

SCHOOL OF COMPUTER AND COMMUNICATION SCIENCES

Applied Data Analysis

Lecture Notes



Dr. CATASTA Michele
Distributed Information Systems Laboratory (LSIR)
michele.catasta@epfl.ch

November, 2016

Contents

1	Introduction	5
1.1	What is Data Science?	5
2	Basic concepts	7
2.1	A taste of "grammar"	7
2.2	Our tools	8
2.3	Panda vs SQL	8
2.4	OnLine Analytical Processing (OLAP cubes)	9
3	Data Wrangling	11
3.1	Diagnosis of the data	12
3.2	Dealing with missing values	12
3.3	General procedure	13
4	Data Variety	14
4.1	Role of Schema	14
4.2	Examples of data	14
4.2.1	XML and DOM	14
4.2.2	JSON	15
4.2.3	Tabular data	16
4.2.4	Log files	16
4.2.5	Binary formats	16
4.3	Processing the data (JSON and XML)	16
4.4	HTML and Web Services	17
4.4.1	HTML	17
4.4.2	Web Services	17
5	Statistics on the Data	19
5.1	Examples of famous mistakes due to statistics	19
5.1.1	Anscombe's quartet: Sensivity of outliers & Robust statistics	19
5.1.2	Simpson's paradox: aggregation of data	19
5.2	Refresh of basic statistics concept	20
5.2.1	Bayes Theorem	20
5.2.2	Random Variables	21
5.2.3	Law of Large Numbers	21
5.2.4	Central Limit Theorem	21
5.3	Most common distributions	21
5.4	Measurement on Samples	23
5.5	Test Statistic	23
5.5.1	Example with t-test	24
5.5.2	Choose the right test	25
5.5.3	Family-wise Error	25
5.5.4	Non-Parametric tests	26
5.5.5	K-S test	26

6 Data Visualization	27
6.1 Two main purposes	27
6.2 Data exploration	27
6.2.1 One variable	27
6.2.2 More than one variable	29
6.3 Moving Towards Interactive Viz	30
6.4 Visualization definitions	31
6.5 Interactive toolkits	36
7 Supervised Learning	37
7.1 Introduction to Machine Learning	37
7.1.1 Different aspects of Machine Learning	37
7.1.2 Supervised vs Unsupervised Learning	38
7.2 More details on Supervised Learning	38
7.2.1 Predicting from Samples	38
7.2.2 Bias and Variance	39
7.3 k-Nearest Neighbors	40
7.3.1 kNN Flavors	42
7.3.2 kNN distance measures	42
7.3.3 Choosing k	43
7.3.4 kNN and the curse of dimensionality	44
7.4 Decision Tree	44
7.4.1 Attribute selection	45
7.4.2 Random Forest	46
7.4.3 Boosted Decision Trees	46
7.4.4 About model transparency	47
7.5 Linear Regression	47
7.5.1 Statistic validation	47

Course content

The purpose of the course is to present multiple topics in the data science field such as *Data Wrangling*, *Data Management*, *Data Mining*, *Machine Learning*, *Visualization*, *Statistics* and *Story telling*. The course has not the presumption to go deeply into each argument. It is due to the extent of the subject and the fact that it is evolving really quickly, hence learning in depth a specific tool will not pay off.

Skills to develop

In this course, you will work, thus develop, the following skills:

Data mining/scraping/sampling/cleaning in order to get an informative, manageable data setlength

Data storage and management in order to be able to access data quickly and reliably during subsequent analysis

Exploratory data analysis to generate hypotheses and intuition about the data

Prediction based on statistical tools such as regression, classification, and clustering

Communication of results through visualization, stories and interpretable summaries

Structure of the notes

The notes of the lectures are put in writing with the aim of summarizing the main topics and concepts illustrated during the classes. To those who are curious, it points to external links that may help you to an in-depth understanding of the field. Each chapter corresponds to a lecture. The hope is that the work could be useful for the current and future students.

1 Introduction

1.1 What is Data Science?

When we talk about Data Science, we often use the term Big Data as the enormous amount of data that exists in the world. But Big Data is not only about collecting huge amount of data. It is challenging but not enough. The real value comes from the insights. The internet companies (Google, Facebook, etc.) understood this many years ago.

An accurate definition of Data Analysis is given by Wikipedia:

Analysis of data is a process of inspecting, cleaning, transforming, and modeling data with the goal of discovering useful information, suggesting conclusions, and supporting decision-making. Data analysis has multiple facets and approaches, encompassing diverse techniques under a variety of names, in different business, science, and social science domains.

[Wikipedia - Data Analysis](#)

Therefore, a Data Scientist has to master different kinds of skills such as **Mathematics**, **Statistics**, **Programming** and the **Domain Expertise**. [Drew Conway's Venn diagram](#), Figure 1, shows the different combination man can obtain with these three skills.

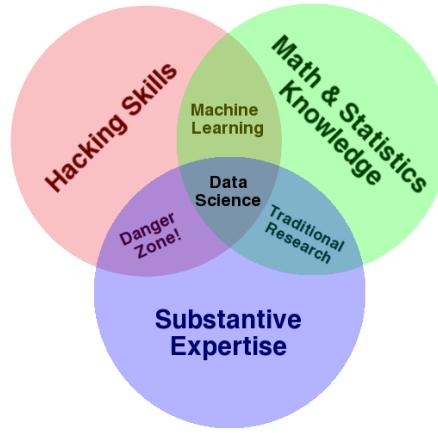


Figure 1: Venn Diagram describing the different combination of skills used by a Data Scientist (by Drew Conway)

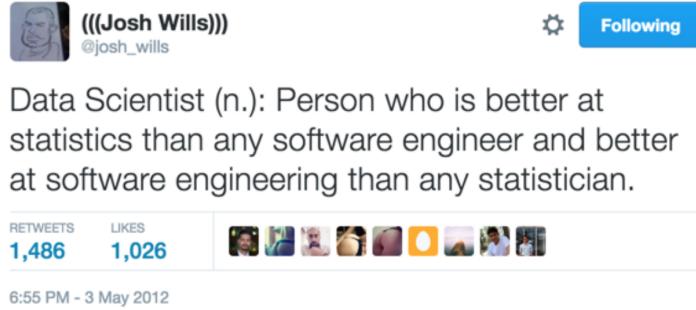
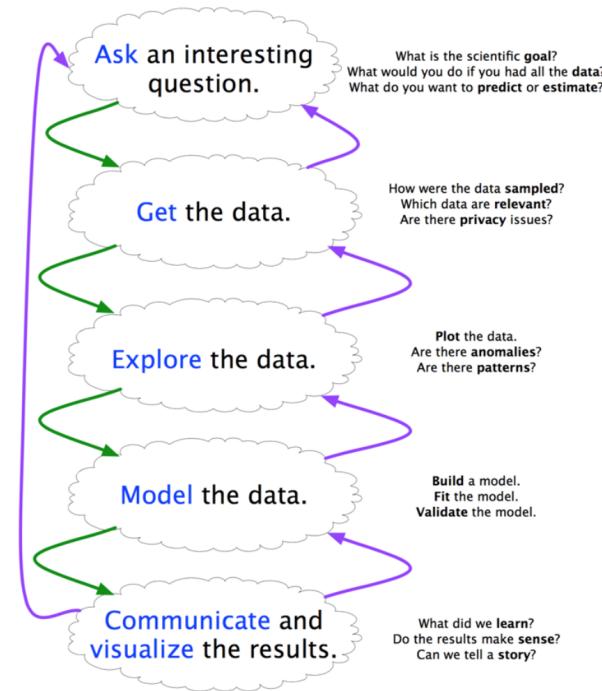


Figure 2: A tweet from Josh Wills, Data Scientist at Slack.

Whether you are interested in knowing what other people think about *Data Science* there are many ongoing [discussions](#).

A more practical definition

Data Science is about the whole processing pipeline to extract information out of data. As such, a Data Scientist **understands and cares about the whole data pipeline**.



A **data pipeline** consists of 3 steps:

1. Preparing to run a model:
Gathering, cleaning, integrating, restructuring, transforming, loading, filtering, deleting, combining, merging, verifying, extracting, shaping
2. Running the model
3. Communicating the results

A “good” Data Scientist will always go back and forth between the steps. The diagram on the left shows exactly what can happen.

2 Basic concepts

2.1 A taste of "grammar"

A data science student is attended to understand the *Grammar of Data Science*. We are going to learn the core data manipulations, so no matter what is the backend is SQL, pandas and R(with dplyr), all share the same *grammar*. For sure having some backgrounds in SQL concepts is a good thing because, as it is very common, people love to make examples with it. Here is a brief refresh of some definitions and concepts that are essential and we need to be aware of.

Let's start with two key concepts that *Structured data* requires:

- **Data model:** a collection of concepts for describing data.
- **Schema:** a description of a particular collection of data, using a given data model.

The most common and ubiquitous approach to manage data is the *Relational model* ([E. F., Ted Codd](#)). It can handle most of the data, so most of it is "reduced" to this model. To have an idea, a counter example is the facebook-like data which requires **graph model**. The *Relational model* is composed by relations. A *relation* is made up two parts:

1. The **Schema** specifies name of relation, plus name and type of each column.
For example, `Students(sid: string, name:string, age:integer)`
2. The **Instance**, *i.e.* the data at a given time.
Definitions:
 - **Cardinality** is the number of rows (= number of items)
 - **Degree or Arity** is the number of fields (= number of attributes)

Database vocabulary

Here follows a list of basic words and operations that should be kept in mind when we talk about *Databases*.

- A **JOIN** is a mean to combine tables based on shared attributes (most of the time some **IDs**). Despite its apparent simplicity beware of the many ways to compute a JOIN and check what is the default JOIN of a language before using it. Every different JOIN operation has implications on the resulting relation. The Figure 3 summarises these possibilities.
- *Aggregation, reduction, and groupby* are the actions of reducing data with a common operation (`sum, count, average, ...`) to summarize them. Remember that you always need to specify the *attribute* you are going to perform the *aggregation* on.

Whether you are not too familiar with *Database* you can go through this [course](#) and look up for what you need.

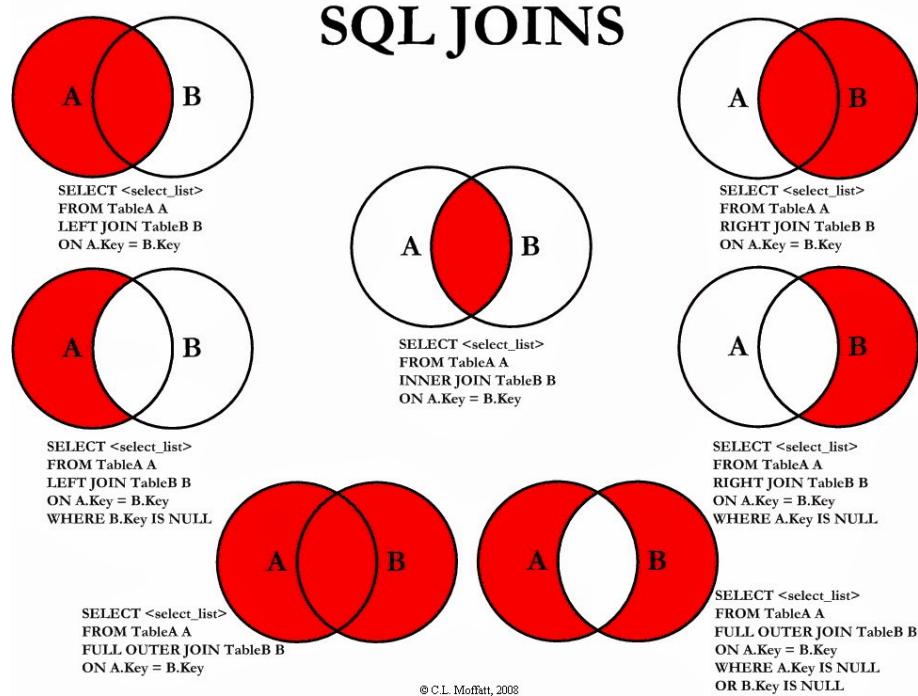


Figure 3: Different ways to join two tables and the related SQL command. [Wikipedia - Join \(SQL\)](#)

2.2 Our tools

During this course and, likely, in your future, to handle data you are going to use a '*magic*' Python's tool that has a black and white coat, with black fur around its eyes: **pandas**. The basic ingredients of our beloved **pandas**:

- **Series** are a name, ordered dictionary
 - keys are indexes
 - built on **numpy.ndarray** (so values can be any Numpy data type)
- **DataFrame** is a table with named column
 - the columns are series
 - it is indeed a dictionary with (columnName → series)

Learn how to use **pandas** and discover the beauty of [IPython Notebooks](#).

2.3 Panda vs SQL

pandas is built to allow easy and fast *data exploration* and not to be a database manager, as SQL is. Thus there are benefits and drawbacks of using it.

Pros	Cons
<ul style="list-style-type: none"> + Lightweight & fast + Great expressiveness (combine SQL + Python) + Easy plot for data visualization (e.g. Matplotlib) 	<ul style="list-style-type: none"> - Tables stored directly in memory - No post-load indexing functionality - No transactions, journalings - Large, complex joins are slower

2.4 OnLine Analytical Processing (OLAP cubes)

OLAP tools enable users to analyze multidimensional data interactively from multiple perspectives. Conceptually, it is like an n-dimensional spreadsheet (a cube) on which we can apply various operations to take decisions.

OLAP cubes are another way to see data tables and are constructed based on them, as shows Figure 4.

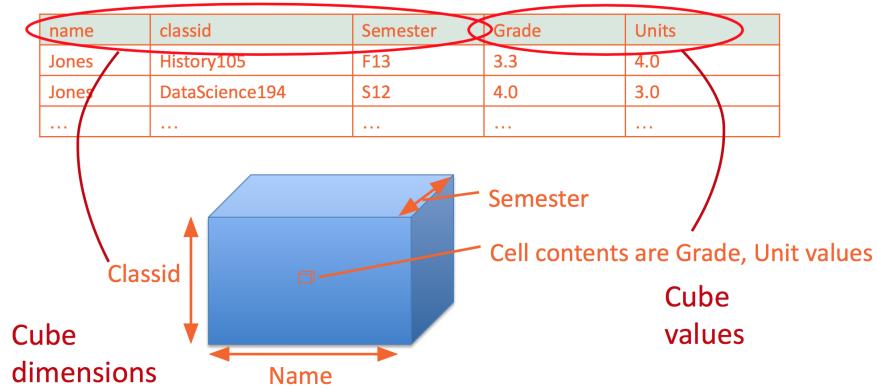


Figure 4: Construction of an OLAP cube from a table.

Operations on OLAP cubes are the following and are illustrated on Figure 5

- *Slicing* fixes one or more variable
- *Dicing* selects a range of one or more variable
- *Drilling up/down* change levels of a hierarchically indexed variable, i.e. "zoom" on a variable and see the subcategories it contains.
- *Pivoting* change the point of view of the cube. Swap an aggregated variable and a detailed one.

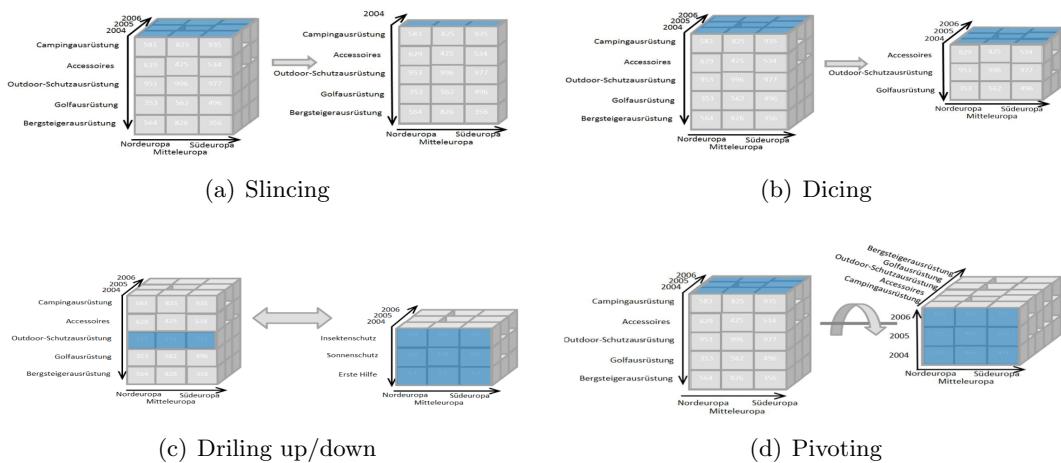


Figure 5: Operations on OLAP cubes

Pros	Cons
+ The main advantage of OLAP cubes is that they are conceptually simpler to understand by a non-scientist person, e.g. a business man who has to take day-to-day decisions based on company's data. Aggregations are limited but cover the main common cases that we can encounter.	- Because of the "on-line" behaviour of this approach, all types of aggregation must be pre-calculated among all combinations of axes which is very expensive in memory and in time (when updating the data)

3 Data Wrangling

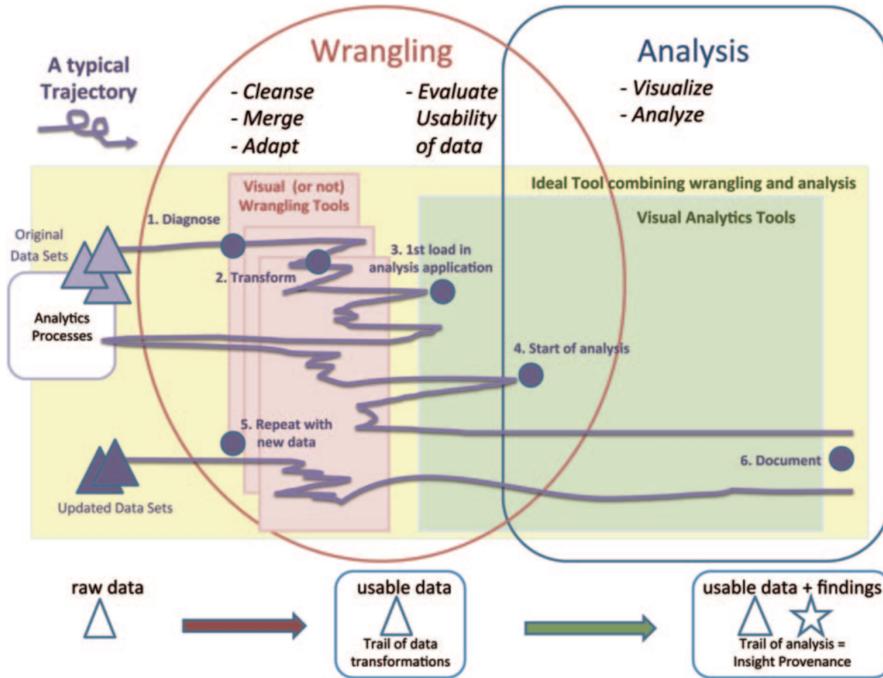


Figure 6: Things do not always happen as expected...

Before any analysis, data need to be transformed from "dirty" to clean and processable data.

Data come from different sources, sometimes collected through different methods over time, with different conventions. Generally, it leads to unwanted anomalies and duplicates. *Data wrangling* goal is to **extract and standardize these raw data**. The best way to do it is to **combine** automation with visualizations in order to proceed with the cleaning.

Here is a *non-exhaustive* list of where data problems can come from:

- *Missing data*
- *Incorrect data*
- *Inconsistent representations of the same data*
- *Non-standardized data (centimeter or inches? Fahrenheit or Celsius?)*
- *Duplicated data*

About 75% of these problems will need **human intervention** to be corrected (by the data-scientist or by crowdsourcing). Some examples of good data leading to horrible conclusion can be found here: [Dirty Data Horror Stories](#).

Even if it seems really dirty, **beware not to over-sanitize the data!** Applying what we can call "defensive programming" is not a good idea because we risk losing any interesting data, keeping only the ones that fit perfectly in our model.

Anyway, a good *Data wrangling* procedure brings about improvements in the efficiency and scale of data importing.

3.1 Diagnosis of the data

One of the most important aspects of Data Wrangling is to **understand** the data and to **find** possible problems. In order to "diagnose" the data, two tools can be used:

- Visualization (A *thoughtful* visualization will always help)
- Basic Statistics

Look out, outliers and missing data can be often identify using a plot. Visualization becomes increasingly difficult when **data gets larger**.

Matrix visualizations of the facebook graph is shown in Figure 7. The Relational visualization, Figure 7(a), does not show any particular problem in the data. But the Time dependant visualization, Figure 7(b), shows that the Facebook API reached its limit while collecting data.

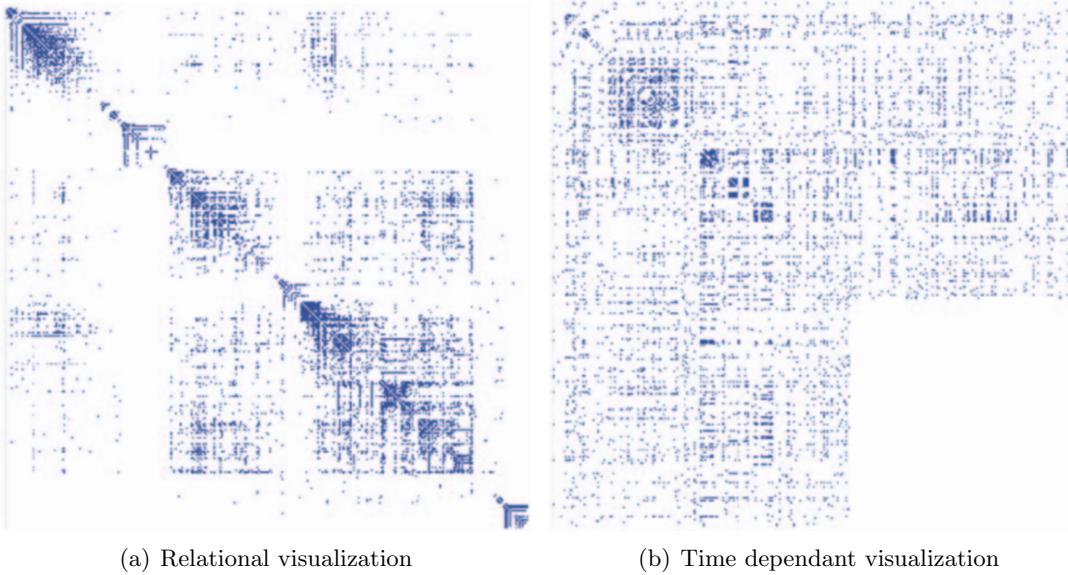


Figure 7: Matrix visualization of the facebook graph.

3.2 Dealing with missing values

Values can often miss from the data we have, because of various events (war, fire, ...). We must detect and correct these values with different methods according to the domain we are working in.

Whatever the method used, it's good to keep track of these changes to know which are original data and which are modified ones.

- Set values to zero Figure 8(a)
- Interpolate based on existing data Figure 8(b)
- Omit missing data Figure 8(c)
- Interpolation with tracks kept Figure 8(d)



Figure 8: To deal with missing values.

3.3 General procedure

Once the data are well wrangled and before trying to analyze them, we must take care of two more steps:

1. **Deal with uncertain data** (can arise from measurement errors, wrong sampling strategies, etc.)
2. **Parse/transform data** (with aggregation and reduction techniques) to obtain meaningful records

As we say in the Introduction, *Data Science* is a mixture of different fields. It often leads to the necessity of working in team where different people have different skills. Working in a team means sharing code, documentation and data. Hence, taking care of them is essential.

4 Data Variety

The “**3 Vs**” of Big Data: *Volume*, *Velocity* and *Variety*. In this course, we don’t address the *Volume* and *Velocity* parts (A course on Database does). Since there is a lot of variety in the data, we need to prepare the data. This flow is called **ETL**:

- **Extract** from the *source(s)*.
- **Transform** data at the source, sink, or in a *staging area*.
- **Load** data into the *sink*.

This variety of the data comes, in a first place, from the many different sources from which we extract them: *files*, *databases*, *logs*, ... Each of these sources uses (or not!) its proper convention and can contain structured (DB), semi-structured (logs) or unstructured (web page) data.

4.1 Role of Schema

The **Schema**, which specifies the *structure* and *types* of data repository, is changing. Traditional databases are **schema-on-write**, *i.e.* you cannot load data into a table without a schema. But new data stores (NoSQL for example) are **schema-on-read** or **schemaless**.

- **Schema-on-write** is typically SQL, where we must create a table before inserting data in our system. Data must scale the defined schema and this is both the strength and weakness of the system. Strength because the data is perfectly oriented and respect the constraints we establish. Weakness because schemas are always subjective in some ways and data (which are perfectly correct) may not fit with it.
- **Schema-on-read** is for instance XML, where you create the schema according to the data you read.
- Youtube and Google Cache where the first **schemaless** data system. Without schema, everything is simply stored as a string and we need a parser to return a typed data.

4.2 Examples of data

4.2.1 XML and DOM

The XML data are used mostly with HTML and specifies the data structure. An XML schema can be applied to interpret the XML data and specifies the **data types**. Figure 9 shows the XML data 9(a) and the schema 9(b) used to parse and type the data.

```

<xs:schema xmlns:xsd="http://www.w3.org/2001/XMLSchema"
elementFormDefault="unqualified">
<xs:complexType name="location">
  <xs:sequence>
    <xs:element name="latitude" type="xsd:decimal"/>
    <xs:element name="longitude" type="xsd:decimal"/>
  </xs:sequence>
</xs:complexType name="location">

<location>
  <latitude>37.78333</latitude>
  <longitude>122.4167</longitude>
</location>

```

(a) XML data

(b) XML schema

Figure 9: Example of XML.

The XML is a text format that encodes **DOM** (Document-Object Models). It's a data structure often used by Web pages. The DOM is tree-structured. An example of a DOM is given in Figure 10.

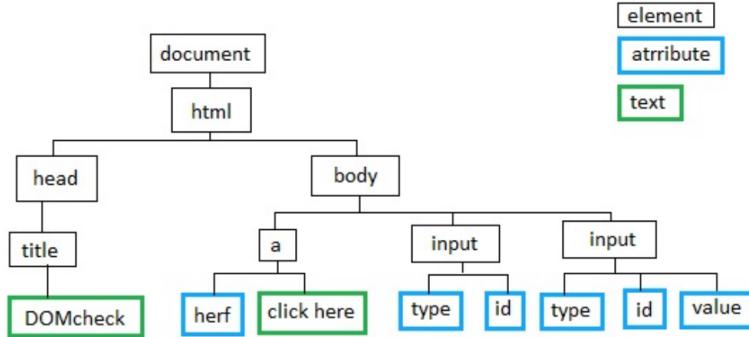


Figure 10: Example of a DOM tree for an HTML Web page.

The XML schema allows a database to interpret the data when running queries. It can do arithmetic or range queries on numerical values, for example.

4.2.2 JSON

JSON stands for Javascript Object Notation. It's a schemaless data (schema support was added later). An example of JSON data is shown in Figure 11

```
{
  "firstName": "John",
  "lastName": "Smith",
  "age": 25,
  "address": {
    "streetAddress": "21 2nd Street",
    "city": "New York",
    "state": "NY",
    "postalCode": "10021-3100" },
  "phoneNumbers": [
    { "type": "home",
      "number": "212 555-1234" },
    { "type": "office",
      "number": "646 555-4567" } ],
  "children": [],
  "spouse": null
}
```

Figure 11: Example of a JSON data.

JSON is typically used to represent **hierarchical data structures** directly in the target language (Javascript or Java at the beginning). The transformation on the data is procedural in the target languages. It is often easier for some tasks, but it can be painful for some of them: for example schema changes.

4.2.3 Tabular data

A Tabular Data is simply data put into a table such as CSV (Comma Separated Value) or TSV (Tab Separated Value). Definition of a table:

- A **table** is a collection of **rows** and **columns**.
- Each row has an **index**.
- Each column has a **name**.
- A **cell** is specified by an (index, name) pair.
- A cell may or may not have a **value**.

It's a very simple yet powerful data type. For example, the sensors usually output data in the form of time series, transformed into a tabular format. However, a system dealing with sensor data should:

- support both long-term (**trend**) and short-term (**real-time**) queries
- have **low latency** but also efficient. It should use **real-time indexing** for longer-term queries.
- support triggers (**alerts**) for a variety of conditions.

Therefore, the **complexity of a data format** does not determine the **complexity of the system required to properly handle it**.

4.2.4 Log files

The log files are simple text files giving information about the process. The daemons, such as `httpd`, `mysqld` or `syslogd`, usually create logs. `syslog` was developed by Eric Allman. It's a way for devices to send event messages to a server that will log all the events. Splunk is a company that built a successful business model around the `syslog` events.

4.2.5 Binary formats

They are often the key to performance because we **avoid expensive parsing**. The modern formats even support nested structures, various levels of schema enforcement, **compression**, etc. Some examples: [Protocol Buffers \(Google\)](#), [Avro \(Apache\)](#), [Parquet \(Apache\)](#), etc.

4.3 Processing the data (JSON and XML)

In order to process XML, we can use the DOM. It can also be used to process JSON data. The DOM is very easy to work with: all the data are directly accessible by links. The problem is that we **might not care about most of the data** and if the data are big, they **might not fit into the RAM**. In order to deal with these two problems, we can use a **SAX** parser which is an event-driven parser. It will find all the **open-close-tag events** in an XML document and will do callbacks to user code.

- + User code can respond to only a subset of events corresponding to the tag it is interested in.

- + User code can correctly compute aggregates from the data rather than create a record for each tag.
- + User code can implement flexible error recovery strategies for ill-formed XML.
 - User code must implement a state machine to keep track of “where it is” in the DOM tree.

For JSON, most parsers construct the “DOM” directly. But there are a few SAX-style parsers: Jackson, JSON-simple, etc. Sometimes **SAX-style is the way to handle ill-formed datasets**, an endless array of objects, for example.

4.4 HTML and Web Services

4.4.1 HTML

Internet contains an “enormous” amount of data. Some crawlers such as Common Crawl datasets contains about 1.82 billion web pages (for 145 TB). We can use different tools to crawl data from the web. Examples for Python: BeautifulSoup, Requests, Scrapy, etc.

Most of the time, the Web pages are considered as unstructured data. But you can find some semi-structured data, *e.g.* Google WebTables. Some big “internet” companies (Google, Yahoo, Yandex and Microsoft) are sponsoring a project called [schema.org](#) to create structured or semi-structured Web pages. A core vocabulary for the type of fields is given. schema.org is more and more used. It’s also used by knowledge bases such as Google Knowledge Graph. [WikiData](#) is a community project to create an open database of structured data taken from Wikipedia.

4.4.2 Web Services

Screen-scraping the content of a large website was possible before, but become more and more difficult nowadays. This is mainly due to the content ”hidden” behind a form or an authentication. Take for example facebook without account, or the IS-academia course page if you do not select a semester. Therefore big companies are providing Web Service APIs¹ to retrieve data from their website. There are two kinds of Web Services:

- The old way: XML-based RPC-style messages: SOAP
- The new way: REST-style stateless interactions, URLs encode state

4.4.2.1 RPC

The SOAP RPC² messages typically encode arguments that are presented to the calling program as parameters and return values. HTTP POST/GET are used to communicate.

¹Application Program Interface: Set of subroutine definitions, protocols, and tools for building software and applications. In this particular case, the APIs are used to retrieve the data from the Web page, *e.g.* Facebook API to retrieve the contacts.

²SOAP = Simple Object Access Protocol, RPC = Remote Procedure Call

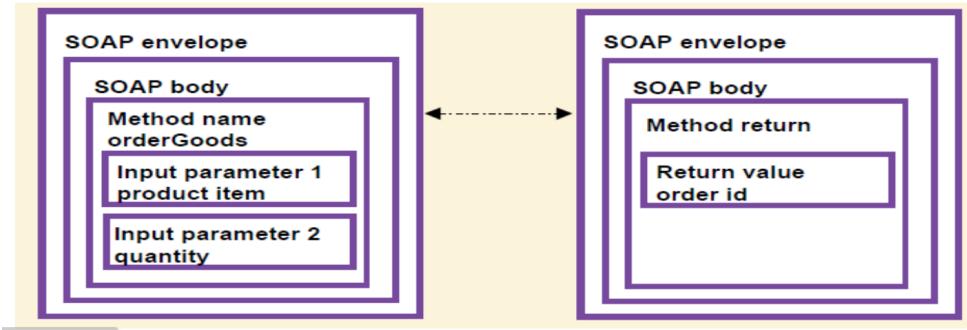


Figure 12: Example of a SOAP RPC exchange.

This kind of procedure (same for XML-RPC) requires a request-response cycle. This often leads to longer “conversations”. The RPC-style is being quickly superseded by newer and more user-friendly technologies.

In **RPC systems**, the design emphasis is on **verbs**. It uses functions such as *getUser()*, *addUser()*, etc.

4.4.2.2 REST

REST³ is a **stateless** client/server protocol. The principles are:

1. Each message in the protocol contains all the information needed by the receiver to understand and/or process it. This constraint attempts to “*keep things simple*” and avoids needless complexity.
2. Set of Uniquely Addressable Resources
 - “*Everything is a Resource*” in a RESTful system
 - Requires universal syntax for resource identification, *e.g.* URI.
3. Set of Well-Defined Operations that can be applied to all resources
 - In the context of HTTP (REST APIs), the primary methods are: **POST**, **GET**, **PUT**, and **DELETE**
These are similar (but not exactly) to the database notion of CRUD (Create, Read, Update, and Delete)
4. The use of Hypermedia both for Application Information and State Transitions
 - Resources are typically stored in a structured data format that supports hypermedia links, such as XHTML or JSON.

In **REST systems**, the design emphasis is on **nouns**. It uses the HTTP Protocols (POST, GET, PUT, and DELETE) a *User*, a *Location*, etc.

³REpresentation State Transfer

5 Statistics on the Data

When we explore and analyze data, it would be great if we only had to look at some statistics numbers and make automatically a conclusion about them. Sadly, it's not the case. At all.

5.1 Examples of famous mistakes due to statistics

5.1.1 Anscombe's quartet: Sensivity of outliers & Robust statistics

The FIG 13 show four different data distribution that present, despite all of that, the same means on x and y , the same variance on x and y , and, thus, the same linear regression function. This is due to the statistics used to define them.

- Min, Max, Mean, Standard Deviation (Std) and Range are sensitive to outliers and then are **not robust statistics**.
- Median, quartils, (and others) are not sensitive and then are said to be **robust statistics**.

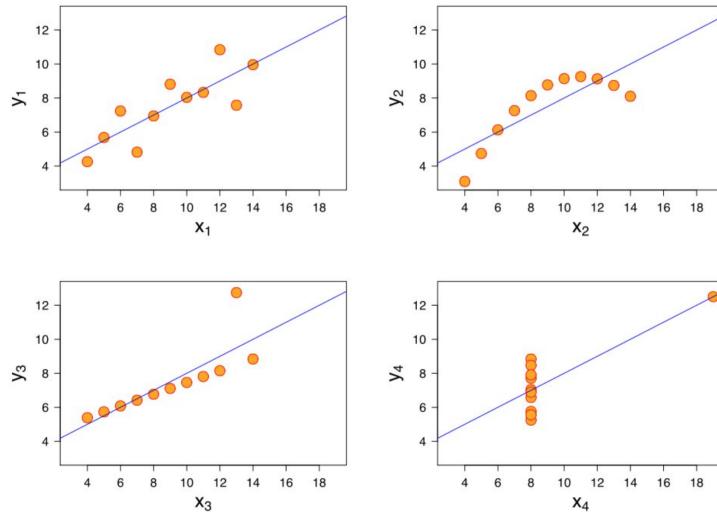


Figure 13: Anscombe's quartet

5.1.2 Simpson's paradox: aggregation of data

Certain tendencies can appear, disappear or even reverse themselves when aggregating the data! This was the case when media started blaming Berkeley of being unfair with women applications (looking at left table of FIG 14). After further investigation (and de-aggregation of the data), it appeared that at the opposite... Berkeley was unfair with men! (Right table of the same FIG).

This paradox comes from the fact that women (according to these tables) tended to apply for more competitive departments, with lower rates of admission. **When aggregating the data, we lost this subtlety and then draw a wrong conclusion.**

Simpson's paradox can appear in a lot of cases and can be very hard to detect. The [wikipedia page of Simpson's paradox](#) describes a lot of examples and, for the ones interested, a great book relates lots of statistical errors that drove to miscarriages of justice: [Leila Schneps and Coralie Colmez, Math on Trial: How Numbers Get Used and Abused in the Courtroom](#)

Department	Men		Women	
	Applicants	Admitted	Applicants	Admitted
Men	8442	44%		
Women	4321	35%		
A	825	62%	108	82%
B	560	63%	25	68%
C	325	37%	593	34%
D	417	33%	375	35%
E	191	28%	393	24%
F	373	6%	341	7%

Figure 14: Berkley admission tables of 1973

5.2 Refresh of basic statistics concept

- **Probabilities:** mathematical theory that describes uncertainty.
- **Statistics:** Set of techniques for extracting useful info from data

Probability and Statistics are related areas of mathematics which concern themselves with analyzing the relative frequency of events. Still, there are fundamental differences in the way they see the world:

Probability deals with predicting the likelihood of future events, while statistics involve the analysis of the frequency of past events.

Probability is primarily a theoretical branch of mathematics, which studies the consequences of mathematical definitions. Statistics is primarily an applied branch of mathematics, which tries to make sense of observations in the real world.

Steven S. Skiena, "Calculated Bets", Cambridge University Press, 2001

5.2.1 Bayes Theorem

The theorem express the very intuitive statement that:

The probability of observing event A and B is the probability of observing B multiplied by the probability of observing A knowing that B occurred.

Mathematically it's expressed as:

$$P(A|B)P(B) = P(A \cap B) = P(B|A)P(A) \quad (1)$$

Or equivalently

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \quad (2)$$

More about Bayes Theorem on [wikipedia](#).

5.2.2 Random Variables

A **random variable** is a quantity that can take various values, each one associated with a probability of apparitions. The sum of these probabilities will always be 1.

$$X: \Omega \rightarrow E \quad (3)$$

Ω being a probability space and E a measurable space (usually $E = \mathbb{R}$).

Any random variable can be described by its **cumulative distribution function**, which describes the probability that the random variable will be less than or equal to a certain value.

Two **independent variables** are defined as

$$\mathbb{P}(A \cap B) = \mathbb{P}(A) \cdot \mathbb{P}(B). \quad (4)$$

or equivalently (by Bayes Theorem)

$$\mathbb{P}(A | B) = \mathbb{P}(A) \quad (5)$$

More about Bayes Theorem on [wikipedia](#).

5.2.3 Law of Large Numbers

The Law of Large Numbers links, in some way, the probability to the statistics. It's, again, a very intuitive statement, even if not so easy to prove (as always in mathematics).

In probability theory, the **law of large numbers** (LLN) is a theorem that describes the result of performing the same experiment a large number of times. According to the law, **the average of the results obtained from a large number of trials should be close to the expected value**, and will tend to become closer as more trials are performed.

[Wikipedia](#)

A common mistake is to deduce that, in the case of playing heads or tails for example, observing a lot of time **heads** increase the probability of observing **tails**. This is absolutely wrong. The variables are perfectly independent and, according to Eq 5, the probability stays exactly 50%. This is the perfect example of confusing probabilities with statistics.

5.2.4 Central Limit Theorem

Central Limit Theorem states that the mean of independent and identically-distributed random variables will converge to **Gaussian Distribution** (Normal Distribution).

5.3 Most common distributions

- **Gaussian Distribution** (fig 15) results from independent and identically-distributed variables $f(x | \mu, \sigma^2) = \frac{1}{\sqrt{2\sigma^2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$ [More on wikipedia](#)
- **Poisson Distribution** (fig 16) describe the observation of events happening in a delimited time-laps. E.g: an event happens in average 4 times each 10 minutes ($\lambda = 4$). What's the probability that it appears after only 3 times in this same interval ($k = 3$)? $p(k) = \frac{\lambda^k}{k!} e^{-\lambda}$ [More on wikipedia](#)

- **Exponential Distribution** (fig 17) describes the time between two events in a Poisson process. $P(x) = \lambda e^{-\lambda x}$ [More on wikipedia](#)
- **Binomial Distribution** (fig 18) describes the discrete distribution on success in a yes/no experiment. (E.g. coin tossing or any win/lose game). $f(k; n, p) = \Pr(X = k) = \binom{n}{k} p^k (1-p)^{n-k}$ [More on wikipedia](#)
- **Multinomial Distribution** generalizes Binomial law. [More on wikipedia](#)
- **Zipf Distribution** is an empirical discrete description of word frequency in a text. [More on wikipedia](#)
- **Pareto Distribution** is the equivalent of Zipf in a continuous space. It allows, amongst other things, to give a theoretical base of the "80-20 principle" (20% of the causes produce 80% of the effects). [More on wikipedia](#)
- **Yule-Simon distribution** describes discrete frequencies of term too. [More on wikipedia](#)

You should understand the distribution of your data before applying a model!

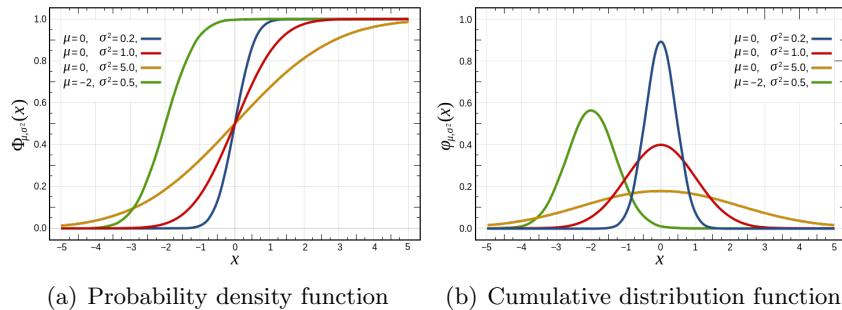


Figure 15: Gaussian distribution

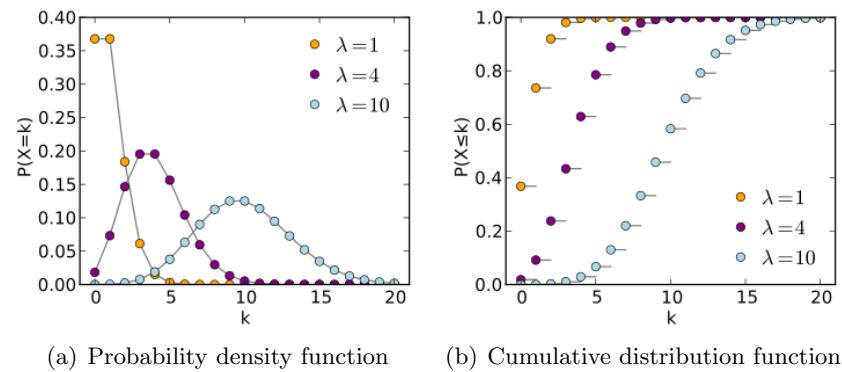


Figure 16: Poisson distribution

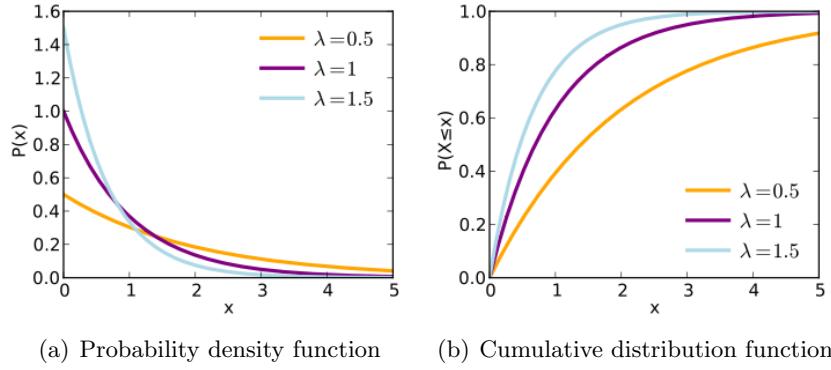


Figure 17: Exponential distribution

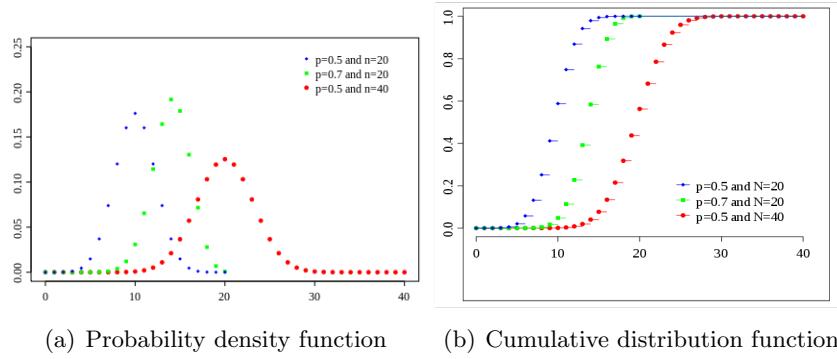


Figure 18: Binomial distribution

5.4 Measurement on Samples

In practice, we (almost) never analyse the entire population. We always work on a subset of it called **sample**. The **variance** is the variation between elements of our sample, that we hope to be the same as the population. The **biases** is the systematic variation between the entire population and the sample we chose.

When randomly select elements of the population to be part of the sample, we have a great chance that the bias is small (i.e. that the distribution of the sample corresponds to the distribution of the population). But do not forget that there is a probability (even if a small one) to select elements that **biased our measures!** This probability can even increase when you clean the data, if you don't do it wisely.

A stupid example could be a study on population education in which, during the cleaning, you remove the answers containing misspelling. Uneducated people are more likely to commit misspelling so, removing them, you artificially bias the sample.

5.5 Test Statistic

(The only good and easy-to-understand explanation about test statistics I ever found is available on [hamelg.blogspot](#))

The idea behind test statistics is instead of proving that our assumption is true, let's calculate the probability that our observations occur by chance (null hy-

pothesis or H_0). If this probability is very low, then there is a good chance that our hypothesis is true!

The probability that this happens by chance is called *pvalue* and we usually consider that if $pvalue \leq 0.05$ our hypothesis is true ($pvalue \leq 0.01$ in some strict cases).

5.5.1 Example with t-test

Let's take the example on FIG 19. The **Null Hypothesis** H_0 represents the distribution of observation we can do, assuming there is no correlation between the values we measured. The **Alternative** is H_A , our hypothesis which states that, at the opposite, there is correlations.

- If the observation we test is $x = 3$, there is **less than 5% probabilities that it was produced by H_0** ($pvalue \leq 0.05$). Our hypothesis H_A is considered true.
- If the observation we test is $x = 0$, there are **more than 5% probabilities that it was produced by H_0** (more or less 40%). Our hypothesis H_A is considered false.

An important thing to notice is that **it does not provide the truth on statistic**, it only provides information about how likely is the null hypothesis! Let's look back to the example

- The $x = 3$ observation **could have been produced by the red area**, meaning that it's part of the small 5% chance of being produced by the H_0 . The test will say that our hypothesis is true, which will be a **false positive**.
- The $x = 0$ observation **could have been produced by the blue area**, meaning that even if H_0 have great chance to produce it, it was in fact produced by H_A . The test will say that our hypothesis is false, which will be a **false negative**.

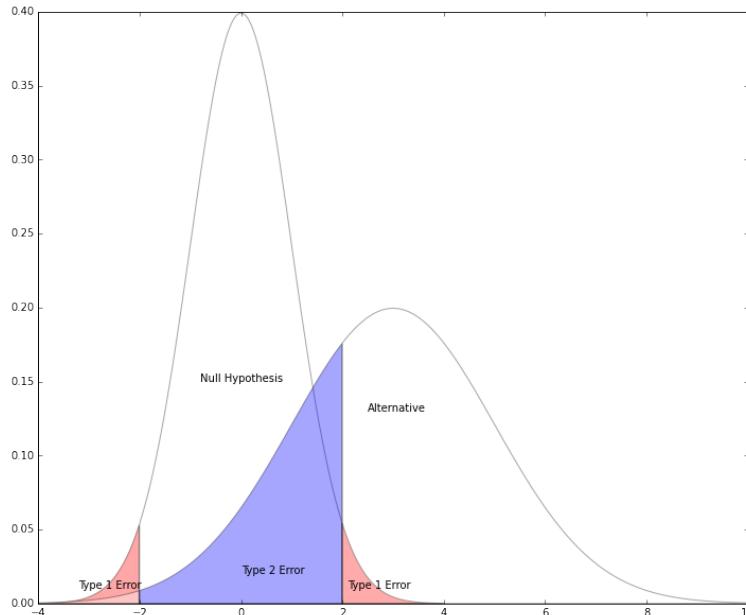


Figure 19: T-Test example

5.5.2 Choose the right test

A lot of tests exist and we must choose wisely which one to use, according to data and hypothesis characteristics. FIG 20 show a decision tree helping to choose the test which suits best our situation.

- Question ?
- Data type ?
- Sample size
- Variance known?
- Variance of several groups equals?
- ...

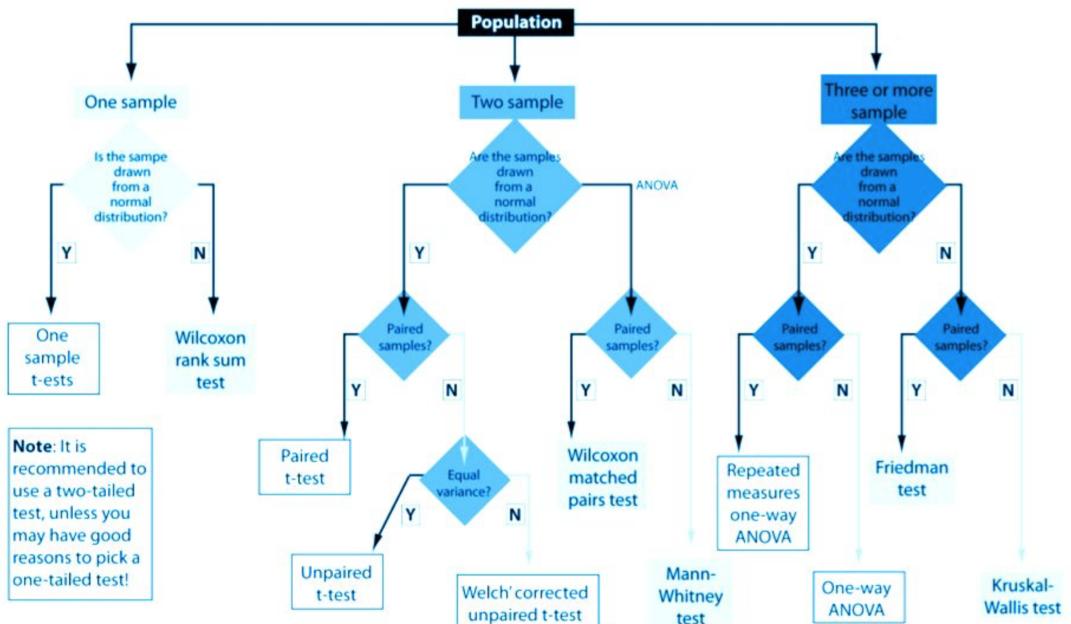


Figure 20: Statistical test decision tree

5.5.3 Family-wise Error

Following this simple math equation, we can figure out that the more experiment we do to test the hypothesis, the more likely we are to find that one of them are spuriously right! This is because the reverse point of view of the test. We are testing the fact that H_0 is unlikely, not directly that H_A is likely.

$$\begin{aligned}
 P(\text{false positive}) &= \alpha = 0.05 \\
 P(\text{true positive}) &= 1 - \alpha = 0.95 \\
 P(\text{true positive on each experiment}) &= (1 - \alpha)^k \\
 P(\text{at least one true positive on one experiment}) &= 1 - (1 - \alpha)^k
 \end{aligned} \tag{6}$$

To counter that, two possible correction exists

- Bonferroni correction : $\alpha_c = \frac{\alpha}{k}$
- Sidak correction: $\alpha_c = 1 - (1 - \alpha)^{1/k}$

5.5.4 Non-Parametric tests

All the tests so far assume that the data are **normally distributed** and that the samples are **independent of each other and all have the same distribution.** (IID) They may be inaccurate if those assumptions are not met. Therefore, make sure the data satisfy the assumptions of the test we're using. Watch out for:

- **Outliers** will corrupt many tests that use variance estimates.
- **Correlated values as samples**, e.g. if you repeated measurements on the same subjective
- **Skewed (bias) distributions** give invalid results.

Some tests make no assumptions and thus can be used on very general cases: **K-S test**, **Permutation test** and **Bootstrap confidence interval**.

5.5.5 K-S test

K-S (Kolmogorov-Smirnov) test is a very useful test for checking whether two (continuous or discrete) distributions are the same.

- In the **one-sided test**, an observed distribution (e.g. some observed values or a histogram) is compared against a reference distribution (e.g., power-law).
- In the **two-sided test**, two observed distributions are compared.
- The K-S statistic is just the **max distance between the CDFs** (Cumulative Distribution Function) of the two distributions.
- The K-S test can be used to test **whether a data sample has a normal distribution** or not.
- Thus it can be used as a sanity check for any common parametric test (which assumes normally distributed data).
- It can also be used to compare distributions of data values in large data pipeline: **Most errors will distort the distribution of a data parameter and a K-S test can detect this.**

This test is expensive! Check for more information on the [wikipedia page](#).

6 Data Visualization

6.1 Two main purposes

In this chapter we are going to talk about visualization in general and then about what it is called interactive visualization. The first thing we do when we talk about visualization is to split it into two different tracks.

- The first one is about *analysis*: you want to support reasoning about information. For instance, when you have a `DataFrame` you can make a plot of the distribution of the attribute in order to identify outliers, missing data and *so forth*. In general with this kind of visualization you can do more like discover structures, quantify values and influences. **This way of using visualization is extremely important for debugging purposes.**
- The second is the *communication* part and it is about informing and persuade people. The key difference in working in *Data Science* and exclusively in *Machine Learning* or *Statistics* is the fact that you don't just stop after getting a good model and evaluating its accuracy. You would make a story that you convey to people. For this reason we have to use visualization that can capture attention, can engage people and can tell a story visually (tell a story using visual tools takes a lot less time) and last but not least, you are focused only on certain aspects omitting others. It is a double-edged sword. That is because, on one hand you have to consider that there is an information overflow that people are suffering in general (we get too many media in which we consume information) so we do not want our visualization conveys more information than a human being can actually get in a few seconds). On the other hand, we have to do it carefully, avoiding omitting some information just because difficult to handle or with, apparently, nonsense.

6.2 Data exploration

In order to do a good *Data exploration* analysis by means of visualization:

- Get familiar with your favorite graphing package:
 - `Matplotlib` which is widely used in `Python`
 - `Seaborn` and `Bokeh` that are two additions on top of `Matplotlib`
 - `D3.js` (`Javascript`) is the most famous framework for interactive graphics
- Get fluent with plotting:
 - Histograms
 - Scatter plots
 - Line and bar plots

6.2.1 One variable

Whenever we want to look at the data we can use histograms, they tell us a lot about the single variable. Once you plot them, you can try to figure out their distribution, for instance we can identify skewed distributions, multimodal or long tail data (Figure 21).

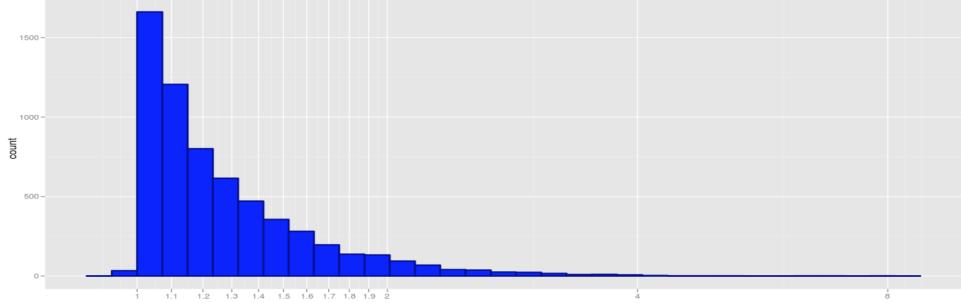


Figure 21: Example of long tail data.

The latter is characterized by a bunch of bins that reveal a lot of occurrences and bars in the tail where we observe a very few occurrences. Many of this long tail data follow a *power-law*. To claim the latter we need to run some test on data that proofs the statistical significance of our hypothesis, otherwise we can just state that it looks like a *power-law*. For a graphical representation:

1. Sort the histogram counts by magnitude, descending.
2. Plot count vs bucket number on a log-log plot.

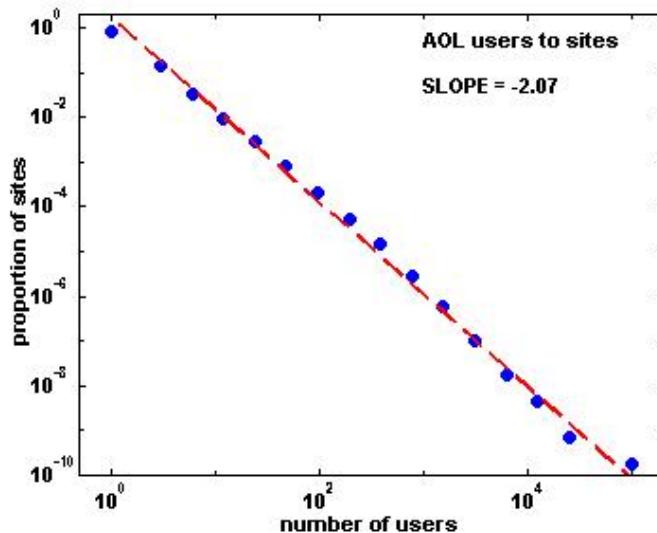


Figure 22: Example power law.

Generally this law is characteristic of social-influence processes, to know more look up for *Preferential attachment*.

The *multinomial* data registers more than one peak in the histogram, it suggests that there are two or more distinct populations of a sample. When you deal with something like this do not guess! Explore further by using, e.g., color and a histogram of multiple populations.

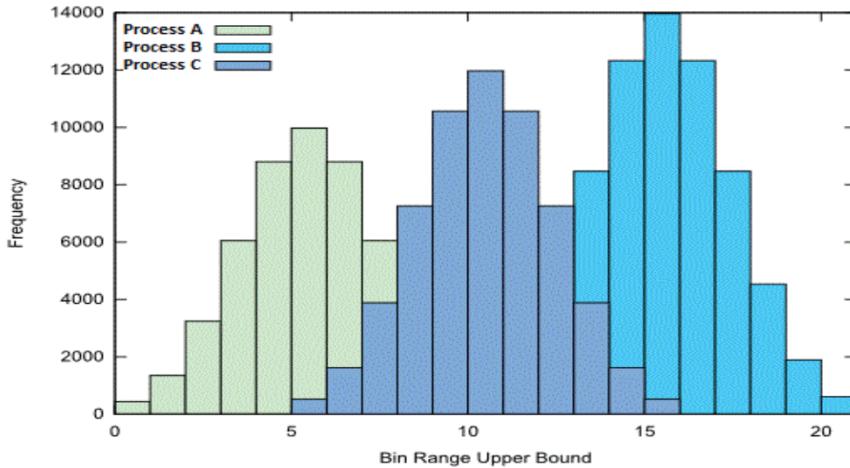


Figure 23: Example of multimodal data.

Sometimes data is weird and is very hard to explain. Also in this case, do not guess! Trace through the data pipeline to find where the strangeness comes from. Usually it is a processing bug. Hence, check your code!

There is a way for a *proactive Weird data Detection*. If data looks normal, take a picture and save it for later, then periodically compare new data with old whenever there is a pipeline update. Generally always try to have a theory of what the data should look like!

6.2.2 More than one variable

Most of the time we are interested in visualizing more than one variable, here a *non-thorough* list of possibilities is listed:

- Two variables
 - *Scatter plots* quickly expose the relationships between two variables
- More than two variables
 - *Stacked plot*: stack variable is discrete, useful to explore data (Figure 24)
 - *Parallel coordinate plot*: one discrete variable, an arbitrary number of other variables (when this number increases it risks becoming very messy), see an example in Figure 25
 - *Radar Chart*: one discrete variable (through the radar design), an arbitrary number of other variables (Figure 26)

When you deal with a high number of variables, a valid idea to visualize in a better way is to reduce the number of variables applying algorithms, this process is called *Dimensionality reduction*, one example is the *PCA*. Intuitively, given twenty different variables, many tend to not variate a lot, *PCA* extracts the couple of attributes that really make the difference allow visualization of high-dimensional continuous data in 2D using principal components. Hence, instead of directly plot multivariate data, try to think whether a dimensionality reduction can be useful.

We argued for analysts is important to form expectations of what the data should look like. This helps against pipeline errors and to identify interesting patterns.

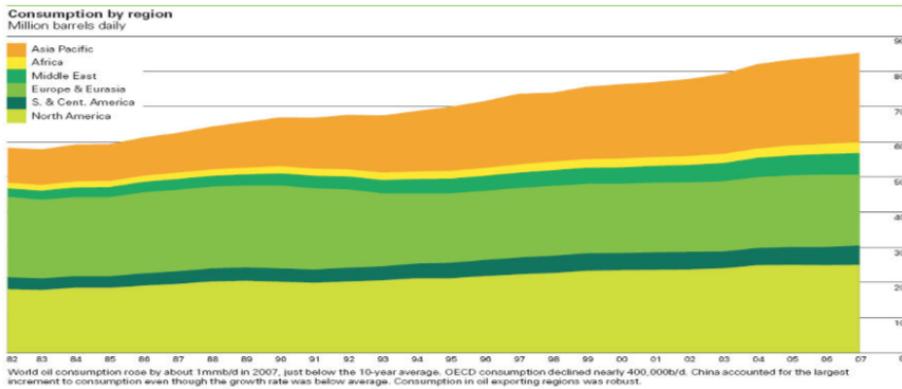


Figure 24: Example of stacked plot.



Figure 25: Example of parallel plot.

But beware of seeing *Martian Canals*: do not see things that are not there. Moreover, an observer should also be attuned to patterns that are not part of his theory, in other words, to expect the unexpected.

6.3 Moving Towards Interactive Viz

Interactive visualization is a new field and it's getting more and more common. Our aim is to deliver results and this has been enabled by the new web technologies and in general by few frameworks essential for the current state of the art. JavaScript plays a very important role in the field. The vast majority of the libraries that allow to do visualization are in [JavaScript](#), so if you know how to use it or if you want to learn how to use it, it is definitely a good tool to have in your toolbar.

A visualization is worth a thousand words! Representing in 2D more than two variables has been being a challenge since a long time ago. Even without the help of the machines, someone tried to do something in [this](#) field. Nowadays the technology allows the *researchers* to go further and to use all their creativity and skills, nevertheless so many efforts should be put in. Lots of concepts have been developed and, for those interested, there are pioneers of the field that should be taken into [consideration](#).

As we already said the visualization has the characteristic of engaging the audience easily and it often results clear and understandable (be careful, not all the graphs and repre-

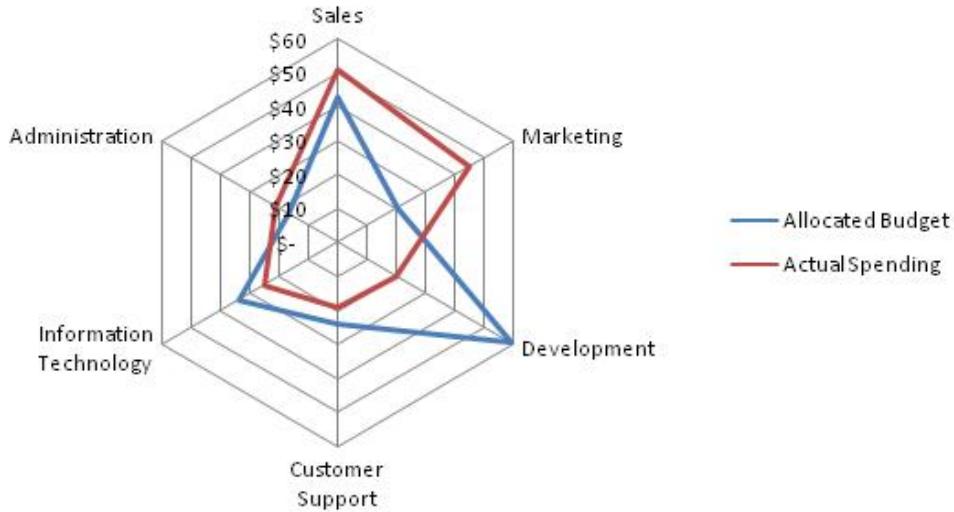


Figure 26: Example of radar plot.

sentations you look at are reliable, fair and proper!!). Hence it can be used to globally describe **phenomena** not easy to understand otherwise. Today, many are the **websites** where you can play with data using visualization.

Visualizing data is becoming a new way to spread information. More than ever, we recognize the existence of *Data journalism*, more data are available, many people have programming skills. Thus, it is simple to find persons who combine both writing and programming skills. There are journals that stand out, such the *New York Times*, *Forbes* and *The Economist*. They build up teams of researchers who are the best experts in the field. Hence, they can be considered a great source of best practices in viz.

6.4 Visualization definitions

There is not a unique way to define visualization, here some definitions that try to include many few aspects are listed:

- *Transformation of the symbolic into the geometric* (McCormick et al. 1987)
- *... finding the artificial memory that best supports our natural means of perception.* (Bertin 1967)
- *The use of computer-generated, interactive, visual representations of data to amplify cognition.* (Card, Mackinlay & Shneiderman 1999)

The 10 rules

When you do visualization you have to take care of the following **rules**:

1. **Show your data:** be careful of showing what you want to show, do not forget the main information;
2. **Use graphics:** glue together descriptions and figures;
3. **Avoid Chartjunk:** display your data in a fancy way, do not add anything that can make the interpretation harder;

4. **Utilize Data-ink** as much as you can, be careful when choosing what keep and remove;
5. **Use labels:** let the people understand what you are talking about;
6. **Utilize Micro/Macro:** an overview does not need so many details as when you zoom in;
7. **Separate Layers:** make more visible what you want the people to focus on;
8. **Use Multiples:** a thing different from the other captures the attention;
9. **Utilize Color** in a way such that data is interpreted;
10. **Understand Narrative:** when you tell a story respect time and space.

Interactive chart design

With interactive charts you can keep things very simple by hiding and dynamically revealing important structure. On an interactive chart, you reveal the information most useful for navigating the chart. The aforementioned rules hold for the interactive charts as well.

The importance of magnitude

Compare areas

Let the reader compare areas is dangerous (Figure 28), avoid it whether possible or try to insert information to be able of making significant comparisons. Related to the capability of distinguishing and understanding magnitudes, in 1984, Cleveland and McGill wrote the paper *Graphical Perception: Theory, Experimentation, and Application to the Development of Graphical Methods* which identifies and analyzes a set of *elementary perceptual tasks* conducted in the moment the reader extract quantitative information from graphs (Figure 27).

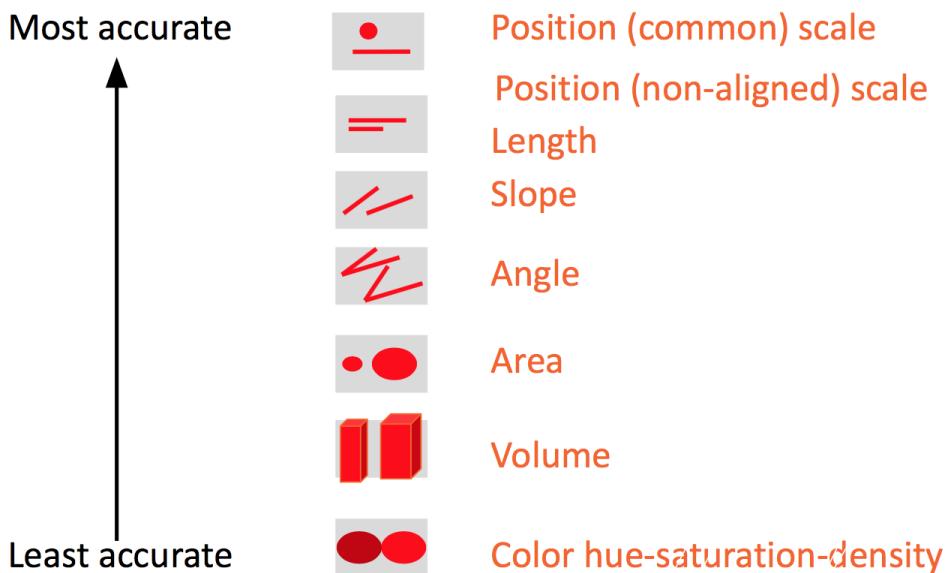


Figure 27: What works and what does not.

These tasks are sorted according to how accurately people perform them.

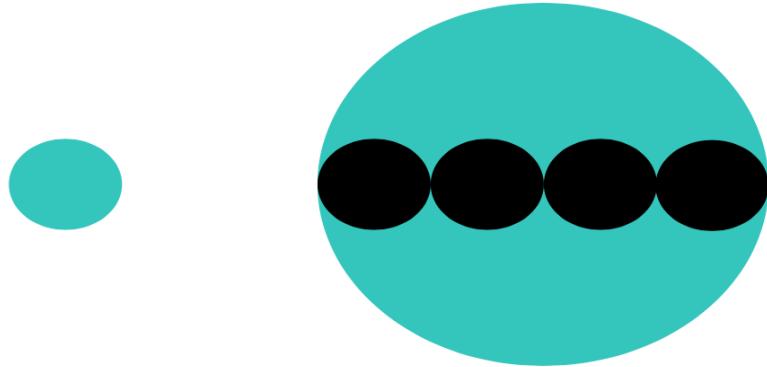


Figure 28: How many times the *little* one is included in the *big* one? (Answer: 16)

Compare colors...

Use a magnitude that allows people to easily read and interpret your data, noticeable differences are required. In 1846 the physicist Ernst Weber, defining I as the intensity of the stimulus and S the sensation, said that

$$\Delta S = k \frac{\Delta I}{I}.$$

It is known as the *Weber's law* and reads out that a variation in the sensation is proportional to the magnitude of the original intensity of the stimulus. So as the base I increase, we require a larger changes in ΔI to notice the change.

...And choose them

Choose colors based on the information you want to convey:

- *Sequential*: colors can be ordered from low to high (Figure 29)
- *Diverging*: two sequential schemes extended out from a critical midpoint value (Figure 30)
- *Categorical*: Lots of contrasts between each adjacent color (Figure 29)



Figure 29: Example of sequential colors.

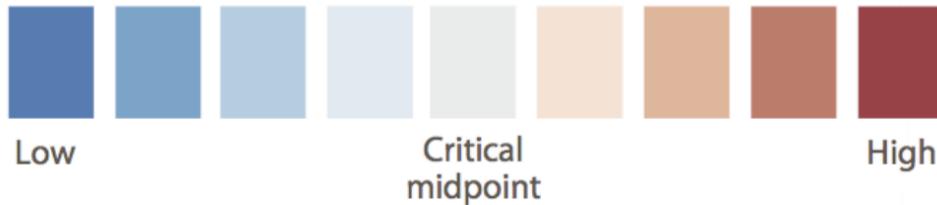


Figure 30: Example of diverging colors.



Figure 31: Example of categorical colors.

The usage of these tools depends on what you want to show. Anyway there are several [online](#) sources that can help you to choose the color scheme according to your purpose.

Use Structure

In 1912 Gestalt outlined principles that describe how our mind organizes individual visual elements into groups, to make sense of the entire visual. When designing a visual, these principles can be used to highlight patterns that are important to us, and downplay other patterns. The Figure illustrates the [principles of Gestalt](#) which is relevant to visualization (Figure 32). Do not concentrate too much information, less is more!

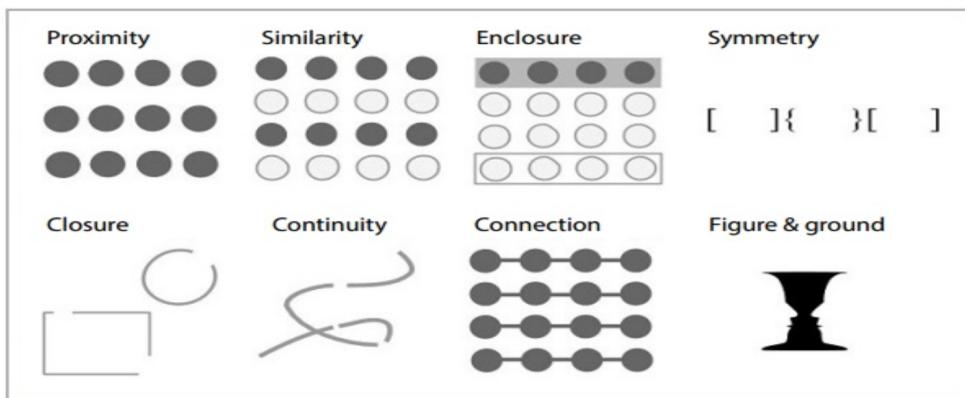


Figure 32: Gestalt's principles.

Here is what we notice from each of the illustrations [[principles of Gestalt](#)]:

- **Proximity:** we see three rows of dots instead of four columns of dots because they are closer horizontally than vertically.
- **Similarity:** we see similar-looking objects as part of the same group.

- **Enclosure:** we group the first four and last four dots as two rows instead of eight dots.
- **Symmetry:** we see three pairs of symmetrical brackets rather than six individual brackets.
- **Closure:** we automatically close the square and circle instead of seeing three disconnected paths.
- **Continuity:** we see one continuous path instead of three arbitrary ones.
- **Connection:** we group the connected dots as belonging to the same group.
- **Figure & ground:** we either notice the two faces, or the vase. Whichever we notice becomes the figure, and the other the ground

These principles allow us to perform many tasks such as reduce the noise from charts, choose the ideal aspect ratio, and show relationships between elements more clearly. Let's look at a dashboard, and see these principles in action.

How to select the right chart

The flowchart below can be helpful to understand the most suitable chart for your purpose.

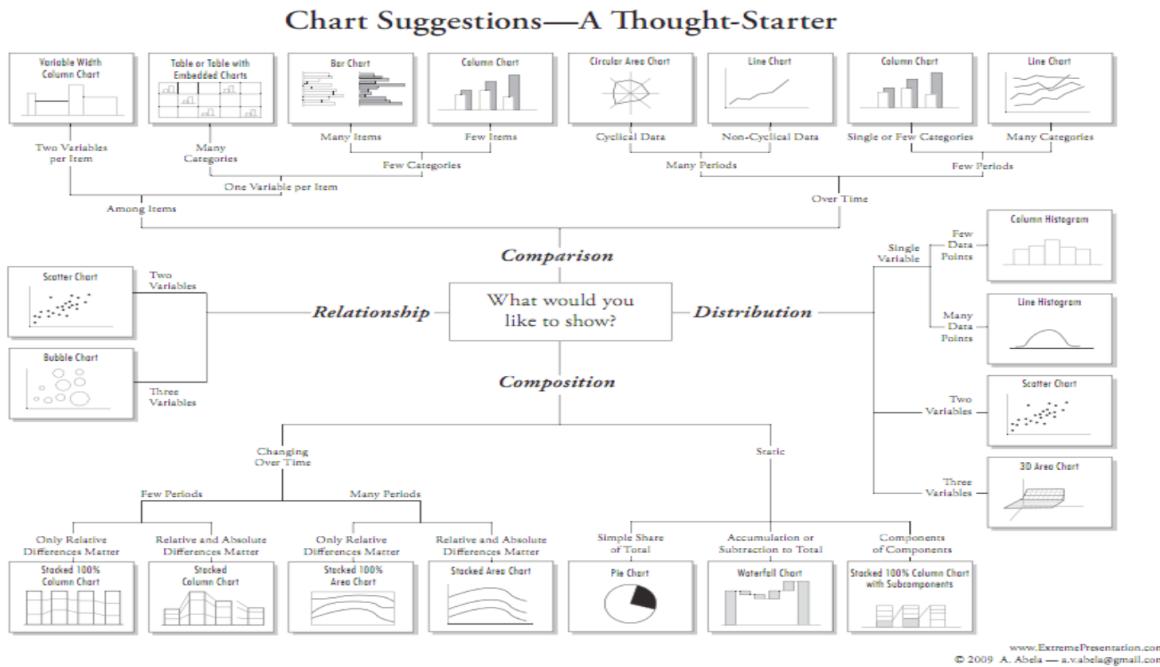


Figure 33: Make your choice.

Instead of using the chart, you can also find sources, like *Juice Analytics*, that let you choose interactively, means some filters, the best chart according to your necessities.

6.5 Interactive toolkits

- **D3** is, without doubt, the most widely used interactive visualization framework, developed around 2011 by Jeff Heer, Mike Bostock and Vadim Ogievetsky. *Notes from the authors:* D3 is intentionally a low-level system. During the early design of D3, we even referred to it as a "visualization kernel" rather than a "toolkit" or "framework";
- **Vega** is a *visualization grammar* developed on top of `d3.js`. It specifies graphics in JSON format;
- **Vincent** is a Python-to-Vega translator;
- **Bokeh** is an independent Viz library focused more heavily on big data visualization. Has both `Python` and `Scala` bindings;

7 Supervised Learning

7.1 Introduction to Machine Learning

Machine Learning is an extended field characterized by many facets. The [Arthur Samuel](#)'s definition can be considered the most meaningful one: “*Field of study that gives computers the ability to learn without being explicitly programmed.*”. The aim of *Machine Learning* is to model into a computer the learning and adapting procedures that characterize the human way of thinking and processing information. Merely, the idea behind is to use computers to apply statistical and optimization algorithms to *automatically* identify pattern in data and/or classify them.

To get an idea of what *Machine Learning* does and consists of, take a look at a [beautiful introduction to Machine Learning](#). In order to capture the essence of this subject, it speaks more than thousand words .

In the end, according to a reductive point of view, we may simply say that Machine Learning is born because we are **lazy** and we let the machine do the “work” for us.

Machine Learning is based on the definition of algorithms that allows the aforementioned procedures. Those algorithms can be distinguished either by the *learning style* (Supervised vs Unsupervised vs Semi-Supervised learning) or by their *similarity*.

In the next part of this chapter, we first give an introduction to *Supervised* and *Unsupervised* learning and then we go deeper into the *Supervised Learning*. If you want to become a Machine Learning Master, you should have a look [here](#).

7.1.1 Different aspects of Machine Learning

When we apply a *Machine Learning* method, one of the things that we are mostly interested in is getting good predictions. This is not the only important aspect of the Machine Learning methods though.

The following list rough out some very important aspects for these methods:

- **Predictive accuracy:** we want our model to return correct result;
- **Speed and scalability:** the model should be efficient in order to be easily applied
 - Time to build the model
 - Time to use the model
 - In memory vs Disk processing
- **Robustness:** the method should not be too sensitive
 - Handling noise
 - Handling outliers
 - Handling missing values
- **Interpretability**
 - Understand the model and its decisions (*black box* vs white box)
 - Compactness of the model

7.1.2 Supervised vs Unsupervised Learning

In Table 7.1.2 we outline some differences/similarities between *Supervised* and *Unsupervised* learning.

The main difference to remark is that for *Supervised* learning, we use a *training* data with **known** labels and we test it on a *test* data **without** labels. For *Unsupervised* learning we do not have any labels. We are just trying to simplify/cluster the samples.

	Supervised	Unsupervised
Variables	Samples X and labels y	Samples X
Learning	Function $y = f(X)$ relate samples and labels. We would like to “learn” f and evaluate it on new data.	We want to compute a function $y = f(X)$ to give a <i>simpler</i> representation of the samples X .
Discrete labels	Classification	Clustering
Continuous labels	Regression	Matrix factorization, Kalman filtering, Unsupervised neural networks
Examples	<ul style="list-style-type: none"> • Is this image a cat, dog, car, house? • How would this user score that restaurant? • Is this email spam? • Is this blob a supernova? 	<ul style="list-style-type: none"> • Cluster some hand-written digit data into 10 classes. • What are the top 20 topics in Twitter right now? • Find and cluster distinct accents of people in Lausanne
Techniques	<ul style="list-style-type: none"> • k Nearest Neighbors • Naïve Bayes • Linear + Logistic Regression • Support Vector Machines • Random Forests • Neural Networks 	<ul style="list-style-type: none"> • Clustering • Topic Models • Hidden Markov Models

Table 1: Summary of the differences between Supervised and Unsupervised learning.

7.2 More details on Supervised Learning

7.2.1 Predicting from Samples

The **samples** are, most of the time, subsets of an infinite population. We are interested in a model that can **describe the whole population**, but since we only have access to a *sample* of it, it is not possible. Therefore we train on a training sample D and we denote the model found by $f_D(X)$, X being the features. Most of the datasets are **samples** from an infinite population, *i.e.* a subset of an **infinite** dataset. We would like to model the **whole population**, but only have access to a sample of it. So, we train on a training sample called D and we denote the model as $f_D(X)$ where X are the features and $y = f_D(X)$ the predictions.

7.2.2 Bias and Variance

The data-generated model $f_D(X)$ is a **statistical estimate** of the true function $f(X)$ (function working for the whole population). Therefore the model is subject to bias and variance.

The **Bias** is defined as the *expected difference* between the prediction of a model $f_D(X)$ and the true labels y :

$$\text{Bias} = \mathbb{E}[f_D(X) - y]$$

The **Variance** is defined as:

$$\text{Variance} = \mathbb{E}[(f_D(X) - \bar{f}(X))^2]$$

where $\bar{f}(X) = \mathbb{E}[f_D(X)]$ being the average prediction on X .

Bias and Variance are very useful to understand if you are doing something wrong. Thus, it is important to understand what you are doing and not just applying “black-boxed” algorithms.

Trade-off between Bias and Variance

The [tradeoff between bias and variance](#) is due to model complexity, see Figure 34.

- **Complex models:** Many parameters, usually lower bias (the model is close to the model that generates the data) but higher variance (the predictions have high variability). It leads to the risk of overfitting. Merely, this kind of models describe well the sample population, likely they do not represent well the entire population though.
- **Simple models:** Few parameters, higher bias (far from the true model) but lower variance (less variability among predictions).

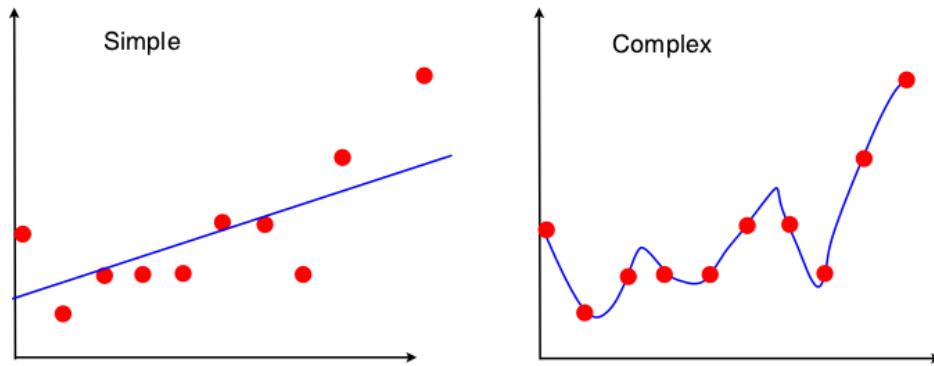


Figure 34: Illustrations of a simple model and a complex model on the same data.

For example, a linear model can only fit a straight line. A high degree polynomial can fit complex curves. Therefore this polynomial will work very well with the samples but not that well with the whole population. Thus a high variance is expected.

In order to take into account this trade-off, we introduce the total expected error is

$$\text{Bias}^2 + \text{Variance}$$

This error **balance** the contributions of the variance and the bias.

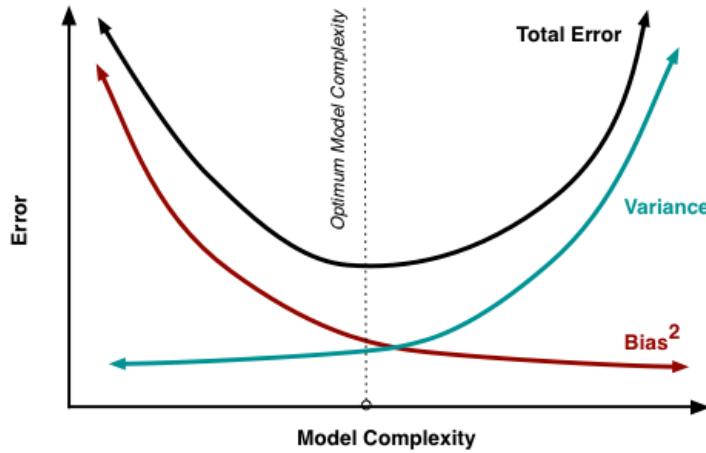


Figure 35: Illustration of the model complexity and the Bias Variance tradeoff. The optimum model complexity is when the total error is minimized.

When the Bias and the Variance are unbalanced, we use the terms:

- **overfitting** when the *Variance* strongly dominates. (Too much variation between models. Hence, the model does not work well on new data)
- **underfitting** when the *Bias* strongly dominates. (The models do not fitting the data well enough)

7.3 k-Nearest Neighbors

The kNN algorithm is a well known method used for classification and regression. The input consists simply of the k closest training examples. The idea of the kNN algorithm is to find the k nearest neighbors of an input using a specific metric. Once we found them, we can give the label of the new input such that it corresponds to the most used label in the neighbors. Figure 36 shows an example with cats and other animals.

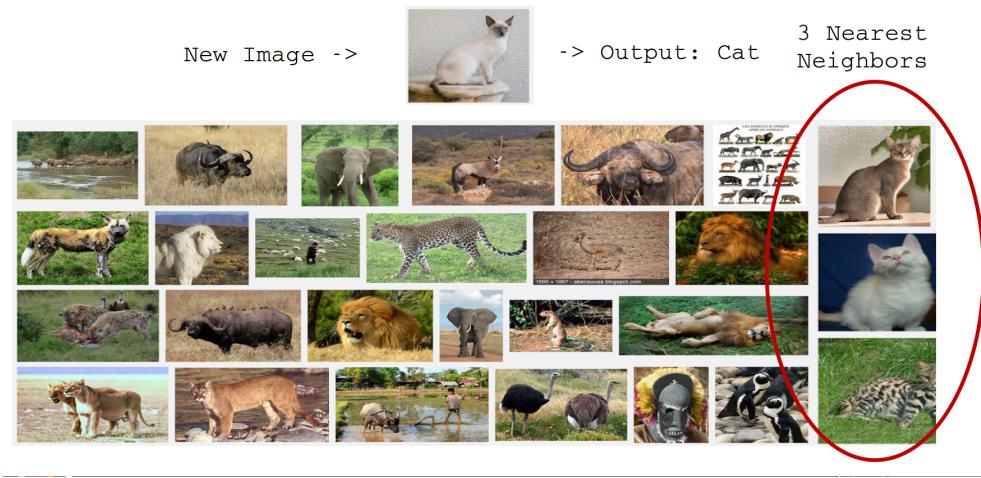


Figure 36: Illustration of the kNN algorithm.

However this very simple algorithm has one issue: the Data is the Model. This implies:

- No training needed.
- The accuracy generally improves with more data.
- Matching is simple and fairly fast if data fits in memory. (Can be run off disk)

Normally, the only parameter is k , the number of neighbors. But two other choices are important:

- Weighting of neighbors (e.g. inverse distance)
- Similarity metric.

7.3.1 kNN Flavors

The kNN algorithm can be used both for regression and classification. Table 7.3.1 gives the similarities/differences of the kNN algorithm for regression and classification.

Classification	Regression
The model is $y = f(X)$ where y is from a discrete set (labels).	The model is $y = f(X)$ where y is a real value.
Given X , we compute y being the majority vote of the k nearest neighbors.	Given X , we compute y being the average value of the k nearest neighbors.
We can also use a weighted vote of the neighbors.	We can also use a weighted average of the neighbors.

Table 2: kNN algorithm used for classification and regression: Differences and similarities. Usually, the weight function is the inverse distance.

7.3.2 kNN distance measures

For the kNN algorithm, we need to use a distance between the neighbors. The choice of the distance function can be very different depending on what you are looking for. We give here some examples:

Euclidean distance Simple, fast to compute.

$$d(x, y) = \|x - y\|$$

Cosine Distance Good for documents, images, etc.

$$d(x, y) = 1 - \frac{x \cdot y}{\|x\| \|y\|}$$

Jaccard Distance For set data

$$d(X, Y) = 1 - \frac{|X \cap Y|}{|X \cup Y|}$$

Hamming Distance For string data

$$d(x, y) = \sum_{i=1}^n (x_i \neq y_i)$$

Manhattan Distance Coordinate-wise distance

$$d(x, y) = \sum_{i=1}^n |x_i - y_i|$$

Edit Distance For strings, especially genetic data. See on [Wikipedia](#) for more information.

Mahalanobis Distance Normalized by the sample covariance matrix – unaffected by coordinate transformations.

$$d(x, y) = \sqrt{(x - y)^T S^{-1} (x - y)}$$

where S is the covariance matrix.

7.3.3 Choosing k

If we choose a **small k**, we will see a low bias but high variance. Figure 37 shows what happens with two different samples if we choose a small k.

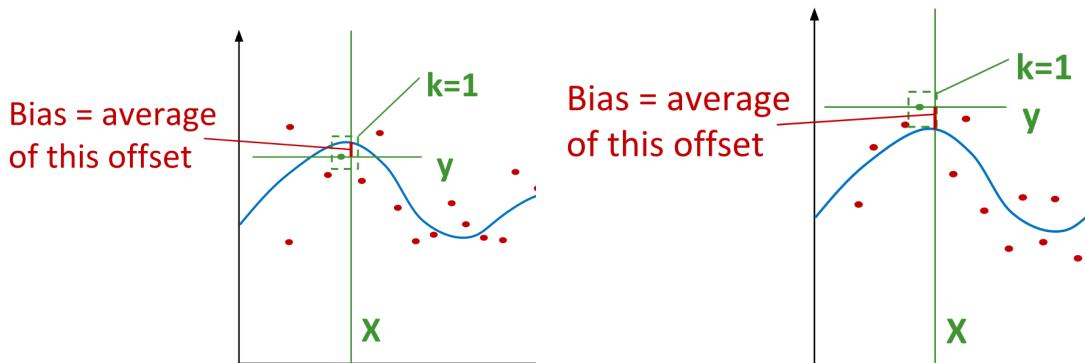


Figure 37: Test on two different samples of the kNN algorithm with $k=1$.

On the other hand if we choose a **large k**, we will see a high bias but low variance. Figure 38 shows what happens with two different samples if we choose a large k.

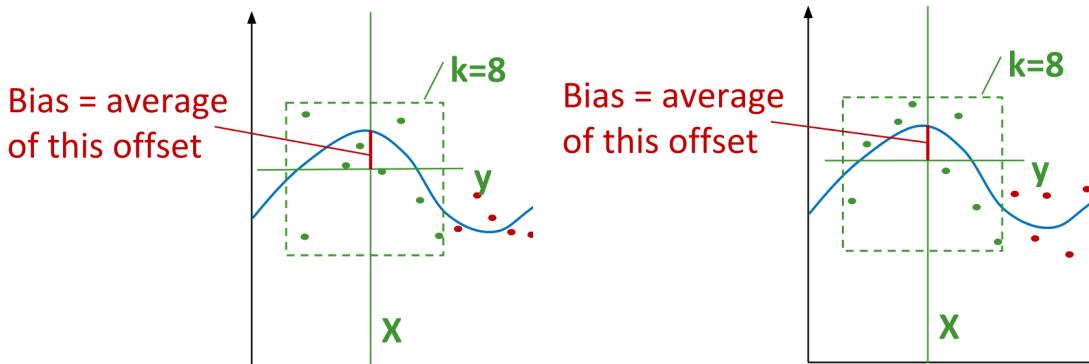


Figure 38: Test on two different samples of the kNN algorithm with $k=8$.

In practice

Use cross-validation! Break data into train, validation and test subsets. For example, you can choose a 60-20-20 % random split.

Predict For each point in the validation set, predict using the k-Nearest neighbors from the training set. Measure the error rate (classification) or the squared error (regression)

Tune Try different values of k, and use the one that gives minimum error on the validation set.

Evaluate test on the test set to measure performance.

7.3.4 kNN and the curse of dimensionality

The curse of dimensionality refers to phenomena that occur in high dimensions, from hundreds to millions, that do not occur in low-dimensional space. Data in high dimensions are much sparser than data in low dimensions. That means there are less points that are very close in the feature space. For example, the Euclidean distance scales as \sqrt{N} with N being the dimension. Thus it is quite surprising that kNN works even in high dimensions. Luckily data are not random points in a high-dimensional cube. They live in **dense clusters** and near **much lower-dimensional surfaces**. Therefore, we can reduce the feature space in many different ways to see the clusters appear.

Even if the Euclidean distance between two points is large they can be very *similar*. For example documents with the same few dominant words (with **tf-idf** weighting) are likely to be on the same topic.

7.4 Decision Tree

Decision Tree (DT) is a basic classifier acting like a **flow-chart having a tree structure**. It's constructed following a top-down approach in which, at each node, the data are split on one of their attribute. The predictions are obtained by following the "if-else" statement of each node and is given by the leaves, once the whole tree is traversed.

The only way to score a DT is by counting the number of right elements it predicts on the test set, since the prediction are not "weighted" by a probability of correctness.

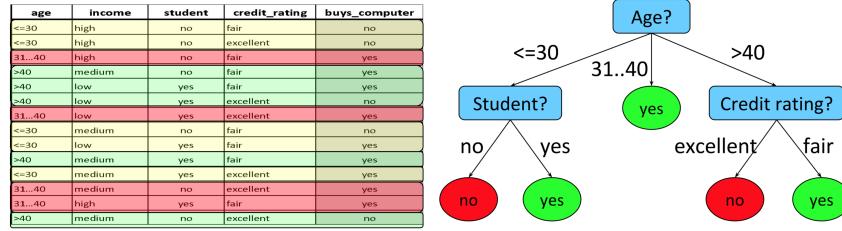


Figure 39: Dataset and the Decision Tree related to it.

Construction (Top-down, divide-and-conquer strategy.)

1. At the beginning, all the data belong to the node
2. Recursively, the (sub)sets are partitioned on their most discriminative attribute (see section 7.4.1)
3. Stop when:
 - A node only contains same labeled data, stop and make it a leaf labeled the same.
 - No more attributes left, assigne the most present
 - No more data left.
 - (A thershold has been defined and is reached)

The DT will continue to add attributes to its decision process until no ones left. As it increases its precision (and then its depth), it starts overfitting the model. A threshold can be defined to stop the construction process earlier and limit this effect.

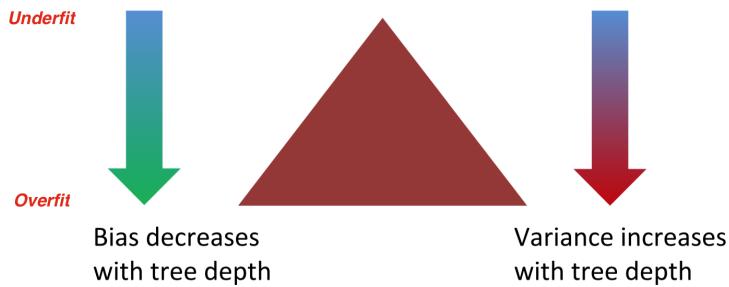


Figure 40: Bias and variance evolution with DT depth

Pros	Cons
+ A first ML approach ;) + Can be enhenced in RF or BDT	- Sensitive to small perturbation - Retrained from scratch when new data are coming - Tend to overfit

7.4.1 Attribute selection

A big part of the DT model creation relies on choosing the good attribute on which to split the data in each node. This decision relies on the concept of entropy, which describe the disorder a system.

For a set S with P positive predictions and N negative ones, its entropy is:

$$H(P, N) = -\frac{P}{P+N} \log_2 \frac{P}{P+N} - \frac{N}{P+N} \log_2 \frac{N}{P+N}$$

Note that:

- If P or $N = 0 \rightarrow H(P, N) = 0$, meaning **no uncertainty at all**
- If $P = N \rightarrow H(P, N) = 1$, meaning **maximum of uncertainty**

Entropy of the attribute A :

$$H(A) = \sum \frac{P_i + N_i}{P+N} * H(P_i, N_i)$$

Gain obtained by splitting the dataset S by attribute A .

$$Gain(A) = H(P, N) - H(A)$$

The gain indicate how a split on a certain attribute will influence our data set. The lower the entropy becomes, the greater is the gain, the more *organised* and *certain* become the data set.

These equations can seem obscure at a first look, the figure 41 illustrates how the entropy of an attribute is calculated and make it easier to understand what represent the equations.

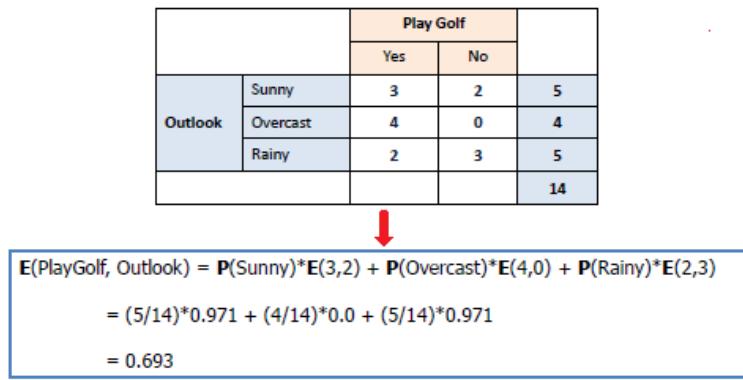


Figure 41: Example of entropy calculation.

7.4.2 Random Forest

A common problem when trying to build a model is to select significant features between all the available one. We tend to think that *the more we have, the better it is*, even knowing the existence of the curse of dimensionality.

Random Forest takes this idea and try to automatize this feature selection by randomly selecting subset of features.

The main idea of Random Forest algorithm is to grow an arbitrary number of **Decision Trees**, each one grown based on a subset of m features, randomly chosen between the

total p of them. It's an example of a **weak learner** saw in the Ensemble method. This weak learner has a lower bias (because of lower number of feature).

Following the **Ensemble method**, the predictions of all these weak learners are then merged together to produce a final prediction (by majority voting for example).

Pros	Cons
+ Popular	- Not state-of-the-art
+ Easy to implement	- Needs many passes over the data
+ Easy to parallelize	- Tend to overfit

7.4.3 Boosted Decision Trees

Variante of Random Forest. Instead of training all DT independently on weak subset, the DT are trained sequentially and emphase incorrectly-labeled instances of the previous tree. This is called **Boosting**.

- Low variance, because of the small trees handling small numbers of features
- Low bias, reduces by the boosting

Opposed to RF that usually trained tens of medium-sized trees, BDT works on smaller trees in greater numbers.

Even if they show good results, their big drayback is their slow execution compared with the parallelized RF.

7.4.4 About model transparency

A recurrent argument of using Decision Tree (DT) or Random Forest (RF) in industry is their transparency compared to state-of-the-art Deep-Neural-Network (DNN). This argument must be carefully taken. Even if by their very nature DT are more understandable by a human than DNN, the more features and Trees we had, the more complicated it becomes. Figure ?? shows the size of a common industry implementation of RF and BT where there are no more possibilities of human understanding.

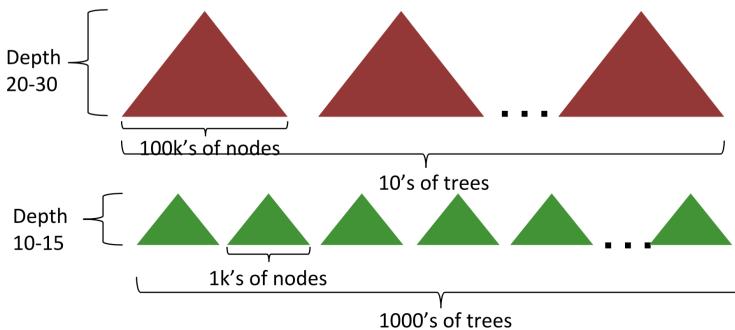


Figure 42: Standard size of RF and BDT implementations. In red: RF with big parallel DT. In green: BDT pipeline with lot of small DT

7.5 Linear Regression

Linear regression model produces a prediction equation:

$$\hat{y} = \hat{\beta}_0 + \sum_{j=1}^p X_j \hat{\beta}_j$$

or in matrix notation

$$\hat{y} = X\hat{\beta}$$

Where X_j are the data and $\hat{\beta}_j$ the characteristic of the model.

7.5.1 Statistic validation

As a linear model can be calculated for every possible existing dataset, it is not enough to calculate it, but the existing of linear relationship between the data must be proved.

7.5.1.1 R^2 -value

R^2 -value describes how much of the total variance is reduced when we include the line as an offset. It computes the distances between the real y and the predicted \hat{y} , and compares them with the distance between real y and the mean \bar{y} .

- if $R^2 = 0$, then there is no difference between the linear model and the trivial mean \bar{y} . Then we conclude that there is not any evidence of linear relationship in our dataset and **we cannot use the model**.
- if $R^2 = 1$, then the data perfectly aligned on the linear regression line and **the model is perfect**.

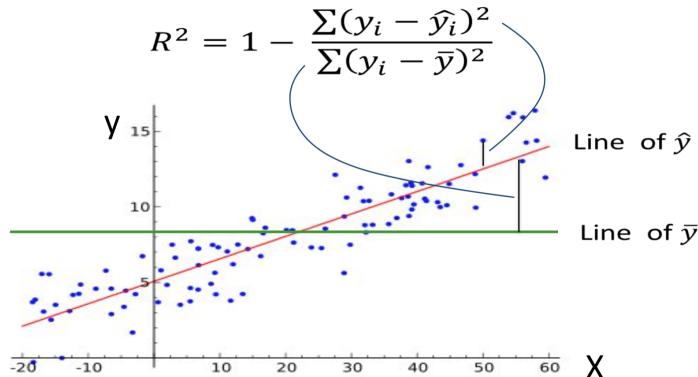


Figure 43: Graphical meaning of R^2 -value.

7.5.1.2 p-value

From the Distribution of Fisher (F-Distribution) we can derive a p-value which is, as usual, the probability that the observed data are produced by the null hypothesis which is, in our case, the hypothesis *no linear relationship*. For $p < 0.05$ we conclude, as usual, that it is very unlikely that the data were produced by the null hypothesis and we then accept the hypothesis *the data are produced by linear relationship*.