

# Introduction to Statistical Learning *with applications in Python*

*Based on “Introduction to Statistical Learning, with applications in R” by Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani*

## Statistical Learning

*what is it?, models, regression, classification, prediction, inference, accuracy, bias, variance*

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# Abstract

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We give a number of examples illustrating what statistical learning is about.

The emphasis is not on particular methods but on the foundational concepts.

# Overview

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- Models
- Prediction & inference
- Accuracy & interpretability
- Bias & Variance
- Regression & classification

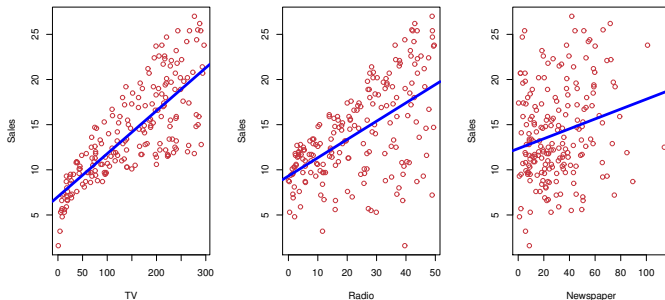
**This sets the stage for the remainder of the course.**

## Example: Advertising

- We are hired to increase the sales of a particular product.
- We are given the **Advertising** data set.
  - **sales** for 200 different markets.
  - advertising budgets for **TV**, **radio** and **newspaper**.
- Our clients can *not directly* influence the sales.
- But they *can* control the advertising budgets.
- We need to determine whether there is an association between advertising and sales.

**This is a typical scenario.**

# Example: Advertising



- The plots display **sales** as a function of the advertising budgets.
- Each plot is a *scatter plot* of **sales** versus a budget.
- We have overlaid a *least squares line* fit on each plot.

**We can already spot some promising relationships.**

## Example: Advertising

- The advertising budgets are *input variables*.
- We denote the input variables with  $X$ .
- We use subscripts to distinguish them.
- For example,  $X_1 = \text{TV}$ ,  $X_2 = \text{radio}$ ,  $X_3 = \text{newspaper}$ .
- The input variables are also called *predictors*, *independent variables*, *features* or simply *variables*.
- $\text{sales}$  is the *output variable*.
- Output variables are also called *dependent variables* or *responses*.
- We denote the output variables with  $Y$ .

**Don't get confused by different names.**

# Models

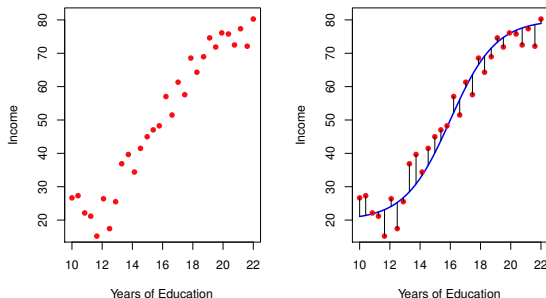
- Suppose we observe a *quantitative* response  $Y$ , and  $p$  different predictors,  $X_1, X_2, \dots, X_p$ .
- We assume that there is some relationship between  $Y$  and  $X$ .
- We can write this in the very general form

$$Y = f(X) + \epsilon$$

- Here  $f$  is a fixed but unknown function of  $X = (X_1, X_2, \dots, X_p)$ .
- And  $\epsilon$  is a random error term, independent of  $X$  with mean zero.
- We say  $f$  represents the *systematic* information that  $X$  provides about  $Y$ .

**This is the most general form of a *model*.**

## Example: Income

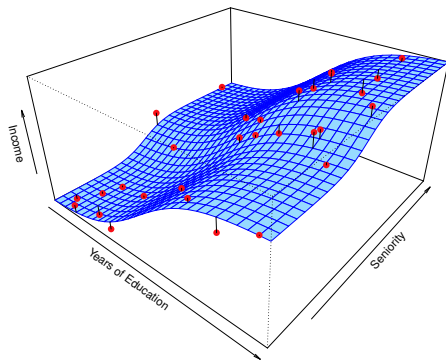


- The figure shows a scatter plot of **income** versus **years of education**.
- The blue curve is the true functional relationship  $f(X) = f(X_1)$ .
- The vertical lines represent the error terms  $\epsilon$ .

**This is a simulated data set.**



## Example: Income



- The figure shows a 3D scatter plot of **income** versus **years of education** and **seniority**.
- The blue surface is the true functional relationship  $f(X) = f(X_1, X_2)$ .
- The vertical lines represent the error terms  $\epsilon$ .

**Visualising higher dimensions is hard.**

# What is Statistical Learning?

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In essence, statistical learning refers to a set of approaches for estimating the function  $f$ .

In this lecture we cover the key theoretical concepts that arise in estimating  $f$ , as well as techniques for evaluating the estimates obtained.

**This equally applies to machine learning.**

## Why estimate $f$ ?

There are two main reasons why we wish to estimate  $f$ .

1. *Prediction*: assuming the inputs  $X$  are readily available, we simply want to predict

$$\hat{Y} = \hat{f}(X)$$

without being interested in the exact form of  $\hat{f}$ .

2. *Inference*: we want to understand the functional relationship

$$Y = Y(X_1, X_2, \dots, X_p)$$

between the predictors and the response.

**We discuss each in more detail.**

## Prediction

- Often the inputs  $X$  are readily available but the response  $Y$  is not.
- Since the error term  $\epsilon$  averages to zero, we can then predict

$$\hat{Y} = \hat{f}(X)$$

where  $\hat{f}$  represents the estimate of  $f$  and  $\hat{Y}$  is the resulting prediction of  $Y$ .

- In this scenario we are not interested in the exact form of  $\hat{f}$ .
- We are mostly concerned with the accuracy of  $\hat{Y}$ .

Here  $\hat{f}$  is often treated as a *black box*. But we don't have to!

# Prediction Accuracy

- The accuracy of  $\hat{Y}$  depends on two quantities:
  1. the *reducible error*
  2. the *irreducible error*
- The reducible error is due to  $\hat{f}$  not being a perfect estimate of  $f$ .  
(We can potentially come up with better statistical learning techniques to improve  $\hat{f}$ ).
- Even if our estimate of the relationship was perfect ( $\hat{f} = f$ ),  
our estimate  $\hat{Y}$  would still have an error!
- This irreducible error is due to our *observations* not being perfect.  
(The error term  $\epsilon$ ).

You have to understand what you can improve and what you can't.

## Prediction Accuracy

- Assuming that  $\hat{f}$  and  $X$  are fixed, we can show that

$$\begin{aligned} E[(Y - \hat{Y})^2] &= E[(f(X) + \epsilon - \hat{f}(X))^2] \\ &= \underbrace{E[(f(X) - \hat{f}(X))^2]}_{\text{Reducible}} + \underbrace{\text{Var}(\epsilon)}_{\text{Irreducible}} \end{aligned}$$

where  $E[(Y - \hat{Y})^2]$  is the average, or *expected value*, of the squared difference between the predicted and the true value of  $Y$ , and  $\text{Var}(\epsilon)$  is the *variance* of the error term  $\epsilon$ .

- The average, or expected value,  $E[z]$  is often written as  $\bar{z}$  or  $\langle z \rangle$ .
- The variance is then  $\text{Var}(z) = \langle (z - \bar{z})^2 \rangle = \langle z^2 \rangle - \langle z \rangle^2 = \overline{z^2} - \bar{z}^2$ .

**All techniques we learn aim to estimate  $f$  while minimising the reducible error.**

# Inference

- We are often interested in *how*  $X_1, X_2, \dots, X_p$  affect  $Y$ .
- We want to estimate  $f$ , but not necessarily predict  $Y$ .
- The aim is to understand the *functional relationship* between  $Y$  and  $X$ .

**We can *not* treat  $\hat{f}$  as a black box in this scenario.**

## Inference: Questions

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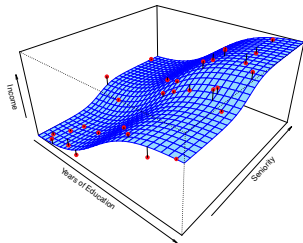
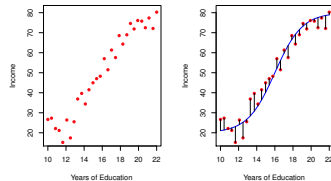
- *Which predictors are associated with the response?*  
We want to identify the *important* predictors.
- *What is the relationship between the response and each predictor?*  
For example, predictors can have positive or negative influence on the response. Any functional relationship can occur, possibly depending on the values of the other predictors.
- *Can the relationship between  $Y$  and each predictor be summarised as a linear equation?*  
It greatly simplifies things when the relationship can be captured by a linear model. Historically, models have been mostly chosen to be linear. However, the true relationships are very rarely linear.

**Linear is good, but rarely true.**



# How do we estimate $f$ ?

- We have  $n$  observations of  $X$  and  $Y$ .
- In the plots on the right  $n$  is 30.
- This is the *training data*.
- We use these observations to *train*, or *teach*, our model how to estimate  $f$ .
- The goal is to find a function  $\hat{f}$  such that  $Y \approx \hat{f}(X)$ , for each observation  $(X, Y)$ .



Statistical learning methods are either *parametric* or *non-parametric*.

# Parametric Methods

1. *Make an assumption about the functional form of  $f$ .*

A very simple assumption is a linear model:

$$f(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$$

With a linear model we only need to estimate  $p + 1$  parameters.

We will cover linear models in great detail in the next lecture.

2. *Use the training data to train, or fit, the model.*

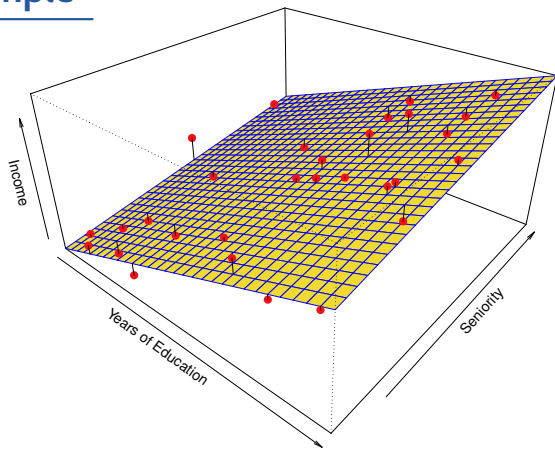
For a linear model we need to estimate the parameters

$\beta_0, \beta_1, \beta_2, \dots, \beta_p$  such that:

$$Y \approx \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \cdots + \hat{\beta}_p X_p$$

**Non-linear models are of course possible, but harder to fit.**

# Linear Model Example



$$\text{income} \approx \hat{\beta}_0 + \hat{\beta}_1 \times \text{years of education} + \hat{\beta}_2 \times \text{seniority}$$

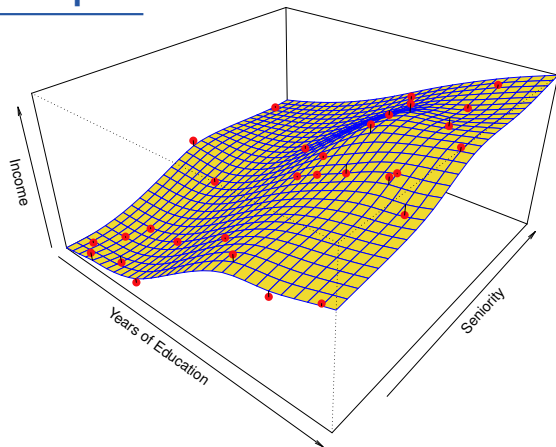
# Non-parametric Methods

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1. *No assumption about the functional form of  $f$  is made.*
  2. *Seek an estimate of  $f$  that smoothly approaches the data points in the training data.*
- + Avoids choosing potentially very wrong models.
  - + Can approximate complex functional relationships.
  - Often needs many more observations for the fit.
  - Prone to over-fitting.

**Oddly, non-parametric methods can have a lot of parameters.**

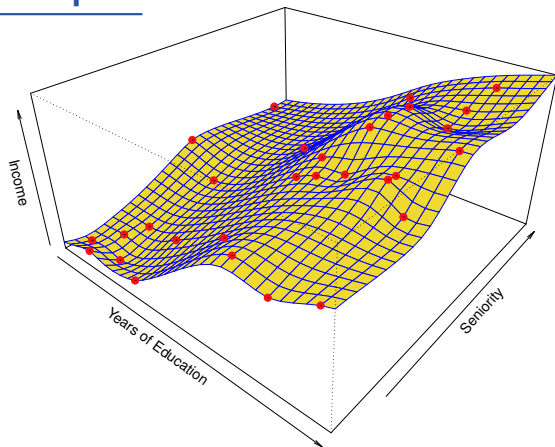
# Non-parametric Example



Approximation to  $f$  to predict **income** using a *thin-plate spline*.

**Better fit to the training data than the linear model.**

## Non-parametric Example



A less smooth spline fit that fits the training data perfectly.

**This is an example of *over-fitting*!**

# Accuracy versus Interpretability Trade-off

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*Why would we choose a less flexible approach?*

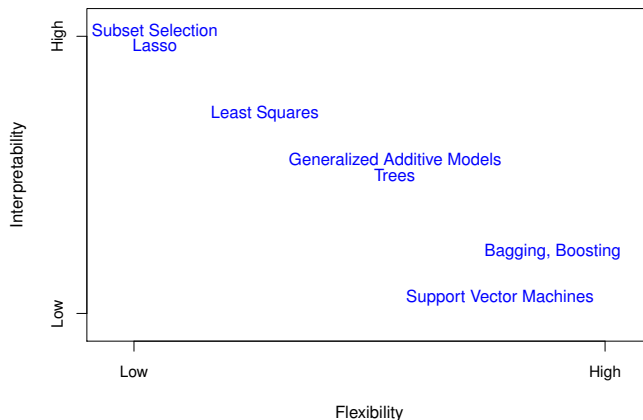
- Interpretability is often desirable (inference).
- For example, in a linear model we can directly infer whether a relationship is positive or negative from the sign of the  $\beta$  coefficient.

*Why would we choose a more flexible approach?*

- We might be mostly interested in the accuracy of our estimate of  $f$  (prediction).
- In the extreme, this is a *black box* approach where we don't care about the interpretation at all.

**This is a *trade-off*, we have to decide.**

# Accuracy versus Interpretability Trade-off



In general, more flexible statistical learning methods have lower interpretability.

**We'll learn more about the methods mentioned in the plot later.**



# Supervised versus Unsupervised Learning

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## *Supervised Learning*

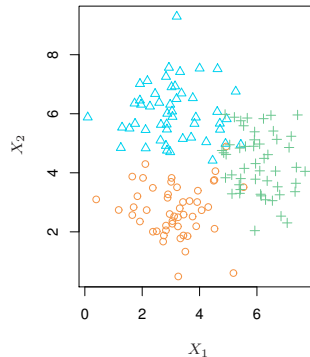
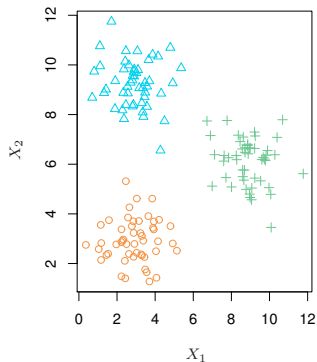
- We have  $n$  observations of the  $p$  predictors  $X_j$  and the corresponding response  $Y$ .
- In this case we can fit a model to the training data.
- The *supervision* comes in through the presence of the known response  $Y$  in the training data.

## *Unsupervised Learning*

- We have  $n$  observations of the  $p$  predictors  $X_j$ , but *no access* to the corresponding response  $Y$  in the training data.
- All we can do is look for *patterns* in the training data.

**This distinction is not always clear-cut.**

# Unsupervised Example



Clustering data involving three groups. Left: little overlap. Right: larger overlap.

**We need to automate this for large data sets.**

# Regression versus Classification

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- Variables, in particular responses, can be *quantitative* or *qualitative*.

## *Quantitative Responses – Regression Problems*

- Gas mileage, crime rate, sales.

## *Qualitative Responses – Classification Problems*

- Sex (male, female), default on debt (yes, no), brand (Apple, Samsung, Blackberry).

**In terms of statistical learning methods the distinction is not crisp.**

# Assessing Model Accuracy

- In this course we introduce a wide range of statistical learning methods.
- Why are we doing this?
- Why not just teach the *best* method?
- No single method dominates all others over all possible data sets.
- It is *our* task to decide which method produces the best results on a given data set.
- We therefore need a way to *measure* how well we are doing.

**There is no free lunch in statistical learning.**

## Measuring Fit Quality

- How can we measure the quality of a fit?
- We need to quantify how close our estimate  $\hat{Y} = \hat{f}(X)$  is to the true values  $Y$ .
- Clearly, the difference between the two is a measure of this, but we don't care about the sign.
- We therefore use the *mean squared error*, MSE:

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{f}(x_i))^2 = E[(Y - \hat{f}(X))^2] = \langle (Y - \hat{f}(X))^2 \rangle$$

Other choices for the *loss function* are possible. This is the most straight-forward and common choice.

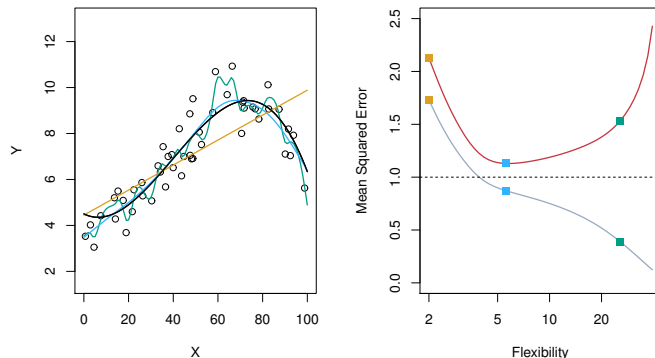
## Measuring Fit Quality

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- We could simply compute the MSE on the training data.
- Most fit, or learning, methods work by minimising the MSE (or another suitable *loss function*) on the training data set.
- However, we want to make predictions on *future* observations, not available at the time of training.
- A better measure of how well we are doing is obtained by computing the MSE on a *test data set* that is *independent* of the training data set.
- We can always produce an independent test data set by only using a subset of the available data for training and the remainder for testing (*cross validation*).

**The MSE from the training data set overestimates the fit quality.**

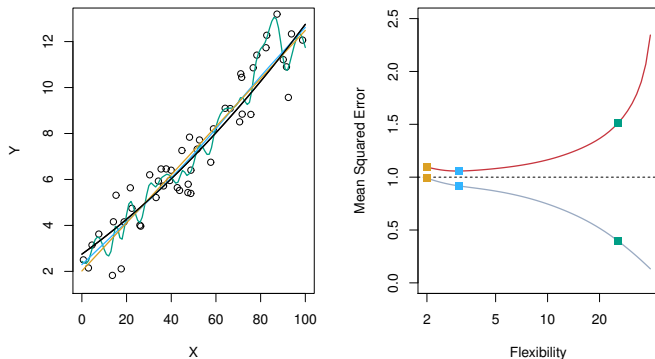
# Measuring Fit Quality: Example 1



Left: true  $f$  (black), linear regression (orange), and spline fits (blue, green).  
Right: training (grey) and test (red) MSE.

**The most flexible model over-fits the training data.**

## Measuring Fit Quality: Example 2

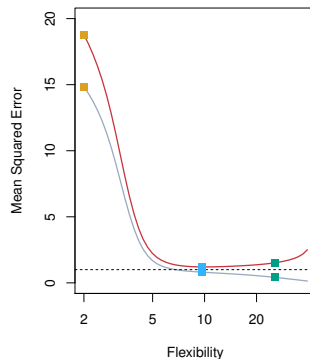
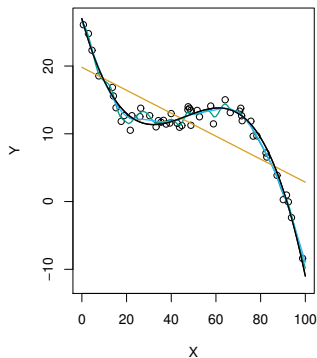


Left: true  $f$  (black), linear regression (orange), and spline fits (blue, green).  
Right: training (grey) and test (red) MSE.

**The truth is more linear, so linear regression does well.**



## Measuring Fit Quality: Example 3



Left: true  $f$  (black), linear regression (orange), and spline fits (blue, green).  
Right: training (grey) and test (red) MSE.

**The truth is highly non-linear, so linear regression does badly.**

# The Bias-Variance Trade-off

- We denote the observations from a test data set as  $(x_0, y_0)$ .
- Then the test data set MSE is:

$$\text{MSE}_{\text{test}} = \langle (y_0 - \hat{f}(x_0))^2 \rangle$$

- We can then show that this can be decomposed like this:

$$\langle (y_0 - \hat{f}(x_0))^2 \rangle = \underbrace{\text{Var}(\hat{f}(x_0)) + (\text{Bias}(\hat{f}(x_0)))^2}_{\text{Reducible}} + \underbrace{\text{Var}(\epsilon)}_{\text{Irreducible}}$$

where the *bias* is:

$$\text{Bias}(\hat{f}(x_0)) = \langle \hat{f}(x_0) \rangle - \langle f(x_0) \rangle$$

In practice, we don't know the true  $f$  and can't compute the bias properly.

# The Bias-Variance Trade-off

- Given the test MSE

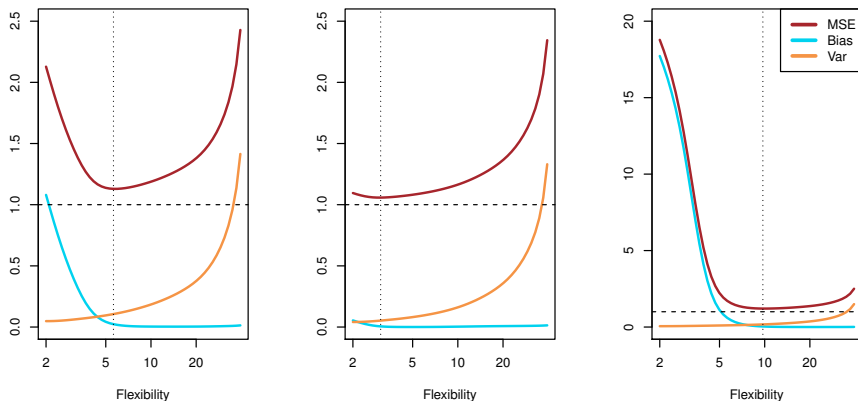
$$\langle (y_0 - \hat{f}(x_0))^2 \rangle = \underbrace{\text{Var}(\hat{f}(x_0)) + (\text{Bias}(\hat{f}(x_0)))^2}_{\text{Reducible}} + \underbrace{\text{Var}(\epsilon)}_{\text{Irreducible}}$$

we want to minimize the variance of  $\hat{f}(x_0)$  *and* the bias.

- This is often not possible at the same time.
- Highly flexible methods can eliminate the bias.
- That does *not* mean they perform better at prediction.

**The bias-variance trade-off translates to a flexibility trade-off.**

# The Bias-Variance Trade-off



The plots correspond to the three example data sets we have seen before.  
(Non-linear, almost linear, highly non-linear).

# The Classification Setting

- As before, we want to estimate  $f$  from the training observations

$$\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$$

and say we train a *classifier*.

- Now the responses  $y_i$  are *qualitative*.
- That is, the  $y_i$  are *labels* denoting the different *classes* the output variable can belong to.
- For example:

$$y = \text{origin}, \text{origin} \in \{\text{US}, \text{EU}, \text{JP}\}$$

**Classifiers usually predict class *probabilities* from observations.**

# Probabilities

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- We need to formalise our notion of *probability*.

We use probabilities to quantitatively express our relative beliefs in various propositions.

- We can hear the mathematicians scream “How can you formalise a *believe*?”.
- Some argue the whole notion is flawed and we can only ever speak of the *frequency* at which events occur in an *ensemble*.
- Of course, we often use observed frequencies to determine probabilities.
- But sometimes the concept of an ensemble does not make much sense.
- We take a pragmatic approach without getting too philosophical about it.

Don't get drawn into heated debates with hard-core frequentists.

## Probabilities: Cook's Rules

- We clearly need a *transitive* property: if we believe (a) more than (b) and (b) more than (c) then we must believe (a) more than (c).

$$P(a) > P(b) \wedge P(b) > P(c) \implies P(a) > P(c), P \in \mathbb{R}$$

- If we specify how much we believe  $X$  to be true we have implicitly specified how much we believe  $X$  to be false. With the conventional norm of one we write this as

$$P(X|I) + P(\bar{X}|I) = 1$$

- If we specify how much we believe  $X$  is true and then how much we believe  $Y$  given  $X$  is true, we have implicitly specified how much we believe  $Y$  and  $X$  are true.

$$P(Y, X|I) = P(Y|X, I) \times P(X|I)$$

These are the quantitative axioms necessary for logical and consistent reasoning.

# Corollaries

## *Bayes' Theorem*

$$P(Y|X, I) = \frac{P(X|Y, I) \times P(Y|I)}{P(X|I)}$$

## *Marginalisation*

$$P(Y|I) = \int_{-\infty}^{+\infty} P(Y, X|I) dX$$

Here ***I*** denotes our background knowledge and assumptions.



# Bayes' Theorem

- The power of Bayes' theorem is that it allows to turn one *conditional probability* into another.
- It relates  $P(X|Y, I)$  to  $P(Y|X, I)$ .
- The importance of this is more obvious when we replace  $Y$  with *hypothesis* and  $X$  with *data*:

$$P(\text{hypothesis}|\text{data}, I) \propto P(\text{data}|\text{hypothesis}, I) \times P(\text{hypothesis}|I)$$

- Note that we have omitted the normalisation factor.

**This relates the probability we are interested in to one we have a chance to measure!**

# Bayes' Theorem

$$P(Y|X, I) = \frac{P(X|Y, I) \times P(Y|I)}{P(X|I)}$$

<i>Term</i>	<i>Name</i>
$P(Y X, I)$	posterior probability
$P(X Y, I)$	likelihood
$P(Y I)$	prior probability
$P(X I)$	evidence

All statistical learning techniques are methods to approximate the posterior probability.

# Classifier Accuracy

- The concepts we have developed for regression also apply to classification.
- We need a way to quantify the accuracy of classifiers.
- We define the *training error rate*:

$$\frac{1}{n} \sum_{i=1}^n I(y_i \neq \hat{y}_i) = \langle I(y_i \neq \hat{y}_i) \rangle, \quad I(y_i \neq \hat{y}_i) = \begin{cases} 1 & y_i \neq \hat{y}_i \\ 0 & y_i = \hat{y}_i \end{cases}$$

- With the convention that  $(x_0, y_0)$  denotes the test observations, the *test error rate* is:

$$\langle I(y_0 \neq \hat{y}_0) \rangle$$

**A good classifier minimises the test error rate.**

# The Bayes Classifier

- The best possible classifier minimises the test error rate on average.
- It assigns each observation to the most likely class given the observed predictors.
- We write the probability of  $Y$  belonging to class  $j$ , given the predictor observation  $x_0$ , as follows.

$$P(Y = j|X = x_0)$$

- In a scenario with two classes (say Up and Down) this classifier predicts  $Y = \text{Up}$  if

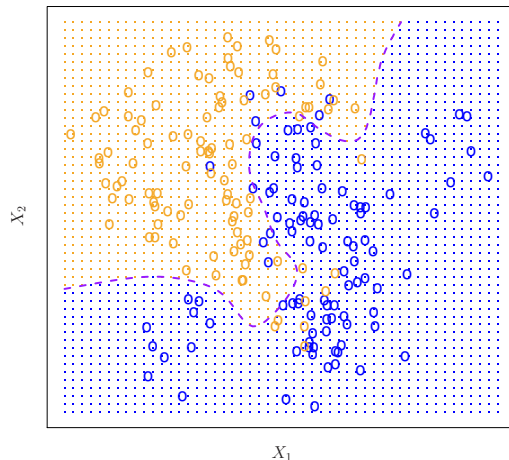
$$P(Y = \text{Up}|X = x_0) > 0.5$$

and  $Y = \text{Down}$  otherwise.

- This is called the *Bayes Classifier* and it is ideal.
- On simulated data we can compute the above probability perfectly.

**No method can do better than this proper Bayesian posterior probability.**

# The Bayes Decision Boundary



A simulated data set with 100 observations. The dashed line is the *Bayes decision boundary*.

## K-Nearest Neighbours

1. Given an integer  $K$  and a test observation  $x_0$ , find the  $K$  observations  $x_i$  in the training data set that are closest to  $x_0$ , denoted by  $\mathcal{N}_0$ .
2. Then estimate the conditional probabilities to observe  $x_0$  from the relative frequencies of the classes in  $\mathcal{N}_0$  (*likelihoods*):

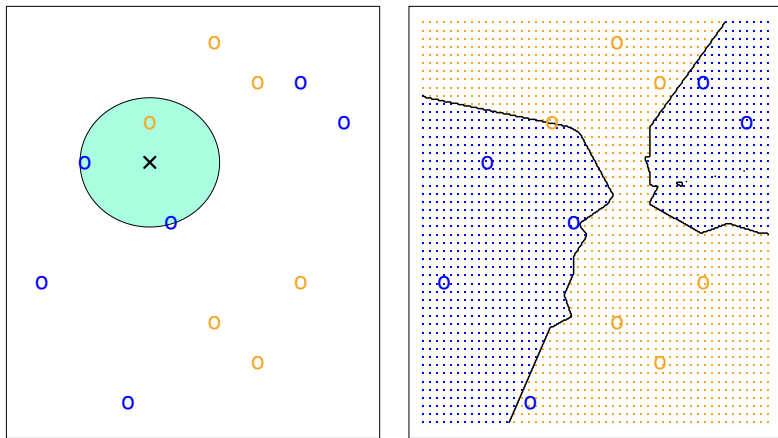
$$P(X = x_0 | Y = j) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} I(y_i = j)$$

3. Finally, use Bayes' theorem to compute the conditional *posterior probability*:

$$P(Y = j | X = x_0) = \frac{P(X = x_0 | Y = j) \times P(Y = j)}{P(X = x_0)}$$

**KNN estimates  $P(Y|X)$ . The flexibility of KNN scales with  $1/K$ .**

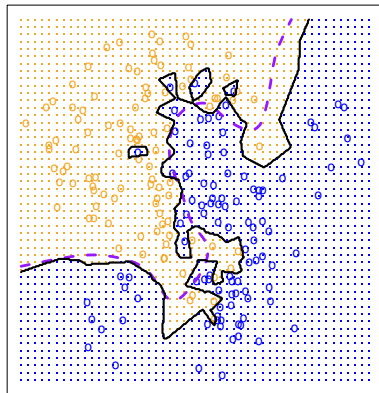
## K-Nearest Neighbours



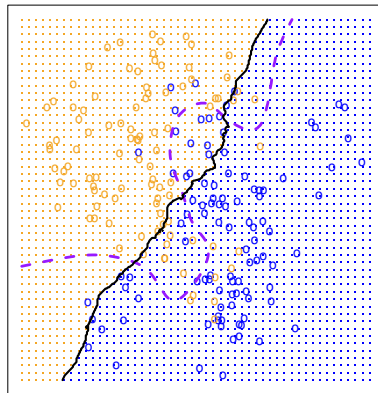
The KNN approach with  $K = 3$ . The black “x” in the left panel is a test observation.

# K-Nearest Neighbours

KNN:  $K=1$



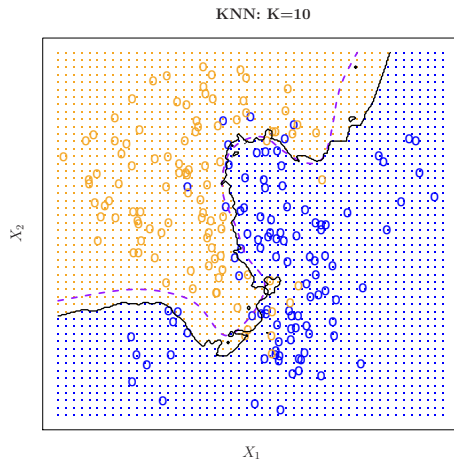
KNN:  $K=100$



A comparison of decision boundaries with  $K = 1$  and  $K = 100$ .

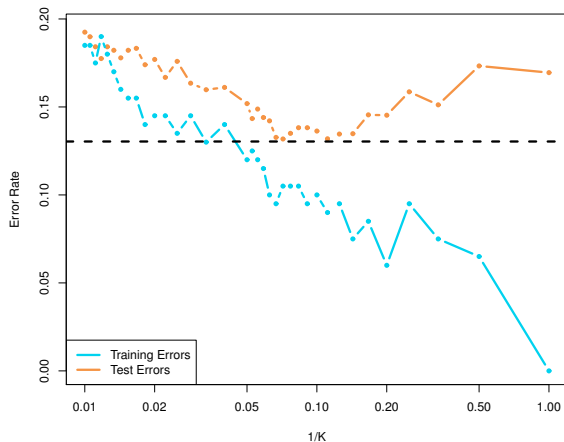


# K-Nearest Neighbours



Comparing to the Bayes decision boundary,  $K = 10$  seems a good choice.

# K-Nearest Neighbours



Flexibility versus model performance on training and test data sets.