

Machine Learning (Semester 1 2024)

Statistical Learning

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Motivation

Building on our statistical knowledge so far, we will see a variety of methods to **better understand data**.

With the massive data sets we nowadays often deal with, this part is essential for drawing conclusions from our data.

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Frequentist vs.
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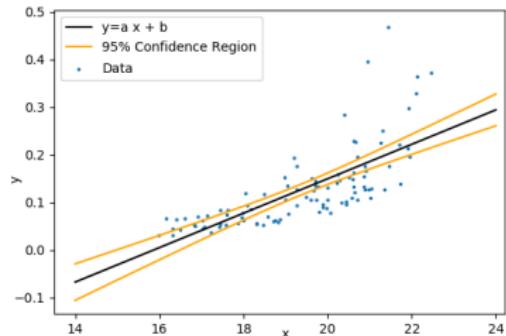
Summary &
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recap: Goal of Statistical Inference

Statistical inference is about **drawing conclusions from data**, specifically determining the properties of a population by data sampling.

Three examples of inference are:

1. What is the best estimate for a (set of) model parameter(s)?



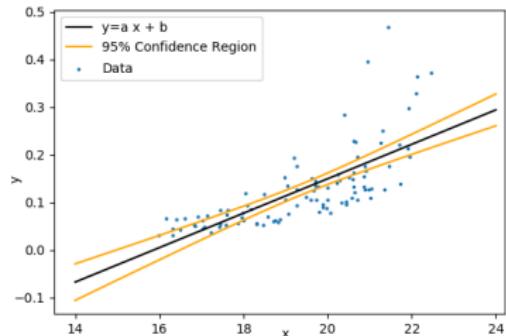
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2. How confident we are about our result?

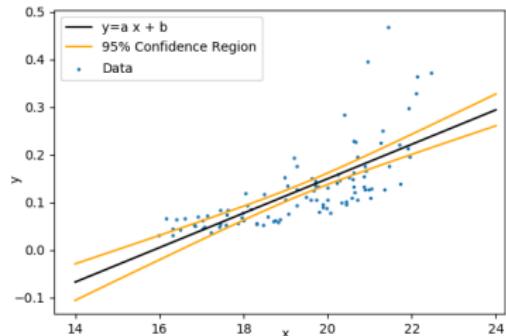


recap: Goal of Statistical Inference

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Three examples of inference are:

1. What is the best estimate for a (set of) model parameter(s)?
2. How confident we are about our result?
3. Are the data consistent with a particular model/hypothesis?



recap: Some Terminology

We study the properties of some **population** by measuring **samples** from that population. The population doesn't have to refer to different objects.

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example: E.g., we may be (re)measuring the position of an object at rest; the population is the distribution of (an infinite number of) measurements smeared by the uncertainty, and the sample are the measurement we've actually taken.

subsequent brightness measurements of a star:

ra dec hjd mag magErr filter

347.66112 -7.39883 2458277.96036 20.083 0.135 g

347.66111 -7.39883 2458280.94526 20.49 0.163 g

347.66111 -7.39881 2458283.94197 19.822 0.116 g

347.66113 -7.39883 2458289.93875 20.361 0.155 g

347.66111 -7.39883 2458377.75728 20.103 0.137 r

347.66111 -7.39883 2458380.84366 20.291 0.151 r

347.66111 -7.39883 2458430.66968 20.471 0.162 r

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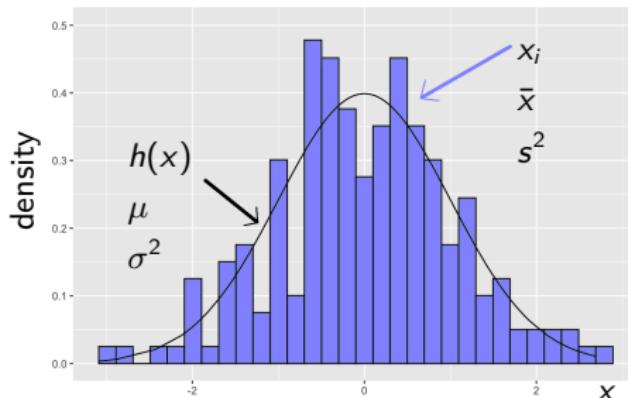
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A **statistic** is any function of the sample. For example, the sample mean is a statistic. But also something like *the value of the first measurement* is also a statistic.

To conclude something about the population from the sample, we use **estimators**. An estimator is a statistic, a rule for calculating an estimate of a given quantity based on observed data.



recap: Some Terminology

There are **point estimators** and **interval estimators**. The point estimators yield single-valued results (example: the position of an object), while with an interval estimator, the result would be a range of plausible values (example: confidence interval for the position of an object).

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Measurements have **uncertainties** (not errors) and we need to account for these (sometimes they are unknown).

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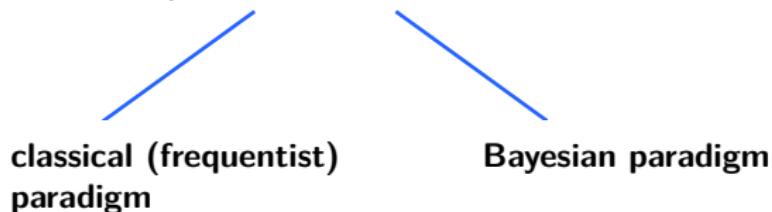
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Frequentist vs. Bayesian Statistical Inference

There are two major statistical paradigms that address the statistical inference questions:



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Frequentist vs. Bayesian Statistical Inference

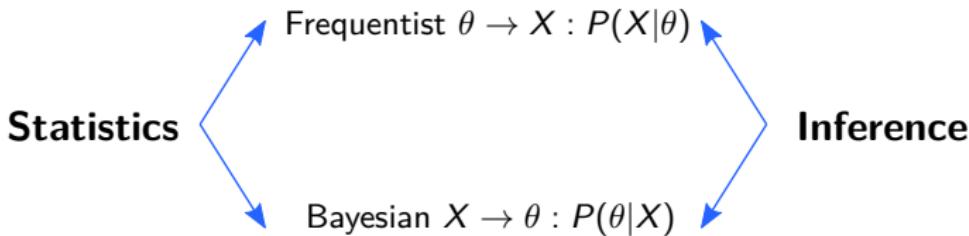
There are two major statistical paradigms that address the statistical inference questions:



	classical (frequentist) paradigm	Bayesian paradigm
Key differences		
Definition of probabilities:	relative frequency of events over repeated experimental trials	probabilities quantify our subjective belief about experimental outcomes, model parameters, or models
Quantifying uncertainty:	confidence levels describe the distribution of the measured parameter from the data around the true value	credible regions derived from posterior probability distributions encode our belief in model parameters

Frequentist vs. Bayesian Statistical Inference

we can summarize this as



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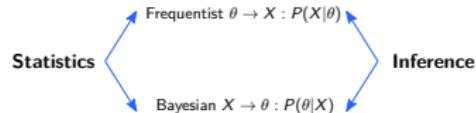
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an example:



A person takes an IQ test (which does not give the “real” IQ but is a way to estimate it, and a possible range of values).

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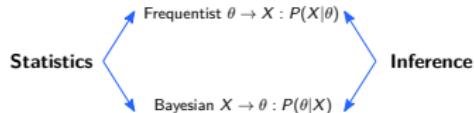
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For a **frequentist**, the best estimator is the **average** of many test results. So, if 5 IQ tests were taken and the sample mean is of 160, then that would be the estimator of that candidate’s true IQ.

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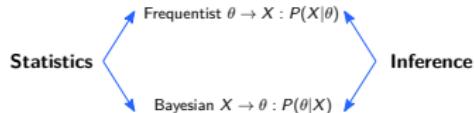
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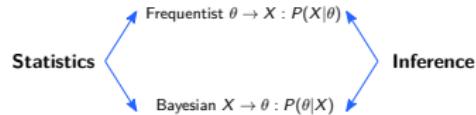
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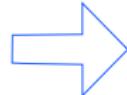
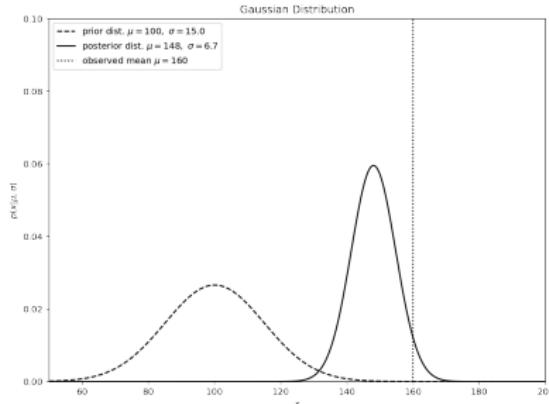
A **Bayesian** would say: *IQ tests are calibrated with a mean of 100, standard deviation of 15 points* and use this as a **prior** information. The Bayesian estimate of that candidate’s person thus would be not 160, but rather 148, or more specifically that $p(141.3 \leq \mu \leq 154.7 | \bar{x} = 160) = 0.683$.

Frequentist vs. Bayesian Statistical Inference

an example:



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we will see an astronomy example later in `lecture_2.ipynb`

Bayesian Statistical Inference

With Bayesian statistics, probability expresses a **degree of belief in an event**. This method is different from the frequentist methodology in a number of ways. One of the big differences is that probability actually expresses the chance of an event happening.

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The Bayesian concept of probability is also more **conditional**. In addition to experiment data to predict probabilities (as in the frequentist case), it also uses **prior knowledge**.

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example: Measuring the flux of a star.

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repeated measurements of flux (from nonvariable star) lead to different values due to the statistical error of the astronomical instrument

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Frequentist: probability only has meaning in terms of a limiting case of repeated measurements

Limit of large numbers: the frequency of any given value indicates the probability of measuring that value.
⇒ probabilities fundamentally related to frequencies of events

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Bayesian:

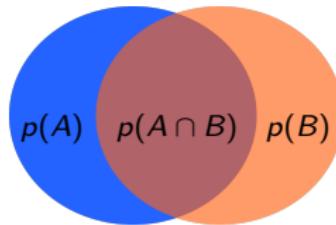
the concept of probability is extended to cover degrees of certainty about statements.

Bayesian approach claims to measure the flux F with a probability $P(F)$: probability as statement of the knowledge of the measurement outcome.
⇒ probabilities fundamentally related to our own knowledge about an event, the **prior**

Bayes' Rule

recap from lecture 1:

If we have two events, A and B , the possible combinations are:

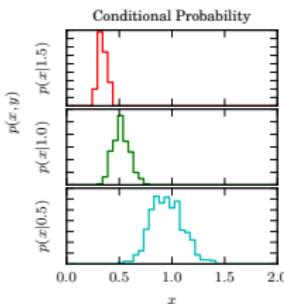
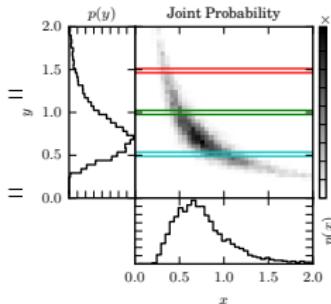


$$p(A \cup B) = p(A) + p(B) - p(A \cap B)$$

$$p(A \cap B) = p(A, B) = p(A|B)p(B) = p(B|A)p(A)$$

We then had seen that the **marginal probability** (projecting onto one axis) is defined as

$$p(x) =$$



Bayes' Rule

Since $p(x|y)p(y) = p(y|x)p(x)$ we can write that

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)} = \frac{p(x|y)p(y)}{\int p(x|y)p(y)dy}$$

which gives

Bayes' Rule:

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)} = \frac{p(x|y)p(y)}{\int p(x|y)p(y)dy}$$

which in words says that

the (conditional) probability of y given x is just the (conditional) probability of x given y times the (marginal) probability of y divided by the (marginal) probability of x , where the latter is just the integral of the numerator.

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The Bayesian Method

The Essence of the Bayesian Method:

- **Probability statements** are not limited to data, but can be made **for model parameters** and models themselves.

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- These pdfs represent our belief spread in what the model parameters are. They have nothing to do with outcomes of repeated experiments (although the shape of resulting distributions can often coincide).

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Bayesian Statistical Inference

frequentist statistical inference:

We calculated a **likelihood** $p(D | M)$.

Bayesian statistical inference:

We instead evaluate the **posterior probability** taking into account prior information and the likelihood.

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We've seen that Bayes' Rule is:

$$p(M | D) = \frac{p(D | M) p(M)}{p(D)},$$

with data D and model $M = M(\theta)$.

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posterior likelihood prior
evidence

prior probability

How probable are the possible values of θ in nature?

likelihood

ties the model to the data:
how likely is the data given θ ?

posterior probability

distribution is updated with information from the data:

what is the probability of different θ values given data and model?

with data D and model $M = M(\theta)$.

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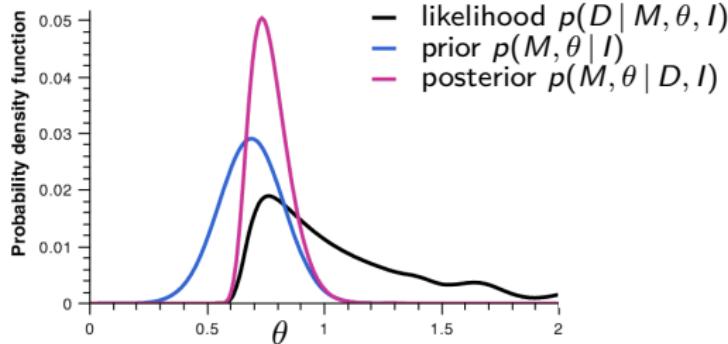
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Bayesian Statistical Inference

The **Bayesian Statistical Inference process** is then

1. formulate the likelihood, $p(D | M, \theta, I)$



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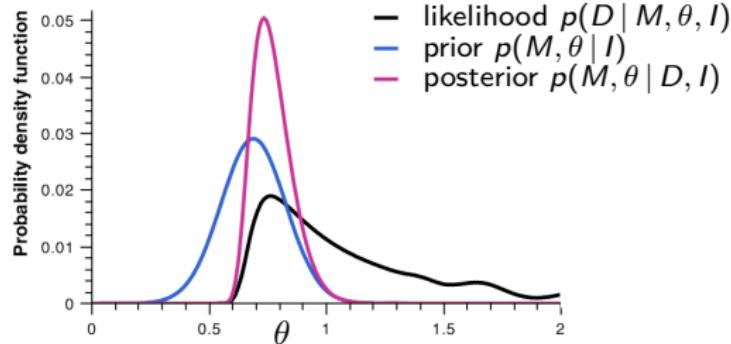
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The **Bayesian Statistical Inference process** is then

1. formulate the likelihood, $p(D | M, \theta, I)$
2. chose a prior, $p(M, \theta | I)$, which incorporates other information beyond the data in D



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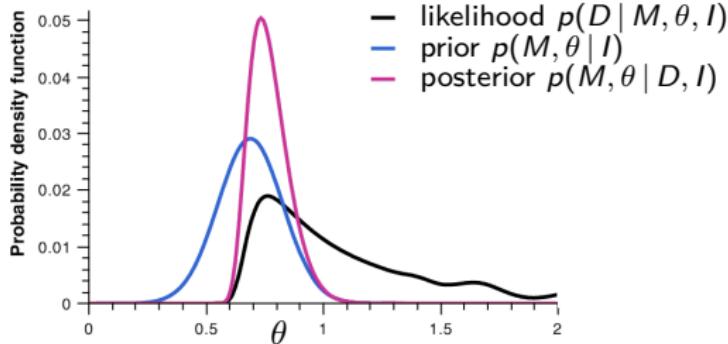
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3. determine the posterior pdf, $p(M, \theta | D, I)$



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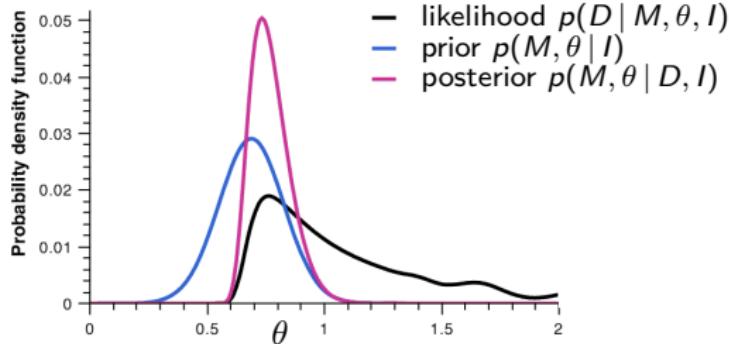
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3. determine the posterior pdf, $p(M, \theta | D, I)$
4. search for the model parameters that maximize $p(M, \theta | D, I)$



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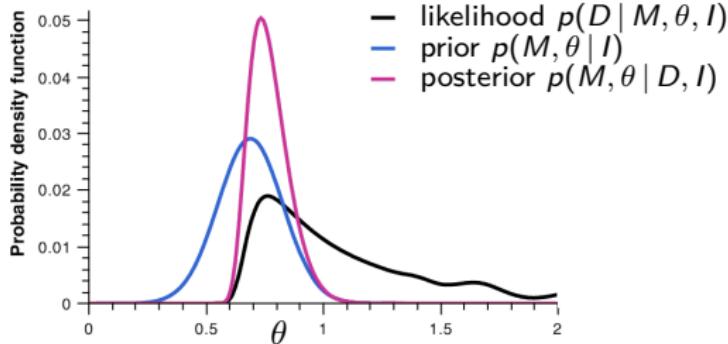
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4. search for the model parameters that maximize $p(M, \theta | D, I)$
5. quantify the uncertainty of the model parameter estimates



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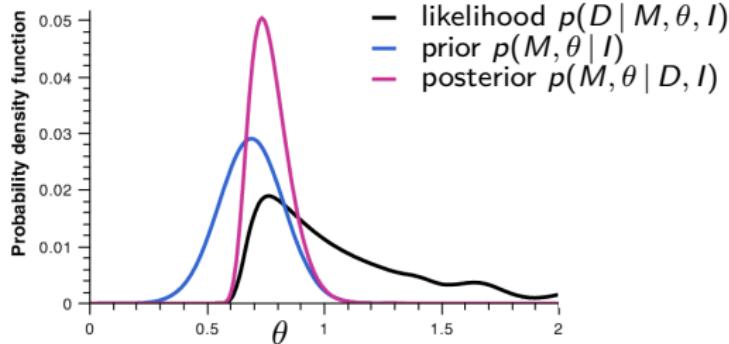
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4. search for the model parameters that maximize $p(M, \theta | D, I)$
5. quantify the uncertainty of the model parameter estimates
6. perform model selection to find best description of the data



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What is Statistical Learning?

Statistical learning refers to methodologies for **understanding data**.

⇒ allows to **uncover hidden correlation patterns**

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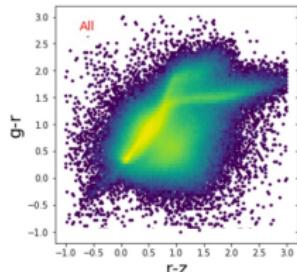
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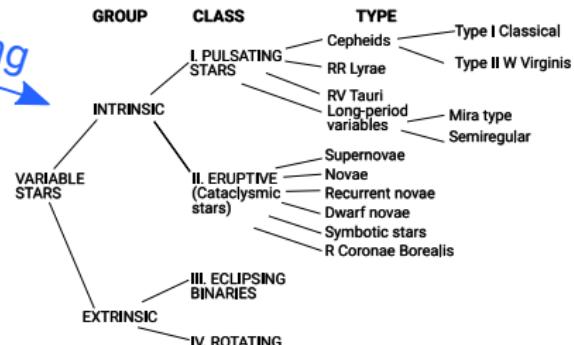
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parameter space of measurements



machine learning

parameter space of astrophysical objects



Unsupervised vs. Supervised Learning

Those methods can be distinguished as follows:

unsupervised learning or “learning without labels”

Clustering:

Find groups that are not defined a priori based on measurements
⇒ members of the same cluster are “close” in some sense

vs.

supervised learning or “learning with labels”

Classification:

Use a priori group labels in analysis to assign new observations to a particular group or class

Regression:

instead of having training data with discrete labels, the “truth” is a continuous property and we are trying to predict the values of that property for the test data

Unsupervised vs. Supervised Learning

supervised learning or “learning without labels”

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Regression:

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example:

The task of determining whether an object is a star, a galaxy, or a quasar is a classification problem: the label is from three distinct categories. On the other hand, we might wish to estimate the age of an object based on such observations: this would be a regression problem, because the label (age) is a continuous quantity.

A Brief History of Statistical Learning

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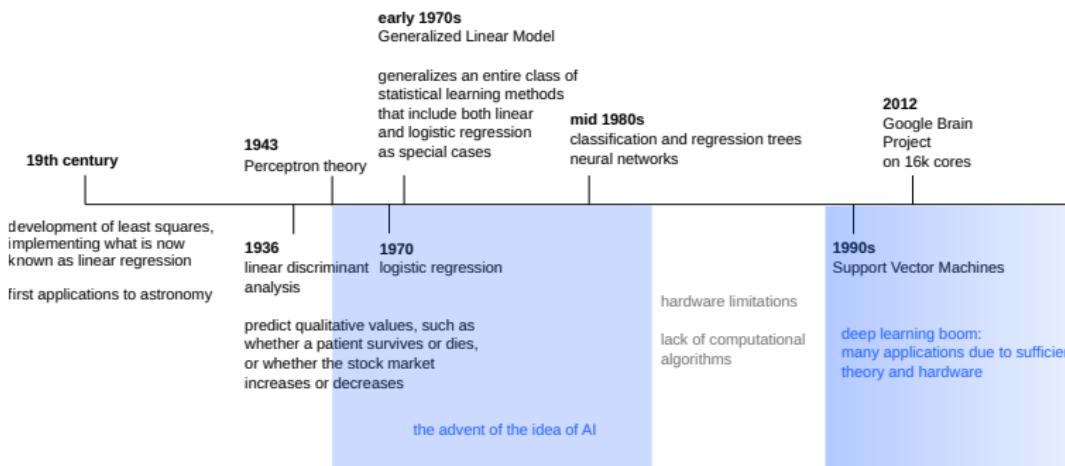
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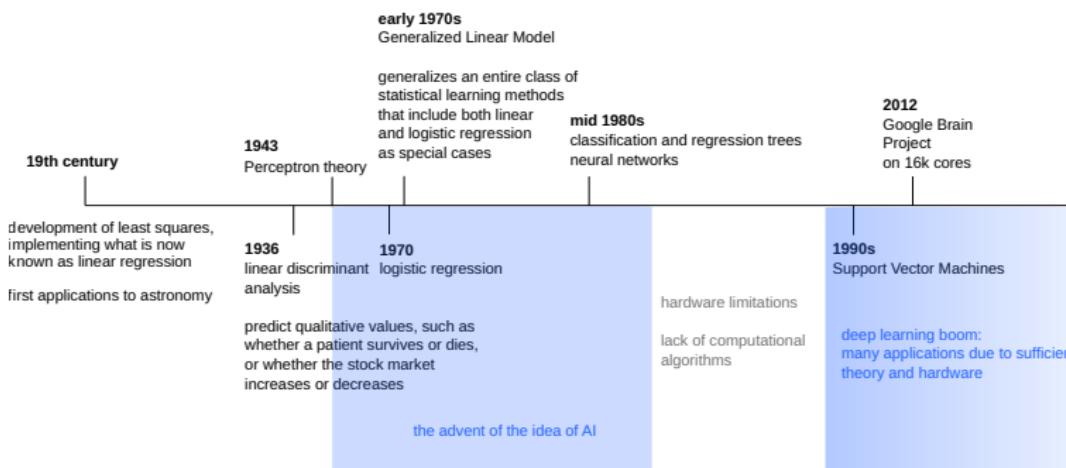
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In recent years, progress in statistical learning has been marked by the increasing availability of powerful and relatively user-friendly software, such as programming libraries for the open-source Python ecosystem.

Notation

The input **variables** (predictors, independent variables, features) are typically denoted using the symbol X , with a subscript to distinguish them.

Example: When we ask which kind of advertisement works best for a product, X_1 might be the TV budget, X_2 the radio budget, and X_3 the internet budget.

The **output variable** is often called the response or dependent variable, and is typically denoted using the symbol Y . In this example, the output variable is sales.

Example: Y might be product sales.

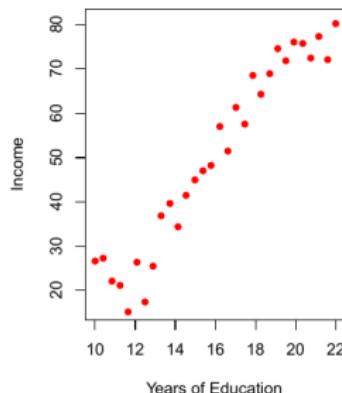
More generally, suppose that we observe a quantitative response Y and we have n different predictors, X_1, X_2, \dots, X_n . We assume that there is some relationship between Y and $X = (X_1, X_2, \dots, X_n)$ which can be written in the very general form $Y = f(X) + \epsilon$.

Here f is some fixed but unknown function of X_1, X_2, \dots, X_n representing the systematic information that X provides about Y , and ϵ is a random error term, which is independent of X and has mean zero.

Another Use Case

As another use case (outside of astronomy), we consider this example from *An Introduction to Statistical Learning: with Applications in Python*. Witten, Hastie, Tibshirani; Springer (<https://www.statlearning.com/>)

The data set consists of income vs. years of education for 30 individuals. The plot of income vs. years suggests that one might be able to predict income using years of education.



source: Fig. 2.2 from
<https://www.statlearning.com/>

Another Use Case

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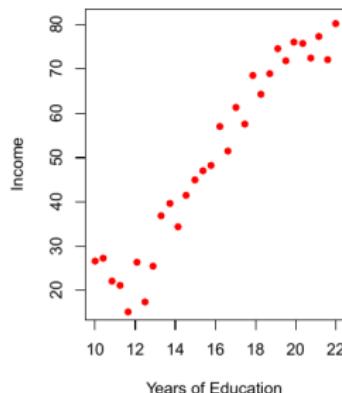
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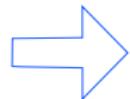
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The unknown function f connecting the input variable to the output variable must be estimated based on the observed points.

Another Use Case

As this data set is *simulated*, f is known and is shown by the blue curve in the right-hand panel:

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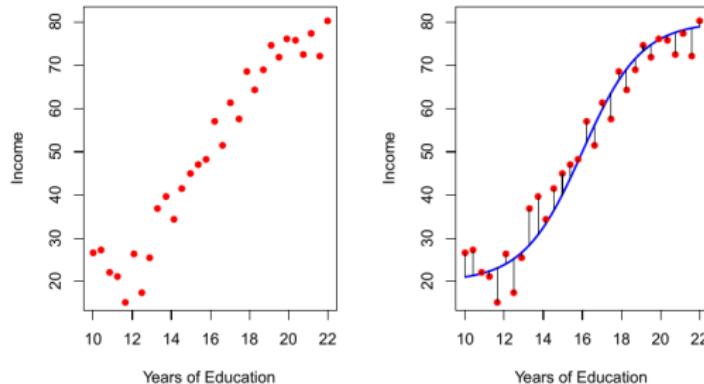
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In this plot, the blue curve is the underlying f .

Vertical lines represent the error terms ϵ . Note that some errors are positive and some are negative. Their overall mean is zero.

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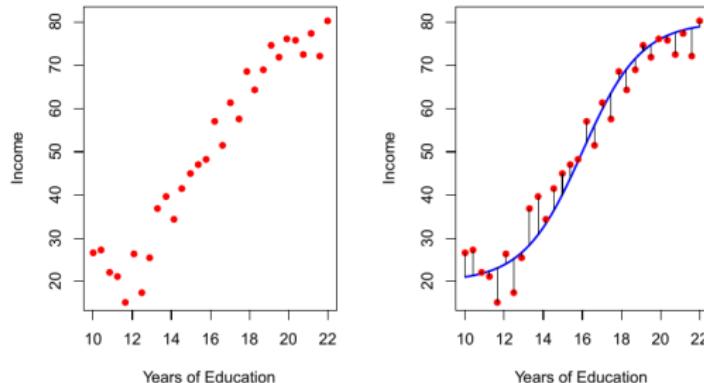
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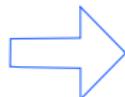
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In this plot, the blue curve is the underlying f .

Vertical lines represent the error terms ϵ . Note that some errors are positive and some are negative. Their overall mean is zero.



Statistical learning refers to a set of approaches for estimating f .

Why Estimate f ?

There are two main reasons why we want to estimate f : prediction and inference.

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Prediction

Often, we have a set of inputs X available, but the output Y cannot be easily obtained.

Based on our assumption of the error term averaging 0, we can predict Y :

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

where \hat{f} represents our estimate for f , and \hat{Y} represents the resulting prediction for Y .

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example:

Suppose that X_1, \dots, X_n are characteristics of a patient's blood sample, and Y is a variable encoding the patient's risk for a severe reaction to a medication. It is natural to try to predict Y using X , to avoid giving at-risk patients the medication.

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Prediction

The accuracy of \hat{Y} as a prediction for Y depends on two quantities: the **reducible error** and the **irreducible error**.

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Prediction

The accuracy of \hat{Y} as a prediction for Y depends on two quantities: the **reducible error** and the **irreducible error**.

\hat{f} will not be a perfect estimate for f - this inaccuracy will introduce the **reducible error**; we can potentially improve the accuracy of \hat{f} by finding a better f .

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Prediction

The accuracy of \hat{Y} as a prediction for Y depends on two quantities: the **reducible error** and the **irreducible error**.

\hat{f} will not be a perfect estimate for f - this inaccuracy will introduce the **reducible error**; we can potentially improve the accuracy of \hat{f} by finding a better f .

However, even with doing that, our prediction is not free from error. This is because Y is also a function of ϵ , which cannot be predicted by X . This is the **irreducible error**.

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Prediction

Consider a given estimate \hat{f} and a set of predictors X , which yields the prediction $\hat{Y} = \hat{f}(X)$.

We assume for the moment that both \hat{f} and X are fixed: now variability only comes from ϵ .

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Prediction

Consider a given estimate \hat{f} and a set of predictors X , which yields the prediction $\hat{Y} = \hat{f}(X)$.

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Then, it is easy to show that

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

where $E(Y - \hat{Y})^2$ represents the **expectation value** of the squared difference between the predicted and actual value of Y , and $\text{Var}(\epsilon)$ represents the **variance** associated with the error term ϵ .

Inference

We are often interested in understanding the **association** between Y and X_1, \dots, X_n . For this we want to estimate f without necessarily making predictions for Y .

Here, we need to know the exact form of \hat{f} .

In this setting, one might want to answer the following questions:

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In this setting, one might want to answer the following questions:

- Which predictors are associated with the response? Often only a small fraction of the available predictors are strongly associated with Y . Identifying them among a large set of possible variables can be extremely useful, depending on the application.

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In this setting, one might want to answer the following questions:

- Which predictors are associated with the response? Often only a small fraction of the available predictors are strongly associated with Y . Identifying them among a large set of possible variables can be extremely useful, depending on the application.
- What is the relationship between the response and each predictor? Some predictors may have a positive relationship with Y , in the sense that larger values of the predictor are associated with larger values of Y . Other predictors may have the opposite relationship.

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- Depending on the complexity of f , the relationship between the response and a given predictor may also depend on other predictors.

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- Depending on the complexity of f , the relationship between the response and a given predictor may also depend on other predictors.
- Can the relationship be adequately modeled with a linear equation, or is the relationship more complicated?

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Prediction vs. Inference

Some modeling could be conducted both with prediction and inference.

example: For real estate prices, one might want to relate home values to inputs such as neighborhood, distance to downtown, crime rates and so forth.

In this case one might be interested in the association between each individual input variable and housing price - for instance, by how much will the price increase for having ocean view? This is an **inference problem**.

Alternatively, one may simply be interested in predicting the value of a home given its characteristics to estimate whether this house is house under- or over-valued? This is a **prediction problem**.

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Prediction vs. Inference

Depending on whether our goal is prediction, inference, or a combination of the two, **different methods** for estimating f may be appropriate.

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For example, **linear models** allow for relatively simple and interpretable inference, but may not yield as accurate predictions as some other approaches. In contrast, some of the highly non-linear approaches that we see later in this course can provide quite accurate predictions for Y , but at the expense of a less **interpretable** model.

How to Estimate f ?

Throughout this course, we will explore many linear and non-linear approaches for estimating f .

We provide an overview of their shared characteristics here before we look at the individual methods.

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In the following, we assume that we have observed a set of n data points. These observations are called the **training data**: we will use these observations to train our method how to estimate f .

Let x_{ij} represent the value of the j th predictor, or input, for observation i , where $i = 1, 2, \dots, m$ and $j = 1, \dots, n$. Correspondingly, let y_i represent the response variable for the i th observation.

Then our training data consist of $\{(x_1, y_1), (x_2, y_2), \dots, (x_m, y_m)\}$ where $x_i = (x_{i1}, x_{i2}, \dots, x_{ip})^T$.

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Then our training data consist of $\{(x_1, y_1), (x_2, y_2), \dots, (x_m, y_m)\}$ where $x_i = (x_{i1}, x_{i2}, \dots, x_{ip})^T$.

Our **goal** is to apply a statistical learning method to the training data in order to estimate the unknown function f : We want to find a function \hat{f} such that $Y \sim \hat{f}(X)$ for any observation (X, Y) .

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Parametric Methods

Most statistical learning methods can be characterized as either parametric or non-parametric.

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Parameteric methods involve a two-step model-based approach:

1. Make an assumption about the functional form of f . For example, assume that f is a linear function of X :

$$f(X) = \beta_0 + \beta_1 X_1 + \dots + \beta_n X_n$$

This greatly simplifies the problem as now only the $n + 1$ coefficients need to be estimated.

2. After selecting a model, the training data are needed to fit or train the model. In the case of the linear model, we need to estimate the parameters $\beta_0, \beta_1, \dots, \beta_n$ such that

$$Y \sim \beta_0 + \beta_1 X_1 + \dots + \beta_n X_n$$

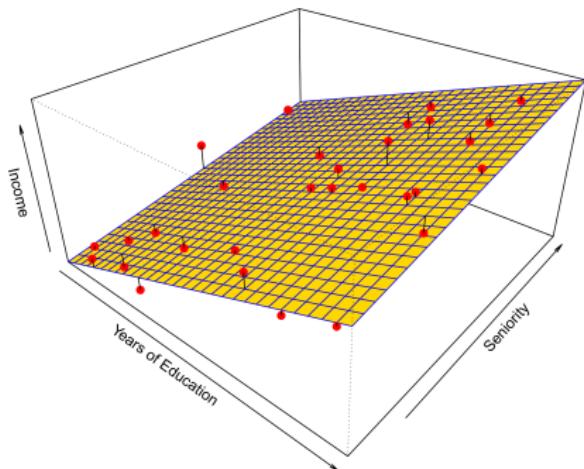
The most common approach is called **least squares**.

Parametric Methods

The **advantage** of the parametric approach is that it is much easier to estimate a set of parameters than to fit an entirely arbitrary function.

The **disadvantage** of the parametric approach is that we have a fixed functional form which usually doesn't match the true form of f .

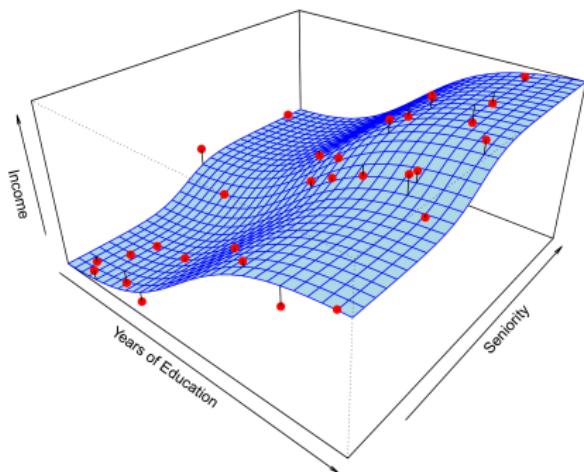
In the following, we see data to which we have fit a linear model of the form $\hat{f} = \beta_0 + \beta_1 X_1 + \beta_2 X_2$:



Linear model fit to data.
The observations are shown in red.
The yellow plane indicates the least-squares fit to the data.
Source: Fig. 2.4 from
<https://www.statlearning.com/>

Parametric Methods

As the data were simulated by drawing from an underlying f we know we can compare how well the fit works:



The blue surface represents the true underlying relationship.
The observations are shown in red.
Source: Fig. 2.3 from
<https://www.statlearning.com/>

We can see that the linear fit misses some features of the functional form of f , i.e. the true f has some curvature that cannot be captured with a linear fit.

Over- and Underfitting

The statistical learning approach tells us what the best-fitting model parameters are, but **not how good the fit actually is.**

If the model isn't well suited for the data, then we should not expect a good fit.

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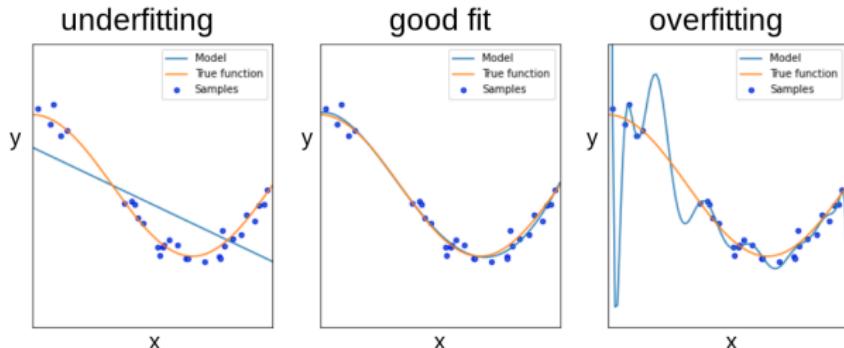
Over- and Underfitting

The statistical learning approach tells us what the best-fitting model parameters are, but **not how good the fit actually is.**

If the model isn't well suited for the data, then we should not expect a good fit.

example:

N points drawn from a linear distribution can always be fitted perfectly with an $N - 1$ order polynomial - which won't help to predict future measurements



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Non-Parametric Methods

In contrast to parametric methods for which the functional form of f is predetermined, **non-parametric methods** do not make explicit assumptions about the functional form.

Instead they try to estimate the functional form of f without too much over- or underfitting.

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Non-Parametric Methods

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The major **advantage** of non-parametric methods over parametric methods:

The potential to accurately fit a wider range of possible shapes for f .

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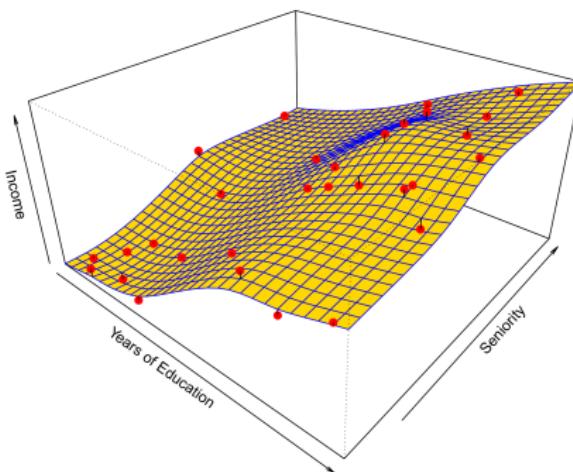
The potential to accurately fit a wider range of possible shapes for f .

The major **disadvantage** of non-parametric methods:

As not reducing the problem of estimating f down to a small set of parameters, a much larger number of observations is required in order to obtain an accurate estimate for f .

Non-Parametric Methods

In the following **example**, we again fit the same data set as shown before, but now with a non-parameteric approach.



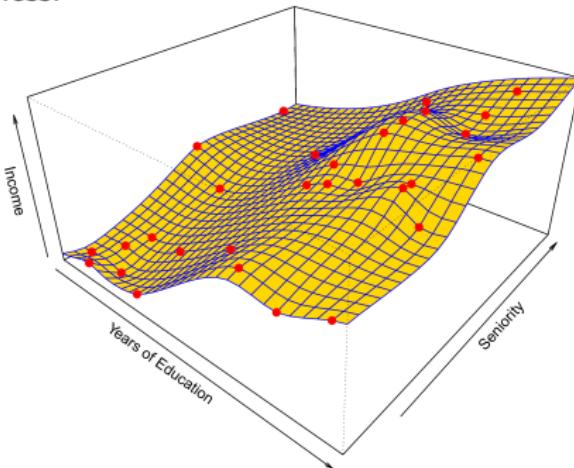
A non-parametric model (thin-plate spline¹, high smooth parameter) is used to estimate f for fitting the data.

Source: Fig. 2.5 from <https://www.statlearning.com/>

¹ *splines* are functions defined piecewise by polynomials

Non-Parametric Methods

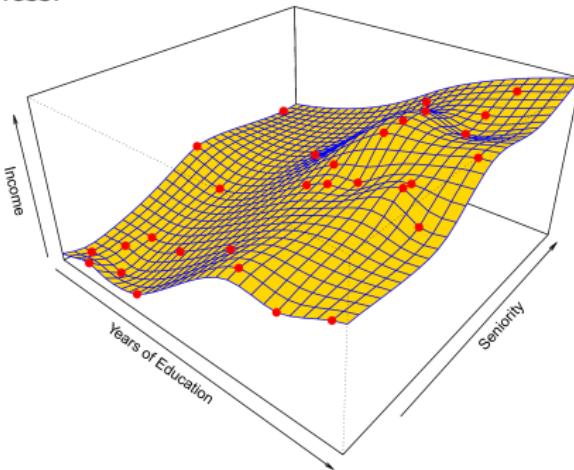
The thin-plate spline has a smoothness parameter that must be selected. The following figure shows the same fit as above but using a lower level of smoothness.



Again a thin-plate spline fit, but with a lower level of smoothness.
Source: Fig. 2.6 from <https://www.statlearning.com/>

Non-Parametric Methods

The thin-plate spline has a smoothness parameter that must be selected. The following figure shows the same fit as above but using a lower level of smoothness.



Again a thin-plate spline fit, but with a lower level of smoothness.

Source: Fig. 2.6 from <https://www.statlearning.com/>

We see that the fit follows the data perfectly. Is this a **good result?**

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Here we know the true underlying function f as these are simulated data. We can compare our fits to that.

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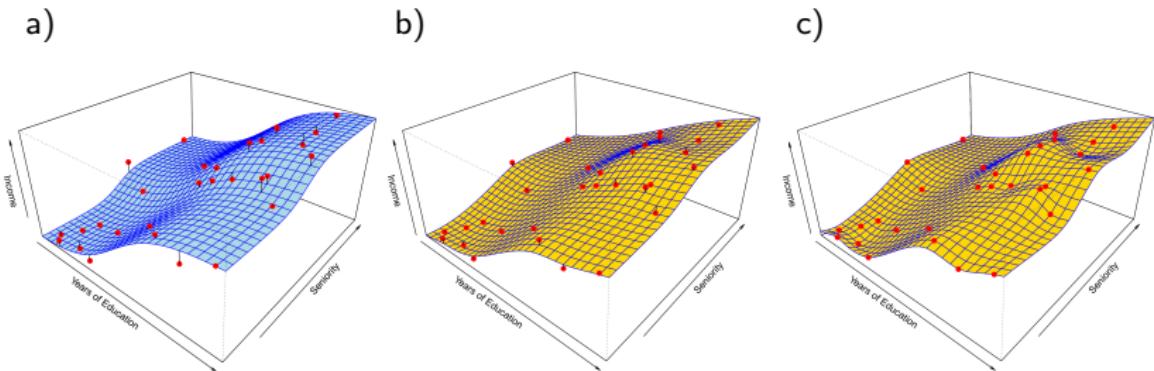
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- a) The true function f .
- b) Thin-plate spline, high smooth parameter.
- c) Thin-plate spline, low smooth parameter.

Non-Parametric Methods

Here we know the true underlying function f as these are simulated data. We can compare our fits to that.

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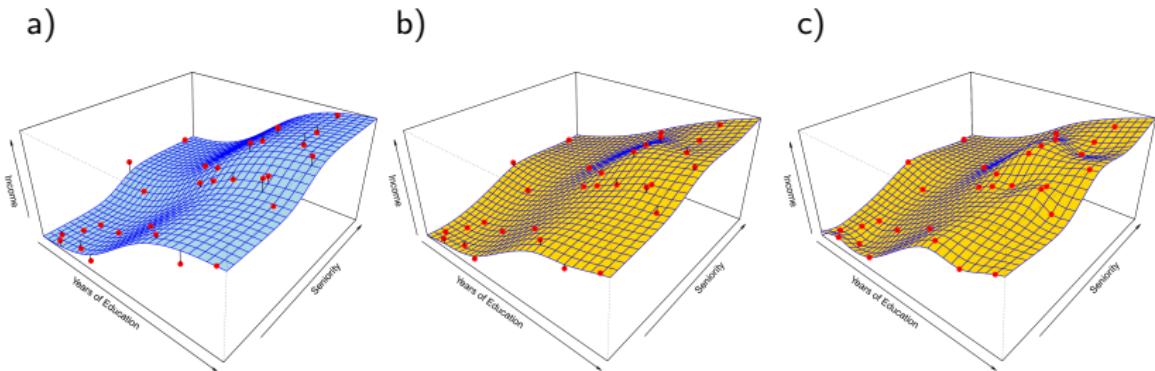
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- a) The true function f .
 - b) Thin-plate spline, high smooth parameter.
 - c) Thin-plate spline, low smooth parameter.
- c) is an example for **overfitting!**

The Trade-Off Between Prediction Accuracy and Model Interpretability

We have seen that some approaches offer less, some offer more flexibility in estimating f .

For example, linear regression can only generate linear functions (lines, planes...), thus being a relatively rigid approach.

Other methods, such as splines, are considerably more flexible because they can generate a much wider range of possible shapes to estimate f .

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Other methods, such as splines, are considerably more flexible because they can generate a much wider range of possible shapes to estimate f .



Why use a more restrictive method instead of a very flexible approach?

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The Trade-Off Between Prediction Accuracy and Model Interpretability

There are several reasons that we might **prefer a more restrictive model**.

If we are mainly interested in inference, then restrictive models are much more interpretable.

For instance, when inference is the goal, the linear model may be a good choice since it will be quite easy to understand the relationship between Y and X_1, X_2, \dots, X_p . In contrast, very flexible approaches, such as splines, can lead to such complicated estimates of f that it is difficult to understand how **any individual predictor** is associated with the response.

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Supervised Versus Unsupervised Learning

Most statistical learning problems fall into one of two categories: supervised or unsupervised. The examples that we have discussed so far in this chapter all fall into the supervised learning domain.

In supervised statistical learning, for each observation of the predictor measurement(s) $x_i, i = 1, \dots, n$ there is an associated response measurement y_i . The goal is to fit a model that relates the response to the predictors (*training*) and from that accurately predicting the response for future observations (*prediction*) or better understanding the relationship between the response and the predictors (*inference*).

Most statistical learning methods we discuss in this course fall into the domain of **supervised learning**.

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Unsupervised Learning

Unsupervised learning is the challenging situation of having a vector of measurements x_i but no associated response y_i .

What sort of statistical analysis is possible?

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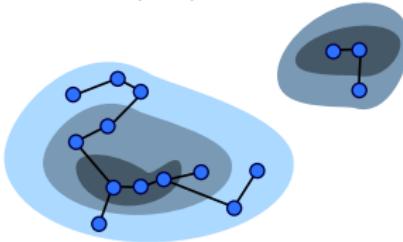
Unsupervised Learning

Unsupervised learning is the challenging situation of having a vector of measurements x_i but no associated response y_i .

What sort of statistical analysis is possible?

We can try to understand the relationships between the variables or between the observations.

A possible statistical tool for this is **cluster analysis (or clustering)** which has the goal of identifying whether the observations x_1, \dots, x_n fall into relatively distinct groups.



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Cluster Analysis

example (outside of astronomy):

In a *market segmentation study* we might observe multiple characteristics (variables) for potential customers, such as ZIP code (or region), family income, and previous shopping habits.

We might believe that the customers fall into different groups, such as customers possibly interested in getting their first credit card or not. If the information about each customer's previous credit card were available, then a supervised analysis would be possible. However, this information is not available as we want to know whether customers are interested in credit cards.

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Cluster Analysis

example (outside of astronomy):

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What we can do is trying to cluster the customers on the basis of the variables measured, in order to identify distinct groups of potential customers. Identifying such groups can be of interest because it might be that the groups differ with respect to some property of interest, such as spending habits.

Cluster Analysis

example (within astronomy):

Gamma Ray Bursts: use properties of GRBs (e.g. location on the sky, arrival time, duration, spectral hardness) to find classes of events
(Mukherjee+1998)

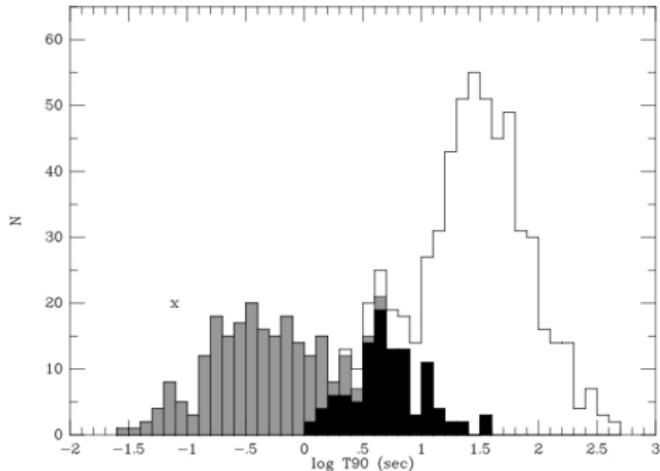


Fig. 5.—Burst types and T_{90} burst duration based on 5-dimensional Average Linkage clustering procedure. Class I = white, Class II = grey and Class III = black. The Class IV outlier is shown as an **x**.

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K-Means Clustering

K-Means Clustering seeks to minimize

$$\sum_{k=1}^K \sum_{i \in C_k} ||x_i - \mu_k||^2$$

where $\mu_k = \frac{1}{N_k} \sum_{i \in C_k} x_i$.

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where $\mu_k = \frac{1}{N_k} \sum_{i \in C_k} x_i$.

The steps are:

1. For a given value of K , initialize K number of centroids randomly and the data points are partitioned into K clusters
2. compute the distance between each of the input to the K centroids and re-assign it to the cluster with the least distance
3. after the re-assignment, update the centroid of each cluster by calculating the mean of the data points in the cluster
4. repeat steps 2 - 3 until there is no re-assignment required

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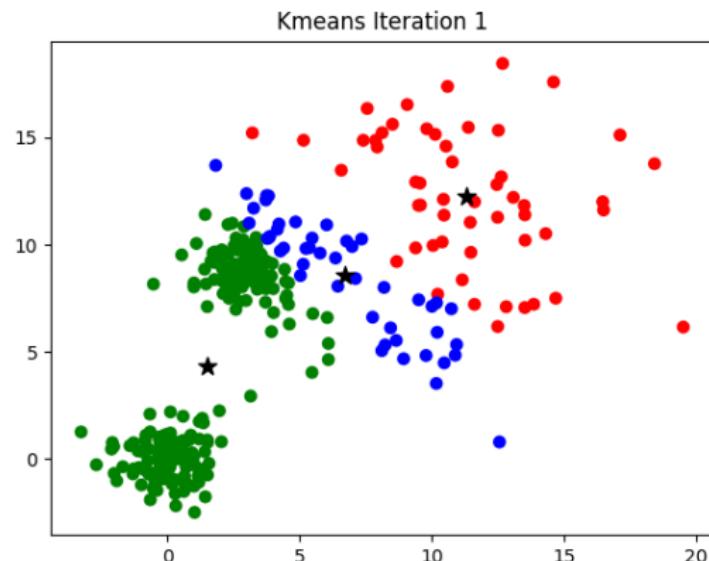
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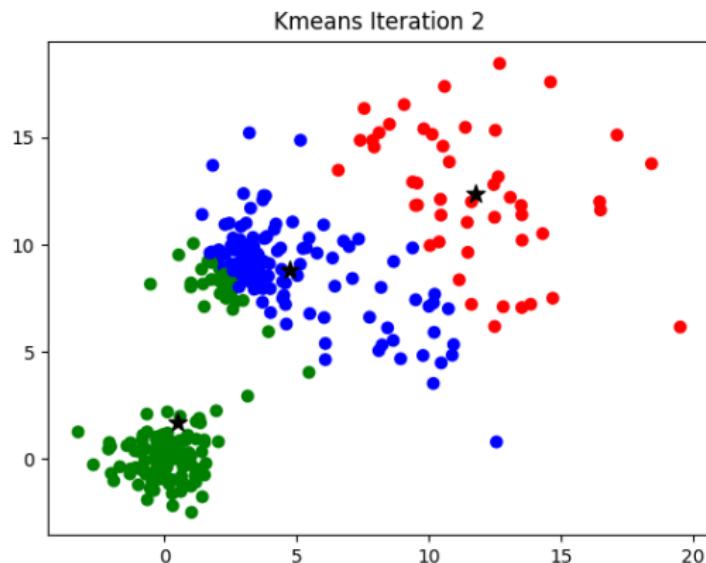
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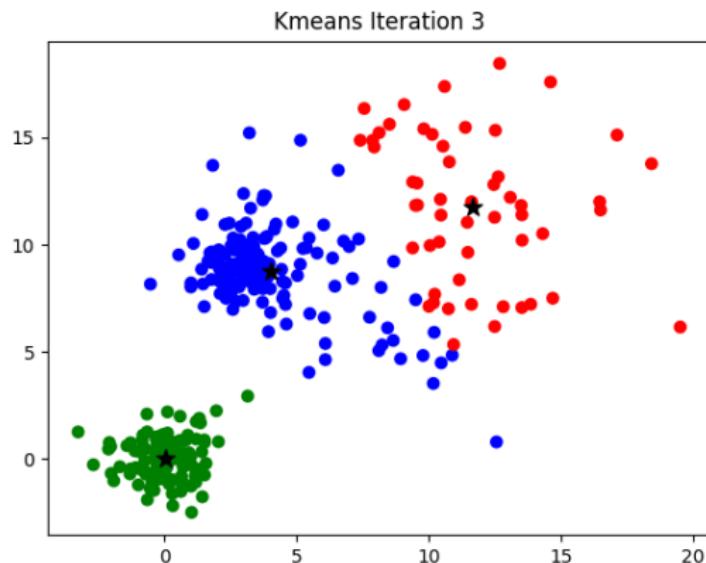
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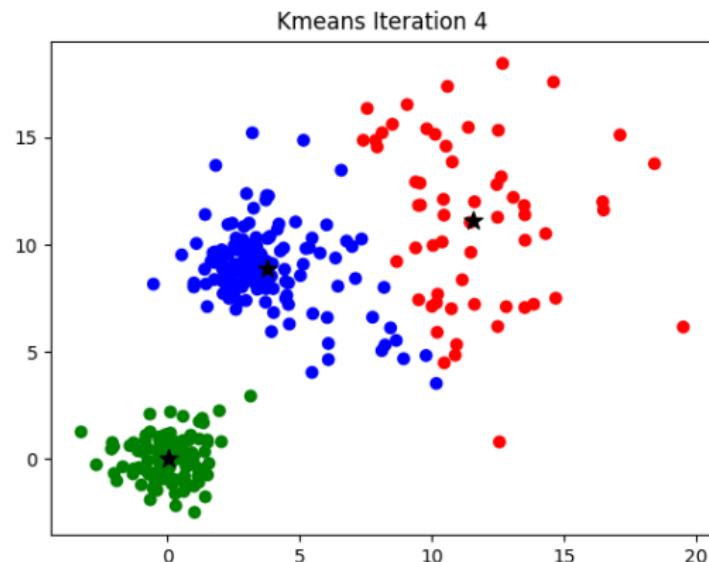
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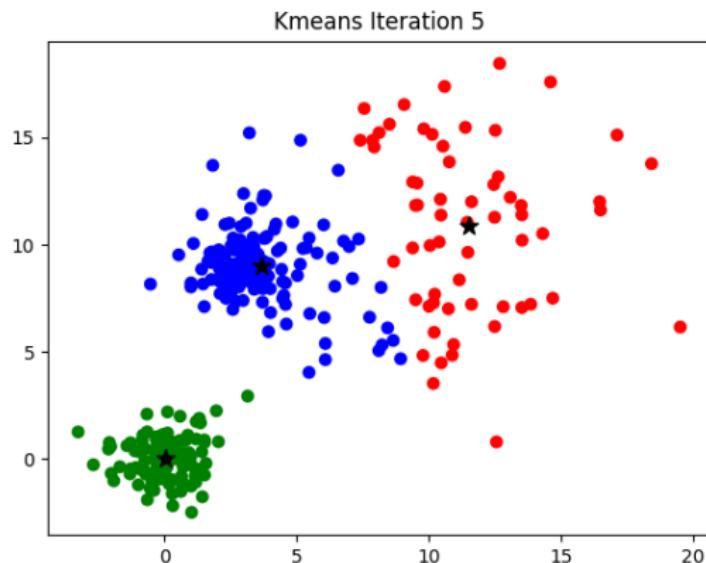
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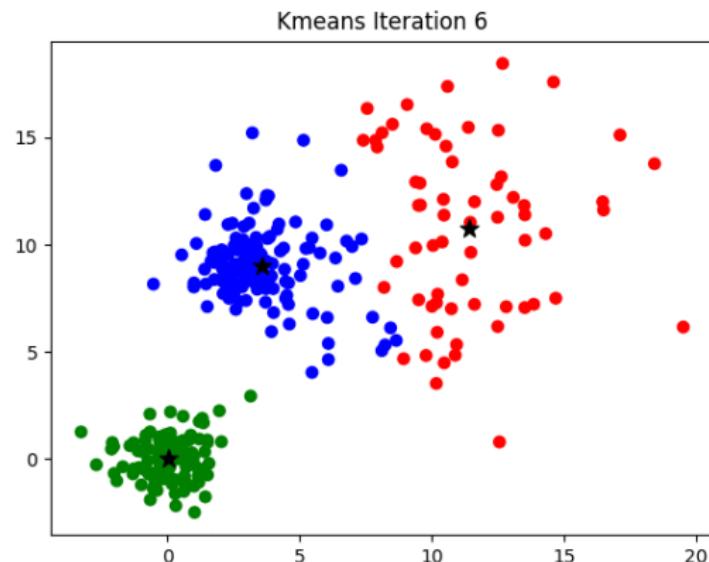
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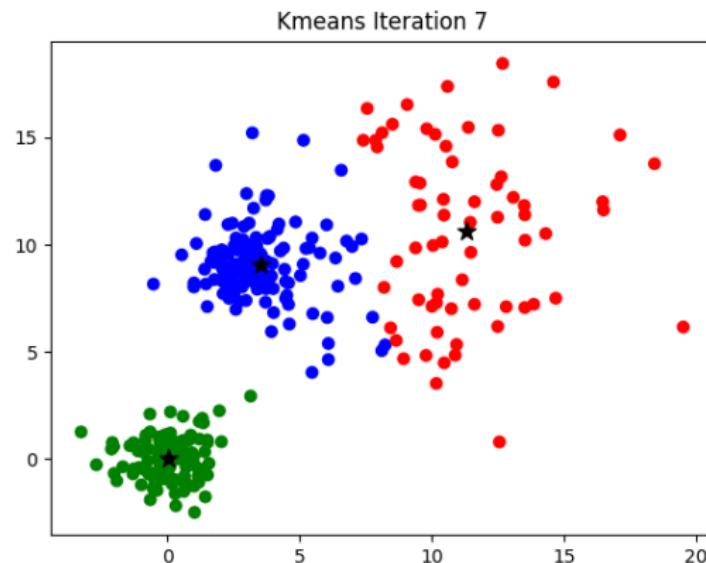
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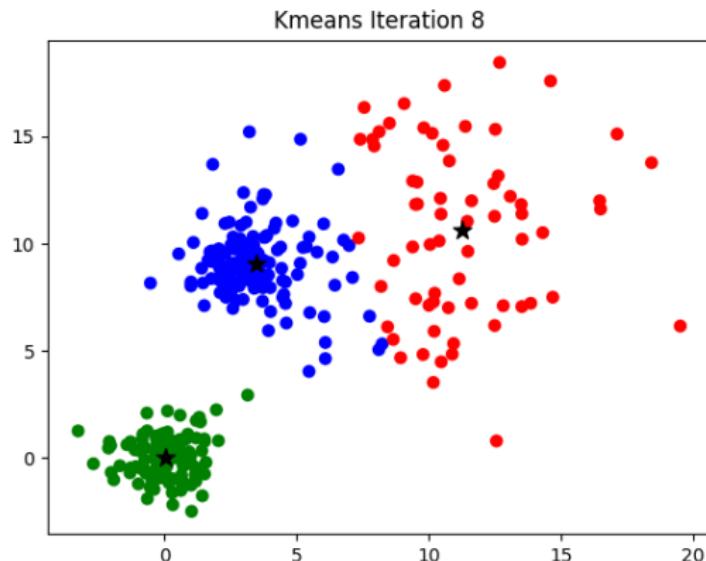
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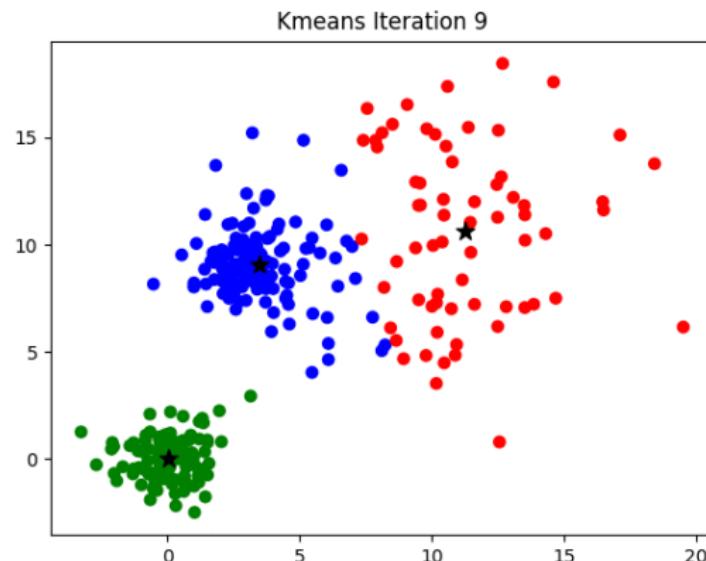
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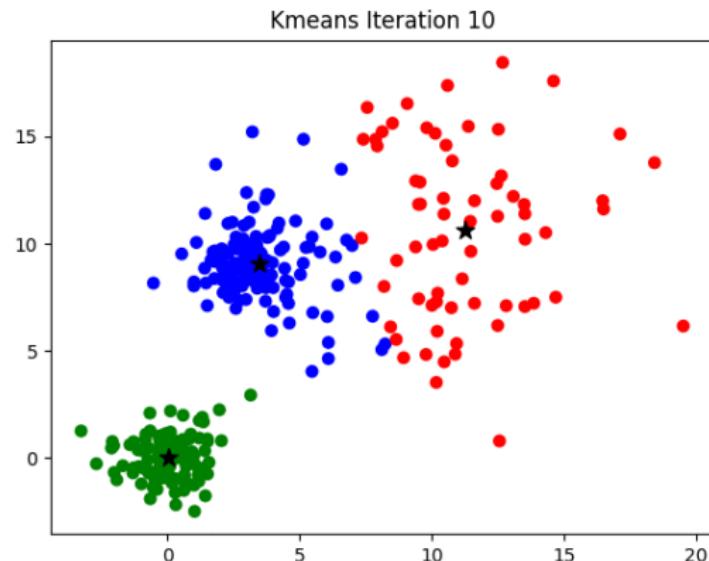
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K-Means Clustering

multidimensional sample, first applying PCA and then a K-Means Clustering

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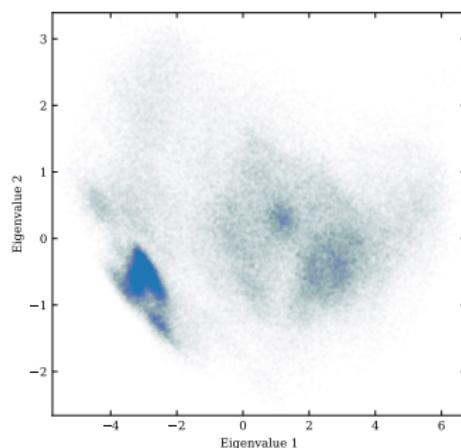
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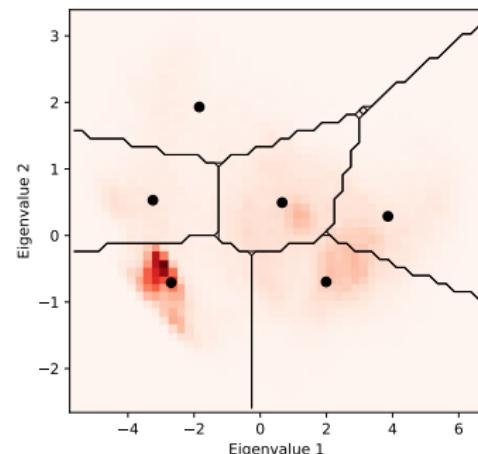
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sample after PCA



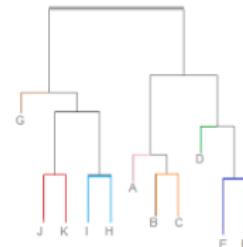
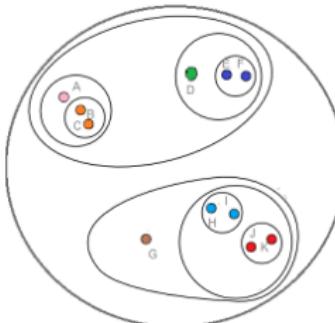
sample after PCA
and *K*-Means Clustering



Hierarchical clustering

Hierarchical clustering is a family of clustering algorithms that build **nested clusters**. This hierarchy of clusters is represented as a **tree (or dendrogram)**. The root of the tree is the unique cluster that gathers all the samples, the leaves being the clusters with only one sample.

The number of clusters aren't specified ahead of time. Instead, hierarchical clustering starts with clusters representing each data point and then the most similar clusters are joined iteratively.



Supervised Versus Unsupervised Learning

When to use which?

Many problems fall naturally into the supervised or unsupervised learning paradigms. However, sometimes the question of whether an analysis should be considered supervised or unsupervised is less clear.

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Suppose we have a set of n observations. For $m < n$ of the observations, we have both predictor measurements and a response measurement. For the remaining $n - m$ observations, we have predictor measurements only.

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Such a scenario can happen if the predictors can be measured rather easily (e.g. in astronomy: photometry), while the corresponding responses are much more difficult/ expensive to measure (e.g. in astronomy: high-resolution spectra).

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Such a scenario can happen if the predictors can be measured rather easily (e.g. in astronomy: photometry), while the corresponding responses are much more difficult/ expensive to measure (e.g. in astronomy: high-resolution spectra).

We refer to this setting as a **semi-supervised learning problem**. We use a statistical learning method that can incorporate the m observations for which response measurements are available as well as the $n - m$ observations for which they are not.

Regression Versus Classification Problems

Supervised learning as a function approximation from samples:

The basic goal of supervised learning is to use the training set S to learn a function f_S that looks at a new x value x_{new} and predicts the associated value of y :

$$y_{pred} = f_S(x_{new})$$

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Regression Versus Classification Problems

Supervised learning as a function approximation from samples:

The basic goal of supervised learning is to use the training set S to learn a function f_S that looks at a new x value x_{new} and predicts the associated value of y :

$$y_{pred} = f_S(x_{new})$$

If y is a real-valued random variable (thus being a quantitative value), we have **regression**.

If y takes values from an unordered finite set (thus being a qualitative categorial variable), we have **classification**.

In two-class (binary) classification problems, we can assign one class a y value of 1, and the other class a y value of 0.

Assessing Model Accuracy

Why is it necessary to introduce so many different statistical learning approaches, rather than just a single best method?

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Assessing Model Accuracy

Why is it necessary to introduce so many different statistical learning approaches, rather than just a single best method?

There is not a single method that's best.

On a particular data set, one specific method may work best, but some other method may work better on a similar but different data set.

We thus must decide based on the given data set which method produces the best results. Selecting the best approach can be one of the most **challenging** parts of performing statistical learning in practice.

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Bayesian Model Comparison

For the **Bayesian** approach to model comparison, we start with Bayes' Theorem,

$$\text{Posterior} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

$$p(M, \theta | D, I) = \frac{p(D | M, \theta, I) \times p(M, \theta | I)}{p(D | I)},$$

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and marginalize over model parameter space θ to obtain the **probability of model M** given data D and prior information I :

$$\begin{aligned} p(M | D, I) &\equiv \int p(M, \theta | D, I) d\theta \\ &= \int \frac{p(D | M, \theta, I) p(M, \theta | I)}{p(D | I)} d\theta \\ &= \frac{p(M | I)}{p(D | I)} \int p(D | M, \theta, I) p(\theta | M, I) d\theta \end{aligned}$$

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Bayesian Model Comparison

To then determine which of two models is better we compute the ratio of the posterior probabilities or the **odds ratio** as

$$O_{21} \equiv \frac{p(M_2|D, I)}{p(M_1|D, I)}.$$

The posterior probability that the model M is correct given data D (a number between 0 and 1) is

$$p(M|D, I) = \frac{p(D|M, I)p(M|I)}{p(D|I)}.$$

We finally get for the odds ratio:

$$O_{21} = \frac{p(D|M_2, I)p(M_2|I)}{p(D|M_1, I)p(M_1|I)} \equiv B_{21} \frac{p(M_2|I)}{p(M_1|I)},$$

where B_{21} is called the **Bayes factor**.

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where B_{21} is called the **Bayes factor**.

The Bayes factor compares how well the models fit the data.
It is a ratio of data likelihoods averaged over all allowed values of the model parameters. For models fitting the data equally well, decision is made based on the priors.

Bayesian Model Comparison

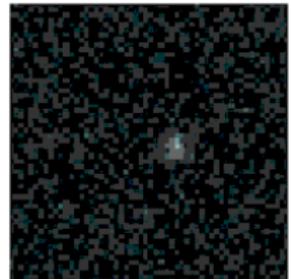
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$$O_{21} = \frac{p(D | M_2, I) p(M_2 | I)}{p(D | M_1, I) p(M_1 | I)} \equiv B_{21} \frac{p(M_2 | I)}{p(M_1 | I)},$$

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example: Consider a noisy image of a source which is equally likely to be a star or a galaxy. The posterior probability that the source is a star will greatly depend on whether we are looking at the Galactic plane or not.



Bayesian Model Comparison

We can compute

$$E(M) \equiv p(D | M, I) = \int p(D | M, \theta, I) p(\theta | M, I) d\theta,$$

where $E(M)$ is called the **marginal likelihood for model M** (or **evidence** or *fully marginalized likelihood*). It quantifies the probability that the data D would be observed if the model M were the correct model.

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Bayesian Model Comparison

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The evidence is a weighted average of the likelihood function, where the prior for model parameters acts as the weighting function.

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How do we **interpret** the values of the odds ratio in practice?

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How do we **interpret** the values of the odds ratio in practice?

Jeffreys (1936, 1961) proposed a scale for interpreting the odds ratio, where $O_{21} > 10$ represents strong evidence in favor of M_2 (M_2 is ten times more probable than M_1), and $O_{21} > 100$ is decisive evidence (M_2 is one hundred times more probable than M_1). When $O_{21} < 3$, the evidence is not worth more than a bare mention.

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caution:

- These are just definitions of conventions, i.e., a way to give a quantitative meaning to qualitative phrases.
- The odds ratio compares the models, it doesn't tell us about the absolute goodness of fit.
Model A can be $100\times$ better than model B (by the odds ratio or another measure), but still don't fit the data well.

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Approximate Bayesian Model Comparison

The full odds ratio can be costly to compute ⇒ **approximate methods** that balance between *goodness of fit* and *model complexity*.

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Approximate Bayesian Model Comparison

Akaike information criterion (AIC)

$$\text{AIC} \equiv -2 \ln[L_0(M)] + 2k + \frac{2k(k+1)}{N-k-1}.$$

with

k : number of model parameters

$L_0(M)$: maximum value of the likelihood function

The term $\frac{2k(k+1)}{N-k-1}$ is sometimes ignored.

The **preferred model** is the one with the minimum AIC value. AIC rewards goodness of fit (as assessed by the likelihood function), but also includes a penalty for an increasing number of parameters to discourages overfitting.

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Approximate Bayesian Model Comparison

Bayesian information criterion (BIC)

The BIC can be derived from the Bayesian odds ratio **by assuming that the likelihood is Gaussian.**

⇒ easier to compute than the odds ratio as it is based on the maximum value of the likelihood, $L_0(M)$, rather than on the integration of the likelihood over the full parameter space (i.e. evidence $E(M)$).

The BIC is for N data points and a model with k parameters:

$$\text{BIC} \equiv -2 \ln[L_0(M)] + k \ln N.$$

The 1st term is equal to the model's χ^2 (under the assumption of normality; note that this is not χ^2 per degree of freedom!).

The 2nd term on the right hand side penalizes complex models relative to simple ones.

Approximate Bayesian Model Comparison

When two models are compared, the model with the smaller BIC/AIC value wins.

If the models are equally successful in describing the data (i.e., they have the same value of $L_0(M)$), then the model with fewer free parameters wins (Occam's razor).

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caution:

Both BIC and AIC are **approximations** and might not be valid if the underlying assumptions (e.g.: Gaussian likelihood) are not met.

⇒ If computationally feasible, compute the odds ratio.

Mean Squared Error

In the **regression** setting, the most commonly-used measure is the mean squared error (MSE), given by

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{f}(x_i))^2$$

where $\hat{f}(x_i)$ is the prediction that \hat{f} gives for the i th observation.

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where $\hat{f}(x_i)$ is the prediction that \hat{f} gives for the i th observation.

The MSE will be small if the predicted responses are very close to the true responses, and will be large if for some of the observations the prediction differs substantially from the true response.

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Mean Squared Error

The MSE is computed using the training data to fit the model. For this reason, it should more accurately be referred to as the training MSE. But: In general, we do not really care how well the method works on the training data. We are interested in the accuracy of the predictions that we obtain when we **apply our method to previously unseen data**.

Suppose we fit our statistical learning method to our training observations $\{(x_1, y_1), \dots, (x_n, y_n)\}$, and we obtain the estimate \hat{f} .

However, we're not interested in whether $\hat{f} \sim y_i$ (training MSE); but we want to know whether $\hat{f}(x_0) \sim y_0$, where (x_0, y_0) is a **previously unseen test observation not within the training set**. This gives us the **test MSE**, and we want to choose the method that gives the lowest test MSE.

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Test and Training MSE



How can we select a method that minimizes the test MSE?

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How can we select a method that minimizes the test MSE?

Optimal case: We have a test data set available (that was not used in training). This is usually the case if we have a large set of observations with response. We can then simply split up our observations into a training and test set.

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Optimal case: We have a test data set available (that was not used in training). This is usually the case if we have a large set of observations with response. We can then simply split up our observations into a training and test set.

Less optimal case: If we have only a low number of observations with response, we might be tempted to simply selecting a statistical learning method that minimizes the training MSE.

Test and Training MSE



How can we select a method that minimizes the test MSE?

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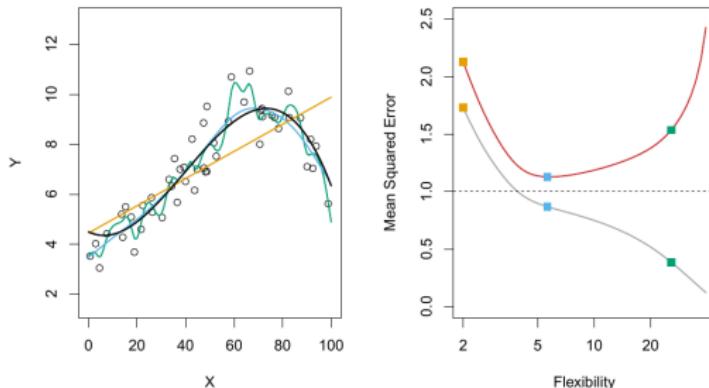
Optimal case: We have a test data set available (that was not used in training). This is usually the case if we have a large set of observations with response. We can then simply split up our observations into a training and test set.

Less optimal case: If we have only a low number of observations with response, we might be tempted to simply selecting a statistical learning method that minimizes the training MSE.

Fundamental problem with this strategy: there is no guarantee that the method with the lowest training MSE will also have the lowest test MSE.

Test and Training MSE

We illustrate this problem on a simple example.

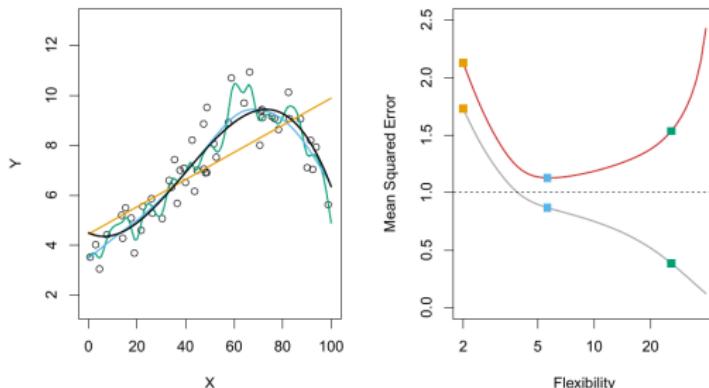


Source: Fig. 2.9 from <https://www.statlearning.com/>

Left: We have generated observations with the true f given by the black curve. The orange, blue and green curves show spline fits obtained using methods with increasing levels of flexibility. As the level of flexibility (degrees of freedom) increases, the curve fit the data more closely.

Test and Training MSE

We illustrate this problem on a simple example.



Source: Fig. 2.9 from <https://www.statlearning.com/>

Right: The curve gives the average training MSE as a function of flexibility. The training MSE declines monotonically as flexibility increases. The red curve gives the test MSE.

The blue curve minimizes the test MSE. The horizontal dashed line indicates $\text{Var}(\epsilon)$, the irreducible error, which corresponds to the lowest achievable test MSE among all possible methods.

Test and Training MSE

When a given method yields a small training MSE but a large test MSE, we are said to be **overfitting the data**. This happens because the statistical learning algorithm is picking up patterns in the data that are just fluctuations rather than by true properties of the unknown function f . In contrary, the test MSE will be very large when overfitting as the supposed patterns that the method found in the training data simply don't exist in the test data.

Note that regardless of whether or not overfitting has occurred, we almost always expect the training MSE to be smaller than the test MSE because most statistical learning methods either directly or indirectly seek to minimize the training MSE. Overfitting refers specifically to the case in which a less flexible model would have yielded a smaller test MSE.

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Model Accuracy for Classification

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Suppose now instead of regression, we seek to estimate f on the basis of training observations where now y_1, \dots, y_n are qualitative. A common approach for measuring the accuracy of \hat{f} is the **training error rate**, the **fraction of incorrect classifications** if we apply our estimate \hat{f} to the training observations:

$$\frac{1}{n} \sum_{i=1}^n I(y_i \neq \hat{y}_i).$$

Here \hat{y}_i is the predicted class label for the i th observation using \hat{f} . $I(y_i \neq \hat{y}_i)$ is an indicator variable that equals 1 if $y_i \neq \hat{y}_i$ (classified incorrectly), and 0 if $y_i = \hat{y}_i$ (classified correctly).

Model Accuracy for Classification

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As in the regression setting, the above gives the training error, whereas we are most interested in the test error rate. The test error rate is given by

$$\text{Ave}(I(y_0 \neq \hat{y}_0)),$$

where \hat{y}_0 is the predicted class label that results from applying the classifier to the test observation with predictor x_0 .

Summary

In this session, we saw an overview about the objectives of statistical learning.

We also saw some applications of classification and regression algorithms, along with methods on how to quantify the quality of fit.

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In the next session, we will focus on the details of **regression algorithms**.

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