

Introduction to Data Science

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January 22, 2024

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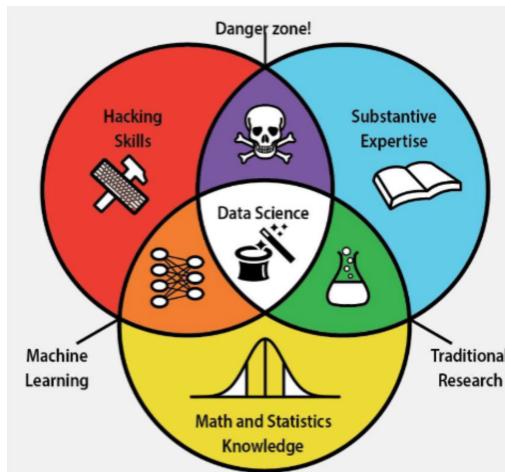
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Introduction

Let's first introduce the general term of data science. It is a new and important discipline that can be viewed as an amalgamation of classical disciplines such as statistics, data mining, databases, and distributed systems, with additional new challenges constantly emerging and making the field highly dynamic and appealing.

The problems grow in terms of size ("Big data") and complexity of the questions to be answered. But the basic job can be summarized as:

- Basic job: Input (data) → Processed by data scientist (with tools) → Output (value)
- Where the skills of a data scientist are the combination of an open mind, human interest, analytical skills, creativity, business-benefiting weighting, etc.
- Or in other terms as can be seen in 0.1



- Data science: due to its interdisciplinary nature requires an intersection of the following abilities (H + M + S)
- Hacking skills (H): necessary for working with massive amounts of electronic data that must be acquired, cleaned, and manipulated
- Math and statistics knowledge (M): to choose appropriate methods and tools to extract insight from data
- Substantive expertise in a scientific field (S): crucial for generating motivating questions and hypotheses and interpreting the results
- Traditional research: in the intersection of M and S
- Machine learning: combines H with M, but doesn't require scientific motivation
- !Danger zone: H and S combined without rigorous methods can beget incorrect analyses

Figure 0.1: Skillset of a data scientist

With the growing importance of data and digitalization, organizations are looking for data scientists, who may outnumber computer scientists in the future. Important is the ability to handle data in any form, so basically the need for an all-around skilled "data wizard". This importance can be further highlighted when looking at the tech development over the past 20 to 30 years. While the hardware got tremendously cheaper, faster, and more compact (20 times faster for MIP = mixed integer programs), also

software has progressed in terms of speed (50 times faster for MIP). Interesting to look at is also the aspect of automation.

Dimensions of data science are:

- The different types of data (structured or unstructured, text, images, events, ...)
- The different types of tasks (supervised or unsupervised, ...)
- Human versus machine (Who does what?)
- Algorithm versus visualization (What is needed?)
- Flexibility versus usability
- Scalability versus quality (exact versus heuristics)
- Responsibility versus utility (accuracy and precision versus fairness, privacy, transparency, ...)

Besides raw data science, interesting to look at is also the connection to process science. The interplay between process and data science (PADS) leads to the term process mining. Imagine the connection as shown in 0.2.

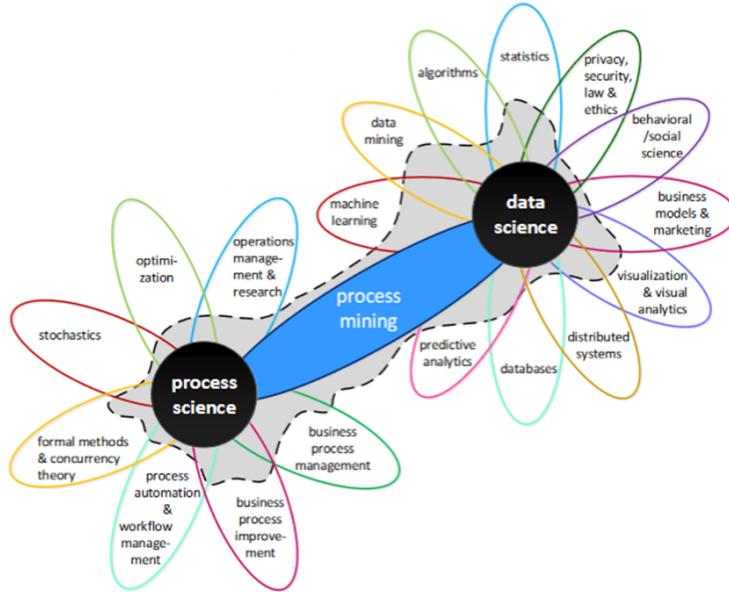


Figure 0.2: Interplay between process science and data science

As the final part of the introduction, we will now see the general covered topics in this course:

- Basic data exploration and visualization
- Decision trees, regression, support vector machines
- Neural networks, evaluation of supervised learning problems, clustering
- Frequent items sets, association rules, sequence mining, process mining, text mining
- Data preprocessing/quality and binning, visual analytics and information visualization
- Responsible data science
- Big data technologies

1 Basics of data science

1.1 Data science pipeline

First, we are going to look at how data is processed in terms of the **data science pipeline** as it can be seen in 1.1.

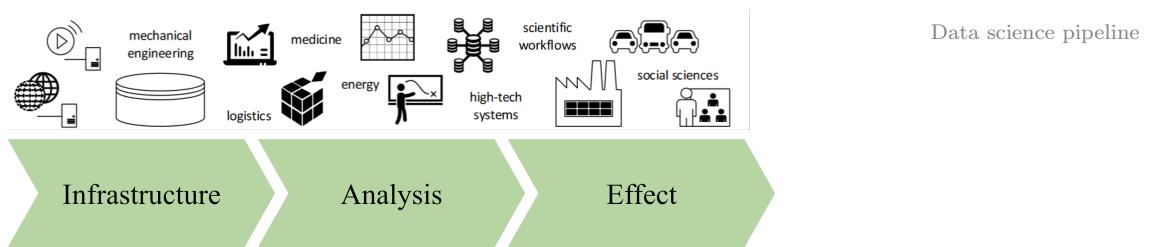


Figure 1.1: Pipeline of data science

Let's look at the individual components. The first step to pay attention to when wanting to handle data is the **infrastructure** with the keywords "**volume and velocity**". The main challenge is making things scalable and instant (responsiveness). Important terms are for example:

- Instrumentation
- Big data infrastructures, distributed systems
- Data engineering (databases and data management)
- Programming
- Security

Next, we have the step of the actual **analysis** concerned with **extracting knowledge** from data. The core challenge can be put as providing answers to known and unknown unknowns. Important terms are for example:

- Statistics, algorithms
- Data and process mining
- Machine learning, artificial intelligence
- Operations research
- Visualization

Finally, we also need to be concerned with the **effect** of our results on people, organizations, and society. The main challenge of this pipeline step is to do **responsibly** perform data handling. Important terms are for example:

- Ethics and privacy, and IT law
- Human-technology interaction
- Operations management
- Business models, entrepreneurship

This course will look into all the steps of the pipeline, but the main focus lies on the data analysis.

Four generic data science questions

The questions vary in their difficulty and prediction into the future:

1. **What** happened?
2. **Why** did it happen?
3. What will happen in the **future**?
4. What is the **best** that can happen?

Important while answering these questions is to keep attention to all three pipeline steps, so not only what analysis we need to perform to answer them, but also how we collect our input (data) and how to deal with our output (result).

1.2 Types of data

Now that we know that we have some kind of data as our input, we need to take a look at what this data can look like. Generally speaking, there are two types:

- Structured data
Unstructured data
- Structured data like age, time, gender, class, etc., and
 - Unstructured data like text, audio, video, etc.

For **structured data** we have a further subdivision into structured data types. The data types depicted in 1.2 will be described in detail.

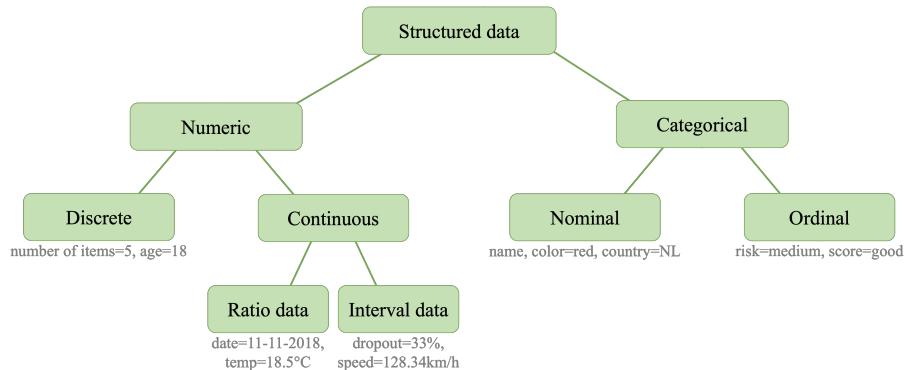


Figure 1.2: Overview structured data types

- Categorical data
Nominal data
Ordinal data
Numerical data
Discrete data
- **Categorical** data can be stored and identified based on names or labels given to them and is also known as "qualitative" data. Matching can be applied, where data is grouped based on similarities.
 - Concretely, **nominal** data or naming data has a label and its characteristic similar to a noun and doesn't imply an order.
 - **Ordinal** data on the other hand is ranked, ordered, or used on a rating scale. This means, you can count and order ordinal data but are not able to measure it.
 - In contrast to categorical data, we also have **numerical** data referring to data in the form of numbers instead of another language or descriptive form. It is also known as "quantitative" data. Important is the ability to be statistically and arithmetically calculated (allowing for $+$, $-$, $>$, $=$, ...).
 - One subtype of numerical data is **discrete** data representing countable items, that are collected in a list (finite or infinite).

- Then, there's also **continuous** data in the form of intervals or ranges. The data represents measurements with their intervals falling on a number line (so counting isn't involved). Continuous data
- Continuous data can now be further distinguished. One subtype is **interval** data where the data can be measured only along a scale at equal distances from each other, so only addition and subtraction operations are allowed. There is no true zero (and hence no \cdot , $/$). Interval data
- And finally, we have **ratio** data describing measurement with a defined (true) zero point. Ratio data

For **unstructured data**, we just take the raw data and interpret it as a stream of bits. This goes for text, audio, images, signals, and videos exactly the same. Examples can be seen in 1.3.

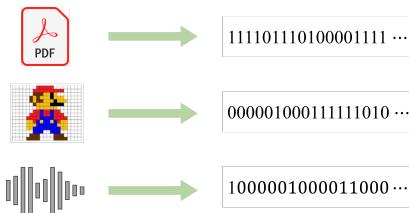


Figure 1.3: Input for unstructured data

Data can now be stored and ordered together by putting it into **tables**. Concretely, columns represent different features (can be different kinds of data types) whereas rows describe data instances (also known as individuals, entities, cases, objects, or records). Examples can be seen in 1.4. Tabular data

feature			
Order id	Product	Price	Date
32424	718 Cayman	66.000	21-10-2018
34535	911 Carrera	102.000	22-10-2018
43555	911 Turbo	154.000	24-10-2018
...

From	To	Message	Image
Sue	Peter	“How are you?”	😊
Peter	Sue	“Very good!”	🎉
Peter	Mary	“Let’s go out.”	💃
...

Ordinal Nominal Ratio data Interval data Nominal Unstructured

Features
Labels

Features can now be raw or derived (e.g. max, min, average, rank, bin, ...). An important aspect is time, as it cannot decrease and we usually want to predict the future based on the past.

An important distinction to be made when it comes to tabular data is whether the items are labeled or not.

- In case of labelled data we have **descriptive features** and a **target feature**. Labelled data
 - The descriptive features are also known as predictor variables or independent variables. Descriptive features

- Target feature
- Alternative names for target features are response variable, dependent variable, or also label.
- Unlabelled data
- Unlabelled data on the other hand doesn't have a selected target feature.

1.3 Supervised and unsupervised learning

Derived from the different kinds of tabular data, we have two fundamental learning paradigms. Exemplary input data and possible results for both paradigms can be seen in 1.5.

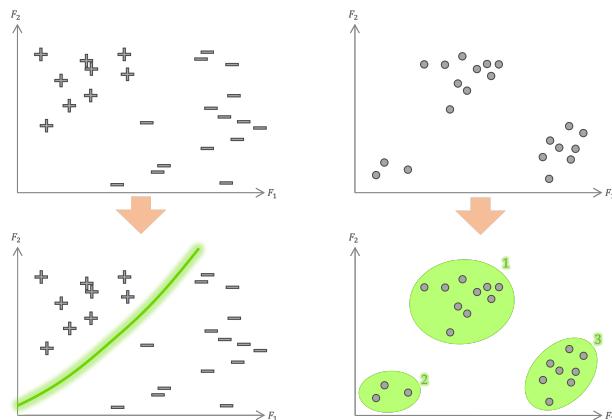


Figure 1.5: Comparing supervised (left) and unsupervised (right) learning

Supervised learning In the case of labeled data, we can apply **supervised learning**. The goal is to find a "rule" in terms of descriptive features explaining the target feature as well as possible. Examples include:

- Hospital environments where the target variable can be "recover" (yes or no), and the descriptive variables can be age, gender, smoking,
- University environments where the target variable can be "drops out" (yes or no), and the descriptive variables can be **mentor**, **prior education**,
- Production environments where the target variable can be "order is delivered in time" (yes or no), and the descriptive variables can be product, agent,

Unsupervised learning In contrast to labeled data, we can also have instances without target labels, where we can only apply techniques of **unsupervised learning**. The goal is to find clusters or patterns.

- Cluster
- **Clusters** are homogeneous sets of instances. Examples include finding similar groups of patients, students, customers, orders, cars, companies, and so on.
- Pattern
- **Patterns** on the other hand reveal hidden structures in the data, so basically the unknown unknowns. Rules of some form can be found in many environments. Examples can look like:
 - Customers who buy bread and butter typically pay by phone.
 - Patients who drink and smoke typically pay the hospital bill earlier than others.
 - Products produced by team A on Monday tend to be returned more frequently by customers.

Interesting to regard is process discovery as a form of unsupervised learning in the way that a process model is just a very sophisticated rule. Important to mention, that this task can get very complex very quickly.

Terminology

Important to see for all of data science: many different names are used to refer to the key disciplines contributing to data science.

- This includes statistics, data analytics, data mining, machine learning, artificial intelligence, predictive analytics, process mining, generative AI, etc.
- Since frequently the same name is used for different concepts (names describe heavily overlapping areas), they really need to be put in context and interpreted accordingly.

The point can be highlighted when looking at scoping machine learning. Here are examples of confusions:

- Sometimes "machine learning" is used as a synonym for "deep neural networks" and sometimes they cover the entire spectrum of learning techniques.
- Neural networks can be used as classifiers. But this doesn't imply that numerous classification techniques developed in data mining are part of machine learning in the narrow sense.

How confusing specifically the arrangement of terms around machine learning is and how fluent and unclear the actual terms are, is depicted in 1.6.

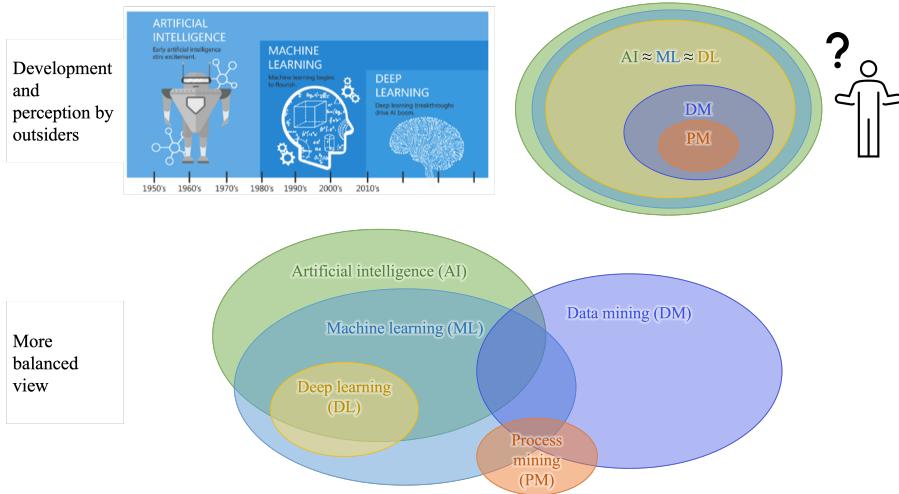


Figure 1.6: Terms around machine learning

1.4 Data science process

There are many different lifecycle models to describe phases in a data science project. This section will give a quick overview of some important ones.

CRISP-DM We'll start with **CRISP-DM** which stands for "Cross-industry standard process for data mining". It was developed in the late 1990s by different involved companies (SPSS, Teradata, Daimler AG, NCR Corporation, Ohra). The process consists of multiple steps playing together as visualized in 1.7

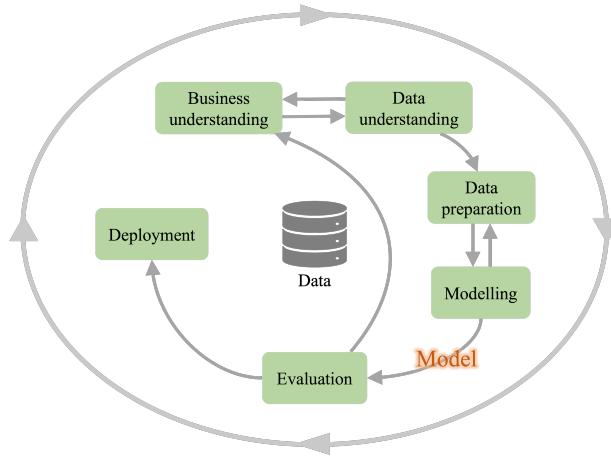


Figure 1.7: CRISP-DM process

Business understanding

Determine business objective
Situation assessment

Background, business objective, business success criteria
Inventory of resources, requirements, assumptions, constraints, risks, contingencies, terminology, costs, benefits

Determine data mining goal
Produce project plan

Data mining goals, data mining success criteria
Project plan, initial assessment of tools and techniques

Data understanding

Collect initial data
Describe and explore data
Verify data quality

Initial data collection report
Data description, exploration report
Data quality report

Data preparation with starting point: data set (with description)

Select data
Clean data
Construct data
Integrate and format data

Rationale for inclusion and exclusion
Data cleaning report
Derived attributes, generated records
Merged/reformatted data

Modeling¹

Select modeling technique
Generate test design
Build model
Assess model

Modeling technique, modeling assumptions
Test design
Parameter settings, models, model description
Model assessment, revised parameter settings

Evaluation

Evaluate results

Review process
Determine next steps

Assessment of data mining results w.r.t. business success criteria, approved models

Review of process
List of possible actions settings

Deployment

Plan deployment

Deployment plan

¹The term "modeling" can be misleading. Meant is the selection and assumptions by a human, or automated learning by a tool or algorithm

Plan monitoring, maintenance
Produce final report
Review project

Monitoring and maintenance plan
Final report and final presentation
Experience documentation

Next, we have the **KDD** (Knowledge Discovery in Databases) process as shown in 1.8.
Another process model also developed by SAS institute is called **SEMMA** consisting of the phases Sample, Explore, Modify, Model, and Assess.

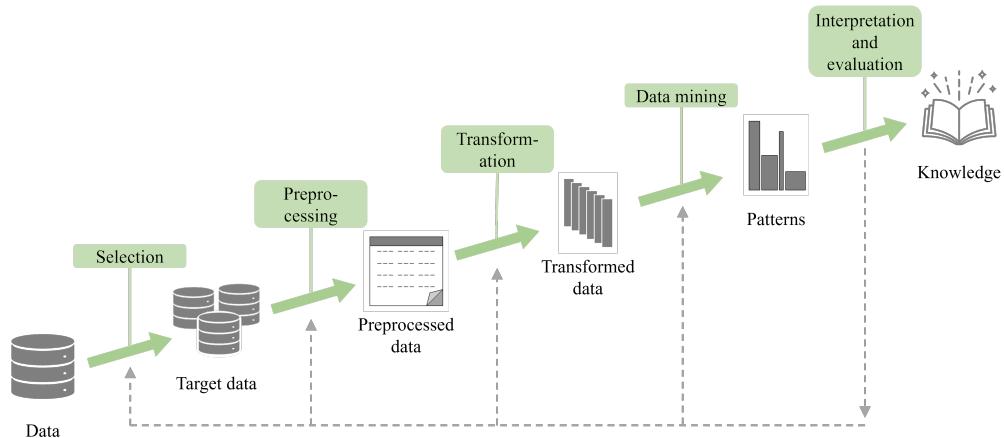


Figure 1.8: KDD process

The next process model is specifically developed for **L* lifecycle model** with multiple stages as shown in 1.9. L* lifecycle model

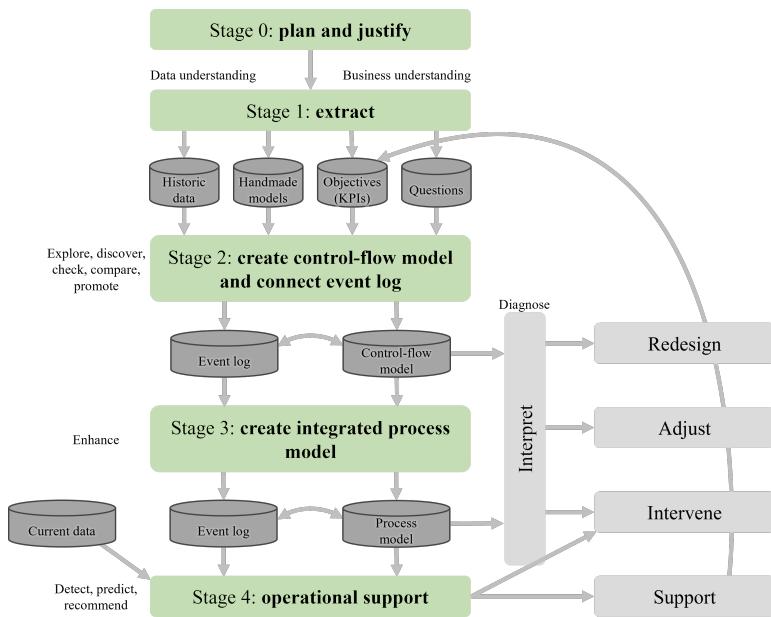


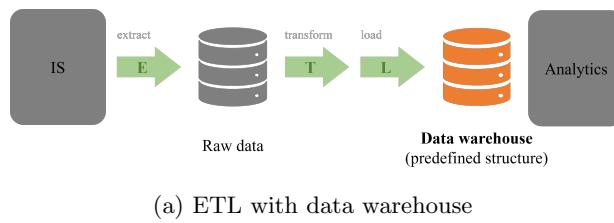
Figure 1.9: L* lifecycle model

Furthermore, we have two methodologies the process model can be related to. Important

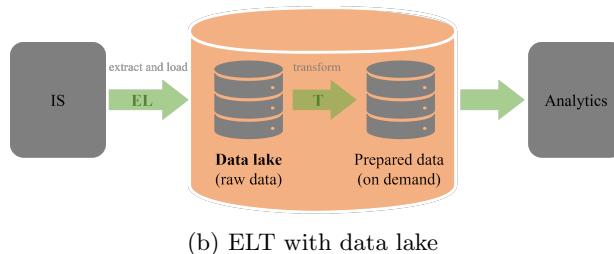
to implement and solidify are improvements in both.

- PDCA
 - **PDCA** stands for Plan-Do-Check-Act and is a never-ending cycle with exactly these steps.
- DMAIC
 - The other one **DMAIC** stands for Define-Measure-Analyze-Improve-Control, with the following subtasks:
 - Define: launch team, establish charter, plan project, gather VOC/VOB, plan for change
 - Measure: document process, collect baseline data, narrow project focus
 - Analyze: analyze data, identify root causes, identify and remove waste
 - Improve: generate, evaluate, and optimize solutions, pilot, plan and implement
 - Control: control the process, validate project benefits

Finally, we have two processes with the same components, but different ordering of the ETL steps as can be seen in 1.10. The short terms for the processes are **ETL** (extract, transform, load) and **ELT** (extract, load, transform).



(a) ETL with data warehouse



(b) ELT with data lake

Figure 1.10: Processes with extraction, transform, and load steps

80/20 rule

As a final note on which steps are usually the most time-expensive: there is a so-called "80/20 rule" stating:

- 80% of a data scientist's time is spent on finding, cleaning, preprocessing, and organizing data. This leaves only 20% to actually perform an analysis.
- On the other hand, we have 20% effort determining 80% of the final result.

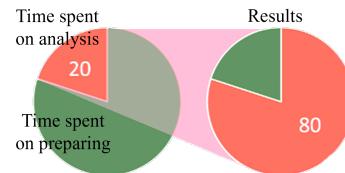


Figure 1.11: 80-20 rule

1.5 Challenges

To finalize the overview and basics of data science, let's look at the typical challenges.

First, we have the challenge of **finding data**. There may be hundreds or thousands of tables (E.g., in the case of SAP the numbers can easily for up to 800'000). But, different entities differ in their relevance, meaning some are less relevant than others.

The next challenge is the **transformation of data**, meaning reorganization of data, filtering, extraction of relevant features, and so on. Not only for transformations, but also in general other challenges are **dealing with big data and streaming data**. The challenge of big data evolved over the last few decades, meaning

- Typical stochastic methods try to solve the problem of saying something about entities given only a small amount of samples, whereas
- Now we have a very high load of data and need to solve the problem of dealing with these large amounts in a correct way.

Also for streaming data, new approaches need to be thought of. Additionally, we also need to **deal with a concept shift**.

Another huge challenge is ensuring **data quality**. This goes especially, since our provided data may be incomplete, invalid, inconsistent, imprecise, and/or outdated. Consider for example timestamps. They might be

- Incomplete (event is missing),
- Invalid (e.g. 14-14-2018),
- Inconsistent (14-07-2018 in contrast to 7-14-2018), or
- Imprecise (only regard part of available data: 2018-09-21^{T13:00:10}).

A very typical problem is **overfitting and underfitting** as it can be seen 1.12.

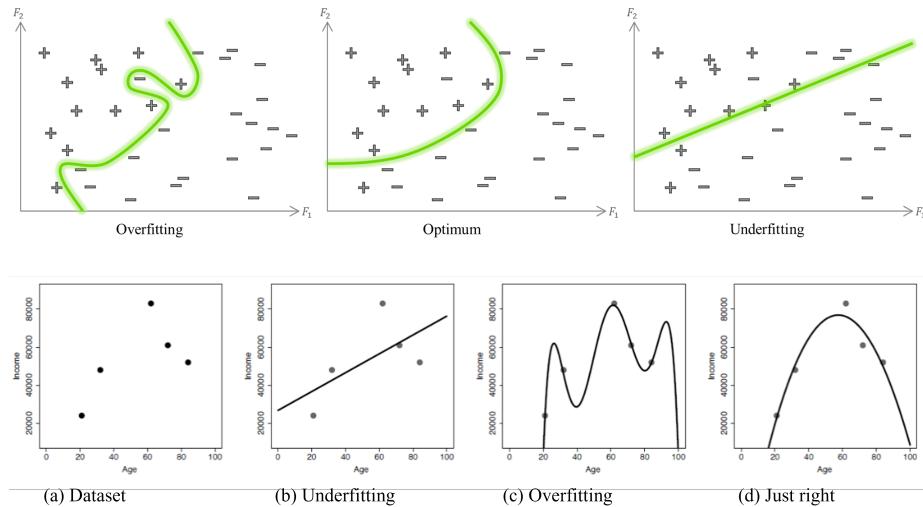


Figure 1.12: Over- and underfitting visualized

The next challenge is the distinction of **correlation and causation**, explicitly that correlation does not imply causation. Consider this example:

- Sunburn and ice cream have a strong correlation. When only these two features are considered, one might derive that either ice cream causes sunburn, or the other way around.
- We know of course, that this is not correct and instead an additional factor causes both phenomena: if the sun is shining, it's warm and people eat ice cream, and also sun directly causes sunburn.

Besides the accuracy of our results, we also need to look into whether our results are valuable. Concretely, **results** should be **made actionable**. This means, that analysis results should be relevant, specific, timely, novel, and clear. Our goal is to go from "data" to "insight" and finally "action". Consider these examples:

- Warning about a traffic jam should come before entering said traffic jam.
- That it's currently raining is not too helpful information. Preferably is a notice ahead of time.

Responsible data science The last, but very important challenge is **responsible data science** (RDS). This includes ensuring of:

- **Fairness**, meaning data science should exclude prejudice (How to avoid unfair conclusions even if they are true?)
- **Accuracy**, so data science without guesswork (How to answer questions with a guaranteed level of accuracy?)
- **Confidentiality** (How to answer questions without revealing secrets?)
- **Transparency** (How to clarify answers such that they become indisputable?)

2 Data visualization and exploration

2.1 Data extraction

Generally, we have a bunch of different data sources, with a multitude of different standards, features, and also information that can be extracted. The general problem is depicted in 2.1.

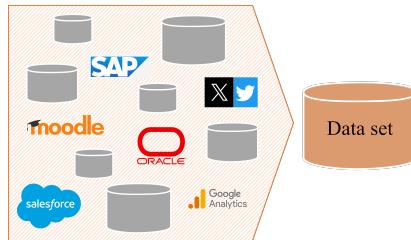


Figure 2.1: Data extraction from different sources

The different datatypes were already analyzed in the previous chapter, but still 2.2 shows a quick recap. Important to mention, that any unstructured data is considered a bit stream.

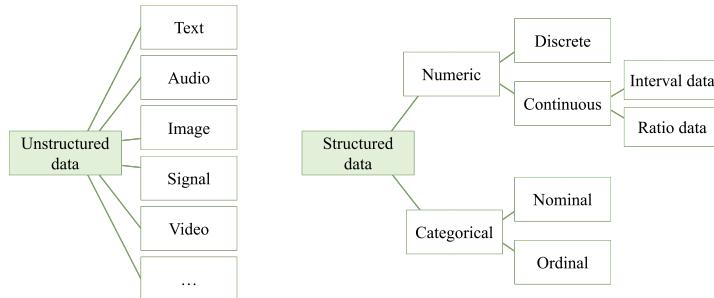


Figure 2.2: Recap: overview types of data

Important when wanting to obtain any object is of course the feature extraction. The data described by features are usually captured in a tabular form, with rows as the instances and columns as the features. There exist some special features:

- **Time** usually always plays a role in data observation, which is why it is usually one of the recorded features.
- Then there are also the **target features**, in contrast to the descriptive features. The concept was introduced in the last section as part of supervised learning.

Importance of visualization

We now looked at how we can represent our data in a very machine-friendly represented way. The following subsection shows, why visualization of data has any importance, even though tabular data already captures the features nicely.

It is important as a human to explore your data before applying mathematical operations to see, which techniques make sense to apply to the provided data. As an extreme example, we will take a look at **Anscombe's quartet** created by Francis Anscombe in 1973.

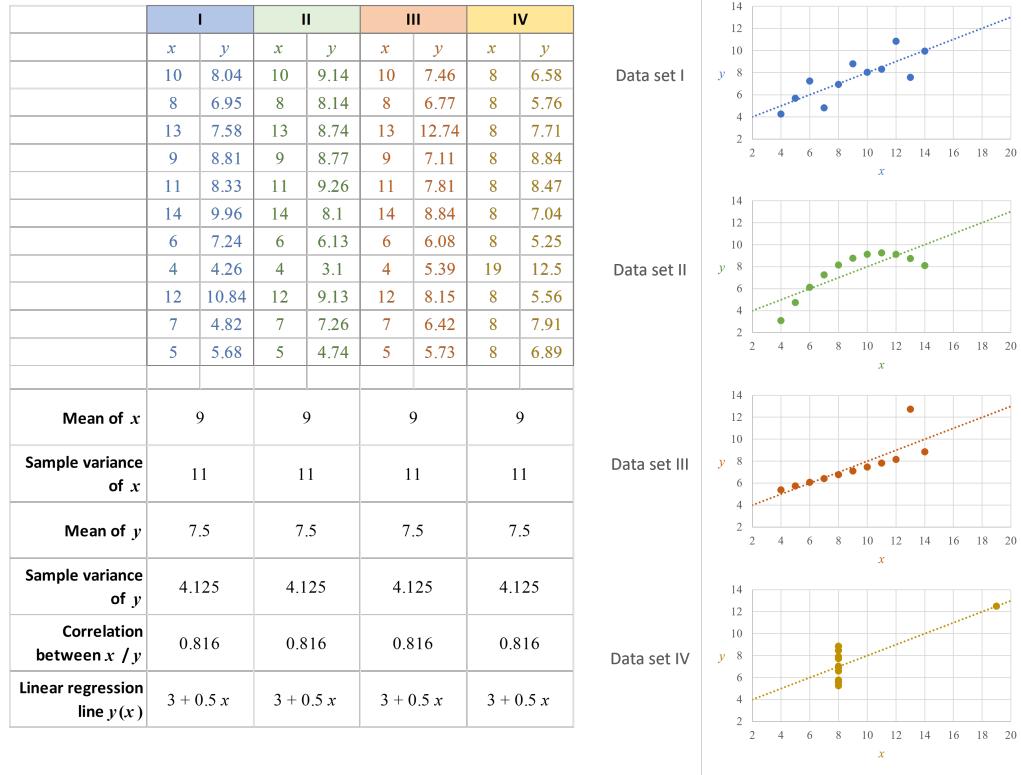


Figure 2.3: Anscombes quartet

- You can see the raw data of all four datasets in the table in 2.3. Since the format isn't human-friendly to read, you might not see any significant differences in the data.
- Now consider applying the evaluation depicted below the data table. As you can see: all of the properties that are evaluated are exactly the same for all datasets.
- BUT, if you visualize the datasets, e.g. as simple scatter plots, you see, how drastically they vary. These show the importance of first exploring your data, to then have a better evaluation foundation for the applied techniques.

The next example highlighting the importance of visualization and especially of a **fitting** and **well-thought-out visualization** is the diagram as shown in 2.4.

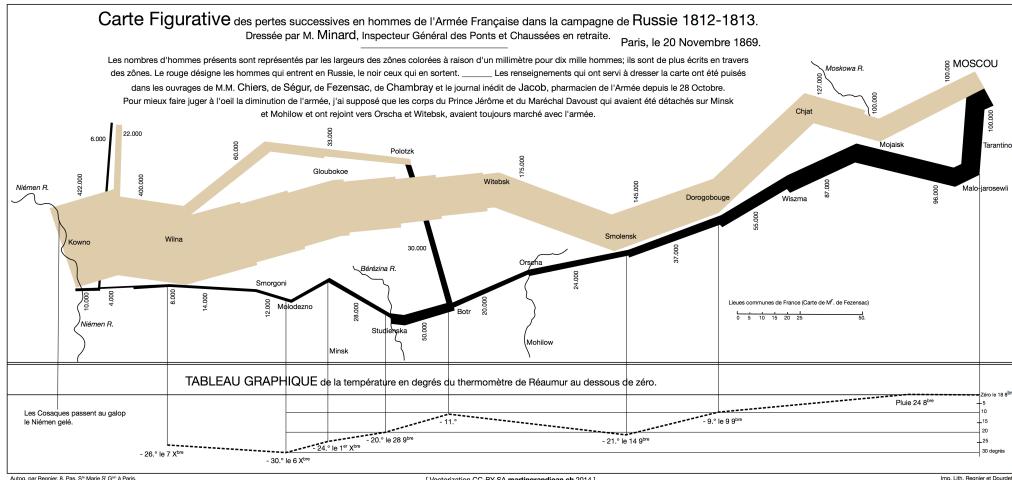


Figure 2.4: Multi-feature visualization (Napoleon's army)

The chart shows the following aspects, which are quite a lot, while still keeping a good overview:

- The number of men in Napoleon's 1812 Russian campaign army,
- Their movements (direction),
- The temperature encountered on the return path,
- All given a specific geographic point.

The final example highlights the importance of visualizing event or process data. In 2.5 we see the plot of different given event data input. With the visualization, some sort of trend, similarities, certain batching areas, etc. can be directly seen.

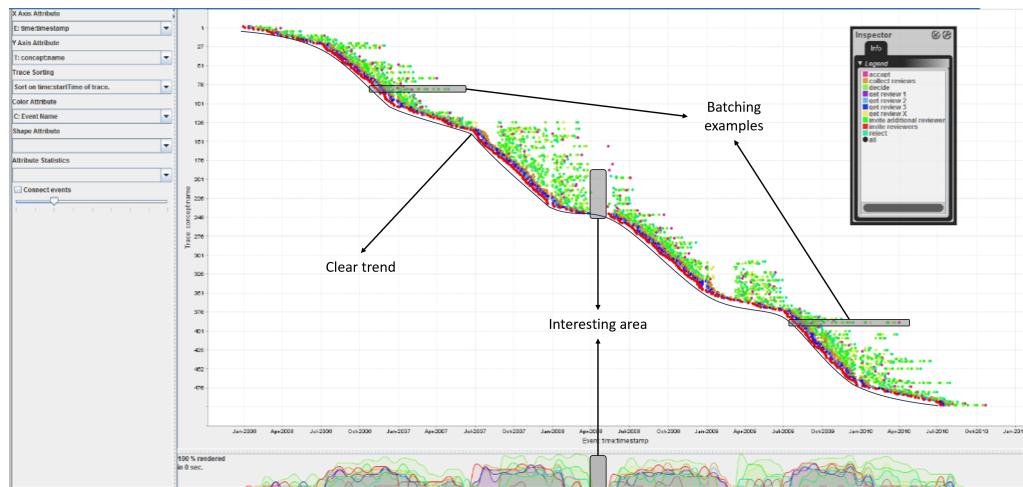


Figure 2.5: Visualization of event data

2.2 Characterizing individual features

As a first step of actual data exploration, we are now going to look at which information we can get from a single data feature. In terms of tabular data: we're going to focus on a single column.

What kind of data we can derive from the feature, depends of course on the data type. Generally deriving features from other ones is of course done best when dealing with structured data. Here, we have two types from which we can derive different properties.

Investigation of
individual
continuous features

From **continuous features**, we can derive

count : Number of instances having this feature

% miss : Percentage of missing information (how many instances don't have this feature)

card : Number of unique values (cardinality)

min : Minimal value over all instances

1st qrt : 25th percentile (largest value of the quarter of instances having the lowest values)

mean : Average value over all instances

median : Middle value of all instances

3rd qrt : 75th percentile (smallest value of the quarter of instances having the highest values)

max : Maximal value over all instances

std. dev : Standard deviation over all instances

Investigation of
individual
categorical feature

From **categorical features**, we can derive²

count : Number of instances having this feature

% miss : Percentage of missing information (how many instances don't have this feature)

card : Number of unique values (cardinality)

mode : Most common value

mode frequ : Frequency of the mode

mode % : Percentage of the mode

2nd mode : Second most common value

2nd mode frequ : Frequency for the second mode

2nd mode % : Percentage of the second mode

To get a better idea of how to get these properties for all of the features, we will look at an example. Consider a table containing information about insurance claims fraud. The dataset contains 500 instances (claims) and a bunch of different features such as type, claim amount, etc. Now first, determine the data type of each feature, and then

²obvious: **min**, **max**, **mean**, etc. can't be computed

create one table for the numerical and one for the categorical features and fill it with the according information. The raw data can be found in 2.6.

ID	TYPE	INC.	MARITAL STATUS	NUM CLMNTS.	INJURY TYPE	HOSPITAL STAY	CLAIM AMNT.	TOTAL CLAIMED	NUM CLAIMS	% SOFT TISS.	CLAIM AMT RCVD.	FRAUD FLAG
1	CI	0		2	Soft Tissue	No	1,625	3250	2	1.0	0	1
2	CI	0		2	Back	Yes	15,028	60,112	1	0	15,028	0
3	CI	54,613	Married	1	Broken Limb	No	-99,999	0	0	0	572	0
4	CI	0		4	Broken Limb	Yes	5,097	11,661	1	1.0	7,864	0
5	CI	0		4	Soft Tissue	No	8869	0	0	0	0	1
6	CI	0		1	Broken Limb	Yes	17,480	0	0	0	17,480	0
7	CI	52,567	Single	3	Broken Limb	No	3,017	18,102	2	0.5	0	1
8	CI	0		2	Back	Yes	7463	0	0	0	7,463	0
9	CI	0		1	Soft Tissue	No	2,067	0	0	0	2,067	0
10	CI	42,300	Married	4	Back	No	2,260	0	0	0	2,260	0
...
300	CI	0		2	Broken Limb	No	2,244	0	0	0	2,244	0
301	CI	0		1	Broken Limb	No	1,627	92,283	3	0	1,627	0
302	CI	0		3	Serious	Yes	270,200	0	0	0	270,200	0
303	CI	0		1	Soft Tissue	No	7,668	92,806	3	0	7,668	0
304	CI	46,365	Married	1	Back	No	3,217	0	0	0	1,653	0
...
458	CI	48,176	Married	3	Soft Tissue	Yes	4,653	8,203	1	0	4,653	0
459	CI	0		1	Soft Tissue	Yes	881	51,245	3	0	0	1
460	CI	0		3	Back	No	8,688	729,792	56	0.08	8,688	0
461	CI	47,371	Divorced	1	Broken Limb	Yes	3,194	11,668	1	0	3,194	0
462	CI	0		1	Soft Tissue	No	6,821	0	0	0	0	1
...
491	CI	40,204	Single	1	Back	No	75,748	11,116	1	0	0	1
492	CI	0		1	Broken Limb	No	6,172	6,041	1	0	6,172	0
493	CI	0		1	Soft Tissue	Yes	2,569	20,055	1	0	2,569	0
494	CI	31,951	Married	1	Broken Limb	No	5,227	22,095	1	0	5,227	0
495	CI	0		2	Back	No	3,813	9,882	3	0	0	1
496	CI	0		1	Soft Tissue	No	2,118	0	0	0	0	1
497	CI	29,280	Married	4	Broken Limb	Yes	3,199	0	0	0	0	1
498	CI	0		1	Broken Limb	Yes	32,469	0	0	0	16,763	0
499	CI	46,683	Married	1	Broken Limb	No	179,448	0	0	0	179,448	0
500	CI	0		1	Broken Limb	No	8,259	0	0	0	0	1

Figure 2.6: Example for single feature investigation (insurance claim fraud)

To investigate the raw data further, let's first extract the resulting feature-describing tables and then also visualize the data. More specifically for the visualization, we're going to show the distributions of the different features. Figure 2.7 shows both the properties of the features and exemplary plots.

- For finite amounts of possible feature classes, simply visualize the distribution as a bar diagram with the different classes as entries on the x-axis. The y-axis can either be the frequency or a percentage.
- For continuous features with continuous variables/ininitely many possible feature values, group items (**binning**) and then visualize the resulting histogram.

Binning

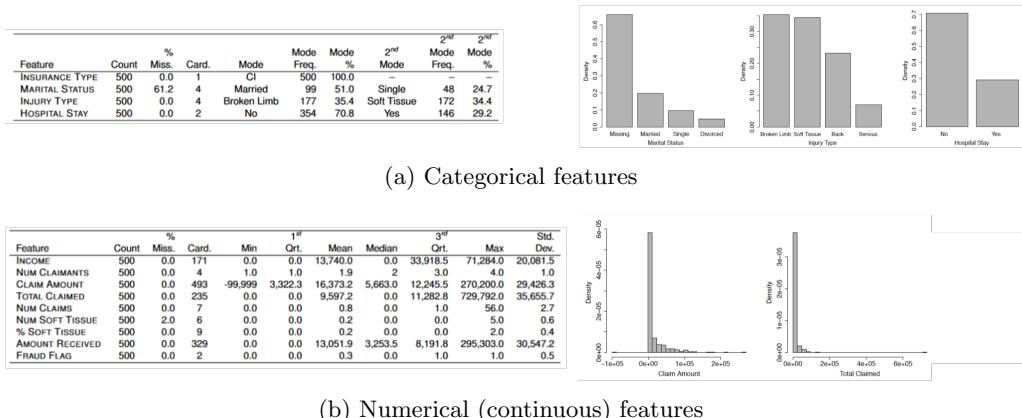


Figure 2.7: Feature-describing table and distribution visualization

Over- and underfitting
for binning

The binning comes with some challenges. When we select the amount of bins with evenly distributed width of each individual bin, we need to be aware not to **over- or underfit**. Examples can be found in 2.8. As one can see:

- In the case of underfitting, the true function is not at all matched.
- In the case of overfitting, there exist very steep valesys, the provided data points are more learned by heart rather than abstracting to a function.

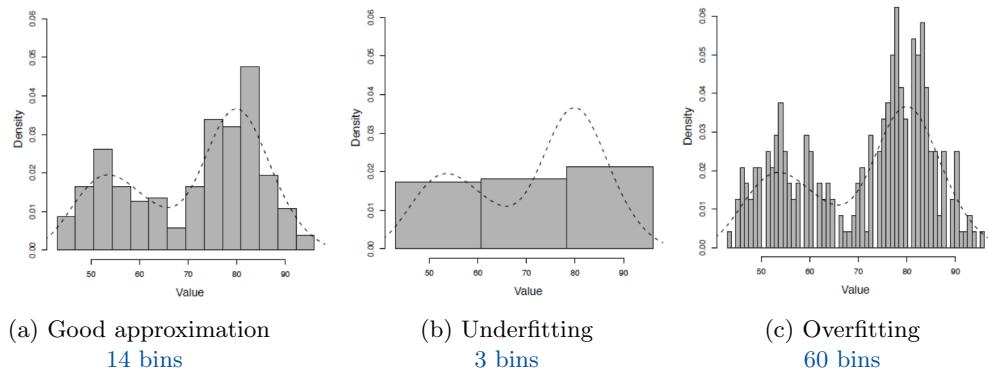


Figure 2.8: Binning for continuous variables

The histograms furthermore can show different types, as depicted in 2.9.

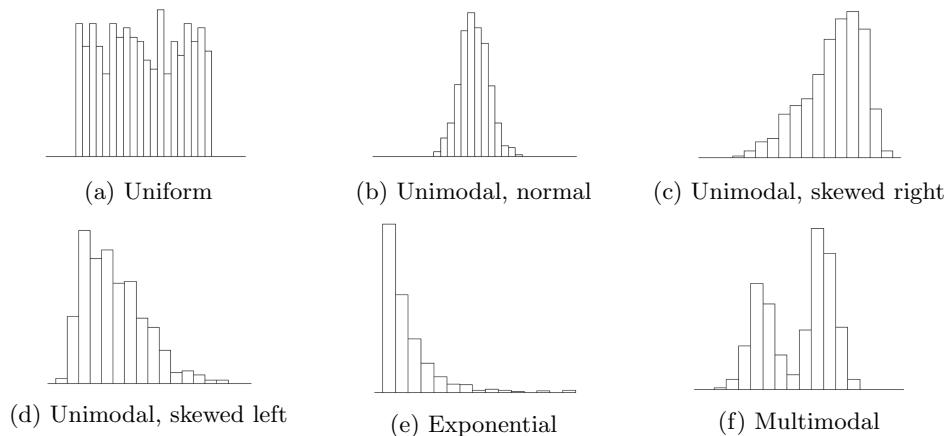


Figure 2.9: Histogram types

Here are some further notes on the types:

- **Uniform** means all items have the same likelihood (within a range).
- **Unimodal** means we have one peak (can be tilted to one side), whereas **multimodal** means there are multiple distinct ones.
- **Exponential** means we have an exponential decrease in the likelihood over all instances.

Normal distribution

One of the types mentioned, we're now gonna investigate a bit further. The **normal distribution** is described by two important variables, whose effects on the distribution are shown in 2.10:

- The **mean** μ , so the expected value also characterizing the peak, and Mean
- The **standard deviation** σ characterizing how narrow the peak, or the distribution Standard deviation around the peak, is.

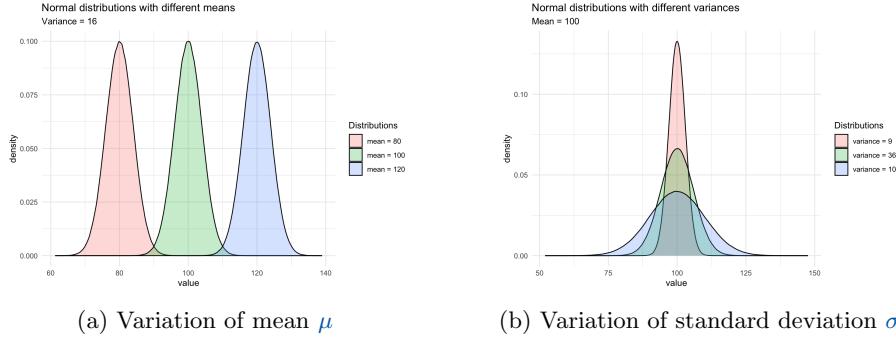


Figure 2.10: Normal distribution

The normal probability distribution over x is defined as:

$$x \sim \mathcal{N}(\mu, \sigma)$$

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right]$$

Interesting are now precise areas we instantly know something about. The **68-95-99.7-rule** tells us, as depicted in 2.11.

68-95-99.7-rule

- 68% of all observations will be within 1σ -distance of the mean,
- 95% of all observations will be within 2σ -distance of the mean, and
- 99.7% of all observations will be within 3σ -distance of the mean

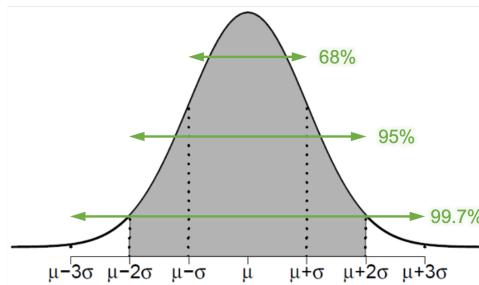


Figure 2.11: 68-95-99.7-rule

From this rule, we can now derive probabilities for different events. Consider the following examples, also visualized in 2.12:

- Example 1 is interested in the amount of defects for some produced item. The tolerance can be defined as within the 2σ -range, so with:
 - **LSL** (lower specification limit) at $\mu - 2\sigma$, meaning only 2.5% of the instances have a larger deviation into the negative direction from the mean than this limit, and
 - **USL** (upper specification limit) at $\mu + 2\sigma$, meaning only 2.5% of the instances have a larger deviation into the positive direction from the mean than this limit.
 Combined, $100\% - 2.5\% - 2.5\% = 95\%$ have a deviation from the mean lying within the defined range.
- Example 2 is interested in how many deliveries are too late. Therefore, it **only** defined an **upper bound** with the USL at $\mu + 2\sigma$. This means, $100\% - 2.5\% = 97.5\%$ of the deliveries are not to late.

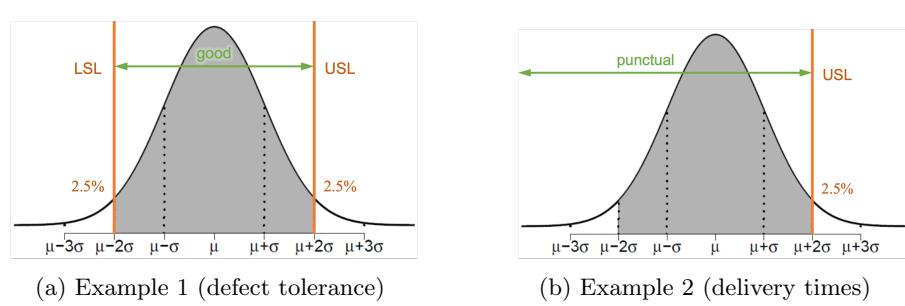


Figure 2.12: Examples for 68-95-99.7-rule

Furthermore, the rule also introduces the term of **six sigma** or also lean six sigma. It basically means that processes operating with "Six Sigma quality" are assumed to have < 3.4 defects per million instances, so $\Pr(\text{error}) = 0.0000034$. It characterizes a process improvement approach. This likelihood is a combination of $\pm 6\sigma$ tolerance and a "drift" of $\pm 1.5\sigma$.

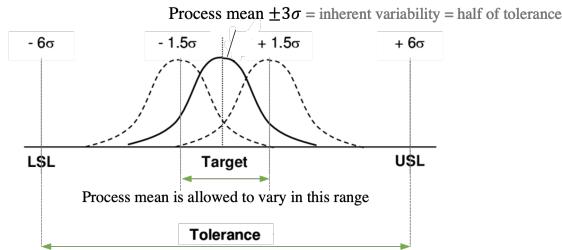


Figure 2.13: Lean six sigma

2.3 Data quality

In the introduction, we already looked at some key challenges regarding data quality. In this subsection, we will investigate and search for solutions for some of the following typical data quality problems in detail:

- **Incompleteness** - missing instances or attributes
- **Invalidity** - impossible values

- **Inconsistency** - conflicting values
- **Imprecision** - approximates or rounded values
- **Outdated** - values based on old observations

For that, we will take a look at missing, invalid, unlikely, and outlier values.

Missing values

Imagine different missing features of some instances. Since some data is missing, we need to deal with this in some way. Here are the possible options:

1. Remove feature completely (for all instances)
2. Only consider instances that have a value (this is done for per-feature-evaluation)
3. Remove all instances that have one of the features missing
4. Repair missing features (imputation)

The problem setting and the possible solutions are visualized in 2.14.

f1	f2	f3	f4	f5
0	1	0	0	0
0		0	0	0
1	1		1	1
1	0	1	1	1
0	0			1

(a) Problem setting

f1	f2	f3	f4	f5
0	1	0	0	0
0		0	0	0
1	0	1	1	1
1	0	1	1	1
0	0			1

f1	f2	f3	f4	f5
0	1	0	0	0
0		0	0	0
1	0	1	1	1
0	0			1

(2) Only consider instances having value
(per feature)

f1	f2	f3	f4	f5
0	1	0	0	0
0		0	0	0
1	0	1	1	1
0	0			1

(3) Remove instances missing at least one feature

f1	f2	f3	f4	f5
0	1	0	0	0
0		0	0	0
1	1	0	1	1
1	0	1	1	1
0	0	0	1	1

(4) Repair values

(b) Possible solutions

Figure 2.14: Missing values

Impossible values

The next typical challenge is impossible values that by some mistake were entered as data. Examples are:

- Wrong date format: instead of **2018-10-18**, we would have **18-10-2018**

- Completely impossible date or time: [2018-13-51, 23:61](#)
- There can be spelling errors, for example for colors: [Blue](#)
- The data type might not make sense with the feature, like the number of members as a float: [6.5 members](#)

The handling of this problem is solved by either manually correcting entries or handling them just as for missing features.

Unlikely values

In contrast to impossible values, unlikely values are theoretically possible, but just not common to appear. Examples are:

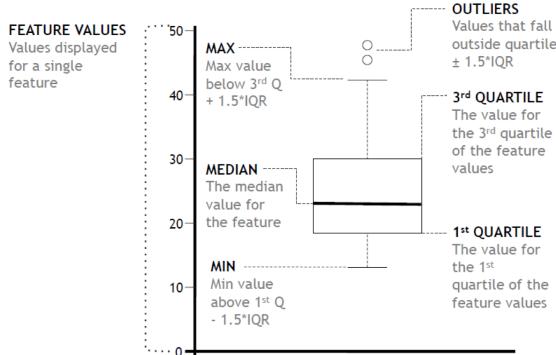
- Age: [123](#) is rather unlikely, but possible
- Price: [120.000\\$](#) in a store where the other prices lie in the range of [5\\$](#) to [150\\$](#)
- Dates: even on dates, where one would usually expect a uniform distribution over months and days, days [1](#) to [12](#) are more frequent than days [13](#) to [31](#)³

Unlikely values, domain knowledge Whether a value is unlikely or not is identified based on **domain knowledge**. They can then be further investigated to see, whether the unlikely value is actually valid.

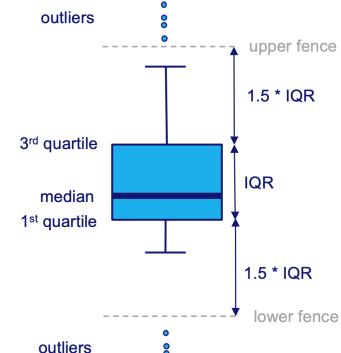
Outlier values

Outlier values In contrast to unlikely values, **outlier values** are identified based on the distribution.

Box plot An especially popular technique to visualize distributions and outliers is **box plots**. They were first introduced by John Tukey in the book "Exploratory data analysis" in 1977. Figure 2.15 shows the properties visualized by a box plot and also how to construct one given a data set.



(a) Properties on a box plot



(b) Construction of a box plot

Figure 2.15: Box plot

Let's first take a look at the properties one can see in the box diagram.

- The **median** value is depicted by the "Bar" in the center.

³NOT the case anymore if date format [DD-MM-YYYY](#) and [MM-DD-YYYY](#) are mixed

- The median is the "middle" value, so the number is halfway between the lowest and highest number.
- The **IQR**, so the interquartile range, covering 50% of the "middle instances" is IQR depicted by the "Box".
 - The first quartile is the number halfway between the lowest and middle number, whereas the third is halfway between the middle and highest number.
 - The IQR is the distance between the first and third quartile.
- The upper whisker indicates the **maximal** value below the $3^{\text{rd}} \text{ quartile} + 1.5 \cdot \text{IQR}$, whereas
- The lower whisker indicates the **minimal** value above the $1^{\text{st}} \text{ quartile} - 1.5 \cdot \text{IQR}$.
- Finally, the **outliers** are drawn separately.

The description already contained a bit of the construction details, which will now be explained in more detail with an example. Consider the (already ordered) data set:

$$\{1: 1, 2: 2, 3: 5, 4: 7, 5: 8, 6: 8, 7: 9, 8: 9, 9: 9, 10: 10, 11: 10, 12: 10, 13: 11, 14: 12, 15: 14, 16: 19, 17: 23\}$$

Then we construct the box diagram like this:

- The median value is 9 (at position 9).
- The first quartile has the value 8 (at position 5), the third one has the value 11 (at position 13) resulting in an $\text{IQR} = 11 - 8 = 3$.
- This means we have an upper fence $11 + 1.5 \cdot 3 = 15.5$, and the upper whisker as the maximum value below this fence at 14 (position 15).
- The lower fence has the value $8 - 1.5 \cdot 3 = 3.5$, the lower whisker therefore the minimum value above this fence value at 5 (position 3).
- Finally, the outliers are 1, 2, 19, 23 (position 1, 2, 16, 17).

Those are all the necessary components to construct the box diagram.

Now, one final detail about box diagrams and also the topic of this paragraph is the handling of the outliers. They can first be removed (meaning remove values above and below the upper and lower fences), and their existence can be indicated by claiming the removed values to these thresholds. The process is shown in 2.16.

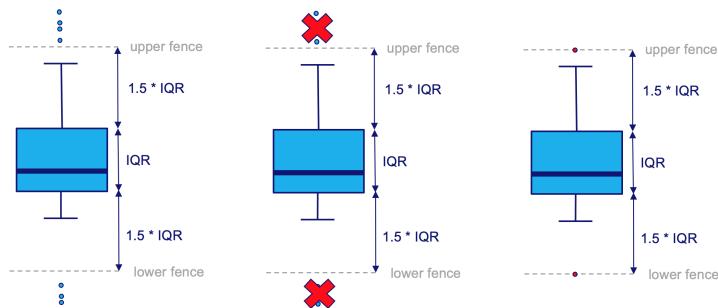


Figure 2.16: Handling outliers in box plots

2.4 Relations among features

So far, we only really looked into features separately. This section will now focus on showing how multiple features are related. We will only consider relating TWO features,

but the techniques are also applicable to more.

Scatter plots

As a first step to see whether a relation exists, first plot the two features. Examples for typical resulting **correlations** are shown in 2.17.

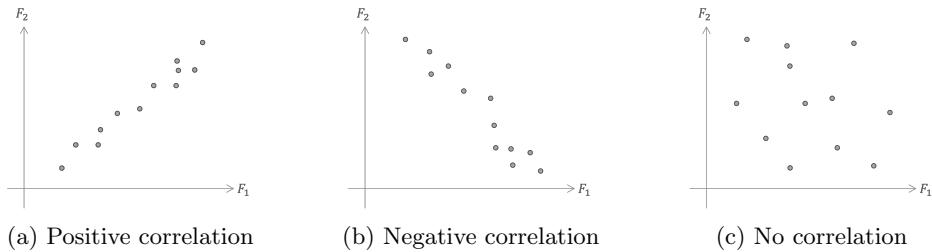


Figure 2.17: Scatter plots visualizing correlations

As an example for detecting correlations, we have a data set about basketball players with different features. The raw data will not be included here. Instead, we will directly look at all correlations of the features simultaneously. This is visualized using a **scatter plot matrix** (SPLOM) as in 2.18.

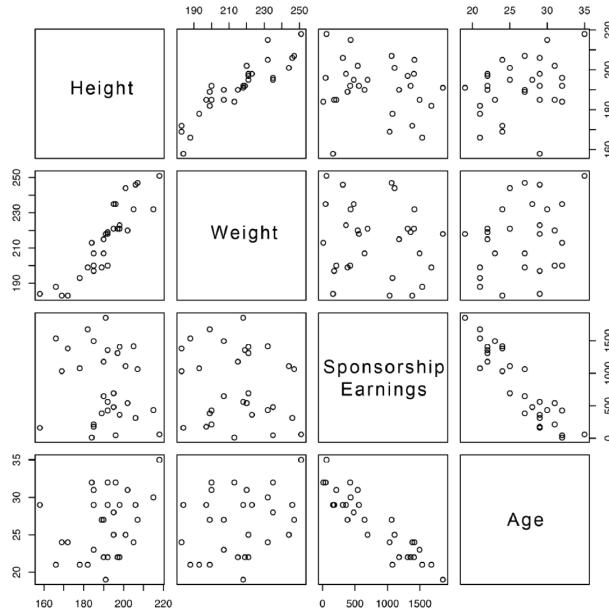


Figure 2.18: Scatter plot matrix for four features

Interesting to see in such a SPLOM is the mirror axis in opposite tiles of the matrix which is an absolutely linear line (so absolute correlation, or identity, as would be displayed if a feature would be displayed on a scatter plot compared to itself). This mirroring doesn't change the nature of a correlation. If feature A is positively correlated to feature B, the same goes in the other direction (equivalently for negative correlation).

Collection of bar plots

Another way to display relations is via a collection of small multiple **bar plots**. Consider the plots in 2.19

Collection of small multiple bar plots

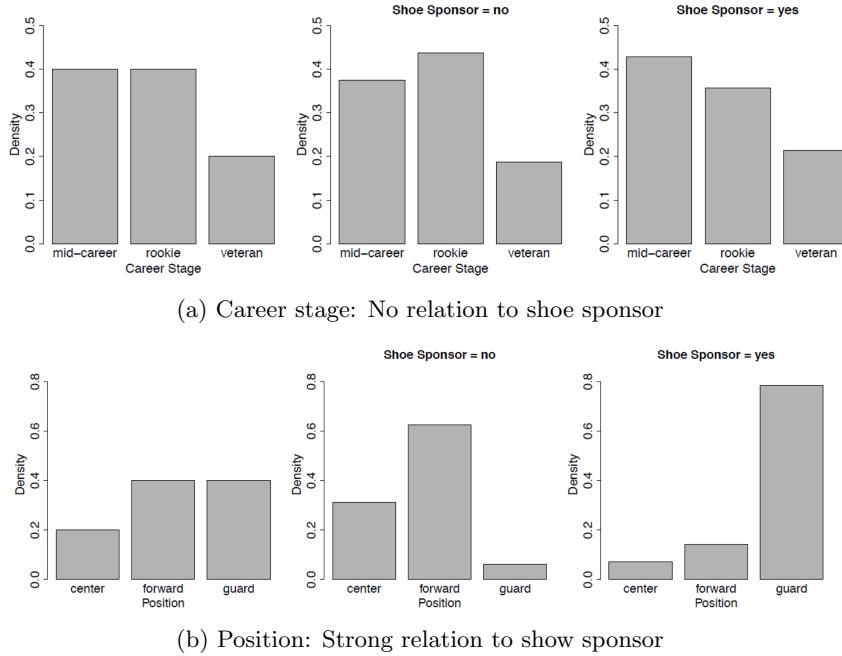


Figure 2.19: Collection of (conditioned) bar plots (Conditioned on shoe sponsor)

No relation is implied when the differently conditioned and non-conditioned bar plots don't show any significant difference, as for the example of career stages. On the other hand, a relation can be seen when the bar plots show specific differences. For example in the position case it can be seen that "guards" are more likely to have a shoe sponsor.

The difference and implied relation can be further highlighted by using **stacked bar plots** that show the conditioned percentage, as can be seen in 2.20.

Stacked bar plots

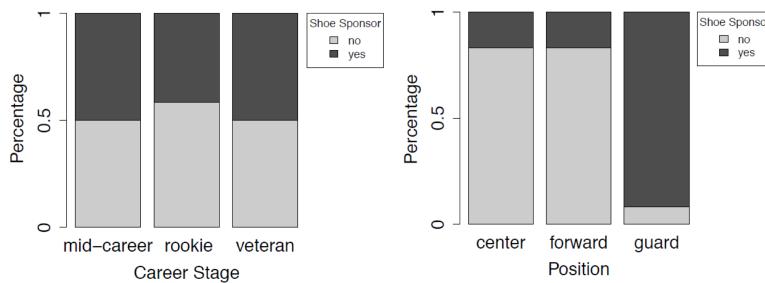
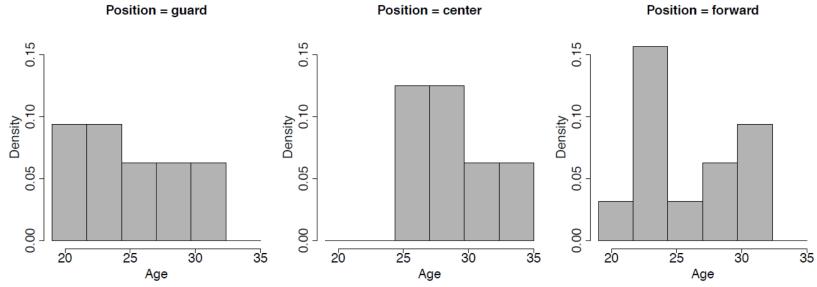


Figure 2.20: Stacked bar plots (for both career and position conditioned on shoe sponsor)

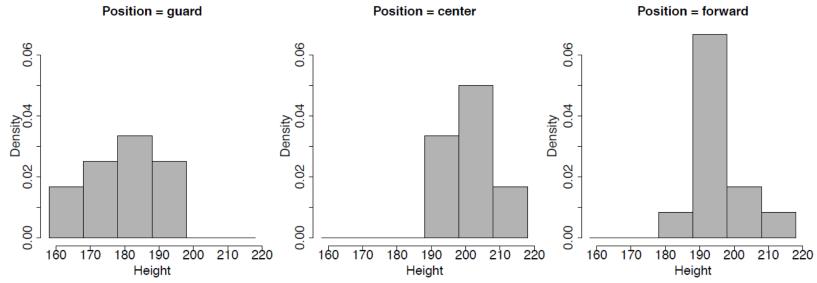
Collection of histograms and box plots

In the case of continuous variables, instead of bar plots, we can use a collection of small multiple **histograms**, as displayed in 2.21.

Collection of small multiple histograms



(a) Age (6 bins): No strong relation to position

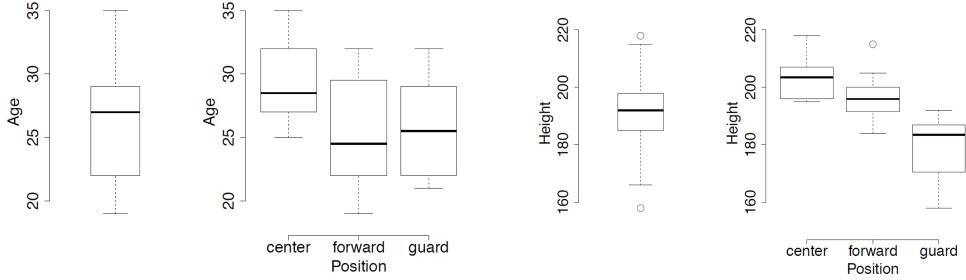


(b) Height (6 bins): Relation to position

Figure 2.21: Collection of (conditioned) histograms (Conditioned on position)

Collection of box plots

Alternatively, **box plots** can be collected and utilized to identify relations. Figure 2.22 conducts the same relation between age or height to position. It further highlights the relatively strict separation of age for individual positions.



(a) Age: Weaker relation to position

(b) Height: Stronger relation to position

Figure 2.22: Collection of (conditioned) box plots (Conditioned on position)

Descriptive statistics

To not only see the relation but also classify it with values, we now introduce some basic descriptive statistics. Based on n values a_1, \dots, a_n , we have the **sample mean** \bar{a} and **sample variance** $var(a)$ and **standard deviation** $sd(a)$ as:

Sample mean

$$\bar{a} = \frac{1}{n} \sum_{i=1}^n a_i$$

Sample variance

$$var(a) = \frac{\sum_{i=1}^n (a_i - \bar{a})^2}{n - 1}$$

$$sd(a) = \sqrt{var(a)} = \sqrt{\frac{\sum_{i=1}^n (a_i - \bar{a})^2}{n-1}}$$

Standard deviation

A quick note on why we divide by $n - 1$ and not n for the calculation of $var(a)$. This is due to the estimated mean \bar{a} instead of actual or true one \hat{a} . Simply put, since we can only estimate, we would rather overestimate the variance (divide by a smaller number) instead of underestimating (divide by a larger number) it. We would call a variance calculated by dividing by n a biased estimator.

To classify the relation between features, based on n pairs of values $(a_1, b_1), \dots, (a_n, b_n)$ we have the **sample covariance** $cov(a, b)$ and the **correlation** $corr(a, b)$ as:

$$cov(a, b) = \frac{1}{n-1} \sum_{i=1}^n ((a_i - \bar{a}) \times (b_i - \bar{b}))$$

Sample covariance

$$corr(a, b) = \frac{cov(a, b)}{sd(a) \times sd(b)}$$

Correlation

Covariance and correlation have the following properties:

$$cov(a, b) \in [-\infty, \infty] \text{ (unbounded)}$$

$cov(a, b)$ is positive (+) if a (\pm) and b (\pm) are the same
negative (-) (\pm) (\mp) are different

$$corr(a, b) \in [-1, 1] \text{ (normalized)}$$

> 0 positively correlated

$corr(a, b) < 0$ if a and b are negatively correlated

$= 0$ independent

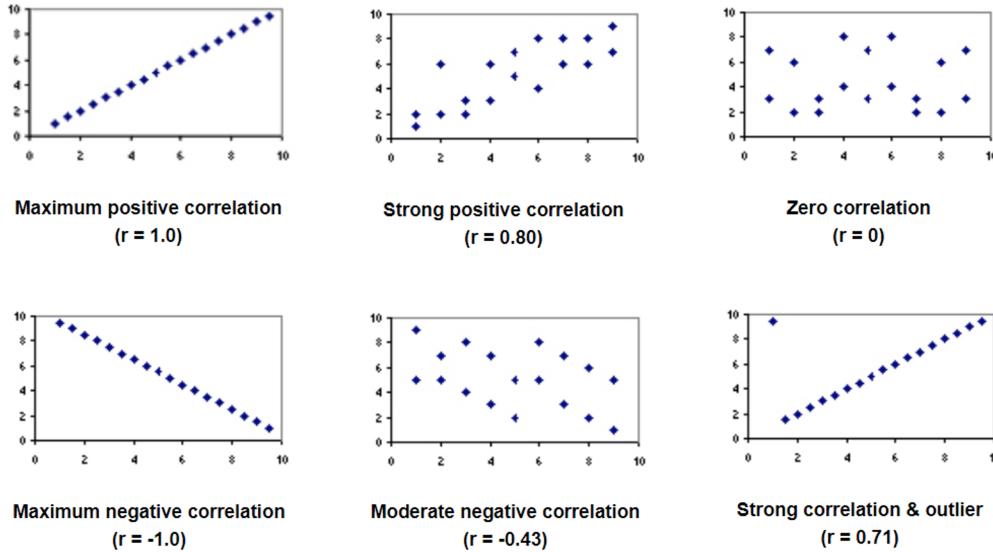


Figure 2.23: Different correlation examples with scatter plot

With the new knowledge, we can expand our previous SPLOM diagram with the **correlation matrix** values. A correlation matrix looks as follows:

$$\text{Correlation matrix} \quad \text{corrmatrix} = \begin{pmatrix} \text{corr}(a, a) & \text{corr}(a, b) & \cdots & \text{corr}(a, z) \\ \text{corr}(b, a) & \text{corr}(b, b) & \cdots & \text{corr}(b, z) \\ \vdots & \vdots & \ddots & \vdots \\ \text{corr}(z, a) & \text{corr}(z, b) & \cdots & \text{corr}(z, z) \end{pmatrix}_{\{a, b, \dots, z\}}$$

with $\text{corr}(f_1, f_2) = \text{corr}(f_2, f_1)$ for all $f_1, f_2 \in \{a, b, \dots, z\}$ making the correlation matrix symmetric.

The updated SPLOM diagram, which basically contains the same information twice (just flipped) now also shows the correlation values as can be seen in 2.24.

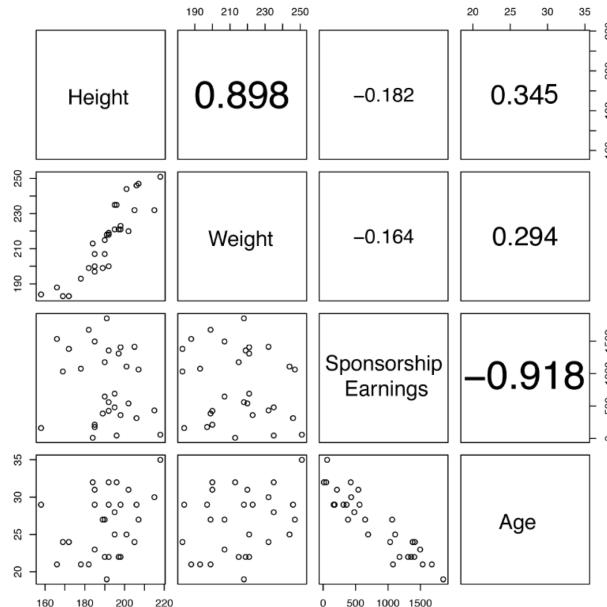


Figure 2.24: Scatter plot matrix of four features with according corr -values

2.5 Preparation for analysis

We now know some techniques to evaluate raw data, feature by feature and the relationship of features. But a very important step before applying analysis is the preparation, consisting of:

- **Normalization** to make things comparable,
- **Binning** to make things categorical, and
- **Sampling** to make data smaller or to change the bias.

Normalization

Normalization Let's first start with normalization. Typically, when applying normalization, values are mapped onto a predefined range while maintaining differences. This predefined

range is usually something like $[0, 1]$ or $[-1, 1]$.

As an example, the following mapping transforms a_i into $a'_i \in [l, h]$ where

- l is the lower bound, h the upper one, and
- We have a complete set of values a with a defined minimum and maximum given.

$$a'_i = \frac{a_i - \min(a)}{\max(a) - \min(a)} \times (h - l) + l$$

Furthermore, we have the **standard score** using the standard deviation to normalize.

$$a'_i = \frac{a_i - \bar{a}}{sd(a)} \in [-\infty, \infty]$$

Standard score

Binning

Next, we have binning of values to **turn continuous** features **into categorical** ones. Bins are a series of ranges. There are two approaches to determine the bins, both visualized in 2.25.

- **Equal-width binning** assumes a fixed width for all bins, where the number of items per bin may vary greatly. Equal-width binning
- **Equal-frequency binning** on the other hand assumes a fixed number of items per bin, but allows a variable width. Equal-frequency binning

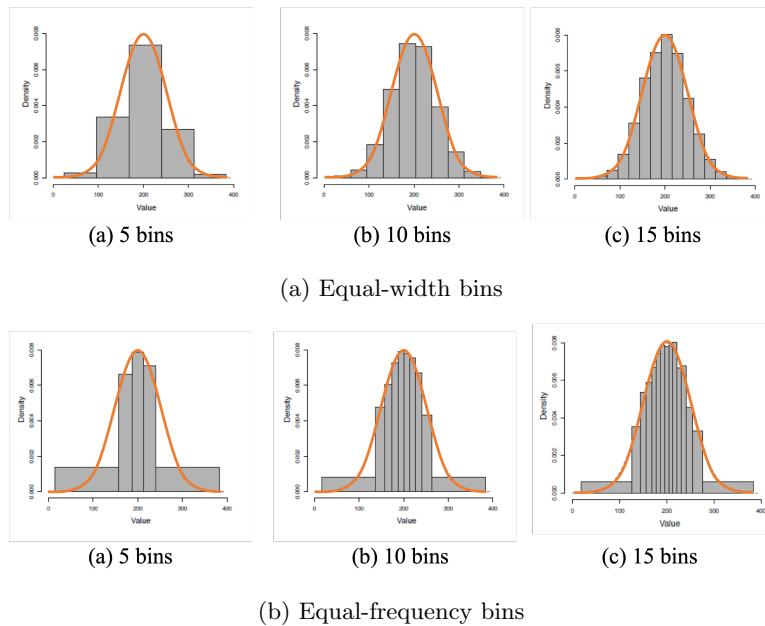


Figure 2.25: Binning with different number of bins

The number of items in a bin is reflected by its surface (need to consider both width and height).

Generally, the number of bins is important as we saw earlier with the problem of over-and under-fitting.

- Underfitting happens when the number of bins is too small, and information gets lost.
- Overfitting on the other hand occurs when the number of bins is too large, leading to sparseness with some (nearly) empty bins in areas where the true function considers items to occur very likely.

Sampling

Sampling Finally, we have the preparation step of sampling (which actually usually comes as the first step). It selects a subset of all available data, and thereby reduces the amount of data. Sampling can remove or introduce a **sample bias**.

There are different **types** of sampling, as depicted in figure 2.26.

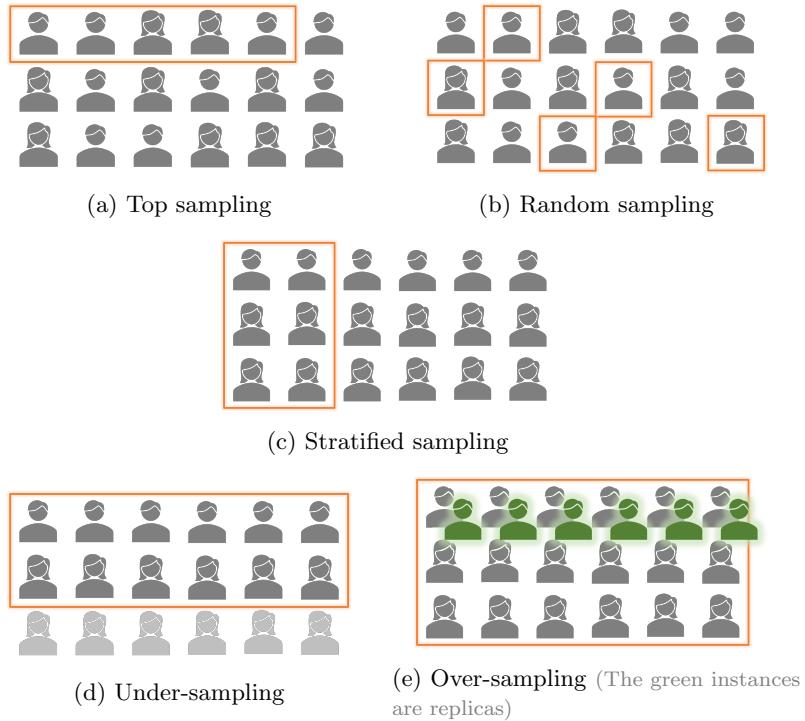
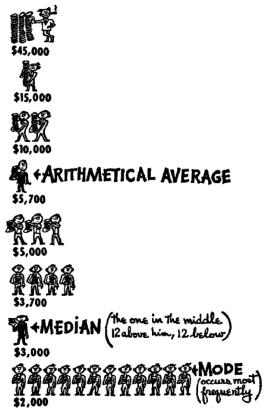


Figure 2.26: Types of sampling

- **Top** sampling takes the first n instances
- **Random** sampling
- **Stratified** sampling where the relative frequencies are ensured to be maintained (e.g. by taking the same percentage from every group)
- **Under**-sampling, where balance between groups is ensured by leaving out instances of over-represented groups.
- **Over**-sampling, where balance between groups is ensured by duplicating under-represented groups.

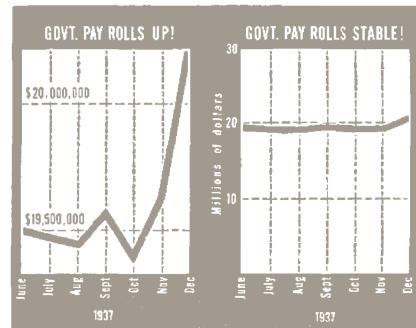
Good and poor visualizations

With statistics and especially visualization, one can really manipulate the view on the provided data, so basically introduces a very strong bias. There's actually a whole book about it, called "How to Lie with Statistics". The following images in 2.27 show some examples.



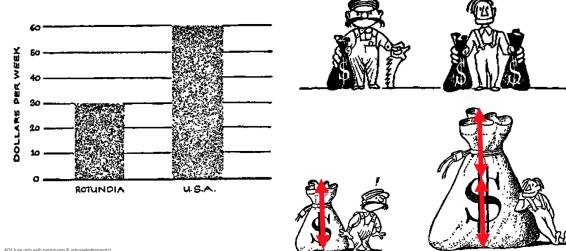
(a) Choosing the middle

- Arithmetical average (gets pumped up by rare but high maximum)
- Median (standing in middle)
- Mode (most frequently occurring)



(b) Tampering with scales

- Easy manipulation of difference perception



(c) Visualizing factor two

- Adjusting the whole volume according to height makes the difference seem more severe than just taking two instances

Figure 2.27: Manipulation of perception via statistics and visualization

As a good example, one can consider the information visualization book "The Visual Display of Quantitative Information" from Edward Rolf Tufte. It encourages the use of **data-rich illustrations** representing all available data such that:

- One can check individual values, while still
- Seeing trends and patterns when looking at the whole.

3 Decision trees

3.1 Statistics versus DM/ML

Statistics have been around for a while. Famous statisticians are for example:

- John Graunt (1620-1674), who studied London's death records around 1660.
 - He was able to predict the life expectancy of a person at a particular age and was the first to create a "life table" with the probability of death for each age.
- Francis Galton (1822-1911), who introduced many core statistical concepts at the end of the 19th century.
 - He (re)invented variance, normal distribution, correlation, linear regression, etc.

Back then, statistics were concerned with the problem of making generalizations based on relatively little data. Since then, the availability of data changed drastically, with now having more of an overload of data. Therefore, more **pragmatic** instead of statistical approaches for handling large amounts of data were introduced to fuel the progress in data science.

- Major breakthroughs in the discovery of patterns and relationships are for example efficiently learning decision trees and association rules.
- By traditional statisticians, these were described as "data fishing", "data snooping", or "data degrading" (Surprisingly, some statisticians claim "owning" the data science field)

Modern statisticians are now also concerned with a more pragmatic approach. Leo Breiman (1928-2005) wrote a paper ("Statistical Modeling: The Two Cultures") about the two main camps of statisticians:

- The "classical statistics camp" (**98%**) assumes nature's behavior to fit some model and focuses on parameter estimation and goodness-of-fit tests.
 - An important aspect of this approach is **hypothesis testing**, which has led to the image of statisticians aiming to prove that nothing can be concluded from basically any given data while still data can be "tortured until confession", creating wrong conclusions.
- The other **2%** of statisticians focus on simply finding a predictive function evaluated by predictive accuracy only (which fits the pragmatic approach).
- John W. Tukey (1915-2000), whose one of those **2%** focussed on practical statistics.
 - This includes **exploratory data analysis** instead of hypothesis testing.
 - For example, he invented boxplots.

So to summarize the concept shift and also the difference between classical statistics and machine learning approaches:

- Before, a small amount of data or only samples of the whole data distribution were available, whereas
- Now, we have a big amount of data or all available data (due to computing power, storage, and tools).
 - The new approach is, therefore, to "let the data speak", since it's there.

Problems, even with this new approach, are:

- Data is always dirty, biased, etc. Fortunately, summarizing it can be surprisingly useful.
- Typical risks, raising the necessity of handling the new approach with care, are:
 - Testing of many hypotheses,
 - Over- or underfitting the data, and
 - Having a bias in the data or the representation.

3.2 Basics of decision trees

A typical decision tree looks as in image 3.1.

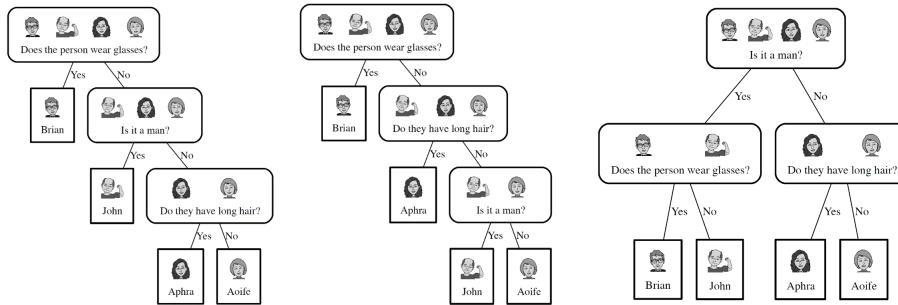


Figure 3.1: Decision tree for person distinction (different grouping)

The example shows that a **decision tree** is built by **grouping** instances step by step. In general, instances are partitioned into **increasingly smaller groups**. Decision tree

- How the groups are formed decides the outcome of the concrete decision tree (different trees are possible).
- For the grouping, keep two goals in mind:
 1. The tree shall be as small and simple as possible.
 2. The leaves shall be homogeneous in terms of the target feature.

The overall **goal of a decision tree** is to explain the target feature in terms of the descriptive features, so we have a supervised learning scenario.

- For categorical features we can differentiate based on the different classes.
- For numerical features, we need to define a threshold or something similar, to make a decision.

The following example in 3.2 (life expectancy given different features) shows the derivation of a (more or less) valid decision tree given tabular example data.

So summarized, a decision tree consists of three different types of nodes:

Decision tree components

- **A root node** referring to all instances,
- **Interior nodes** partitioning the set of instances based on a descriptive feature, and
- **Leaf nodes** that have a label (the target feature value) that hopefully corresponds to a homogeneous group of instances with the same label.

How the partitioning influences the size and therefore efficiency of the decision tree can

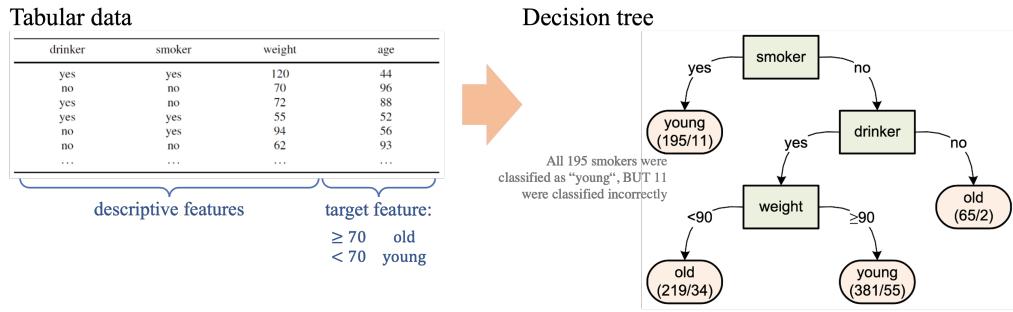


Figure 3.2: Example for deriving a decision tree from tabular data (life expectancy)

be seen in the example in 3.3. Both the good and bad partitioning options classify the observed instances correctly, but one is more simple and seems better. While investigating the example, keep the following keywords in mind:

- Avoid overfitting
- Apply Occam's razor (problem-solving principle recommending searching for explanation constructed with the smallest possible set of elements = simplest solution is best one)
- Prefer shallow trees

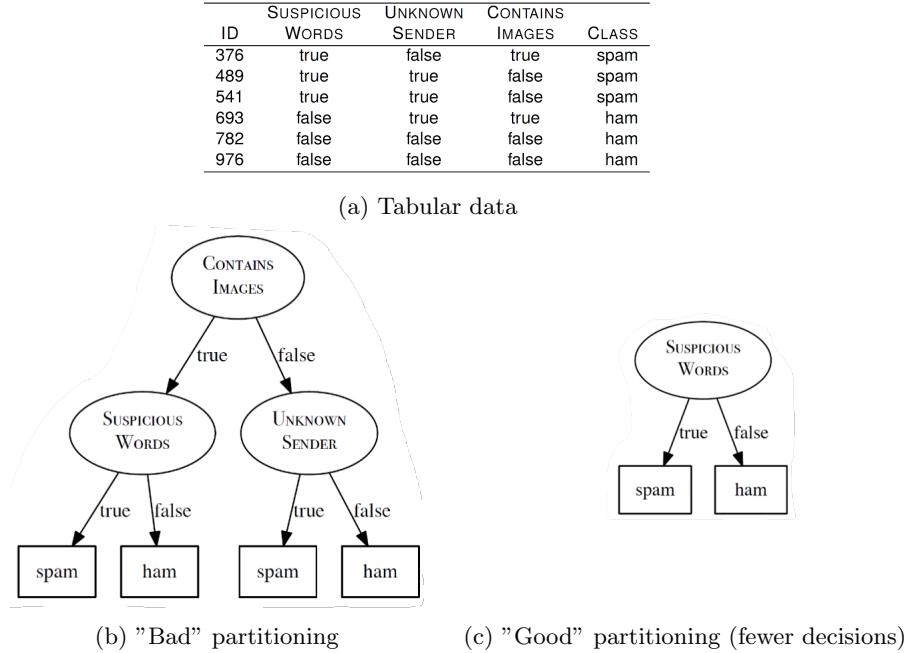


Figure 3.3: Example for different partitioning results on the same problem (both correct)

3.3 Entropy

As a main motivation of why we need the term entropy, let's first look at the idea of **information gain**. This can be applied to decision trees and asks for improvement

in knowledge with each partitioning step, so better predictability of class labels in the nodes. This implies more homogenous interior nodes with every layer as visualized in the example in 3.4.

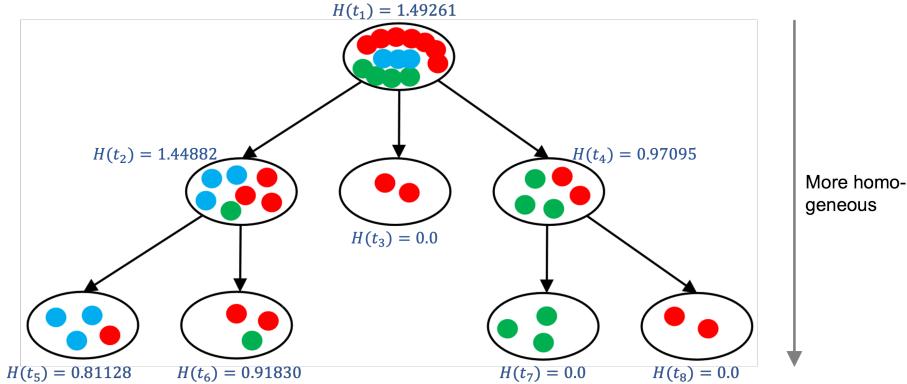


Figure 3.4: Idea of information gain and entropy intuition

Next, we'll take a look into the intuition of the term **entropy**. Figure 3.4 also displays Entropy the entropy values. As one can see in the example:

- Entropy **measures the impurity** in a set.
- With higher entropy, the **uncertainty in guessing** a class label grows.
- For a low entropy, the information gained when investigating the according data set is not very high, basically the data is "compressable". Entropy therefore also indicates **incompressibility**.
- Or put alternatively: entropy represents the number of bits needed to encode one instance knowing the population it comes from.

All of these statements are summarized in the formula:

$$H(t) = - \sum_{i=1}^n (\Pr[t = i] \cdot \log_s(\Pr[t = i]))$$

The minus occurs, since $\log_s(\frac{1}{x}) = -\log_s(x)$. In this course, we will always take the logarithmic base $s = 2$.

For a better understanding, we will calculate the entropy for three example sets from figure 3.4.

Example	Distribution over colored dots
1: high entropy value	$n_{\text{red}} = 7, n_{\text{blue}} = 3, n_{\text{green}} = 4$, so $n = 14$ $\Rightarrow H(t_1) = -\left(\frac{7}{14} \cdot \log_2\left(\frac{7}{14}\right) + \frac{3}{14} \cdot \log_2\left(\frac{3}{14}\right) + \frac{4}{14} \cdot \log_2\left(\frac{4}{14}\right)\right) = 1.49261$
2: middle-high entropy value	$n_{\text{red}} = 2, n_{\text{blue}} = 0, n_{\text{green}} = 3$, so $n = 5$ $\Rightarrow H(t_4) = -\left(\frac{2}{5} \cdot \log_2\left(\frac{2}{5}\right) + \frac{3}{5} \cdot \log_2\left(\frac{3}{5}\right)\right) = 0.97095$
3: minimal entropy value	$n_{\text{red}} = 0, n_{\text{blue}} = 0, n_{\text{green}} = 3$, so $n = 3$ $\Rightarrow H(t_7) = -\left(\frac{3}{3} \cdot \log_2\left(\frac{3}{3}\right)\right) = 0$

Now that we have seen an example, we can easily see the **bounds of entropies**.

Bounds on H

- The lowest possible entropy value yields when all instances have the same value, then $H(t) = 0$.
 - Then there is no impurity at all, no uncertainty when guessing, and the information in the data is highly compressible.
- The highest possible entropy value yields when we have an even distribution over all possible values, then $H(t) = -n\left(\frac{1}{n} \cdot \log_2\left(\frac{1}{n}\right)\right) = \log_2(n)$ is maximized
 - E.g., for 3 possible values: $\log_2(3) \approx 1.58$
 - Then there is the highest possible impurity, highest uncertainty when guessing, and the information in the data is incompressible.

Our goal when building decision trees is to have **pure leaves**, or the lowest possible average over the entropies of all leaves. With the entropy, we can now also put a number to the concept of information gain or loss, as can be seen in 3.5. When we have to select the next decision dividing an interior node, we select the features partitioning into groups with the least **remaining entropy** rem , which is the weighted average over all subnodes.

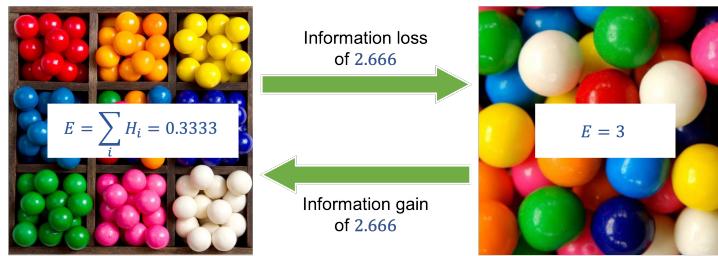


Figure 3.5: Example for information gain and loss

3.4 ID3 algorithm

We now know about the core concepts and components for building decision trees. The following algorithm introduces a standard procedure to build decision trees.

ID3 ID3, short for **iterative Dicchotomiser 3**, was developed by Ross Quinlan in 1986 and is a predecessor of algorithms like C4.5. The key idea is the following:

1. Calculate the entropy of every attribute using the data set D .
2. Split the set D into subsets using the attribute with the minimal resulting entropy.
 - Meant is the entropy after splitting using this attribute.
 - Equivalent formulation: choose the attribute maximizing the information gain.
3. Make a decision tree node containing that attribute.
4. Recurse on the subsets using the remaining attributes.

More formally, the algorithm looks as follows in pseudocode. We will afterward investigate certain details of the algorithm 3.1.

- Detail 1: three different reasons to stop
 - All instances have the same classification (labeled with consensus value)
 - No features are left (labeled with majority value)
 - Data set is empty (labeled with the majority value of the parent node)

```

1 Require: set of descriptive features  $\mathbf{d}$ 
2 Require: set of training instances  $\mathcal{D}$ 
3
4 // Different reasons to stop
5 if all instances in  $\mathcal{D}$  have the same target level  $C$  then
6   return DecisionTree(leaf_node with label  $C$ )
7 else if  $\mathbf{d}$  is empty then
8   return DecisionTree(leaf_node with the label of majority target level in  $\mathcal{D}$ )
9 else if  $\mathcal{D}$  is empty then
10  return DecisionTree(leaf_node with label of the majority target level of the immediate parent
    node)
11
12 else
13   // Pick feature
14    $\mathbf{d}[best] \leftarrow \arg \max_{d \in \mathbf{d}} IG(d, \mathcal{D})$ 
15   make a new node  $Node_{\mathbf{d}[best]}$  and label it with  $\mathbf{d}[best]$ 
16   partition  $\mathcal{D}$  using  $\mathbf{d}[best]$ 
17   remove  $\mathbf{d}[best]$  from  $\mathbf{d}$ 
18
19   // Create subproblems
20   for each partition  $\mathcal{D}_i$  of  $\mathcal{D}$  do
21     grow a branch from  $Node_{\mathbf{d}[best]}$  to the decision tree created by rerunning ID3 with  $\mathcal{D} = \mathcal{D}_i$ 

```

Listing 3.1: ID3 algorithm code

- Detail 2: which feature to select
 - The feature should be picked that maximizes the information gain.
 - A feature can't be picked more than once along the path from the root.
- Detail 3: subproblems are created based on the selected feature, building the decision tree in a divide-and-conquer fashion.
 - The amount of subproblems is dependent on the selected feature.

The ID3 algorithm has a lot of variations, from which we're gonna take a look at some.

Alternative information gain notions

Information gain (IG) aims to measure the improvement in purity, predictability, and compressibility. Instead, it is also possible to select a feature maximizing:

- The information gain ratio (GR), or
- The Gini index ($Gini$)

The standard information gain notion favors features with many values since a split in many subsets increases the entropy. The **information gain ratio** on the other hand addresses:

$$GR(d, \mathcal{D}) = \frac{IG(d, \mathcal{D})}{-\sum_{l \in levels(d)} \Pr[d = l] \cdot \log_2(\Pr[d = l])}$$

Basically: make absolute value relative

Another alternative is the **Gini index** measuring impurity in an alternative way. Specifically, it uses the expected misclassification rate when guessing based on the observed

Information gain ratio
 GR

Gini index $Gini$

distribution:

$$Gini(t, \mathcal{D}) = 1 - \sum_{l \in levels(t)} \underbrace{\Pr[t=l]^2}_{\text{Probability of guessing the wrong label}} \underbrace{\text{Guess } t=l \text{ with probability } \Pr[t=l] \text{ and with probability } \Pr[t=l] \text{ this is right}}$$

A comparison of all the evaluation metrics can be found in figure 3.6.

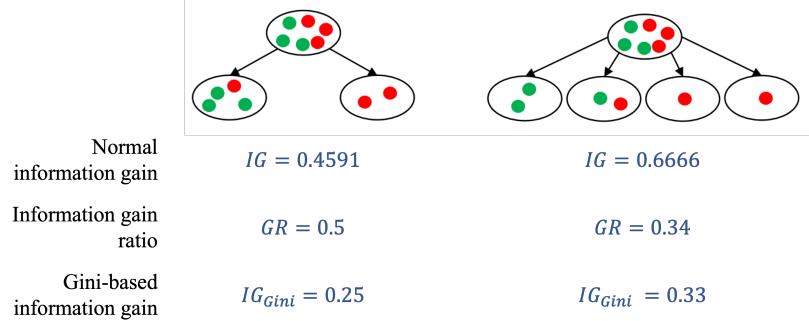


Figure 3.6: Comparison of IG , GR , and $Gini$

Pruning decision trees

When applying the ID3-algorithm to build decision trees, two possible problems can occur: The decision tree overfits the data, or is too complex or deep. For those problems, there are now two solution directions:

- Pre-pruning, so an early stopping, functioning forwards, and
- Post-pruning, so a reduced error, functioning backward.

Pre-pruning We'll first take a deeper look into **pre-pruning**, where at some point the procedure of creating subtrees is **stopped** at which point the label is determined via majority vote. There are many possible stopping criteria, for example, lower bounds on the number of instances or on the information gain.

The trees resulting from pre-pruning may not be consistent with respect to the data. But they generalize and therefore avoid overfitting nicely. So the procedure is very efficient, but strong dependencies at lower levels of the tree might be missed.

Post-pruning Next, let's investigate **post-pruning**, where first the whole decision tree is built and then some branches are **cut-off** that don't add too much information. One common approach for cutting off is to

- First split the data in a **training set** and a **validation/test set**,
- Built the decision tree based on the training set, and then
- Measure the performance of each split based on the validation/test set (e.g., count misclassified instances).

Ensembles

The final extension works with **ensembles**, where:

Ensembles

- Instead of creating a single decision tree, a set of trees called a "model ensemble" is created.
- The models should complement each other.
- Different models can then "vote" on a label (votes may be weighted).

The concept relates to the "wisdom of the crowds" and aims at avoiding overfitting. The multiple trees may give different answers. Multiple trees can give different answers, then a "compromise" should be found, so the most frequent value or average is selected. There are many variations of this idea.

The first implementation of ensembles is called **boosting** where an iterative correction in a sequential manner happens.

Boosting

- The correction happens by changing the data set based on previous misclassifications.
- Wrongly classified instances get a higher weight for training the next model.
- This creates a sequence of models, that combined lead to a (rather) correct classification.

The second implementation is called **bagging** where data is split upfront allowing a parallel rather than sequential model training. We alter the original data set by adjusting the rows (so the instances).

Bagging

- Each model is based on a random sample of the data set.
- The idea is, that models are avoided depending on a specific sample in the data set. This is supposed to avoid that learning in decision trees is very sensitive to small variations.
- How the training bags are created has a lot of variants. Instances can for example be removed, or other duplicated, etc.

A third implementation called **subspace sampling** takes a similar approach as bagging, but instead of altering the rows, the columns so the features are adjusted.

Subspace sampling

- Each model is based on a random set of descriptive features.
- The idea is that overfitting is less likely and also the training process is faster when focussed on just a few features instead of the whole feature space.
- The similarity to (instance) bagging is highlighted with the alternative name "feature bagging".

A fourth implementation combines feature and instance bagging and is called **random forest**. All three bagging strategies are also visualized in 3.7.

Random forest

Finally, all of the ensemble methods can be combined in many possible combinations.

- When we have multiple classifiers (e.g. implemented as decision trees), they can be combined by voting or averaging.
- This often leads to a higher accuracy on unseen data and avoids overfitting.

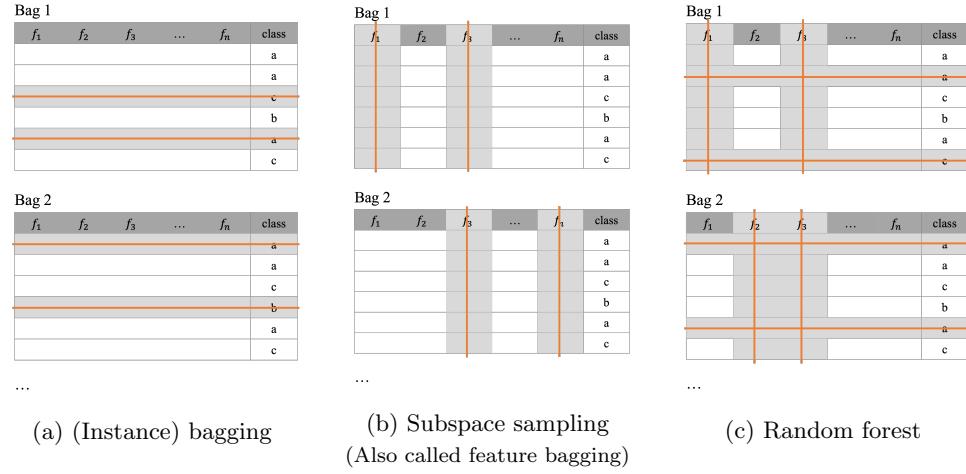


Figure 3.7: Different ensemble bagging implementations

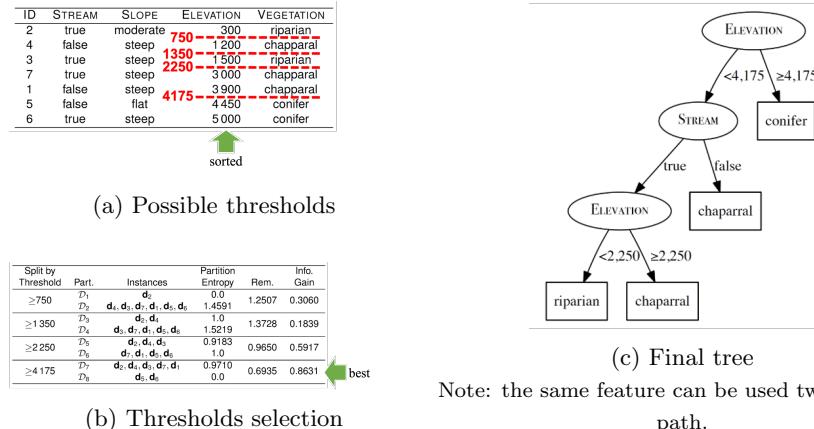
3.5 Dealing with continuous variables

So far we mainly assumed categorical features, for both the descriptive and target features. Now, we also want to take a look at how to deal with continuous features. Remember, that generally continuous features can be tuned into categorical ones using binning.

First, let's look at **continuous descriptive features**. The challenge is to determine suitable boundaries, where also an infinite number of thresholds is possible. The approach is:

- Sort the instances based on the continuous feature and then look for changes in class labels.
- Points where class label changes happen are candidate thresholds.
- The threshold with the highest information gain is selected.

How this works is visualized as an example in 3.8.



Note: the same feature can be used twice along a path.

Figure 3.8: Building a decision tree with a continuous descriptive feature

Next, consider a **continuous target feature**. Here, we want to find descriptive features that "nicely" partition the target feature axis.

- How to distinguish and evaluate different classifications can be seen in 3.9
- Impurity is measured by the variance within a partition (so a leaf in the decision tree)
- But the split can't use the target feature as a decision. Instead, the weighted variance after the split is used as a performance criterion
 - The smaller, the better.
 - $\text{var}(t, \mathcal{D}) = \frac{1}{n-1} \sum_{i=1}^n (t_i - \bar{t})^2$

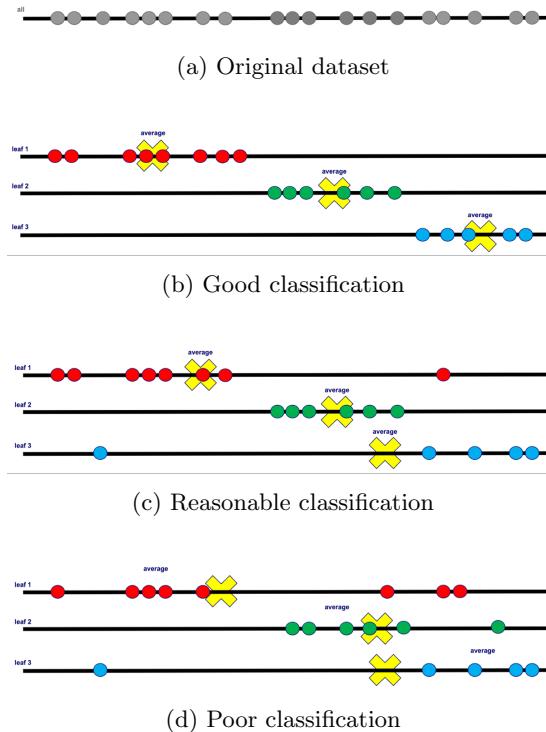


Figure 3.9: Level of validity of different classifications for a continuous target feature

It's important to keep track of over- and underfitting, as visualized in 3.10. Generally, variance gets smaller when the sets get smaller, so the measure leans towards overfitting. This can be avoided by stopping early enough.

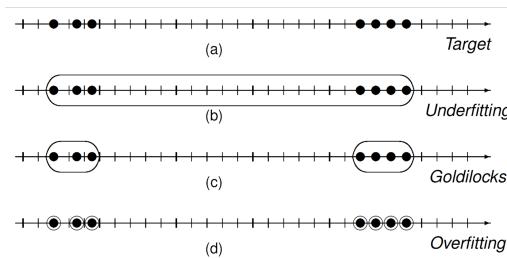


Figure 3.10: Over- and underfitting in continuous target feature classification

The **predicted value**, so the output of the decision tree, is the **average** value within a (leaf) node.

To be able to still use the ID3-algorithm, the decision for $\mathbf{d}[best]$ needs to be adjusted.

- Instead of $\mathbf{d}[best] \leftarrow \arg \max_{d \in \mathbf{d}} IG(d, \mathcal{D})$, we will
- Base the split on the feature lowering the weighted variance within the subtrees as much as possible, so $\mathbf{b}[best] \leftarrow \arg \min_{d \in \mathbf{d}} \sum_{l \in levels(d)} \frac{|\mathcal{D}_{d=l}|}{|\mathcal{D}|} \cdot var(t, \mathcal{D}_{d=;})$

In general, there are some extensions of ID3 implementing different ideas presented throughout this chapter:

- ID3 is the original.
- C4.5 can also deal with continuous features, missing values, implements post-pruning, etc. (C5.0 extends this further)
- J48 is an open-source implementation of C4.5.
- CART (classification and regression trees) use the Gini index, can handle continuous features, and can deal with missing values.
- CAID (Chi-square automatic interaction detector) relies on the Chi-square test to determine the best next split at each stop.

4 Regression

In the next three chapters, we'll look at **error-based learning**. In general, this learning approach functions as follows:

- We have a **parameterized prediction model** which is initialized with random parameters.
- An **error function** is then used to evaluate the performance of this model when it makes predictions for instances in a training dataset.
- Based on the results of the error function, the parameters are **iteratively adjusted** to create a more and more accurate model.

There are different approaches to realizing error-based learning:

- Regression (covered in this section)
- SVMs (covered in the next section)
- Neural networks (covered in a later section)
- Genetic algorithms, or other evolutionary approaches

We'll start with **regression** and the following basic idea.

Regression

Our model: $f : \text{descriptive features} \rightarrow \text{target features}$

Goal: find f minimizing $\text{error}(\text{prediction}, \text{observed data})$

When we compare this approach to decision trees, we see:

- Decision trees were initially developed for categorical features and then extended to continuous features.
- Regression followed the reverse path, which means it's most **suitable for continuous data**.
- Still, both are supervised learning techniques.

4.1 Simple linear regression

Consider the following simple example where we have:

- Rental price p_r as our target feature, and
- Size s as our descriptive (continuous) feature

We assume a linear dependency $p_r = b + a \cdot s$ and now want to base our prediction of the rental prize on the size. The example will guide us through this subchapter.

The **general problem** is given as follows:

General problem
regression

- We have given n data rows in a set \mathcal{D} with a target feature t and descriptive features $\mathbf{d} = (d[1], d[2], \dots, d[m])$, and
- We want to find a regression function M_w with a constant weight and a weight for each feature, where
- We predict $\text{pred}(t) = M_w(\mathbf{d}) = M_{(w[0], w[1], \dots, w[m])}(d[1], d[2], \dots, d[m])$

In our example, we only have one descriptive feature $\mathbf{d} = (d[1])$, two weights $w =$

$(w[0], w[1])$, and the regression function is linear, so $\mathbb{M}_{\mathbf{w}}(d) = \underbrace{w[0]}_{p_r} + \underbrace{w[1]}_b \cdot \underbrace{d[1]}_s$.

What can be seen is that the weights $\mathbf{w} = (w[0], w[1])$ define the linear function. Our goal is now to find the weights such that the resulting function has the "smallest error". There are different ways to characterize the error with different **error metrics**:

Error metrics
 Sum of squared errors
 L_2

- Sum of squared errors

$$L_2(\mathbb{M}_{\mathbf{w}}, \mathcal{D}) = \frac{1}{2} \cdot \sum_{i=1}^n (t_i - \mathbb{M}_{\mathbf{w}}(d_i))^2$$

- For each instance: compute the error, then square it
- Compute the sum of the results
- Finally, take half (\rightarrow end result)

Mean squared error
 MSE

- Mean squared error

$$MSE(\mathbb{M}_{\mathbf{w}}, \mathcal{D}) = \frac{1}{n} \cdot \sum_{i=1}^n |t_i - \mathbb{M}_{\mathbf{w}}(d_i)|^2$$

Root mean squared error
 $RMSE$

- Root mean squared error

$$RMSE(\mathbb{M}_{\mathbf{w}}, \mathcal{D}) = \sqrt{\frac{1}{n} \cdot \sum_{i=1}^n |t_i - \mathbb{M}_{\mathbf{w}}(d_i)|^2}$$

Mean absolute error
 MAE

- Mean absolute error

$$MAE(\mathbb{M}_{\mathbf{w}}, \mathcal{D}) = \frac{1}{n} \cdot \sum_{i=1}^n |t_i - \mathbb{M}_{\mathbf{w}}(d_i)|$$

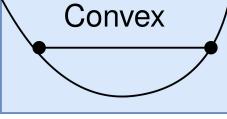
All of the introduced error metrics express the same idea, but usually, L_2 is chosen since it has a simple derivative. We'll take a look at the **partial derivative of error**, concretely of L_2 (here, i refers to the training instance, and j to one of the multiple descriptive features)

$$\begin{aligned} \frac{\delta}{\delta \mathbf{w}[j]} L_2(\mathbb{M}_{\mathbf{w}}, \mathcal{D}) &= \frac{\delta}{\delta \mathbf{w}[j]} \frac{1}{2} \sum_{i=1}^n (t_i - \mathbb{M}_{\mathbf{w}}(d_i))^2 \\ &= - \sum_{i=1}^n ((t_i - \mathbb{M}_{\mathbf{w}}(d_i)) \cdot d_i[j]) \end{aligned}$$

Using this derivate, we can now find the weights minimizing the error.

- Brute force, meaning we try as many values as possible for the weights, isn't feasible in practice (not even for simple linear case).
- But we can use that our error surface is convex and therefore has a global minimum, enabling faster methods.
 - Take the partial derivatives (for linear case: $\delta/\delta \mathbf{w}[0] L_2(\mathbb{M}_{\mathbf{w}}, \mathcal{D})$, and $\delta/\delta \mathbf{w}[1] L_2(\mathbb{M}_{\mathbf{w}}, \mathcal{D})$)
 - Find the correct values for all partial derivatives to result in zero (Needs to be the case for an actual global minimum)

One important thing to mention, the convex property of a function is very useful here:

- 
 - One local minimum = global minimum
 - Gradient descent works

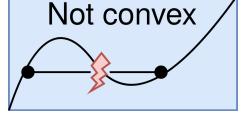

 - Multiple local minima, so global minimum harder to find
 - Gradient descent might fail

Figure 4.1: Convex vs. non-convex functions

The technique we can use to quickly find the global minimum is **gradient descent**. For convex functions we know, that we will always end up in the global minimum. Still, there is the open question of which direction to walk to:

- Take the steepest way down, which is known since there is a derivative of the function.
- This leads to a lower point point on each step and therefore converges.

An important decision to make is the **step size**:

Gradient descent

Step size

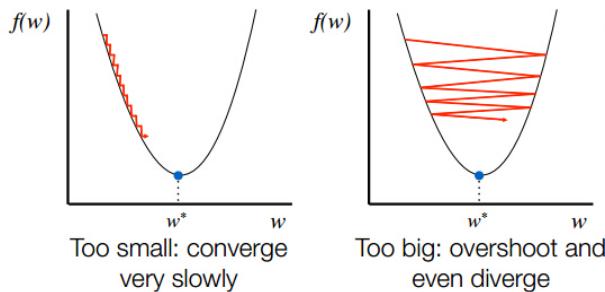


Figure 4.2: Step size for gradient descent

4.2 Multiple descriptive features

We now assume a feature consisting of multiple elements:

$$\begin{aligned}
 M_{\mathbf{w}}(\mathbf{d}) &= \mathbf{w}[0] + \mathbf{w}[1]\mathbf{d}[1] + \cdots + \mathbf{w}[m]\mathbf{d}[m] \\
 &= \mathbf{w}[0] + \sum_{j=1}^m \underbrace{\mathbf{w}[j]}_{\substack{\text{weight of the } i\text{-th feature } d[j]}} \mathbf{d}[j] \\
 &= \sum_{j=0}^m \mathbf{w}[j] \underbrace{\mathbf{d}[j]}_{\substack{\text{with } d[0]=1}} \\
 &= \underbrace{\mathbf{w} \cdot \mathbf{d}}_{\substack{\text{dot product of vectors}}}
 \end{aligned}$$

In particular, this means we have $m+1$ -dimensional vectors \mathbf{d}_i and \mathbf{w} with m as the number of features. This notational convenience extends the normal feature vector \mathbf{d}'_i

by $\mathbf{d}_i[0] = 1$. With n instances, we therefore have the error function:

$$L_2(\mathbb{M}_{\mathbf{w}}, \mathcal{D}) = \frac{1}{2} \sum_{i=1}^n (t_i - \underbrace{\mathbf{w} \cdot \mathbf{d}_i}_{=\mathbb{M}_{\mathbf{w}}(\mathbf{d}_i)})^2$$

With our now introduced multiple descriptive feature vector, we can write down the **sketch of the overall algorithm** of regression:

```

1  Require: set of descriptive features  $\mathcal{D}$ 
2  Require: learning rate  $\alpha$  (controls how quickly algorithm converges)
3  Require: function  $\Delta_{error}$  (determines the direction in which to adjust given weight  $\mathbf{w}[i]$  to move
   down the slope of an error surface determined by  $\mathcal{D}$ )
4  Require: convergence criterion (indicating when the algorithm has been completed)
5
6   $\mathbf{w} \leftarrow$  random starting point in weight space // randomly pick initial point
7  repeat
8    for each  $\mathbf{w}[j] \in \mathbf{w}$  do
9      // run downhill in steepest direction with speed  $\alpha$ 
10      $\mathbf{w}[j] \leftarrow \mathbf{w}[j] + \alpha \Delta_{error}(\mathcal{D}, \mathbf{w})[j]$ 
11  until convergence occurs // stop when improvements become too small

```

Listing 4.1: Sketch of regression algorithm

For Δ_{error} we typically choose $\frac{\delta}{\delta \mathbf{w}[j]} L_2$. This means:

- If the derivative is positive, lower the weight $\mathbf{w}[j]$,
- If the derivative is negative, increase the weight $\mathbf{w}[j]$,
- While $\alpha > 0$ determines the speed in both cases.
- Line 10 in 4.1 would then result in $\mathbf{w}[j] \leftarrow \mathbf{w}[j] - \alpha \sum_{i=1}^n (t_i - \mathbf{w} \cdot \mathbf{d}_i) \mathbf{d}_i[j]$

4.3 Interpretation of results

For the one-feature case, the interpretation isn't difficult. We can simply see, that the target feature has some linear dependence on the descriptive feature. E.g., in our earlier example: the rental price has a "direct" dependency on the size.

It becomes more difficult when **interpreting results for multiple descriptive features**. This is due to the potentially completely different ranges of those features. The weights change dramatically when the units change (e.g. when changing cm^2 to m^2). This shows that the weight itself is irrelevant, only the sign has meaning.

Significance test An alternative approach is the **significance test**.

In a simple version of this, we have:

- Create a regression model using k descriptive features and measure the error Δ' .
- Create k regression models leaving out one descriptive feature at a time and measure the error Δ_i for $i \in [k]$.
- The difference in error $|\Delta' - \Delta_i|$ indicates the significance of feature i for $i \in [k]$

In a more complex way (no need to know details), we follow this approach:

- Null hypothesis: the feature does *not* have a significant effect on the model.

- Null hypothesis is rejected when *p-level* is too small ($1 - 5\%$) → a smaller p-value indicates a more important feature.
- In statistical hypothesis testing:
 - p-value or probability value: the probability of obtaining test results at least as extreme as results actually obtained during testing
 - Assumes a correct null hypothesis
 - Very small p-value means: such an extreme observed outcome is very unlikely under the null hypothesis

4.4 Handling categorical features

So far we assumed features (both descriptive and target) are continuous. In this chapter, we'll look at categorical descriptive and target features.

- E.g., {true, false}, {A, B, C}, or similar

For **categorical descriptive features**, we'll introduce $\{0, 1\}$ -features for every possible value, which is called **one hot encoding**.

One hot encoding

- E.g., for {A, B, C}: A= (1, 0, 0), B= (0, 1, 0), C= (0, 0, 1)

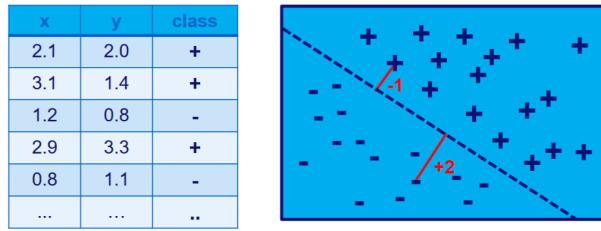
Next to one hot encoding, we have **single numeric value encoding**:

- Binary values {true, false} which can be translated to $\{0, 1\}$.
- Also, categorical variables with a clear order (ordinal) like {good, average, poor} can be translated to $\{1.0, 0.5, 0.0\}$.

Possible issues are:

- Adding order to unordered categorical variables resulting in nonsense
 - E.g., simple encoding applied to country names maps numbers to countries (but no natural order exists)
- All encodings are approximations, so intermediate values will be considered possible by the "regression machine"
- One hot encoding discards dependencies
 - Say if A= 1 then logically B= 0, but B= 0.66 is also possible
- Approach may introduce many additional features, making the problem computationally expensive

For a **categorical target feature** we can try to derive a numerical (continuous) feature. The naive approach is to find a line separating the results (try to find a line s.t. $\text{wd} = 0$). The line then performs more of a separation than a prediction.



Target feature is +/- label, and not the value on the y-axis

Figure 4.3: Separating target feature (alternative to prediction)

This means, we can use the $\{0, 1\}$ idea for encoding the two categories (+/-). The model then also produces either 0 or 1:

$$M_w(\mathbf{d}) = \begin{cases} 1 & \text{if } \mathbf{w} \cdot \mathbf{d} \geq 0 \\ 0 & \text{else} \end{cases}$$

After this step, do business as usual e.g. by minimizing the sum of squared errors.

- Notice that in this naive approach, we don't use the distance to the decision boundary yet.
- But this would be desirable to make the decision surface continuous or smooth and thereby more applicable to gradient descent.

4.5 Logistic regression

Logistic regression will help us make a 0/1-decision continuous and smooth.

Logistic function First, we need the **logistic function**:

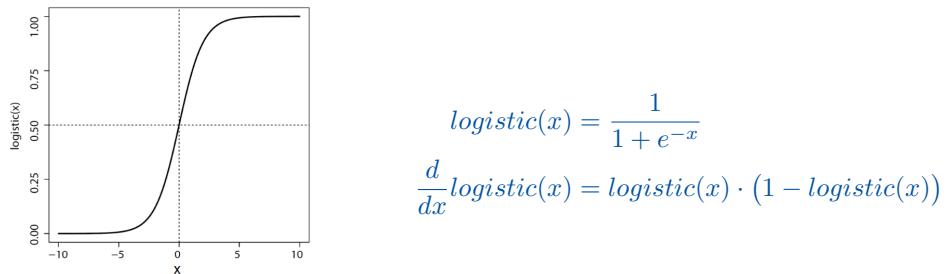
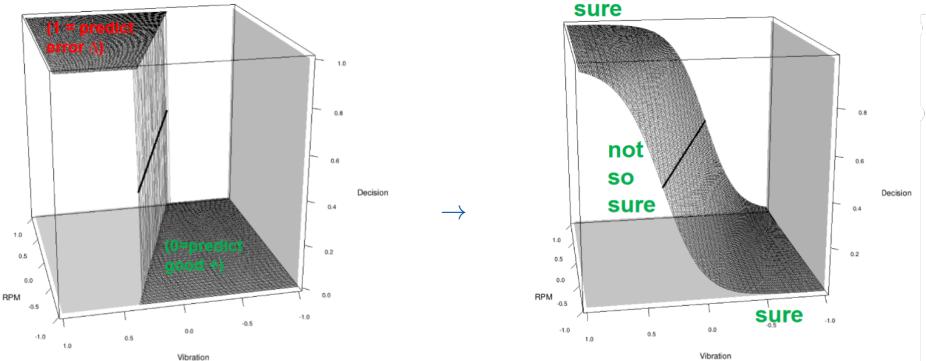


Figure 4.4: Logistic function

- Here, $e = 2.7182818\dots$ is Euler's number
- Any value is mapped on a value between 0 and 1
 - $logistic(0) = 0.5$, $logistic(-\infty) = 0$, $logistic(+\infty) = 1$
- 0 and 1 are quickly approached, therefore we can use it as a "smooth binary value"

Logistic regression So now, we can use **logistic regression** instead of a hard 0/1-decision.



$$\mathbb{M}_w(\mathbf{d}) = \begin{cases} 1 & \text{if } \mathbf{w} \cdot \mathbf{d} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbb{M}_w(\mathbf{d}) = \text{logistic}(\mathbf{w} \cdot \mathbf{d})$$

Figure 4.5: Difference 0/1 and logistic

The probabilistic interpretation looks as follows:

- $P[t = 'faulty' | \mathbf{d}] = \mathbb{M}_w(\mathbf{d})$
- $P[t = 'good' | \mathbf{d}] = 1 - \mathbb{M}_w(\mathbf{d})$
- And the system is more sure about the decision, the further it is away from the separating line.

4.6 Extensions (non-linear and multinomial)

Non-linear functions that can't be separated by a line can still be handled by using linear machinery. The basic idea for that is to transform the data in advance, leading to the following formula:

$$\mathbb{M}_w(\mathbf{d}) = \sum_{k=0}^b \mathbf{w}[k] \phi_k(\mathbf{d})$$

- Data in non-linear relationships is transformed *before* applying the linear machinery.
- For that, apply "basis functions" ϕ_k like $\phi_0(x) = 1$, $\phi_1(x) = x$, $\phi_2(x) = x^2$, etc.

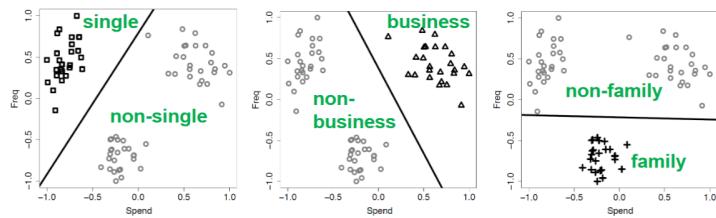
For the case of **multinomial regression**, we look at the problem where categorical data is not binary. As a solution for n possible classes, we can split the decision into n models (per class i one model, classifying as "is class i " or "is not class i "). Those can then be combined back again into one model.

Non-linear relationship

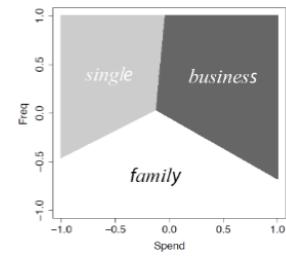
Multinomial regression



(a) Original problem



(b) Binary classification



(c) Resulting model (multinomial classification)

Figure 4.6: Combining binary (one-versus-rest) models to multinomial regression

5 Support vector machine (SVM)

5.1 Basic functionality

Let's suppose we have the following dataset where

- Our target feature has two possible classes: sun and cloud.
- We have two descriptive features: x and y

The data set is separable, and our goal is now to find the best hyperplane (a line here) separating the two classes.

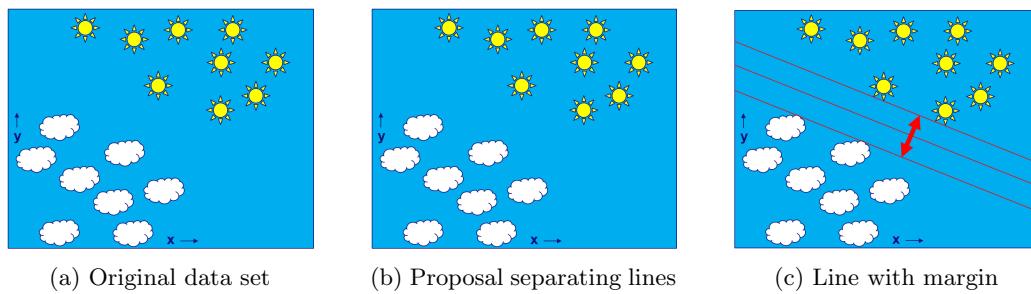
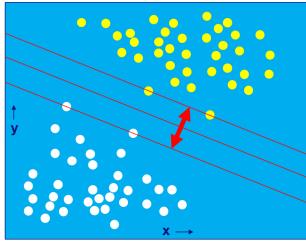


Figure 5.1: Example for SVM

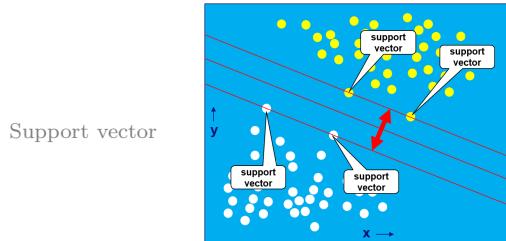
We need to determine which proposal lines are better than others. The idea to determine this is that the degrees of freedom become less when the separating hyperplane gets thicker. The best hyperplane is:

- The best-separating hyperplane is the one fitting between the data points with the maximal thickness (= safety margin).
- Therefore, SVMs also tend to be more robust than logistic regression.

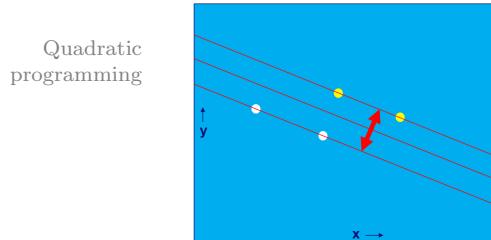
Consider now a more abstract data set:



(a) Data set with hyperplane and safety margin



(b) Support vectors



(c) Reduced problem

We have instances that are (atomic) points in an n -dimensional space.

Support vectors (SV) are the boundary points → only those matter.

Define a **QP** problem (quadratic programming) to make (compared to logistic regression):

- Things more efficient
- It less sensitive to outliers
- Reduce the risk of overfitting

But, there are applications where logistic regression works better.

Figure 5.2: SVM basic idea

The dimension of the separating hyperplane is always $n - 1$ where n is the dimension of the space.

- One descriptive feature → hyperplane is a point (of dimension $0 = n - 1$)
- Two descriptive features → hyperplane is a line (of dimension $1 = n - 1$)
- Three descriptive features → hyperplane is a plane (of dimension $2 = n - 1$)
- ...

For $n > 3$, the problem can't be visualized anymore, but SVMs also work for very large n .

- This is in contrast to logistic regression, which gets too complex at large n

Hyperplane The technical definition of the **hyperplane** is as follows:

$$\vec{w} \cdot \vec{x} + b = \underbrace{\vec{w}_1 x_1 + \vec{w}_2 x_2 + \cdots + \vec{w}_n x_n}_{\vec{x} = (x_1, x_2, \dots, x_n)} + b = 0$$

$$\vec{w} = (w_1, w_2, \dots, w_n)$$

At least one of the weights is non-zero. The hyperplane then splits the n -dimensional into two disjoint parts:

- $\vec{w} \cdot \vec{x} + b \geq 0$
- $\vec{w} \cdot \vec{x} + b < 0$

There are some cases where the dataset is not separable.

- This can be due to **outliers**. A solution for this problem is to relax the problem by allowing violating instances → but they then add a penalty.
- Alternatively, there can also be a **structural** problem (not linearly separable in n -dimensional space). The idea to solve this problem is to try whether the problem is linearly separable in a higher-dimensional space, which then also includes feature design.

We need to make some further definitions to completely formalize the SVM approach. We'll first look at **vectors** like $\vec{x} = (x_1, x_2, \dots, x_n)$.

Vector

- The vector **length** is defined as

Vector length

$$\|\vec{x}\| = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}$$

- The vector **direction** is the normalized vector of length one, so

Vector direction

$$\vec{w} = \frac{\vec{x}}{\|\vec{x}\|} = \left(\frac{x_1}{\|\vec{x}\|}, \frac{x_2}{\|\vec{x}\|}, \dots, \frac{x_n}{\|\vec{x}\|} \right)$$

- To extend the length of a vector without changing its direction, multiply the vector with a constant

$$q\vec{x} = (q \cdot x_1, q \cdot x_2, \dots, q \cdot x_n)$$

- The dot product on the other hand allows the multiplication of two vectors:

$$\vec{x} \cdot \vec{y} = \sum_{i=1}^n x_i y_i = \underbrace{\|\vec{x}\| \cdot \|\vec{y}\| \cdot \cos \theta}_{\text{with angle } \theta \text{ between } x, y} \in \mathbb{R}$$

- The dot product is heavily influenced by the angle between the two vectors and therefore also tells their linear dependency.
- For orthogonal vectors $\cos \theta = 0$, for vectors with the same direction $\cos \theta = 1$ and for angles in the opposite direction $\cos \theta = -1$

Now, let's look deeper into the definition of a hyperplane. Our hyperplane is defined by

$$\begin{aligned} \vec{w} \cdot \vec{x} + b &= 0 \\ \iff \sum_{i=1}^n w_i x_i + b &= 0 \end{aligned}$$

where

- $\vec{x} = (x_1, x_2, \dots, x_n)$ are free variables,
- $\vec{w} = (w_1, w_2, \dots, w_n)$ is the direction vector of the hyperplane (no-zero),
- And the hyperplane is fully defined by \vec{w} and b

Further interesting to see:

$$\begin{aligned} \text{For } q \in \mathbb{R} \setminus \{0\} : \quad \vec{w} \cdot \vec{x} + b = 0 &\iff \sum_{i=1}^n w_i x_i + b = 0 \\ &\iff q \vec{w} \cdot \vec{x} + qb = 0 \iff \sum_{i=1}^n q w_i x_i + qb = 0 \end{aligned}$$

The hyperplane splits a set of data points in the following way. Assume we have N data points $X_N = \{\vec{x}_i = (x_{i,1}, x_{i,2}, \dots, x_{i,n}) \mid i \in N\}$. Then, for \vec{x}_i calculate $f(\vec{x}_i) := \vec{w} \cdot \vec{x}_i + b = \sum_{j=1}^n w_j x_{i,j} + b$, and

$$\text{Classify as positive if } f(\vec{x}_i) \geq 0 \text{ negative if } f(\vec{x}_i) < 0$$

Note the ongoing confusion of whether above or below the hyperplane is defined as positive, e.g. by multiplying \vec{w} and b with $q = -1$

By splitting the data as described above, we introduce two possible classes for each \vec{x}_i , namely $y_i \in \{-1, 1\}$. If our hyperplane (\vec{w}, b) **separates** a dataset X_N **perfectly**, then:

$$\text{Perfectly separating hyperplane} \quad \text{For all instances } (\vec{x}_i, y_i) : \begin{array}{ll} y_i = +1 & \implies f(\vec{x}_i) \geq 0 \\ y_i = -1 & \implies f(\vec{x}_i) < 0 \end{array}$$

But actually, there might be many "perfect" hyperplanes. The one we would like to pick is the one that maximizes the distance of the hyperplane to the nearest point. For that, we of course first need to define the **distance between a point and a hyperplane**. Assume, we have the following setting:

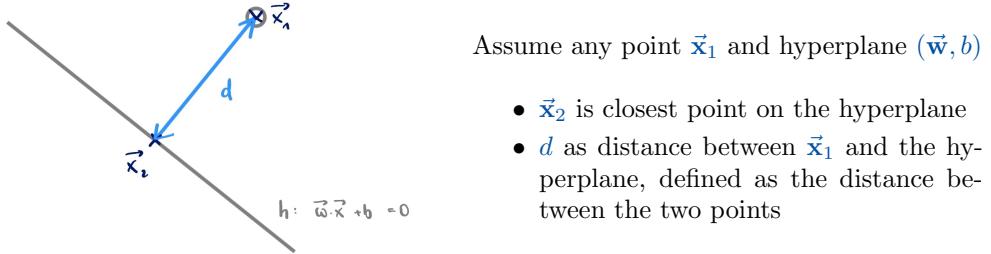


Figure 5.3: Distance between a point and the hyperplane

As can be seen in figure 5.3, we have the closest point defined as the point that can be found by following an orthogonal path and seeing which point is on the hyperplane:

$$\begin{aligned} \underbrace{\vec{x}_1 = \vec{x}_2 + \lambda \vec{w}}_{\text{orthogonal path}} \text{ and } \underbrace{\vec{w} \cdot \vec{x}_2 + b = 0}_{\vec{x}_2 \text{ is on hyperplane}} \\ \implies \vec{w} \cdot (\vec{x}_1 - \lambda \vec{w}) + b = 0 \\ \implies d = \|\lambda \vec{w}\| \end{aligned}$$

Next, we try to get rid of the λ in the computation of $d = \|\lambda \vec{w}\|$. For that, just rewrite

the formula for the calculation of \vec{x}_2 :

$$\begin{aligned}
 & \vec{w} \cdot (\vec{x}_1 - \lambda \vec{w}) + b = 0 \\
 \implies & \vec{w} \cdot \vec{x}_1 + b = \lambda \vec{w} \cdot \vec{w} = \lambda \|\vec{w}\|^2 \\
 \implies & \lambda = \frac{\vec{w} \cdot \vec{x}_1 + b}{\|\vec{w}\|^2} \\
 \implies & d = \left\| \left(\frac{\vec{w} \cdot \vec{x}_1 + b}{\|\vec{w}\|^2} \right) \cdot \vec{w} \right\| \\
 & = \left| \frac{\vec{w} \cdot \vec{x}_1 + b}{\|\vec{w}\|^2} \right| \|\vec{w}\| = \left| \frac{\vec{w} \cdot \vec{x}_1 + b}{\|\vec{w}\|} \right|
 \end{aligned}$$

So finally, we can formulate how to calculate the **optimal hyperplane**:

Optimal hyperplane

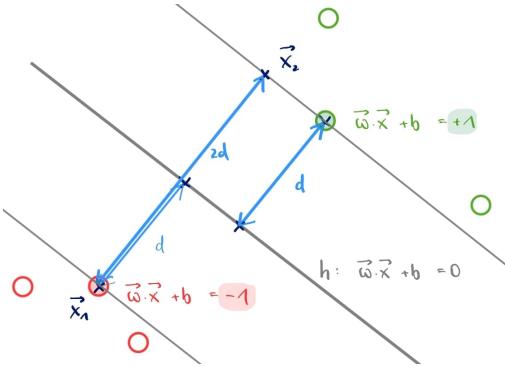
Given $\{(\vec{x}_i, y_i) \in \mathbb{R}^n \times \{-1, 1\} \mid 1 \leq i \leq m\}$

Find (\vec{w}, b) such that for any $1 \leq i \leq m$: If $y_i = +1$, then $\vec{w} \cdot \vec{x}_i + b \geq 0$
If $y_i = -1$, then $\vec{w} \cdot \vec{x}_i + b < 0$

And maximize $\min_{1 \leq i \leq m} d_i$ with: $d_i = \left| \frac{\vec{w} \cdot \vec{x}_i + b}{\|\vec{w}\|} \right|$

Alternatively, we could normalize the distance to one, such that the resulting situation is as depicted in 5.4.

- This rescaling can be performed since the hyperplane formulation doesn't change when multiplying with a constant q .
- The support vectors yield the result $\vec{w} \cdot \vec{x}_i + b = \pm 1$.



The support vectors are on the lines (positive and negative support vectors)

Figure 5.4: Normalized distance

Also, the classification is adjusted to

$$\left. \begin{array}{l} \text{If } y_i = +1, \text{ then } \vec{w} \cdot \vec{x}_i + b \geq +1 \\ \text{If } y_i = -1, \text{ then } \vec{w} \cdot \vec{x}_i + b \leq -1 \end{array} \right\} \rightarrow \text{can be combined to: } \forall i : y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1$$

Optimal hyperplane normalized

Our goal is still to maximize the smallest $d = \|\lambda \vec{w}\|$. In our alternative formulation, we want to formalize this goal only with the help of the shifted hyperplanes $\vec{x} \cdot \vec{x} + b = \pm 1$:

- Choose an arbitrary support vector \vec{x}_1 (let's say on $\vec{x} \cdot \vec{x} + b = -1$)

- Now take the corresponding $\vec{x}_2 = \vec{x}_1 + 2\lambda\vec{w}$ on the other support-vector-line (so $\vec{w} \cdot \vec{x} + b = +1$)
- This leads to the following equations to be solved:

$$\begin{aligned}\vec{w} \cdot \vec{x}_1 + b &= -1 \\ \vec{w} \cdot (\vec{x}_1 + 2\lambda\vec{w}) + b &= +1\end{aligned}$$

- This can be further readjusted to:

$$\begin{aligned}\implies \vec{w} \cdot \vec{x}_1 + b + \vec{w} \cdot 2\lambda\vec{w} &= +1 \\ \implies -1 + \vec{w} \cdot 2\lambda\vec{w} &= +1 \\ \implies \vec{w} \cdot 2\lambda\vec{w} &= +2 \\ \implies \lambda &= \frac{1}{\vec{w} \cdot \vec{w}} = \frac{1}{\|\vec{w}\|^2}\end{aligned}$$

- So, we can replace:

$$\text{Maximize } d = \|\lambda\vec{w}\| = \frac{1}{\|\vec{w}\|^2} \|\vec{w}\| = \frac{1}{\|\vec{w}\|}$$

Minimize $\|\vec{w}\|$ under the constraints stated before

So, the reformulated problem is:

Reformulated: SVM problem

$$\begin{aligned}\text{Given a set of } m \text{ instances } \{(\vec{x}_i, y_i) \in \mathbb{R}^n \times \{-1, 1\} \mid 1 \leq i \leq m\} \\ \min_{\vec{w}, b} \|\vec{w}\| \text{ s.t. } \forall i : y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1\end{aligned}$$

For technical reasons, a common variant of this problem is the convex quadratic optimization problem

Convex quadratic optimization problem

$$\begin{aligned}\text{Given a set of } m \text{ instances } \{(\vec{x}_i, y_i) \in \mathbb{R}^n \times \{-1, 1\} \mid 1 \leq i \leq m\} \\ \min_{\vec{w}, b} \frac{1}{2} \|\vec{w}\|^2 \text{ s.t. } \forall i : y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1\end{aligned}$$

- This problem is easier to solve than the original linear formulation (maximizing $\min_{1 \leq i \leq m} d_i$)
- The concrete solution or techniques for finding solutions are not covered here, but assume they exist

Another reformulation of the problem is the Wolfe dual Lagrangian problem which is important for the "kernel trick":

Wolfe dual Lagrangian problem

$$\begin{aligned}\text{For } \vec{w} = \sum_{i=1}^m \alpha_i y_i \vec{x}_i \text{ and } \alpha_i \geq 0, i = 1, \dots, m \\ \max_{\alpha} \quad \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j \vec{x}_i \cdot \vec{x}_j \\ \text{subject to} \quad \sum_{i=1}^m \alpha_i y_i = 0\end{aligned}$$

5.2 Non-linear decision boundaries

5.3 Using kernels