# Introduction to Statistical Learning

INF 552, Machine Learning for Data Informatics

University of Southern California

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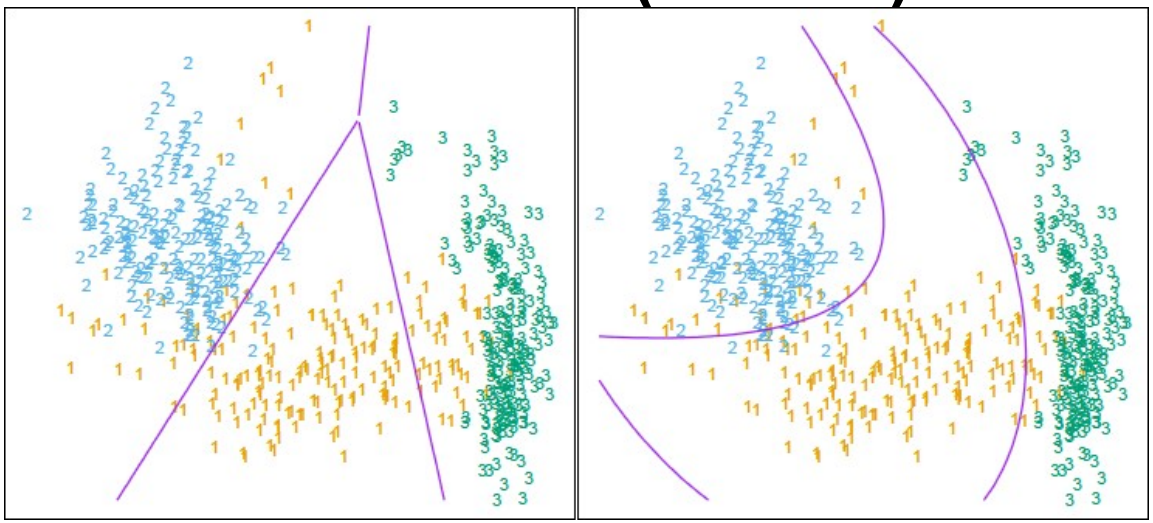
# Lesson 3
# Classification

Linear and Logistic Regression:

LDA, QDA

k-NN (k Nearest Neighbors)

optimal separating hyperplane – will be discussed later (SVM)



# Classification

- Qualitative variables take values in an *unordered* set $C$, such as:

  eye color $\in$ {brown, blue, green}
  digit $\in$ {0, 1, ...,9}
  email $\in$ {spam, ham}.

- Given a feature vector $X$ and a qualitative response $Y$ taking values in the set $C$, 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. $C(X) \in C$.

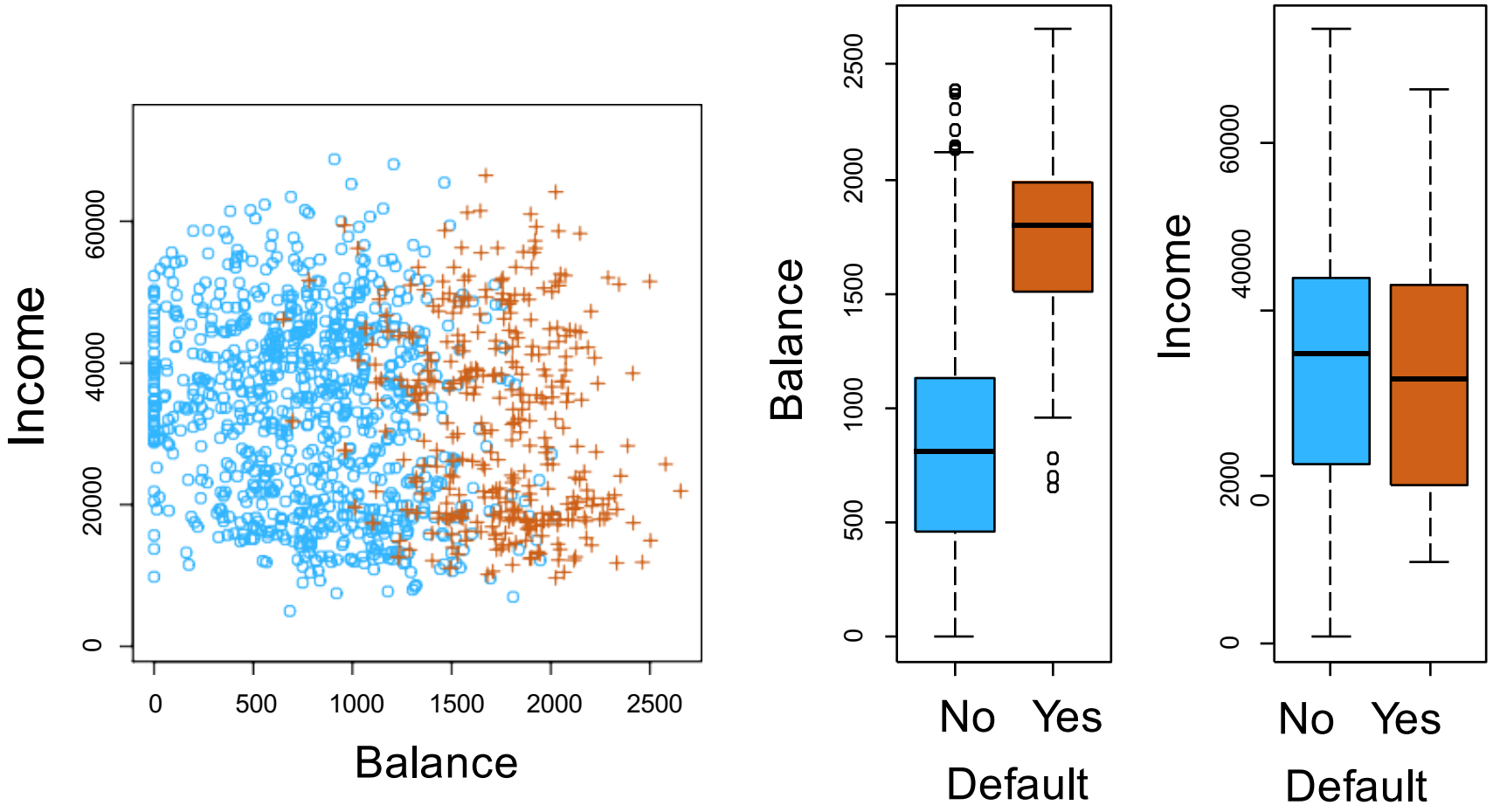
# Classification

- Often we are more interested in estimating the *probabilities* that $X$ belongs to each category in $C$.

# Case: Credit Card Default Data

- To predict customers that are likely to default
- Possible *X* variables are:
  - Annual Income
  - Monthly credit card balance
- The *Y* variable (Default) is categorical: Yes or No
- How do we check the relationship between *Y* and *X*?

# Example: Credit Card Defualt



# 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 $\hat{Y} > 0.5$?

# Can we use Linear Regression?

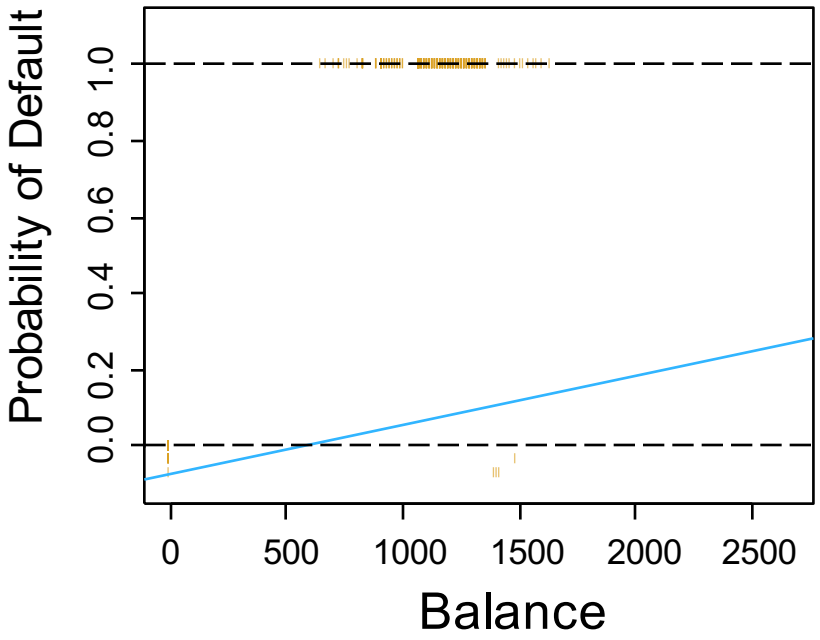
Can we simply perform a linear regression of $Y$ on $X$ and classify as Yes if $Y > 0.5$?

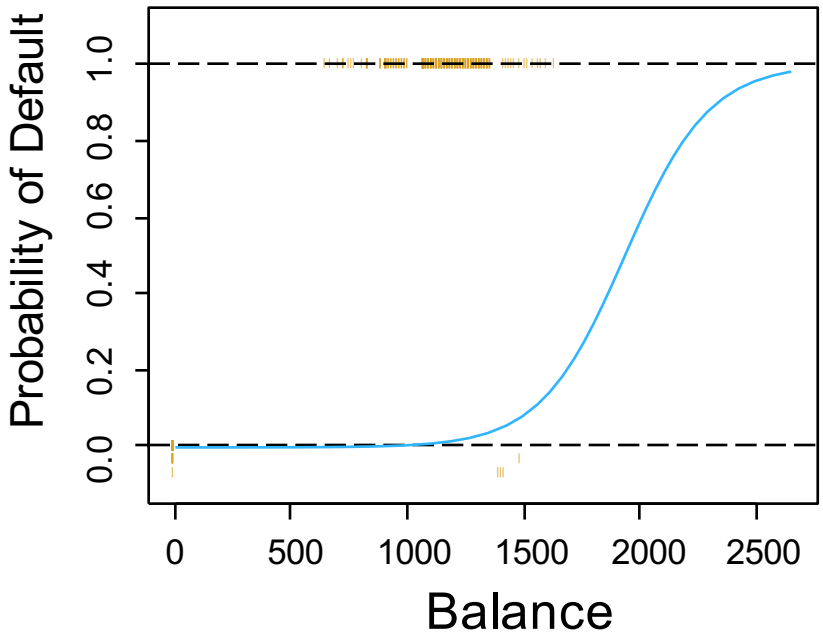
- In this case of a binary outcome, linear regression does a good job as a classifier, and is equivalent to *linear discriminant analysis* which we discuss later.
- Since in the population $E(Y|X = x) = \Pr(Y = 1|X = x)$, we might think that regression is perfect for this task.

# Can we use Linear Regression?

- 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.

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

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.

# Linear Regression continued

- 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.

# Multi-Class and Multi-Label Problems

**Multiclass classification** means a classification task with more than two classes; e.g., classify a set of images of animals which may be horses, birds, or fish.

Multiclass classification makes the assumption that each sample is assigned to one and only one label: an animal can be either a horse or a bird but not both at the same time.

# Multi-Class and Multi-Label Problems

**Multilabel classification** assigns to each sample a set of target labels. This can be thought as predicting properties of a data-point that are not mutually exclusive, such as topics that are relevant for a document.

A text might be about any of religion, politics, finance or education at the same time or none of these.

# Binary Classification

A binary classification task assigns only one of the two possible classes to each observation.

Because multi-class and multi-label classification tasks can be performed using binary classification techniques, many times we focus on binary classification.

# 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

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

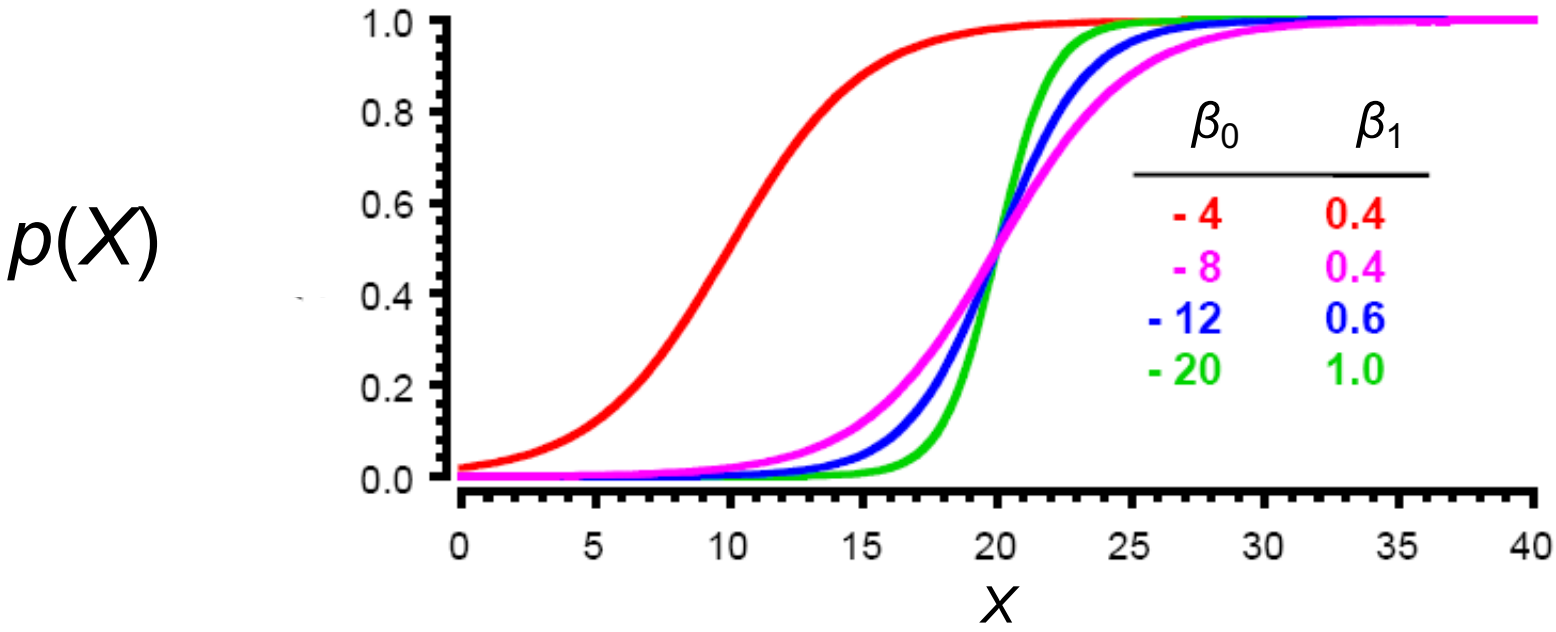
($e \approx 2.71828$ is a mathematical constant [Euler's number.])
It is easy to see that no matter what values $\beta_0$, $\beta_1$ or $X$ take, $p(X)$ will have values between 0 and 1.

# Sigmoid Function

Parameters control shape and location of sigmoid curve

- $\beta_0$ controls location of midpoint
- $\beta_1$ controls slope of rise

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




When x=- $\beta_0$/ $\beta_1$ , $\beta_0$+ $\beta_1$x=0; thus $p(X) = 0.5$

# Logistic Regression

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

A bit of rearrangement gives

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

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

# Definition of Odds

- The probability of an event divided by the probability of its complement is called its odds.
- Example: The probability of winning in a casino is 1%. What is the odds of winning in that casino?

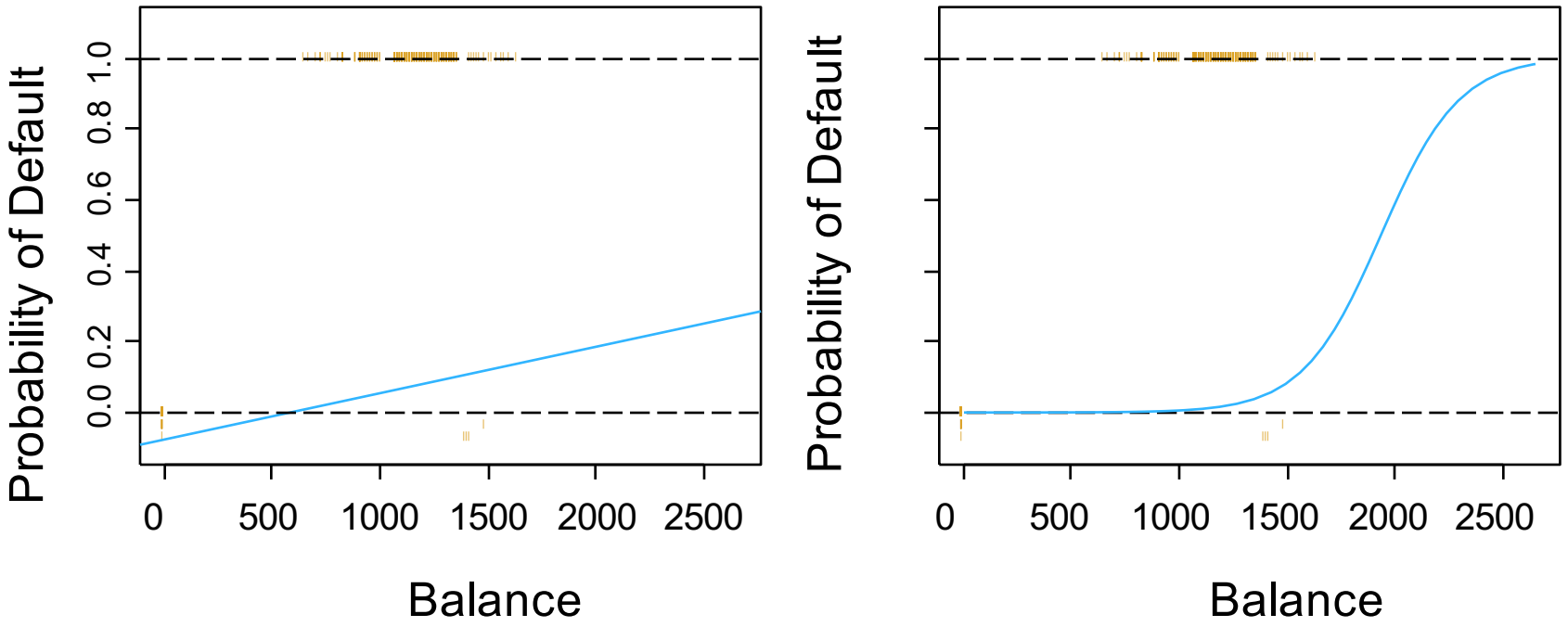
$$O(W)=Pr(W)/(1-Pr(W))$$
$$=0.01/0.99=1/99$$

# Logit Model

Therefore, the logit model is trying to predict the log of odds of a model as a linear combination of the predictor(s):

$$\log(O(Y=1|X=x))=\beta_0+\beta_1 X$$

# Linear versus Logistic Regression




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

# Class as A Bernoulli Random Variable

One can see class in a binary classification problem as a Bernoulli random variable that can take two values 0 and 1:

$$\Pr(Y=1|X=x) = p(x)$$

$$\Pr(Y=0|X=x) = 1-p(x)$$

This can be rewritten as:

$$p_Y(y) = \Pr(Y = y) = [p(x)]^y [1 - p(x)]^{1-y}, y = 0,1$$

# Independent Sample of Bernoulli Variables

Assume that we have an *independent* sample whose classes are $Y_1 = y_1, Y_2 = y_2, \ldots, Y_N = y_N$

The *joint probability mass* function of this independent sample is:

$$p(y_1, y_2, \ldots, y_N) = \Pr(Y = y_1, Y = y_2, \ldots, Y = y_N) =$$

# Independent Sample of Bernoulli Variables

The assumption is that the probability that $Y = y_i$ is a function of the features $X = x_i$

So

# Independent Sample of Bernoulli Variables

The joint probability mass function is a function of $\beta_0$, $\beta_1$ and is called the likelihood function, given the data samples.

# Maximum Likelihood: Simple Example

Your friend gives you a biased coin and tells you that he is sure that the probability of Heads is either 0.1 or 0.5. You flip the coin 100 times and see 90 Heads. What would be your best estimate of the probability of heads, given that you are sure that your friend is right?

# Maximum Likelihood: Simple Example

What would be your best estimate of the probability of heads, given that you are sure that your friend is right?

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This simple example motivates us to estimate parameters from data samples by maximizing their likelihood.

# Maximum Likelihood

We use maximum likelihood to estimate the parameters $\beta_0$, $\beta_1$.

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

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.

# Maximum Likelihood

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

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

# Are the coefficients significant?

- We perform a hypothesis test to see whether $\beta_0$ and $\beta_1$ are significantly different from zero.
- A Z test is used instead of a T test, but the p-value is interpreted similarly
- The p-value for balance is very small, and estimate of $\beta_1$ is positive, so we are sure that if the balance increase, then the probability of default will increase as well.

| | 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 |

# Predictions

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

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

# Predictions

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 |

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

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

# Logistic regression with several variables

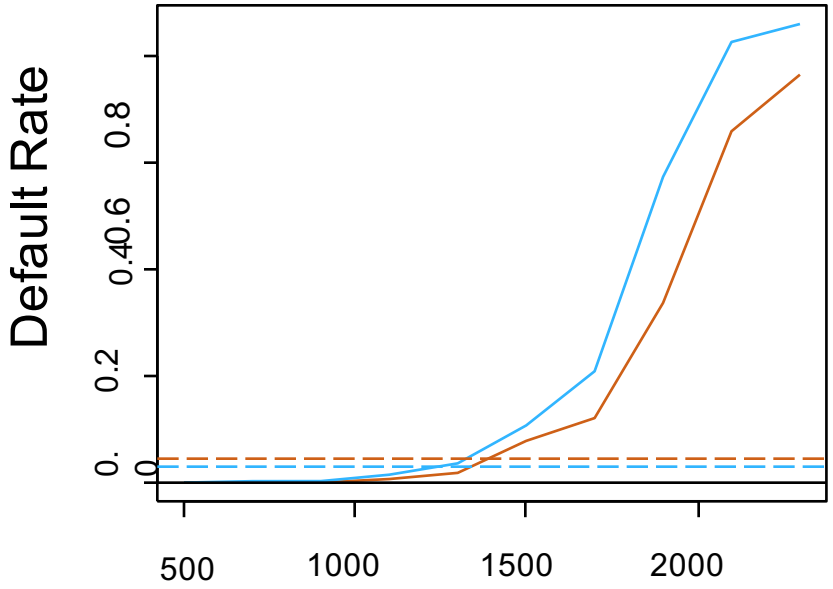
$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$

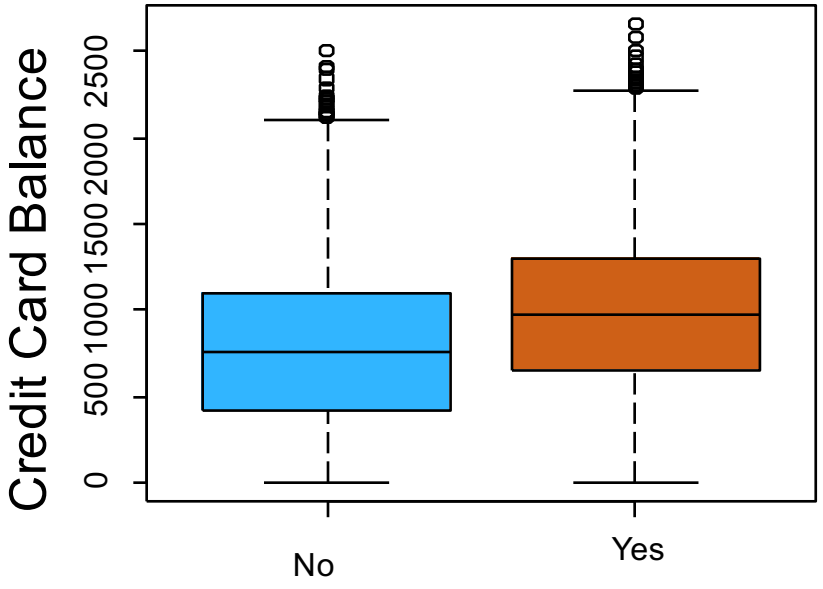
$$p(X) = \frac{e^{\beta_0+\beta_1 X_1+\cdots+\beta_p X_p}}{1+e^{\beta_0+\beta_1 X_1+\cdots+\beta_p X_p}}$$

| | 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?

# 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.

# To whom should credit be offered?

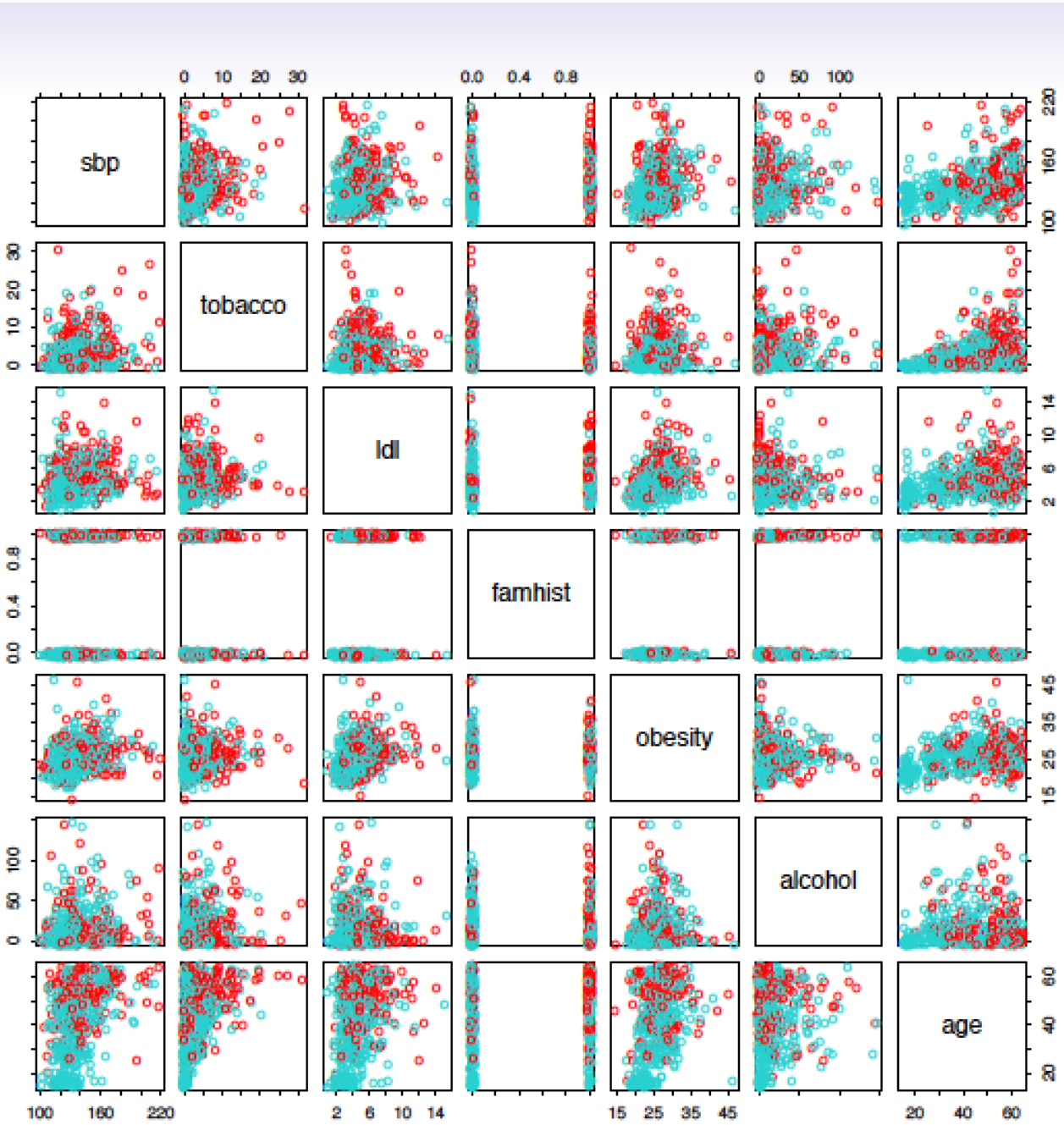
- A student is riskier than non students if no information about the credit card balance is available
- However, that student is less risky than a non student with the same credit card balance!
- Example of data-driven decision-making

# 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%.

# Example: South African Heart Disease

- 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
```

# Class Imbalance

- Intuitively, a dataset is imbalanced when members of certain class(es) are rare.
- The lack of observations of certain classes does not always imply their irrelevance.
- For example, in medical studies of rare diseases, the small number of infected patients (cases) conveys the most valuable information for diagnosis and treatments.

# Types of Imbalance

- Formally, an imbalanced dataset exhibits one or more of the following properties:
  - **Marginal Imbalance**. A dataset is marginally imbalanced if one class is rare compared to the other class. In other words, $\Pr(Y=1) \approx 0$.

# Types of Imbalance

**Marginal Imbalance**.

Such imbalance typically occurs in data sets for predicting click-through rates in online advertising, detecting fraud or diagnosing rare diseases.

# Types of Imbalance

- Formally, an imbalanced dataset exhibits one or more of the following properties:
  - ***Conditional Imbalance***. A dataset is conditionally imbalanced when it is easy to predict the correct labels in most cases. For example, if $X \in \{0,1\}$, the dataset is conditionally imbalanced if $\Pr(Y=1 \mid X=0) \approx 0$ and $\Pr(Y=1 \mid X=1) \approx 1$.

# Subsampling (Down-sampling)

- Typically in such problems, the statistical noise is primarily driven by the number of representatives of the rare class
- We might hope to remedy the problem by subsampling the training set in a way that enriches for the rare class.

# Subsampling (Down-sampling)

However, if the training set is randomly sampled to be balanced, the test set should be sampled to be more consistent with the state of nature and should reflect the imbalance so that honest estimates of future performance can be computed.

# Upsampling

- Ling and Li (1998 ) provide an approach to up-sampling in which cases from the minority classes are sampled with replacement until each class has approximately the same size.
- Some minority class samples may show up in the training set with a fairly high frequency

Ling C, Li C (1998). "Data Mining for Direct Marketing: Problems and solutions." In "Proceedings of the Fourth International Conference on Knowledge Discovery and Data Mining," pp. 73–79.

# SMOTE

- The *synthetic minority over-sampling technique* (SMOTE) is a data sampling procedure that uses both up-sampling and down-sampling, depending on the class
- To up-sample for the minority class, SMOTE synthesizes new cases. To do this, a data point is randomly selected from the minority class and its K -nearest neighbors (KNNs) are determined.

Chawla N, Bowyer K, Hall L, Kegelmeyer W (2002). "SMOTE: Synthetic Minority Over–Sampling Technique." Journal of Artificial Intelligence Research,16 (1), 321–357.

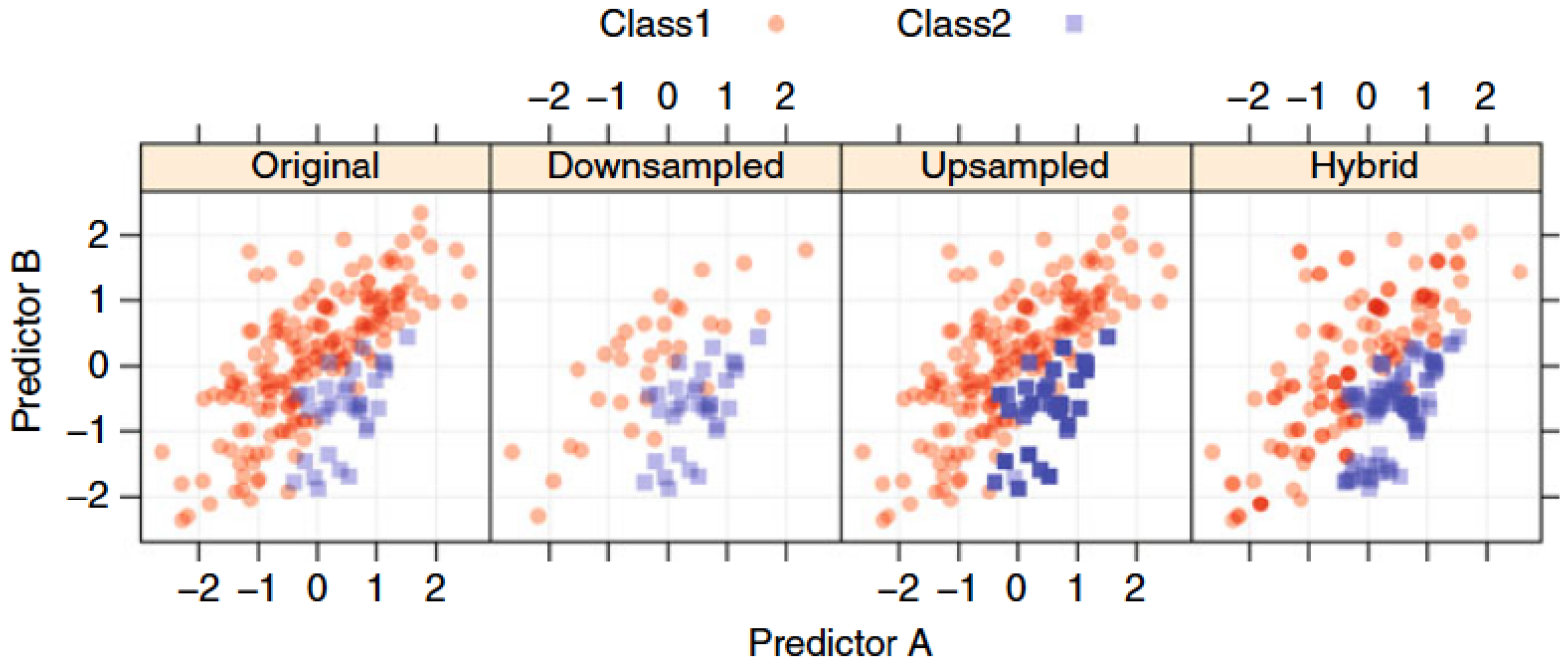
# SMOTE

- The new synthetic data point is a random combination of the predictors of the randomly selected data point and its neighbors.
- SMOTE can down-sample cases from the majority class via random sampling.
- Three operational parameters:
  - the amount of up-sampling,
  - the amount of down-sampling,
  - and the number of neighbors

Chawla N, Bowyer K, Hall L, Kegelmeyer W (2002). "SMOTE: Synthetic Minority Over–Sampling Technique." Journal of Artificial Intelligence Research,16 (1), 321–357.

# SMOTE

From left to right: The original simulated data set and realizations of a down-sampled version, an up-sampled version, and sampling using SMOTE



# 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.

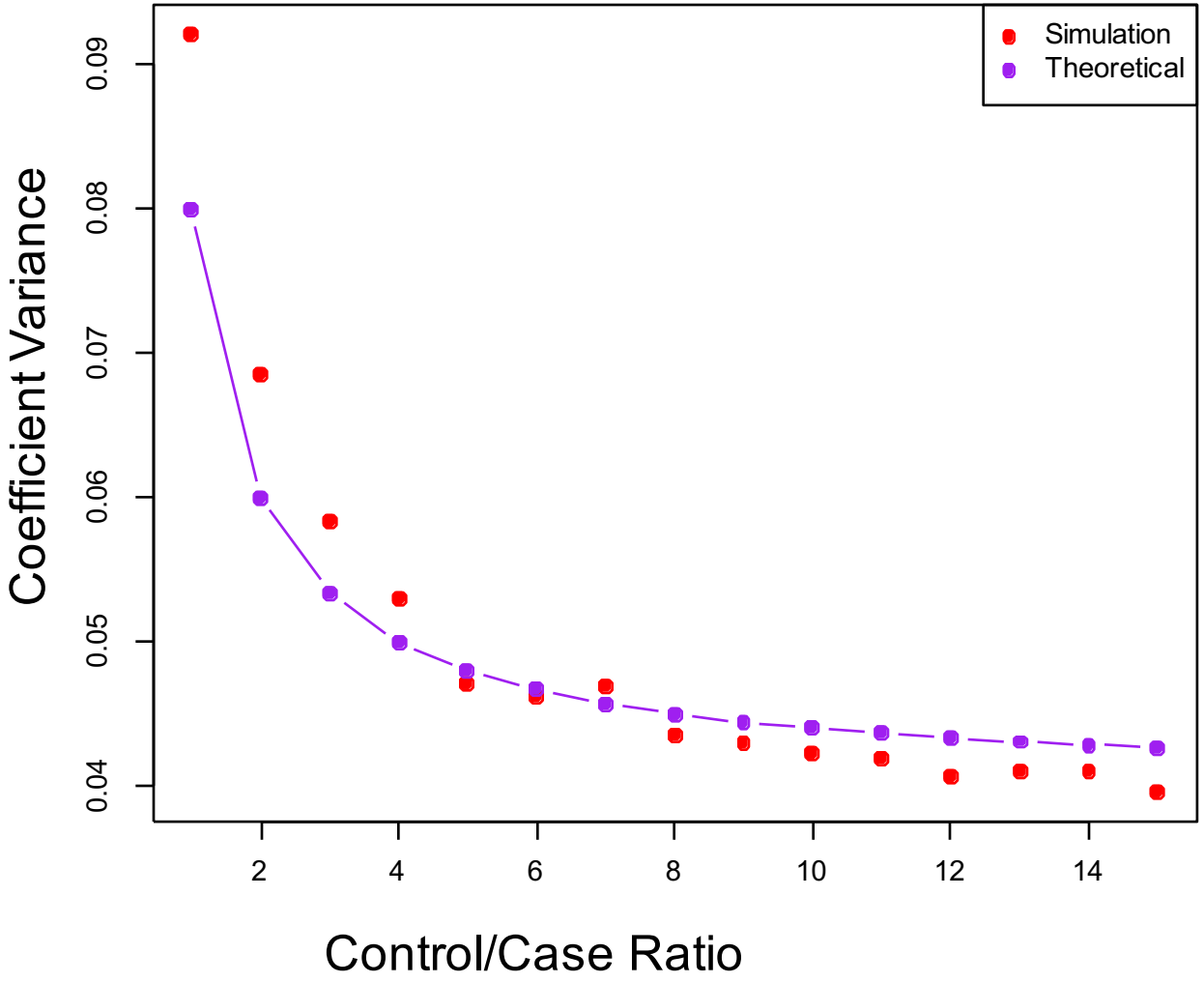
# Case-control sampling and logistic regression

- 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.

# 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

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

# Logistic regression with more than two classes

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

Here there is a linear function for *each* class. (Examine the logit model) Multiclass logistic regression is also referred to as *multinomial regression*.

# Logistic regression with more than two classes

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

The students will recognize that some cancellation is possible, and only $K-1$ linear functions are needed as in 2-class logistic 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.

# 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 probablistic modeling. Here we focus on a simple result, known as Bayes theorem:

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

# Bayes theorem for classification

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

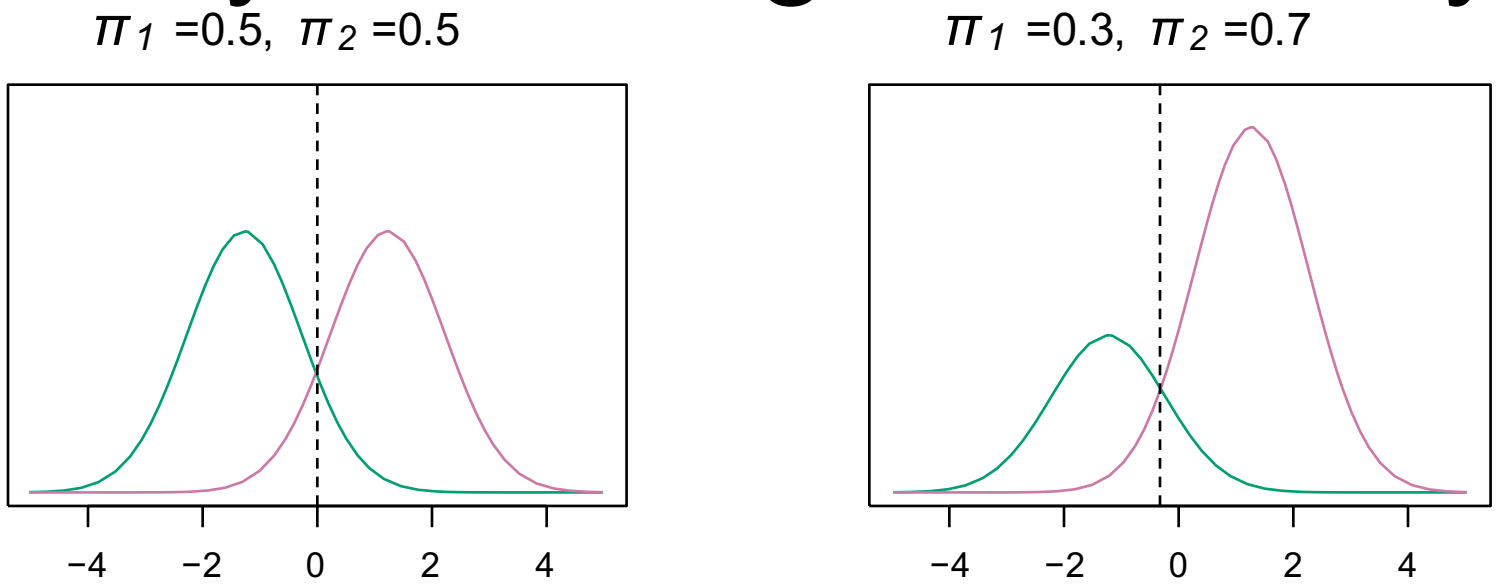
One writes this slightly differently for discriminant analysis:

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

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




- 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?

- 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.

# Why discriminant analysis?

- 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.

# Why discriminant analysis?

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

# Linear Discriminant Analysis when $p = 1$

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

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

Happily, there are simplifications and cancellations.

# Linear Discriminant Analysis when $p = 1$

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

Happily, there are simplifications and cancellations.

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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 $x$.

# Discriminant functions

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

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

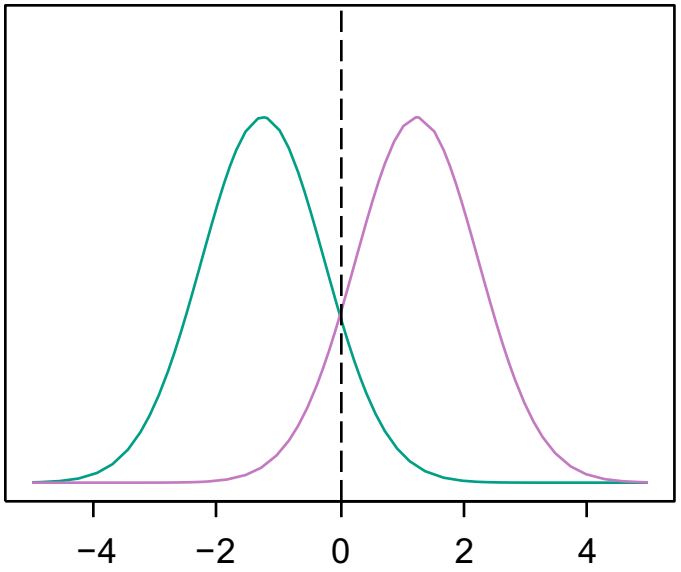
$$x = \frac{\mu_1 + \mu_2}{2}$$

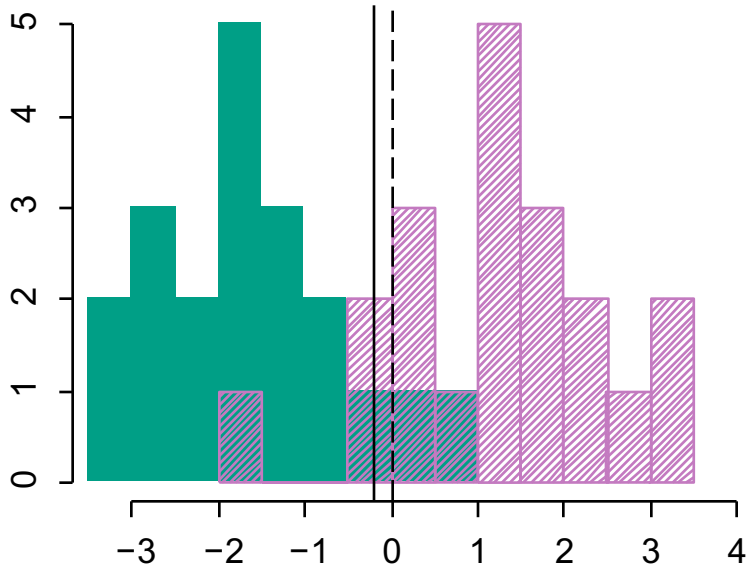
(show this)

# Discriminant functions

(show this)

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




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

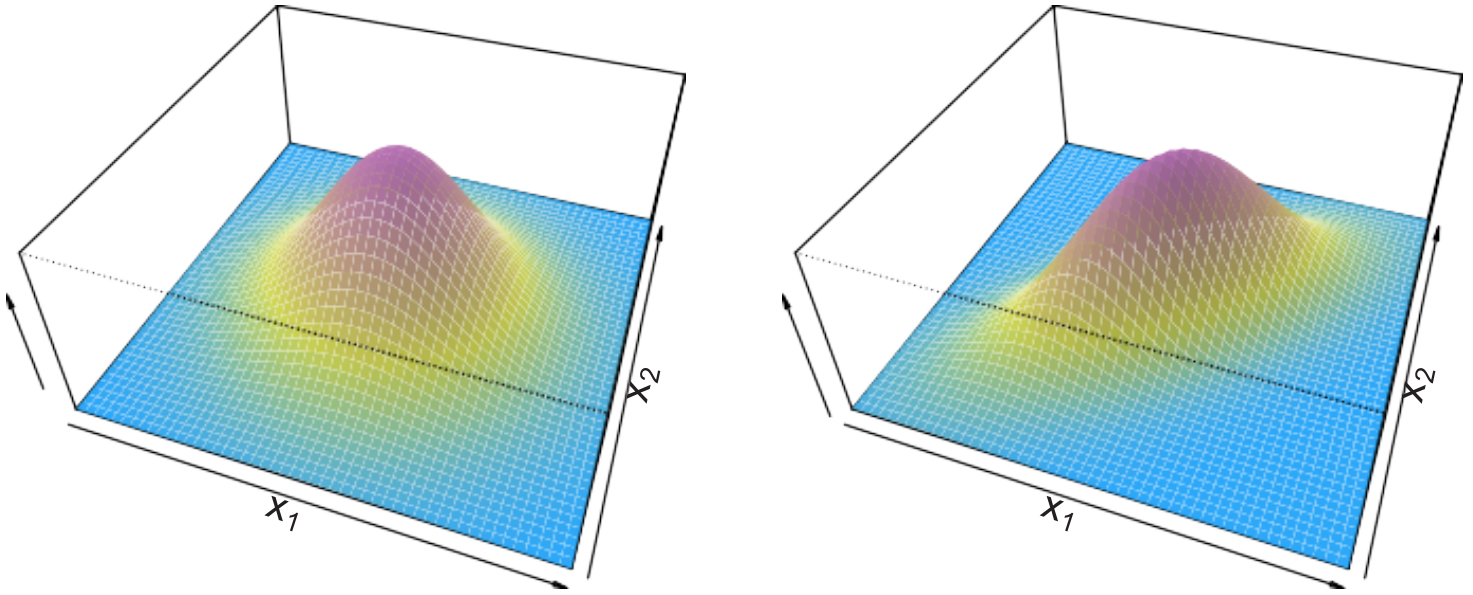
Typically we don't know these parameters; we just have the training data. In that case we simply estimate the parameters and plug them into the rule.

# Estimating the parameters

$$\begin{aligned}
\hat{\pi}_k &= \frac{n_k}{n} \\
\hat{\mu}_k &= \frac{1}{n_k} \sum_{i:\, y_i = k} x_i \\
\hat{\sigma}^2 &= \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:\, y_i = k} (x_i - \hat{\mu}_k)^2 \\
&= \sum_{k=1}^{K} \frac{n_k - 1}{n-K} \cdot \hat{\sigma}_k^2
\end{aligned}$$

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 $p > 1$




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

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

# Linear Discriminant Analysis when $p > 1$

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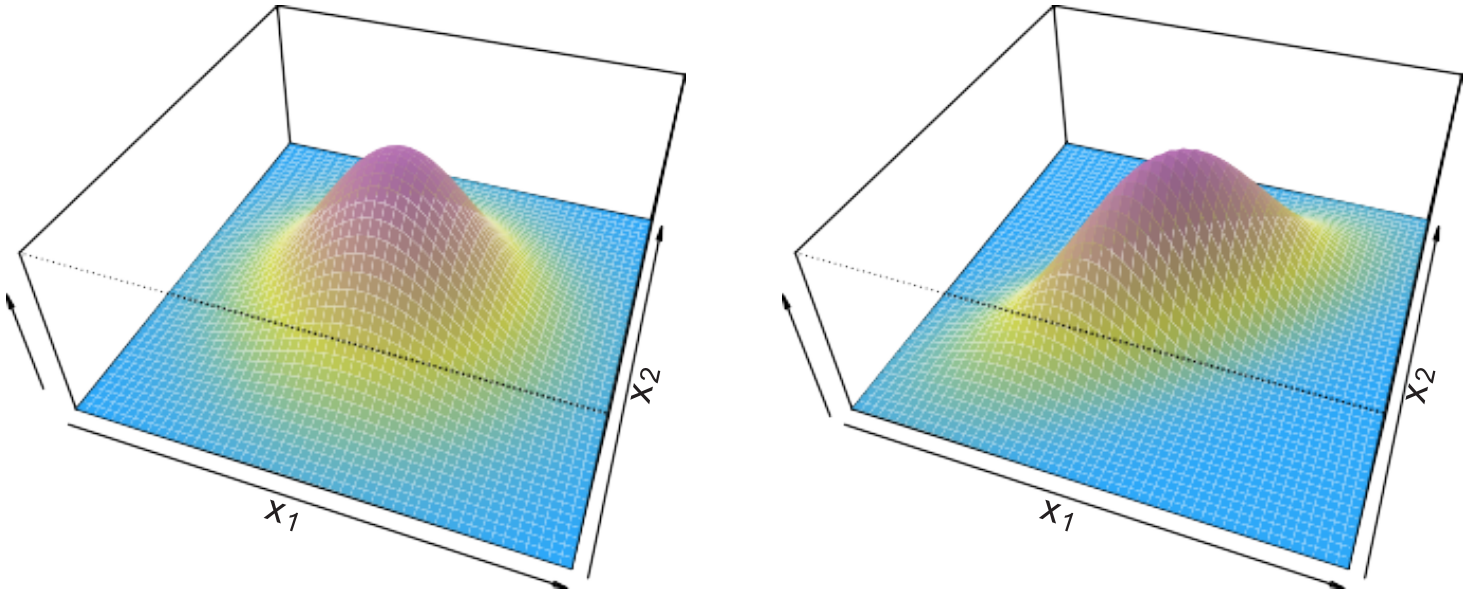
Discriminant function: $\delta_k(x) = x^T \mathbf{\Sigma}^{-1} \mu_k - \frac{1}{2} \mu_k^T \mathbf{\Sigma}^{-1} \mu_k + \log \pi_k$

# Linear Discriminant Analysis when $p > 1$

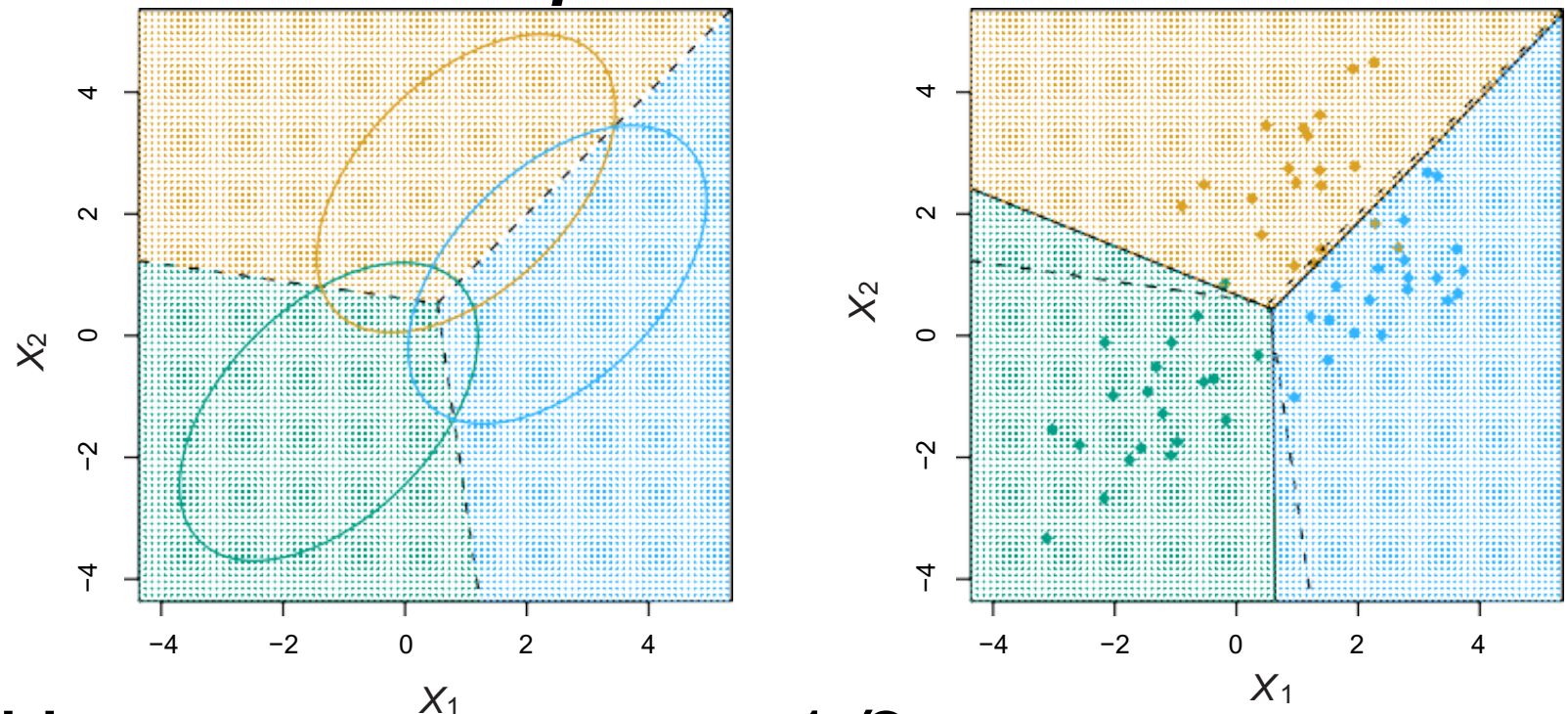



Despite its complex form,

$\delta_k(x) = c_{k0} + c_{k1}x_1 + c_{k2}x_2 + \ldots + c_{kp}x_p$

is a linear function.

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



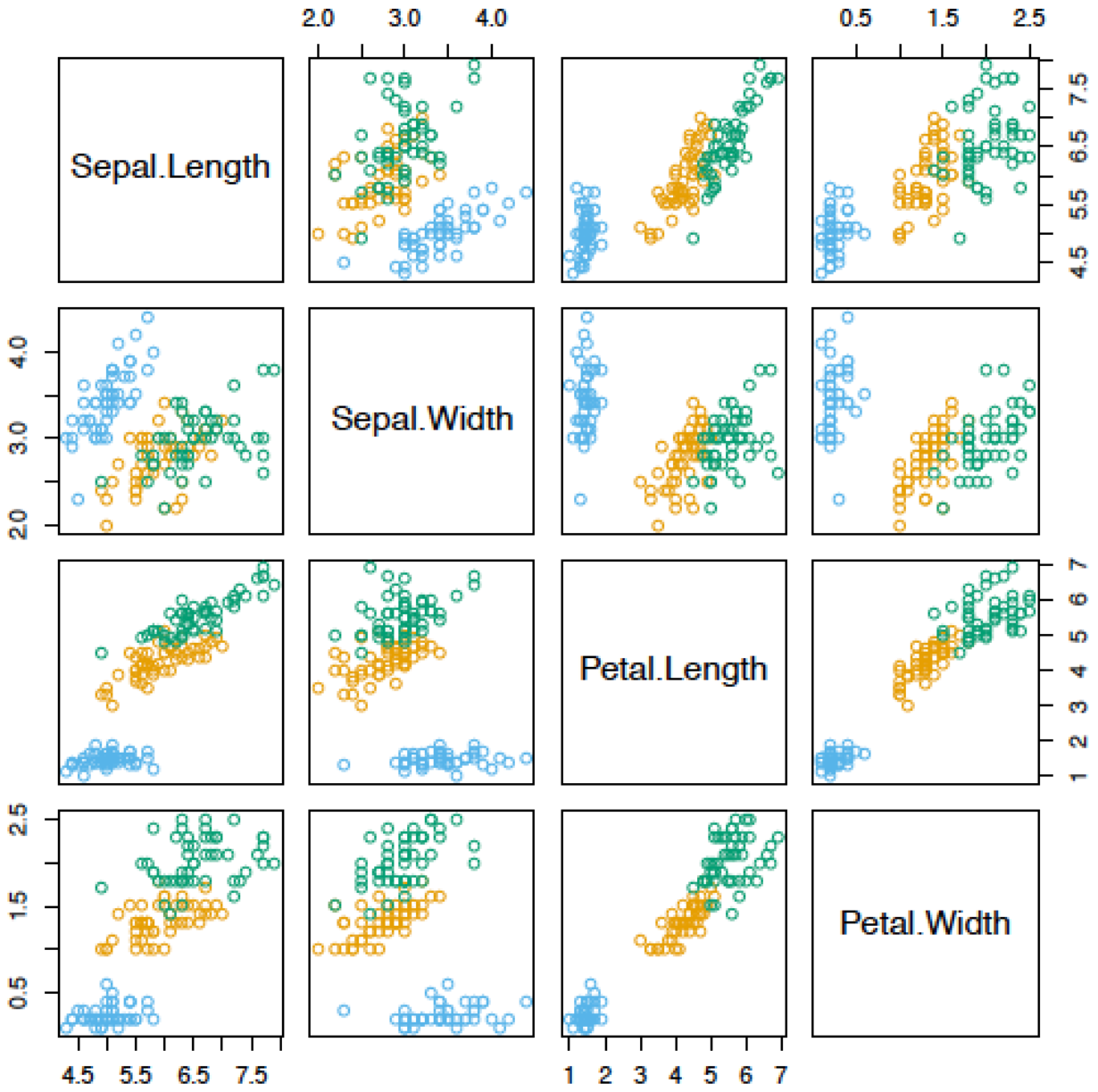

- Here $\pi_1 = \pi_2 = \pi_3 = 1/3$.
- The dashed lines are known as the *Bayes decision boundaries*. Were they known, they would yield the fewest misclassification errors, among all possible classifiers.

# Fisher's Iris Data

4 variables
3 species
50 samples/class

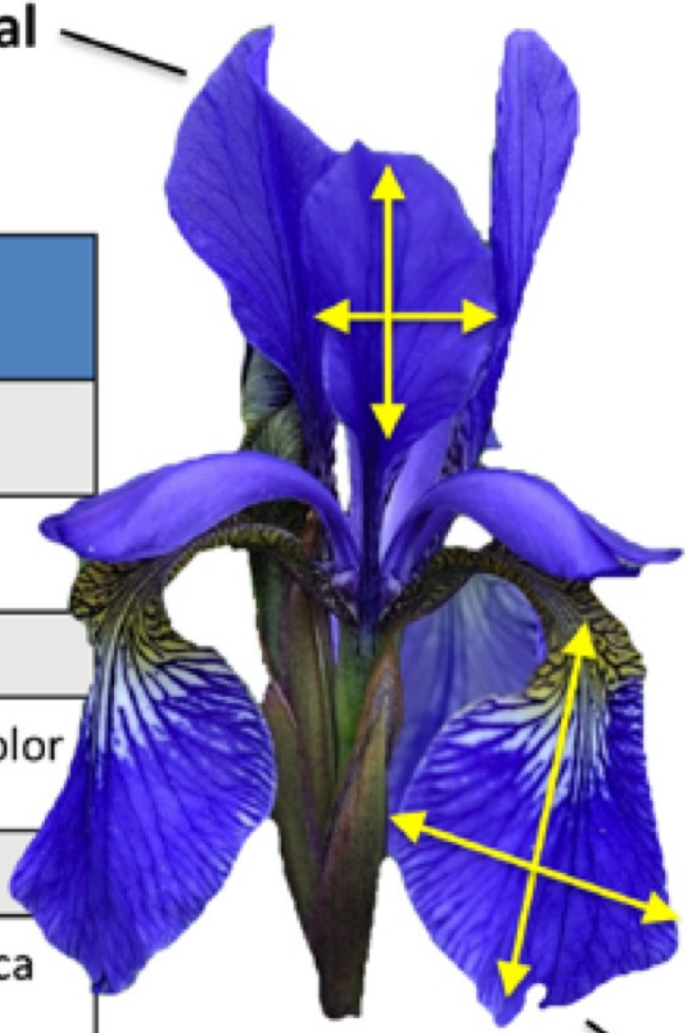
- Setosa
- Versicolor
- Virginica

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



**Samples**
(instances, observations)

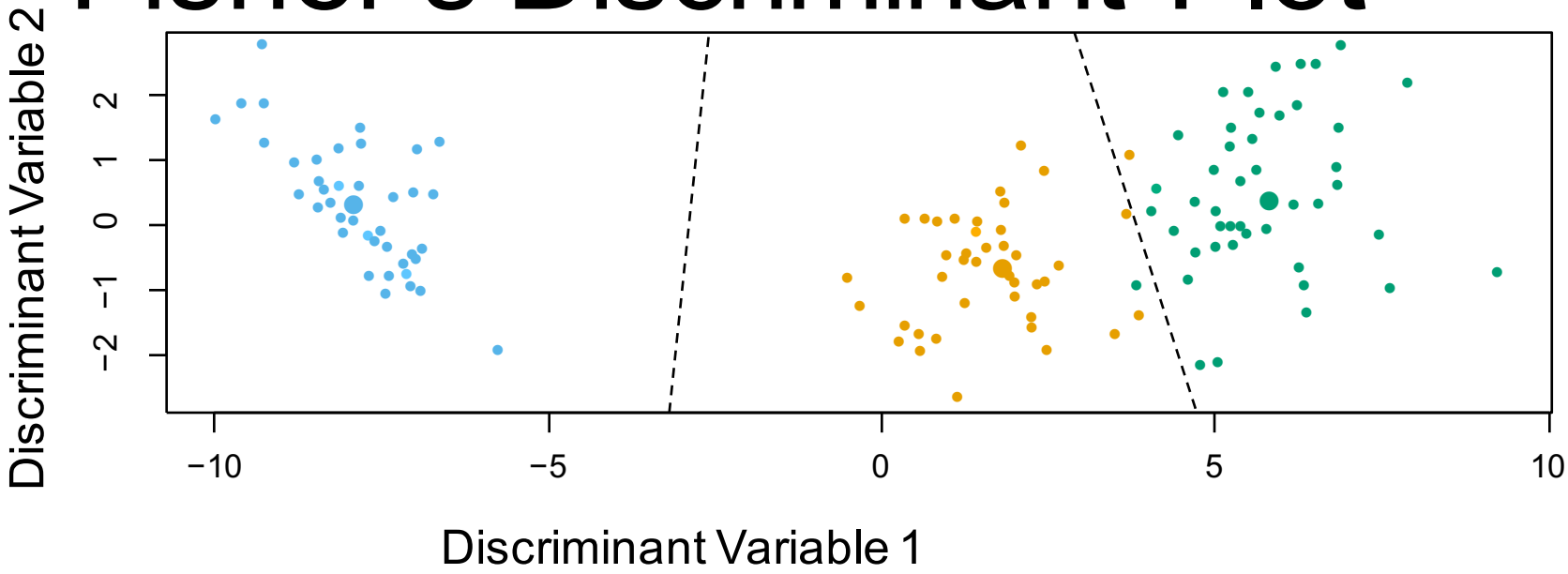
| | Sepal length | Sepal width | Petal length | Petal width | Class label |
|---|---|---|---|---|---|
| 1 | 5.1 | 3.5 | 1.4 | 0.2 | Setosa |
| 2 | 4.9 | 3.0 | 1.4 | 0.2 | Setosa |
| ... | | | | | |
| 50 | 6.4 | 3.5 | 4.5 | 1.2 | Versicolor |
| ... | | | | | |
| 150 | 5.9 | 3.0 | 5.0 | 1.8 | Virginica |




**Features**
(attributes, measurements, dimensions)

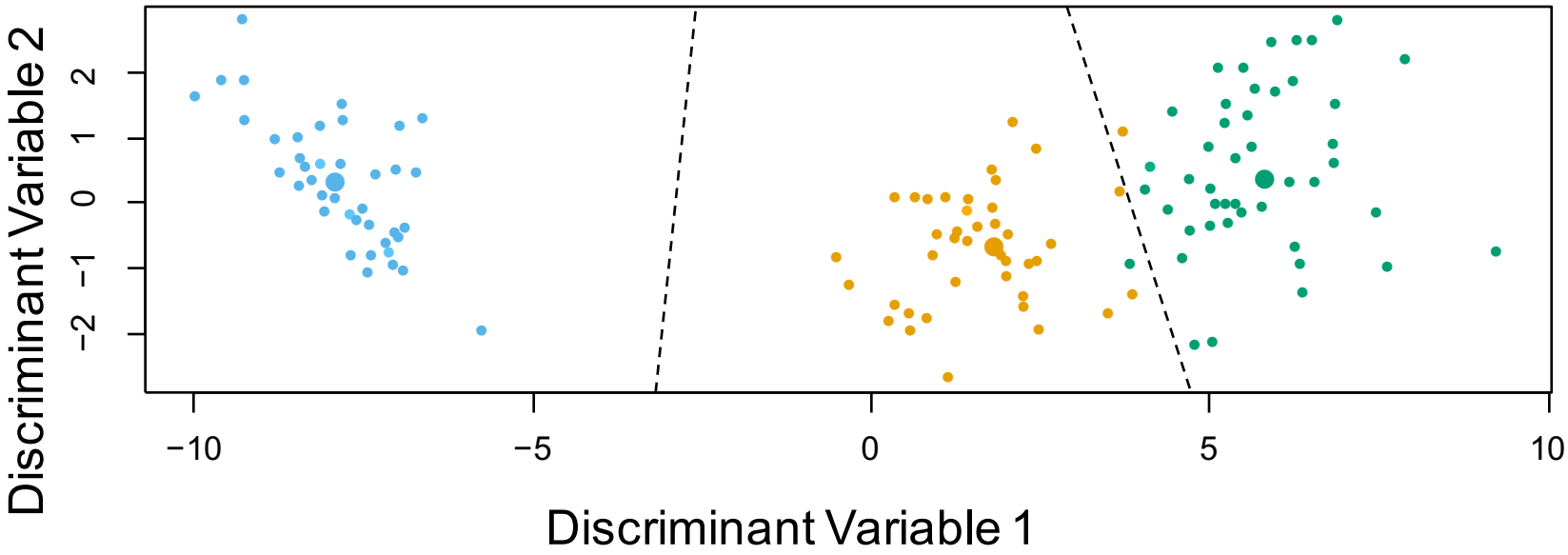
**Class labels**
(targets)

# Fisher's Discriminant Plot




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

# Fisher's Discriminant Plot




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 vizualizing 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:

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

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

# From $\delta_k(x)$ to probabilities

- 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* | | |
|---|---|---|---|---|
| | | 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!

# LDA on Credit Data

**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

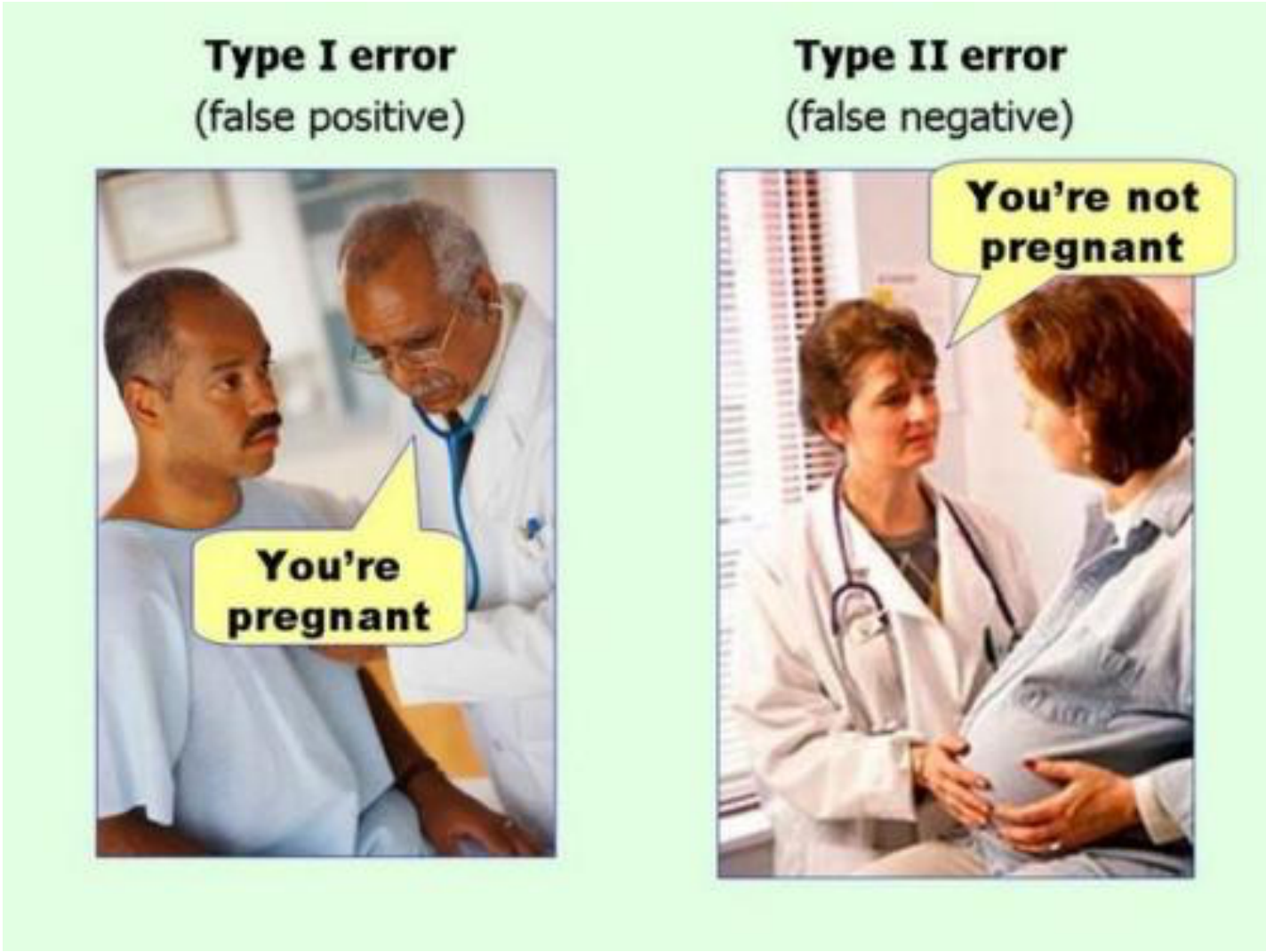
**Some caveats:**

- 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!
- This is because of class imbalance!

# Types of errors

- False positive (type I error) rate: The fraction of negative examples that are classified as positive — 0.2% in example.
- False negative (type II error) rate: The fraction of positive examples that are classified as negative — 75.7% in example.

# Types of errors




https://chemicalstatistician.files.wordpress.com/2014/05/pregnant.jpg?w=500

# Measures for Different Types of Error

The sensitivity or recall of a binary classifier is the rate that the event of interest is predicted correctly for all samples having the event, or

$$TP/P=TP/(TP+FN)$$

It is also called the True Positive Rate (TPR) or Hit Rate (HR).

- What proportion of credit card defaults did we detect?

# Measures for Different Types of Error

The specificity of a binary classifier is the rate that non-events are predicted correctly for all non-event samples or

TN/N=TN/(TN+FP)

It is also called the True Negative Rate (TNR).

- What proportion of credit card non-defaults did we detect?

# Types of errors

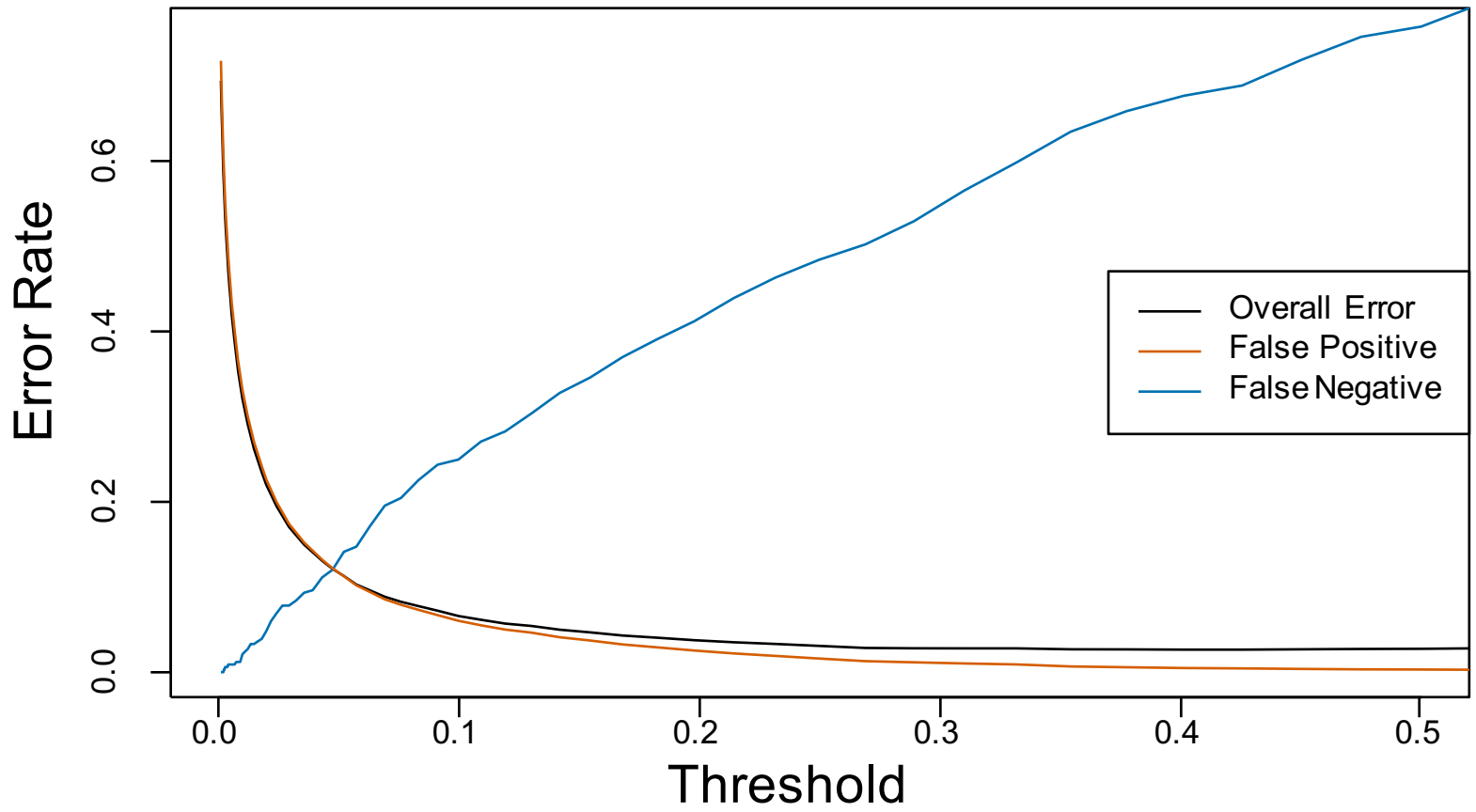
We produced the confusion matrix for credit data by classifying to class Yes if

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

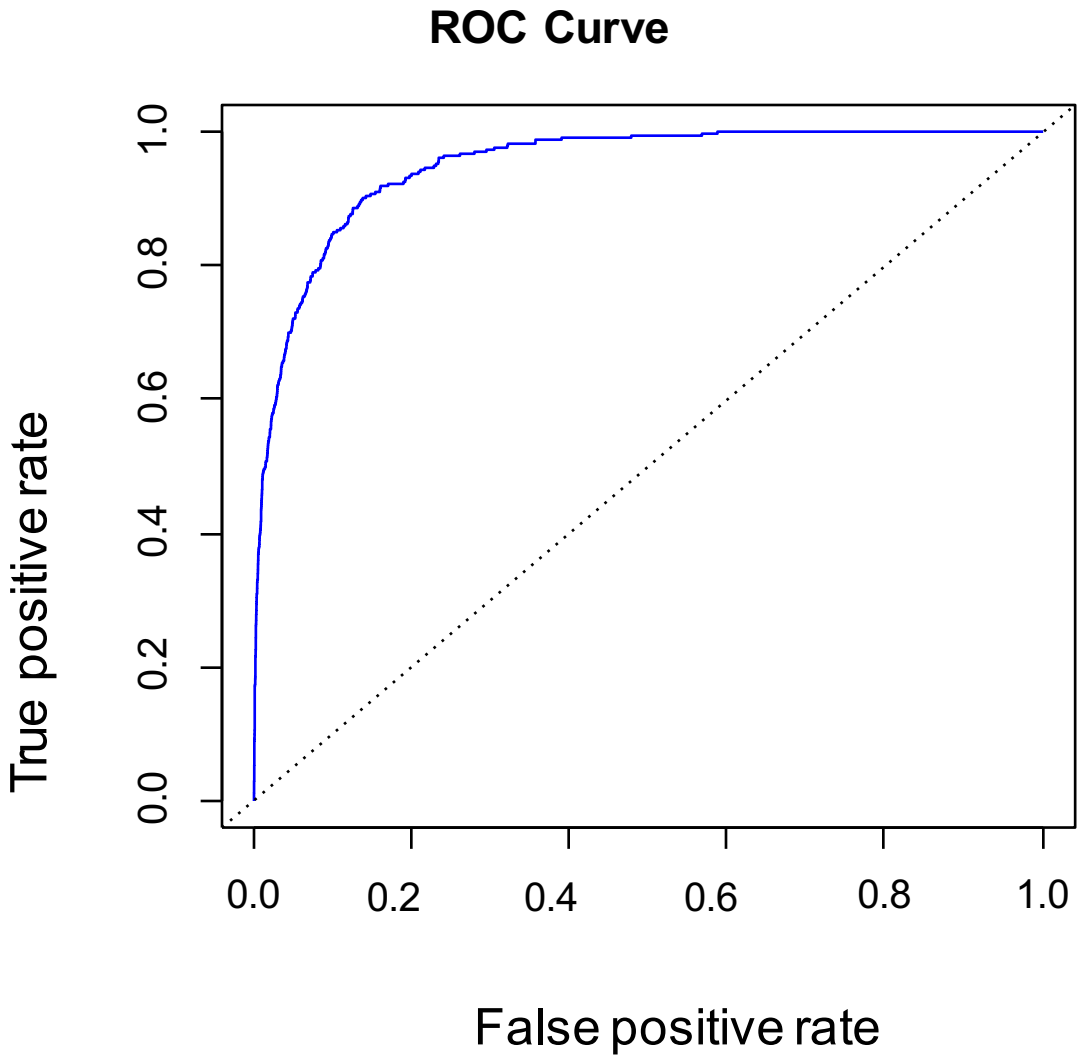
We can change the two error rates by changing the threshold from 0.5 to some other value in [0, 1]:

$\hat{Pr}(\text{Default} = \text{Yes} | \text{Balance}, \text{Student}) \geq$ *threshold*, and vary *threshold*.

# Varying the *threshold*




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




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.

# Measures for Different Types of Error

The precision or the positive predictive value of a binary classifier is the ratio of true positives with respected to all detected positives.

Precision= PPV=TP/(TP+FP)

Of those defaults that we detected, what proportion actually defaulted?

# Measures for Different Types of Error

The negative predictive value of a binary classifier is the ratio of true negatives with respect to all detected negatives.

NPV=TN/(TN+FN)

Of those non-defaults that we detected, what proportion actually did not default?

# Measures for Different Types of Error

The F1 score or F measure of a binary classifier is the harmonic mean of precision and recall:

$$F = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

# Measures for Different Types of Error

F1 Score: seeks a balance between Precision (ratio of true positives to all detected positives) and Recall (True Positive Rate).

F1 Score might be better than accuracy if we seek a balance between Precision and Recall AND there is a class imbalance (large number of Actual Negatives).

# Measures: Training or Testing?

Note that all of the measures used to evaluate types of error can be computed over both training and test sets.

# 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 $\mathbf{\Sigma}$ 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 $\mathbf{\Sigma}_k$ in each class, we get *quadratic discriminant analysis*.

# Other forms of Discriminant Analysis

- With Gaussians but different $\boldsymbol{\Sigma}_k$ in each class, we get *quadratic discriminant analysis*. Let's show it for $p$=1.

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

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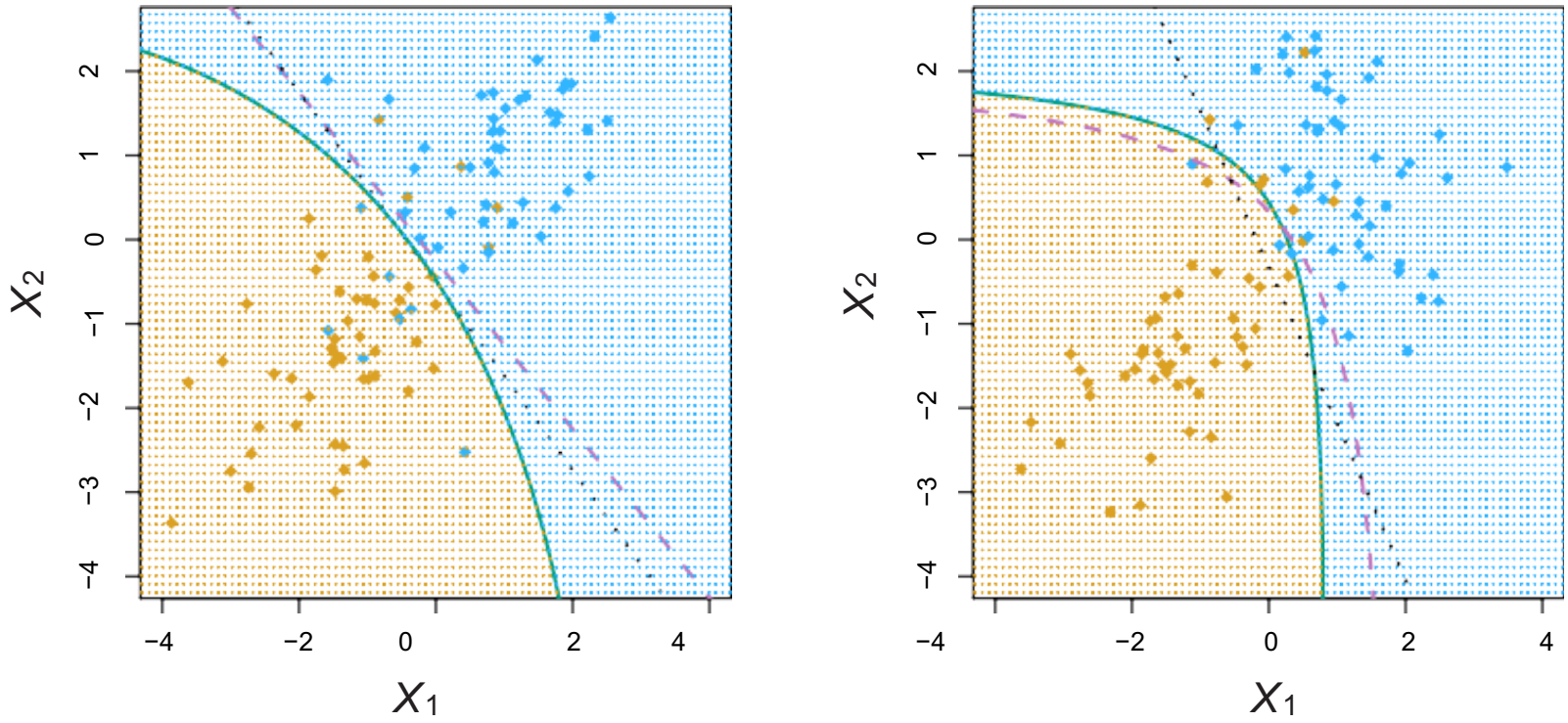
# Other forms of Discriminant Analysis

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

- With $f_k(x) = \prod_{j=1}^{p} f_{jk}(x_j)$ (conditional independence model) in each class we get *naïve Bayes*. For Gaussian this means the $\mathbf{\Sigma}_k$ are diagonal.
- Many other forms, by proposing specific density models for $f_k(x)$, including nonparametric approaches.

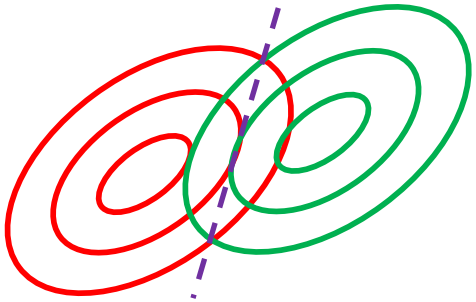
# Quadratic Discriminant Analysis



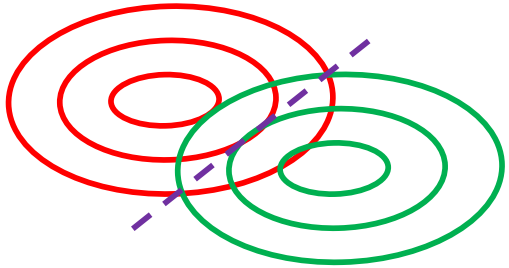

$$\delta_k(x) = -\frac{1}{2}(x-\mu_k)^T\mathbf{\Sigma}_k^{-1}(x-\mu_k) + \log\pi_k$$

Because the $\mathbf{\Sigma}_k$ are different, the quadratic terms matter.

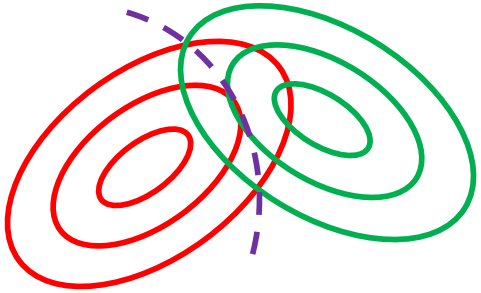
# Models for Class Covariances



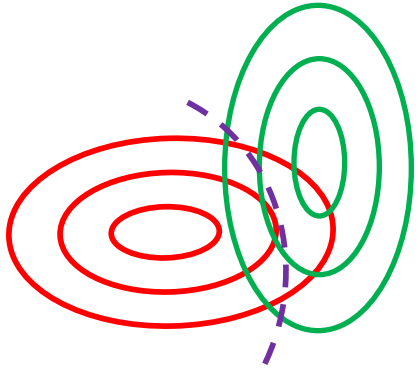
`'linear'`:
all classes have same covariance matrix $\boldsymbol{\Sigma}_k$
linear decision boundary



`'diaglinear'`:
all classes have same diagonal covariance matrix $\boldsymbol{\Sigma}_k$
linear decision boundary



`'quadratic'`:
classes have different covariance matrices $\boldsymbol{\Sigma}_k$
quadratic decision boundary



`'diagquadratic'`:
classes have different diagonal covariance matrices $\boldsymbol{\Sigma}_k$
quadratic decision boundary

# Logistic Regression versus LDA

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

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

So it has the same form as logistic regression.

The difference is in how the parameters are estimated.

# Logistic Regression versus LDA

.

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.

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 $K > 2$.
- Naïve Bayes is useful when $p$ is very large.
- See Section 4.5 for some comparisons of logistic regression, LDA and KNN.

# Naïve 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 naïve Bayes assumes each $\mathbf{\Sigma}_k$ is diagonal:

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

- 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, naïve Bayes often produces good classification results.

# Bayesian: Classify to the highest density

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

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

- $f_k(x) = \Pr(X = x|Y = k)$ 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 $k$.

# Bayesian: Classify to the highest density

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

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

- 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

$\pi_k f_k(x) = \Pr(Y = k) \Pr(X = x|Y = k)$ .

# Bayesian classifiers

Easy to estimate priors $\pi_k$ from data. (*How?*)
The real challenge: how to estimate
$f_k(x) = \Pr(X = x | Y = k)$
$= \Pr(X = (x_1, x_2, \ldots, x_p) | Y = k)$

# Bayesian classifiers

How to estimate
$f_k(x_1, x_2, \ldots, x_p) = \Pr(X = (x_1, x_2, \ldots, x_p) | Y = k)$

- In the general case, where the attributes $x_j$ have dependencies, this requires estimating the full joint distribution $f_k(x_1, x_2, \ldots, x_p)$ for each class $k$ in $C$.
- There is almost never enough data to confidently make such estimates.

# Naïve Bayes classifier

Assume independence among attributes $x_j$ when class is given:

$$f_k(x_1, x_2, \ldots, x_p) = f_k(x_1)\ f_k(x_2)\ \ldots\ f_k(x_n)$$

Usually straightforward and practical to estimate $f_k(x_i) = \Pr(X_i = x_i | Y = k)$ for all $x_j$ and $k$.

New sample is classified to $Y=k$ if

$$\pi_k \prod_i f_k(x_i) \text{ is maximal.}$$

# How to estimate $f_k(x_i) = \Pr(X_i = x_i | Y = k)$ from data?

| *Tid* | Refund | Marital Status | Taxable Income | Evade |
|---|---|---|---|---|
| 1 | Yes | Single | 125K | No |
| 2 | No | Married | 100K | No |
| 3 | No | Single | 70K | No |
| 4 | Yes | Married | 120K | No |
| 5 | No | Divorced | 95K | Yes |
| 6 | No | Married | 60K | No |
| 7 | Yes | Divorced | 220K | No |
| 8 | No | Single | 85K | Yes |
| 9 | No | Married | 75K | No |
| 10 | No | Single | 90K | Yes |

Class priors:

$\pi\hat{}_k = N_k / N$

$\pi$ ( No ) = 7/10

$\pi$ ( Yes ) = 3/10

For discrete attributes:

$\Pr\hat{}$ ( $X_i = x_i$ | Y=$k$ ) = | $x_{ik}$ | / $N_k$

where | $x_{ik}$ | is number of instances in class $k$ having attribute value $x_i$

Examples:

$\Pr\hat{}$( Status = Married | No ) = 4/7

$\Pr\hat{}$ ( Refund = Yes | Yes ) = 0

# How to estimate $f_k(x_i)$ from data?

For continuous attributes:

Discretize the range into bins

replace with an ordinal attribute

Two-way split: ( $x_i$ < v ) or ( $x_i$ > v )

replace with a binary attribute

Probability density estimation:

- assume attribute follows some standard parametric probability distribution (usually a Gaussian)
- use data to estimate parameters of distribution (e.g. mean and variance)
- once distribution is known, can use it to estimate the conditional probability $\Pr(X_i = x_i | Y = k)$

# How to estimate $f_k(x_i)$ from data?

| Tid | Refund | Marital Status | Taxable Income | Evade |
|---|---|---|---|---|
| 1 | Yes | Single | 125K | No |
| 2 | No | Married | 100K | No |
| 3 | No | Single | 70K | No |
| 4 | Yes | Married | 120K | No |
| 5 | No | Divorced | 95K | Yes |
| 6 | No | Married | 60K | No |
| 7 | Yes | Divorced | 220K | No |
| 8 | No | Single | 85K | Yes |
| 9 | No | Married | 75K | No |
| 10 | No | Single | 90K | Yes |

Gaussian distribution:

$$f_k(x_i) = \Pr(X_i = x_i | Y = k) = \frac{1}{\sqrt{2\pi\sigma_{ik}}} e^{-\frac{(x_i - \mu_{ik})^2}{2\sigma_{ik}}}$$

one for each ( $x_i$, $k$ ) pair

For ( Income | Class = No ):

sample mean = 110

sample variance = 2975

$$\Pr(\text{Income} = 120 \mid \text{No}) = \frac{1}{\sqrt{2\pi}(54.54)} e^{-\frac{(120-110)^2}{2(2975)}} = 0.0072$$

# Naïve Bayes classifier

Problem: if one of the conditional probabilities is zero, then the entire expression becomes zero.

This is a significant practical problem, especially when training samples are limited.

Ways to improve probability estimation:

$$\text{Original}: p(x_j \mid C_i) = \frac{N_{ji}}{N_i}$$

$$\text{Laplace}: p(x_j \mid C_i) = \frac{N_{ji} + 1}{N_i + c}$$

$$\text{m-estimate}: p(x_j \mid C_i) = \frac{N_{ji} + mp}{N_i + m}$$

c: number of levels in class $C_i$

p: prior probability

m: parameter

# Summary of Naïve Bayes

Robust to isolated noise samples.

Handles missing values by ignoring the sample during probability estimate calculations.

Robust to irrelevant attributes.

*NOT* robust to redundant attributes.

- Independence assumption does not hold in this case.
- Use other techniques such as Bayesian Belief Networks (BBN).