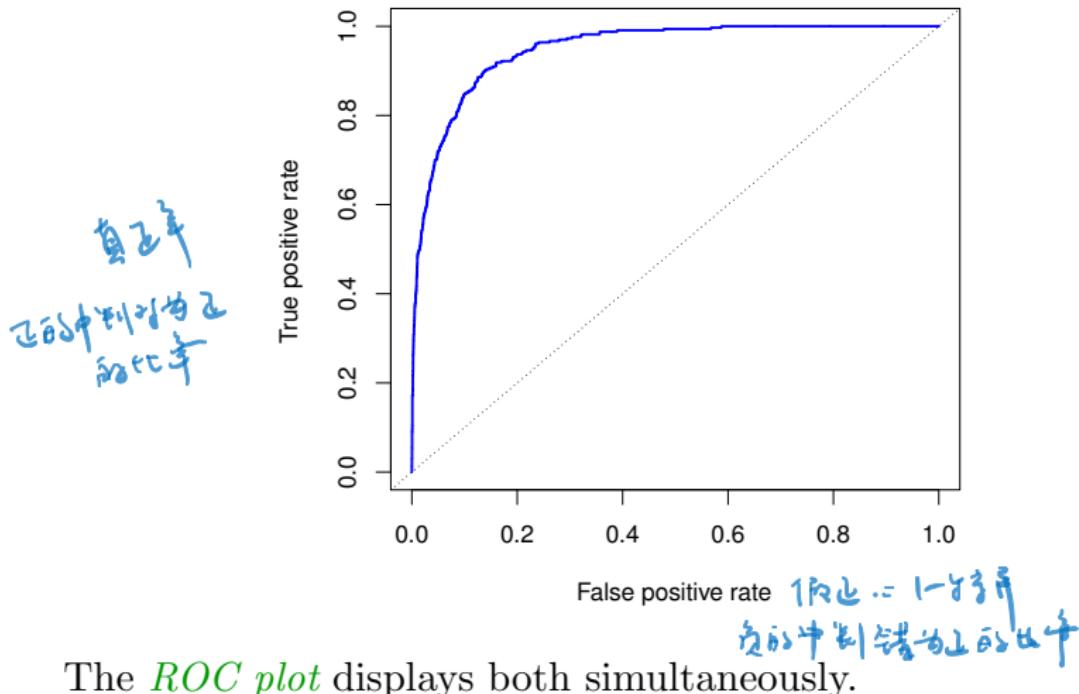
以关心的为正(违约)  
关心其违约性

## Varying the threshold



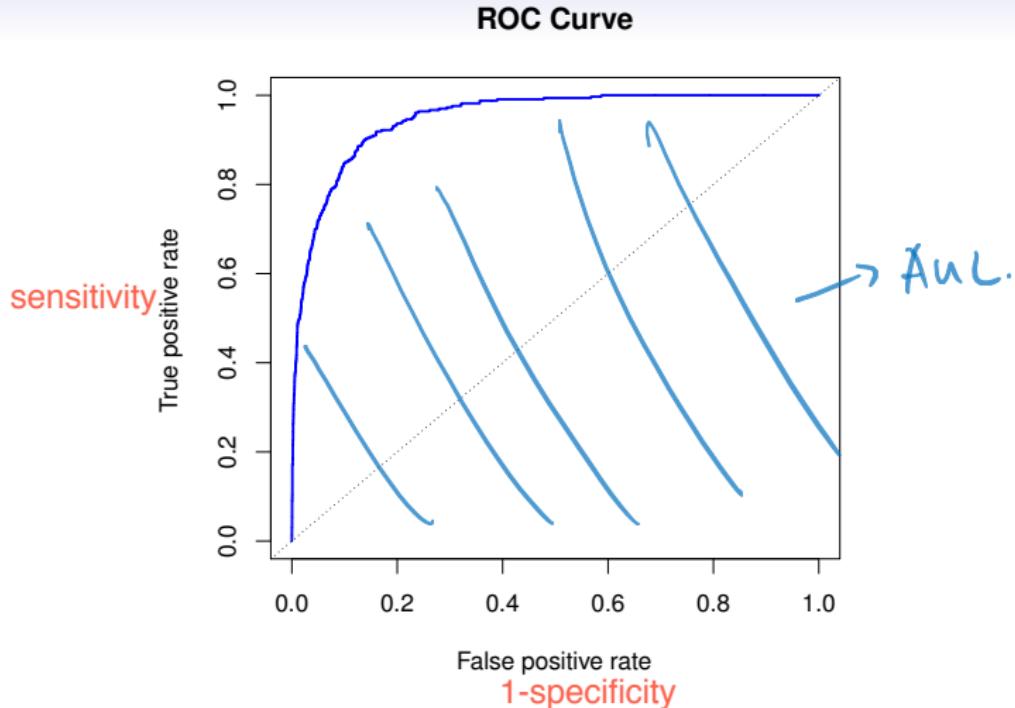
In order to reduce the false negative rate, we may want to reduce the threshold to 0.1 or less.

## ROC Curve



The *ROC plot* displays both simultaneously.

## ROC: receiver operating characteristics



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.

True  
 P N  
 Pre P TP FP  
 N FN TN

## LDA

True  
 P N  
 N FN TN  
 P FN TP

False pos =  $\frac{FP}{TN+FP}$   
 True pos =

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

似然率  
 =  $\frac{\text{真阳性}}{\text{真阴性} + \text{假阳性}}$   
 真阳性 + 假阳性  
 = 真实的阳性中  
 判断为正的比列。

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.

似然率：真实阳性判为正 =  $\frac{TP}{TN+FP} = 1 - \text{Specificity}$   
 真正率：真实正例判为正 =  $\frac{TP}{TP+FN} = \frac{TP}{TP+FP} = \text{Sensitivity} = \text{Recall}$

真正率：  
 $= \frac{TP}{P} = \frac{TP}{TP+FN} = \frac{\text{真正例}}{\text{真正例} + \text{假阳性}} = \text{真实的正例中判断为正的比列。}$

## 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  $\Sigma$  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  $\Sigma_k$  in each class, we get *quadratic discriminant analysis*.

## Other forms of Discriminant Analysis

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- With  $f_k(x) = \prod_{j=1}^p f_{jk}(x_j)$  (conditional independence model) in each class we get *naive Bayes*. For Gaussian this means the  $\Sigma_k$  are diagonal.

## Other forms of Discriminant Analysis

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When  $f_k(x)$  are Gaussian densities, with the same covariance matrix  $\Sigma$  in each class, this leads to linear discriminant analysis. By altering the forms for  $f_k(x)$ , we get different classifiers.

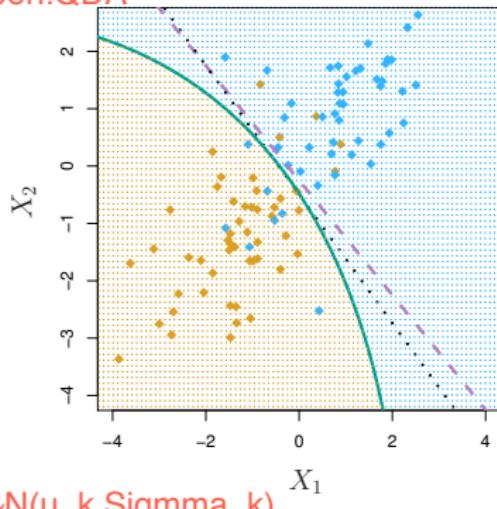
- With Gaussians but different  $\Sigma_k$  in each class, we get *quadratic discriminant analysis*. (QDA 高斯分析但各类协方差不同.)
- With  $f_k(x) = \prod_{j=1}^p f_{jk}(x_j)$  (conditional independence model) in each class we get *naive Bayes*. For Gaussian this means the  $\Sigma_k$  are diagonal. (朴素贝叶斯：各维独立。高斯，协方差对角阵。)  
很多时  
反面效果好。  
• Many other forms, by proposing specific density models for  $f_k(x)$ , including nonparametric approaches.

# Quadratic Discriminant Analysis

purple: Bayes decision boundary

black: LDA

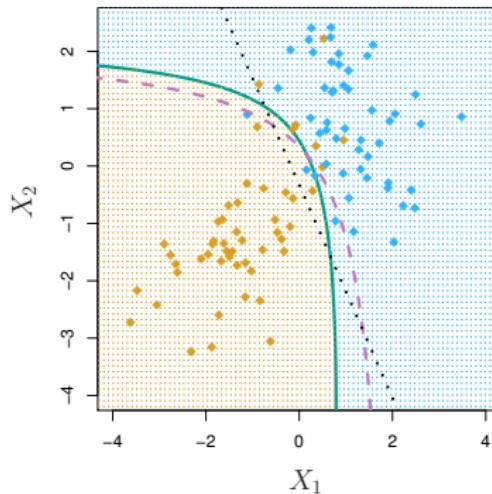
green:QDA



$X \sim N(\mu_k, \Sigma_k)$

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

Because the  $\Sigma_k$  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  $\Sigma_k$  is diagonal:

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

可用于混合特征(定性、定量)  
定性变量  
用其概率分布  
作为  $f_j(x_j)$   
(频率)

- 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.

LDA 与 Logistic 在二分类时仅参数估计方法不同

## Logistic Regression versus LDA

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

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The difference is in how the parameters are estimated.

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

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- Logistic regression uses the conditional likelihood based on  $\Pr(Y|X)$  (known as *discriminative learning*).
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- Despite these differences, in practice the results are often very similar.

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So it has the same form as logistic regression.

The difference is in how the parameters are estimated.

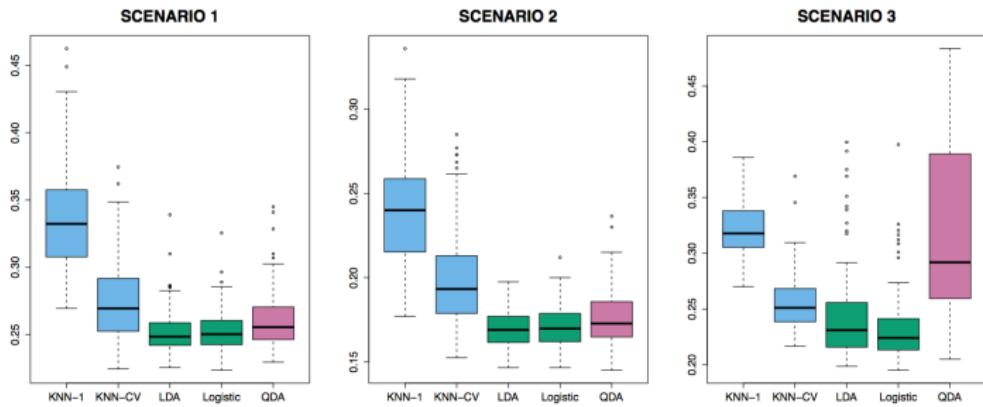
- Logistic regression uses the conditional likelihood based on  $\Pr(Y|X)$  (known as *discriminative learning*).
- LDA uses the full likelihood based on  $\Pr(X, Y)$  (known as *generative learning*).
- Despite these differences, in practice the results are often very similar.

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

## Comparision of classification methods

- $p = 2$
- Scenario 1: There were 20 training observations in each of two classes. The observations within each class were uncorrelated random normal variables with a different mean in each class.
- Scenario 2: Details are as in Scenario 1, except that within each class, the two predictors had a correlation of 0.5.
- Scenario 3: We generated  $X_1$  and  $X_2$  from the  $t$ -distribution, with 50 observations per class. The  $t$ -distribution has a similar shape to the normal distribution, but it has a tendency to yield more extreme points that is, more points that are far from the mean. In this setting, the decision boundary was still linear, and so fit into the logistic regression framework. The setup violated the assumptions of LDA, since the observations were not drawn from a normal distribution.

# LDA

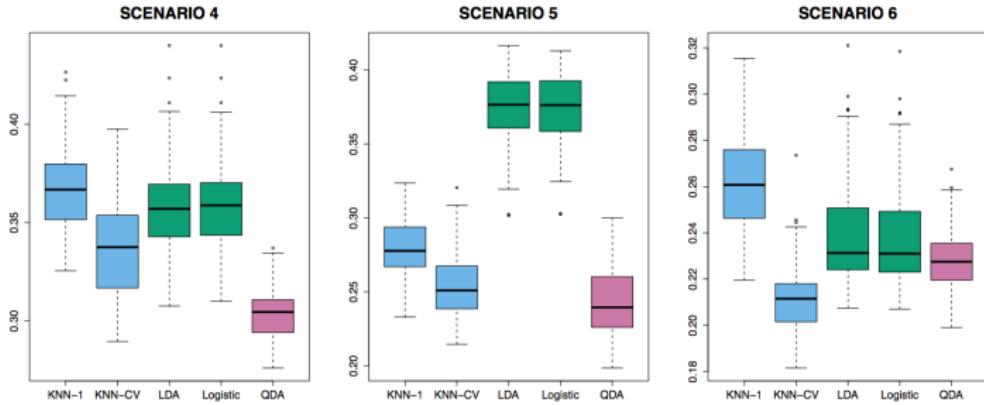


**FIGURE 4.10.** Boxplots of the test error rates for each of the linear scenarios described in the main text.

## Comparision of classification methods

- Scenario 4: The data were generated from a normal distribution, with a correlation of 0.5 between the predictors in the first class, and correlation of 0.5 between the predictors in the second class.
- Scenario 5: Within each class, the observations were generated from a normal distribution with uncorrelated predictors. However, the responses were sampled from the logistic function using  $X_1^2$ ,  $X_2^2$ , and  $X_1 \times X_2$  as predictors. Consequently, there is a quadratic decision boundary.
- Scenario 6: Details are as in the previous scenario, but the responses were sampled from a more complicated non-linear function. As a result, even the quadratic decision boundaries of QDA could not adequately model the data.

# LDA



**FIGURE 4.11.** Boxplots of the test error rates for each of the non-linear scenarios described in the main text.

# 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.
- See Section 4.5 for some comparisons of logistic regression, LDA and KNN.