DATA SCIENCE PROJECT

AN INDUCTIVE LEARNING APPROACH

F.A.N. VERRI

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WIP

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Disclaimer: This version is a work in progress. Many parts of the book have been drafted with the help of GitHub Copilot and may not be revised yet by the author. The author is not responsible for any misinformation contained in this version of the book.

Book cover image was created with the assistance of Gemini and DALL·E 2.

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About this book

I intend to make this book forever free and open-source. You can find (and contribute to) the source code at github.com/verri/dsp-book.

If you like this book, consider *buying me a coffee* at buymeacoffee.com/verri. All donations are used to improve this book, including editing and proofreading.

If you find any typos, grammar errors, incomplete material or have any suggestions, please open an issue at github.com/verri/dsp-book/issues.

Students can found a printable version (A4 paper, double-sided, short-edge spiral binding) of this book at comp.ita.br/~verri/dsp-book-print.

This book comprises the lectures notes of the course PO-235 Data Science Project. I hope someday it becomes an actual book. For now, beware many typos, grammar errors, ugly typesetting, disconnected material, etc.

Also, it is important to highlight that:

- This is not a Machine Learning book, and I do not intend to explain how specific ML algorithms work.
- This contains some kind of introductory material on data science. Although I introduce the fundamental concepts, I expect you have strong mathematical and statistics background.
- An artificial constraint I have imposed in the material (for the sake of the course) is that I only consider *predictive methods*, more specifically inductive ones. I do not address topics such as clustering, association-rules mining, transductive learning, anomaly detection, time series forecasting, reinforced learning, etc.

I have decided to work on this material because the books I like on data science are either

- too broad and too shallow, in the sense they hide many mathematical foundations and focus on just explaining what data science is and where it is applied;
- too tool-centric, in the sense that they focus only on a specific toolbox or programming language; or
- too machine-learning-y, exposing the functioning of some machine learning algorithms and missing the foundations of learning and/or practical aspects.

So...I expect my approach on the subject provide:

- awareness of all steps in a data science project;
- deeper focus (than most books) on data handling, describing the semantics of dataset operators instead of restraining ourselves with a specific tool;
- deeper focus (than most books) on *why* machine learning works, increasing awareness of its pitfalls and limitations;

- deeper focus (than most books) on correct evaluation and validation (pre-deployment) of machine learning models.

This book will probably cover the following material:

- Brief history of data science.
- Background topics.
- Fundamental data concepts.
- Stages in a data science project.
- Data handling.
- Inductive learning and principles of statistical learning theory.
- Experimental planning for data science.
- Model evaluation and Bayesian analysis.
- Documentation and deployment.
- Ethical and legal issues in data science.
- Privacy-preserving computational approaches.

Course plan

In the following, I present the course plan for PO-235 and CMC-16.

Any questions about the classes should be sent via Google Classroom. If your question is of general interest, please use the main stream. If your question is personal and about a specific assignment or grade, please use the private stream.

PO-235 Data science project

Course plan (2024)
Prof. Filipe A. N. Verri

Important: Only graduate students are allowed to take this course.

Number of students: Approx. 20

Course load: 3–0–0–4

Requirements: Advanced programming skills, strong statistics background, and beginner-level machine-learning skills.

Course program: Brief history of data science. Fundamental data concepts. Stages in a data science project. Data Infrastructure. Data integration from multiple sources. Data engineering and shaping. Inductive learning and principles of statistical learning theory. Application of machine learning models in real-world problems. Experimental planning for data science. Model evaluation and Bayesian analysis. Documentation and deployment. Ethical and legal issues in data science. Privacy-preserving computational approaches.

Goals: Providing the theoretical background and the practical concepts to develop an end-to-end data science project for an inductive task.

Teaching methodology: Expository classes in common classroom, using whiteboard, slide presentations, coding examples, books and scientific papers. Supplementary didactic materials will be available in Google Classroom. The development of the case study will happen during home study hours, including programming and scientific paper writing. All classes will be given in English. Students are encouraged to ask questions in English, but Portuguese is also allowed. All written and oral assignments must be in English.

Grading: Two individual written tests in the 1st quarter (T_1 and T_2) and another in the 2nd quarter (T_3). Also, a group activity that includes writting a scientific paper (optional), developing a data science product, and a 30 minutes presentation (L).

Final grades will be calculated as

$$1^{\text{st}}\ \text{Q} = \sqrt{T_1 T_2}, \qquad 2^{\text{nd}}\ \text{Q} = \sqrt{T_3 L}, \qquad \text{Exam} = L.$$

Case study: At most 6 groups will be formed. Each group will be responsible for a case study. Students must choose a real-world problem and develop a data science project, including data collection, data handling, inductive learning, validation, documentation, and deployment. The results must be presented in a 30 minutes presentation. Extra points will be given to groups that write a scientific paper about the case study. The trained models must be incorporated in a data science product, such as a web application, a mobile application, or a web service.

Bibliography:

- N. Zumel and J. Mount (2019). *Practical Data Science with R*. 2nd ed. Manning.
- H. Wickham, M. Çetinkaya-Rundel, and G. Grolemund (2023). *R for Data Science: Import, Tidy, Transform, Visualize, and Model Data*. 2nd ed. O'Reilly Media.
- J. D. Kelleher and B. Tierney (2018). *Data science*. The MIT Press.

The first two books — Zumel and Mount (2019) and Wickham, Çetinkaya-Rundel, and Grolemund (2023) — are available online for free.

Any required extra material will be made available in Google Classroom.

Calendar: The expected schedule is presented below.

1st Quarter	
Week	Topics
1	Brief history of data science (chapter 1) Preliminaries (chapter 2)
2	**Written test**
3	Fundamental data concepts (chapter 3)
4	Stages in a data science project (chapter 4)
5 6	Statistical learning theory (chapter 5)
6 7	Data handling (chapter 6)
8	**Written test**

2nd Quarter	
Week	Topics
1	Evaluation (chapter 7)
2	Experimental planning (chapter 8)
3	Ethics, privacy and legal issues (chapter 9)
4	**Written test**
5 6	Project discussion
7 8	**Presentations**

Case studies will be presented during exam weeks. At most 3 case studies will be presented per day, with 30 minutes for each presentation and 20 minutes for questions.

CMC-16 Data science practices

Course plan (2024)
Prof. Filipe A. N. Verri

Important: Only ITA's undergraduate students are allowed to take this course.

Number of students: Approx. 20 (no more than 40 students)

Course load: 2–0–1–5

Requirements: CMC-13 or CMC-15

Course program: Brief history of Data Science. Stages in a Data Science project. Tidy Data. Data integration from multiple sources. Data engineering and shaping. Inductive learning and statistical learning theory. Experimental planning for Data Science. Model evaluation and Bayesian Analysis. Documentation and deployment. Privacy-preserving computational approaches.

Goals: Further studying the practical aspects of Data Science (in relation to CMC-13) and providing the mathematical foundations to ensure the correct usage of Data Science techniques.

The specific goals are:

- Understanding the steps and people involved in a Data Science project;
- Developing an end-to-end case study, including data collection, data transformation, inductive learning, validation, documentation, and deployment; and
- Critically evaluate the results and implications of the case study.

Teaching methodology: Expository classes in common classroom, using whiteboard, slide presentations, coding examples, books and scientific papers. Supplementary didactic materials will be available in Google Classroom. The development of the case study will happen during laboratory classes and home study hours.

Grading: One individual written test in the 1st and another in the 2nd quarter. Software development and oral presentation about the case study (in groups) for the final exam.

Case study: At most 6 groups will be formed. Each group will be responsible for a case study. Students must choose a real-world problem and develop a data science project, including data collection, data handling, inductive learning, validation, documentation, and deployment. The results must be presented in a 30 minutes presentation. The trained models must be incorporated in a data science product, such as a web application, a mobile application, or a web service.

Bibliography:

- N. Zumel and J. Mount (2019). *Practical Data Science with R*. 2nd ed. Manning.
- H. Wickham, M. Çetinkaya-Rundel, and G. Grolemund (2023). *R for Data Science: Import, Tidy, Transform, Visualize, and Model Data*. 2nd ed. O'Reilly Media.
- J. D. Kelleher and B. Tierney (2018). *Data science*. The MIT Press.

The first two books — Zumel and Mount (2019) and Wickham, Çetinkaya-Rundel, and Grolemund (2023) — are available online for free.

Any extra material will be made available in Google Classroom.

Calendar: The expected schedule is presented below.

1st Quarter	
Week	Topics
1	Brief history of Data Science
2	Stages in a Data Science project
3	Tidy Data and data integration from multiple sources
4	Data engineering and shaping
5	Inductive learning and statistical learning theory
6	
7	Case study discussion and definitions
8	**Written test**

2nd Quarter	
Week	Topics
1	Model evaluation
2	Experimental planning for Data Science
3	Bayesian Analysis
4	Documentation and deployment
5	Privacy-preserving computational approaches
6	**Written test**
7	**Presentations and discussions**
8	

1

Brief history of data science

"Begin at the beginning," the King said gravely, "and go on till you come to the end: then stop."

— Lewis Carroll, *Alice in Wonderland*

There are many points-of-view about the beginning of data science. For the sake of contextualization, I separate the topic in two approaches: the history of the term itself and a broad timeline of data-driven sciences highlighting the important figures in each age.

I believe that the history of the term is important to understand the context of the discipline. Along the years, the term has been used to label rather different fields of study. Before I present my view on the term, I present the views of two important figures in the history of data science: Peter Naur and William Cleveland.

Moreover, studying the main facts and figures in the history of data-driven sciences enables us to understand the evolution of the field and hopefully to guide us to evolve it further. Most of the important theories and methods in data science have been developed simultaneously in different fields, such as statistics, computer science, and engineering. The history of data-driven sciences is long and rich. I present a timeline of the ages of data handling and the most important markers of data analysis.

I do not intend to provide a comprehensive history of data science. I aim to provide enough context to support the development of the material in the following chapters, sometimes avoiding directions that are not relevant in the inductive learning context.

Chapter remarks

Contents

Context

- The term “data science” is recent and has been used to label rather different fields.
- The history of data-driven sciences is long and rich.
- Many important theories and methods in data science have been developed simultaneously in different fields.
- The history of data-driven sciences is important to understand the evolution of the field.

Objectives

- Understand the history of the term “data science.”
- Understand the major milestones in the history of data-driven sciences.
- Identify important figures in the history of data-driven sciences.

Takeways

- We have evolved both in terms of theory and application of data-driven sciences.
- There is no consensus on the definition of data science (including which fields it encompasses).
- However, there is enough evidence to support data science as a new science.

1.1 The term "data science"

The term data science is recent and has been used to label rather different fields of study. In the following, I emphasize the history of a few notable usage of the term.

Peter Naur (1928 – 2016) The term "data science" itself was coined in the 1960s by Peter Naur (/naʊə/). Naur was a Danish computer scientist and mathematician who made significant contributions to the field of computer science, including his work on the development of programming languages[1]. His ideas and concepts laid the groundwork for the way we think about programming and data processing today.

Naur disliked the term computer science and suggested it be called datalogy or data science. In the 1960s, the subject was practised in Denmark under Peter Naur's term datalogy, which means the science of data and data processes.

He coined this term to emphasize the importance of data as a fundamental component of computer science and to encourage a broader perspective on the field that included data-related aspects. At that time, the field was primarily centered on programming techniques, but Naur's concept broadened the scope to recognize the intrinsic role of data in computation.

In his book[2], "Concise Survey of Computer Methods", he parts from the concept that *data* is "a representation of facts or ideas in a formalised manner capable of being communicated or manipulated by some process."[3] Note however that his view of the science only "deals with data [...] while the relation of data to what they represent is delegated to other fields and sciences."

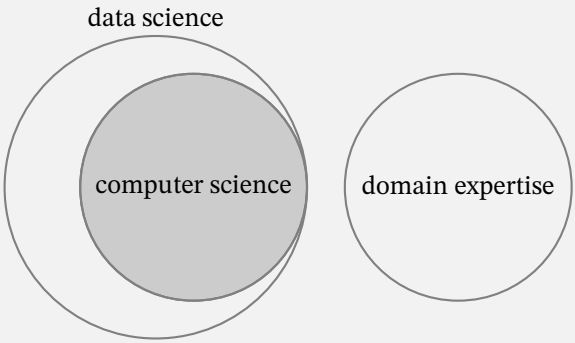
It is interesting to see the central role he gave to data in the field of computer science. His view that the relation of data to what they represent is delegated to other fields and sciences is still debatable today. Some scientists argue that data science should focus on the techniques to deal with data, while others argue that data science should encompass the whole business domain. A depiction of Naur's view of data science is shown in fig. 1.1.

[1] He is best remembered as a contributor, with John Backus, to the Backus–Naur form (BNF) notation used in describing the syntax for most programming languages.

[2] P. Naur (1974). *Concise Survey of Computer Methods*. Lund, Sweden: Studentlitteratur. ISBN: 91-44-07881-1. URL: http://www.naur.com/Conc.Surv.html.

[3] I. H. Gould (ed.): 'IFIP guide to concepts and terms in data processing', North-Holland Publ. Co., Amsterdam, 1971.

Figure 1.1: Naur's view of data science.



For Naur, data science studies the techniques to deal with data, but he delegates the meaning of data to other fields.

William Cleveland (born 1943) In 2001, a prominent statistician used the term "data science" in his work to describe a new discipline that comes from his "plan to enlarge the major areas of technical work of the field of statistics[4]." In 2014, that work was republished[5]. He advocates the expansion of statistics beyond theory into technical areas, significantly changing statistics. Thus, it warranted a new name.

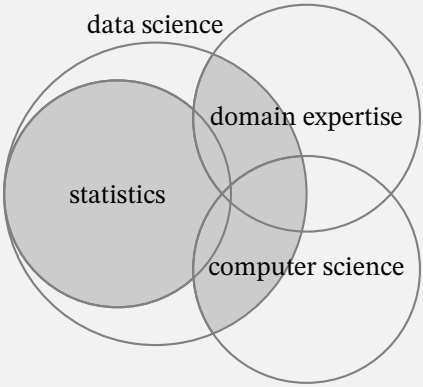
As a result, William Swain Cleveland II is credited to define data science as it is most used today. He is a highly influential figure in the fields of statistics, machine learning, data visualization, data analysis for multidisciplinary studies, and high performance computing for deep data analysis.

In his view, data science is the "modern" statistics, where it is enlarged by computer science methods and domain expertise. An illustration of Cleveland's view of data science is shown in fig. 1.2. It is important to note that Cleveland never defined a explicit list of computer science fields and business domains that should be included in the new discipline. The main idea is that statistics should rely on com-

[4]W. S. Cleveland (2001). "Data Science: An Action Plan for Expanding the Technical Areas of the Field of Statistics". In: *ISI Review*. Vol. 69, pp. 21–26.

[5]W. S. Cleveland. Data Science: An Action Plan for the Field of Statistics. Statistical Analysis and Data Mining, 7:414–417, 2014. reprinting of 2001 article in ISI Review, Vol 69.

Figure 1.2: Cleveland's view of data science.



For Cleveland, data science is the "modern" statistics, where it is enlarged by computer science and domain expertise.

putational methods and that the domain expertise should be considered in the analysis.

Buzzword or a new science? Be aware that scientific literature has no consensus on the definition of data science, and it is still considered by some to be a buzzword[6].

Most of the usages of the term in literature and in the media are either a rough reference to a set of data-driven techniques or a marketing strategy. Naur (fig. 1.1) and Cleveland (fig. 1.2) are among the few that try to carefully define the term. However, both of them do not see data science as an independent field of study, but an enlarged scope of an existing science. I disagree; the social and economical demand for data-driven solutions led to an evolution in our understanding of the challenges we are facing. As a result, we see many "data scientist" being hired and many "data science degrees" programs emerging.

In chapter 3, I dare to provide a (yet another) definition for the term. I argue that its object of study can be precisely established to support it as a new science.

[6] Press, Gil. "Data Science: What's The Half-Life of a Buzzword?". Forbes. Available at https://www.forbes.com/sites/gilpress/2013/08/19/data-science-whats-the-half-life-of-a-buzzword/

1.2 Timeline and historical markers

Kelleher and Tierney (2018)[7] provides an interesting timeline of data-driven methods and influential figures in the field. I reproduce it here with some changes, including some omissions and additions. On the subject of data analysis, I include some of the exceptional remarks from Vapnik (1999)[8].

I first address data handling — which I include data sources, collection, organization, storage, and transformation —, and then data analysis and knowledge extraction.

1.2.1 Timeline of data handling

The importance of collecting and organizing data goes without saying. Data fuels analysis and decision making. In the following, I present some of the most important milestones in the history of data handling.

Figure 1.3: Timeline of the ages of data handling.

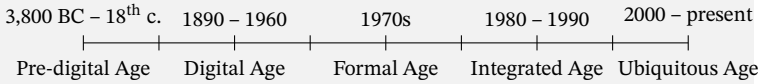


Figure 1.3 illutrates the proposed timeline. Ages are not strict boundaries, but rather periods where some important events happened. Also, observe that the timescale is not linear. The Pre-digital Age is the longest period, and one could divide it into smaller periods. My choices of ages and their boundaries are motivated by didactic reasons.

Pre-digital age

We can consider the earliest records of data collection to be the notches on sticks and bones to keep tracking of passing of time. The Lebombo bone, a baboon fibula with notches, is probably the earliest known mathematical object. It was found in the Lebombo Mountains located between South Africa and Eswatini. They estimate it is more than 40,000 years old. It is conjectured to be a tally stick, but its exact purpose is

[7] J. D. Kelleher and B. Tierney (2018). *Data science*. The MIT Press.

[8] V. N. Vapnik (1999). *The nature of statistical learning theory*. 2nd ed. Springer-Verlag New York, Inc. ISBN: 978-1-4419-3160-3.

unknown. Its 29 notches suggests that may have been used as a lunar phase counter. However, since it is broken at one end, the 29 notches may or may not be the total number[9].

Another important milestone in the history of data collection is the record of demographic data. One of first known census was conducted in 3,800 BC in the Babylonian Empire. It was ordered to assess the population and resources of his empire. Records were stored on clay tiles[10].

Since the early forms of writing, humanity abilities to record events and information increased significantly. The first known written records date back to around 3,500 BC, the Sumerian archaic (pre-cuneiform) writing. This writing system was used to represent commodities using clay tokens and to record transactions[11].

"Data storage" was also a challenge. Some important devices that increased our capacity to register textual information are the Sumerian clay tablets (3,500 BC), the Egyptian papyrus (3,000 BC), the Roman wax tablets (100 BC), the codex (100 AD), the Chinese paper (200 AD), the printing press (1440), and the typewriter (1868).

Besides those improvements in unstructured data storage, at least in the Western and Middle Eastern world, there are no significant advances in structured data collection until the 19th century. (A Eastern timeline research seems much hard to perform. Unfortunally, I left it out in this book.)

I consider a major influential figure in the history of data collection to be Florence Nightingale (1820 – 1910). She was a passionate statistician and probably the first person to use statistics to influence public and official opinion. The meticulous records she kept during the Crimean War (1853 – 1856) were the evidence that saved lives — part of the mortality came from lack of sanitation. She was also the first to use statistical graphics to present data in a way that was easy to understand. She is credited with developing a form of the pie chart now known as the polar area diagram. She also reformed healthcare in the United Kingdom and is considered the founder of modern nursing; where great part of the work was to collect data in a standardized way to quickly draw conclusions[12].

[9] P. B. Beaumont and R. G. Bednarik (2013). In: *Rock Art Research* 30.1, pp. 33–54. URL: https://search.informit.org/doi/10.3316/informit.488018706238392.

[10] C. G. Grajalez et al. (2013). "Great moments in statistics". In: *Significance* 10.6, pp. 21–28. DOI: 10.1111/j.1740-9713.2013.00706.x.

[11] G. Ifrah (1998). *The Universal History of Numbers, from Prehistory to the Invention of the Computer*. First published in French, 1994. London: Harvill. ISBN: 1 86046 324 x.

[12] C. G. Grajalez et al. (2013). "Great moments in statistics". In: *Significance* 10.6,

Digital age

In the modern period, several devices were developed to store digital[13] information. One particular device that is important for data collection is the punched card. It is a piece of stiff paper that contains digital information represented by the presence or absence of holes in predefined positions. The information can be read by a mechanical or electrical device called a card reader. The earliest famous usage of punched cards was by Basile Bouchon (1725) to control looms. Most of the advances until the 1880s were about the automation of machines (data processing) using hand-punched cards, and not particularly specialized for data collection.

However, the 1890 census in the United States was the first to use machine-readable punched cards to tabulate data. Processing 1880 census data took eight years, so the Census Bureau contracted Herman Hollerith (1860 – 1929) to design and build a tabulating machine. He founded the Tabulating Machine Company in 1896, which later merged with other companies to become International Business Machines Corporation (IBM) in 1924. Later models of the tabulating machine were widely used for business applications such as accounting and inventory control. Punched card technology remained a prevalent method of data processing for several decades until more advanced electronic computers were developed in the mid-20$^{\text{th}}$ century.

The invention of the digital computer is responsible for a revolution in data handling. The amount of information we can capture and store increased exponentially. ENIAC (1945) was the first electronic general-purpose computer. It was Turing-complete, digital, and capable of being reprogrammed to solve a full range of computing problems. It had 20 words of internal memory, each capable of storing a 10-digit decimal integer number. Programs and data were entered by setting switches and inserting punched cards.

For the 1950 census, the United States Census Bureau used the UNIVAC I (Universal Automatic Computer I), the first commercially produced computer in the United States[14].

It goes without saying that digital computers have become much more powerful and sophisticated since then. The data collection process

pp. 21–28. DOI: 10.1111/j.1740-9713.2013.00706.x.

[13] Digital means the representation of information in (finite) discrete form. The term comes from the Latin digitus, meaning finger, because it is the natural way to count using fingers. Digital here do not mean electronic.

[14] Read more in https://www.census.gov/history/www/innovations/.

has been easily automated and scaled to a level that was unimaginable before. However, "where" storing data is not the only challenge. "How" to store data is also a challenge. The next period of history addresses this issue.

Formal age

In 1970, Edgar Frank Codd (1923 – 2003), a British computer scientist, published a paper entitled "A Relational Model of Data for Large Shared Data Banks"[15]. In this paper, he introduced the concept of a relational model for database management.

A relational model organizes data in tables (relations) where each row represents a record and each column represents an attribute of the record. The tables are related by common fields. Codd showed means to organize the tables of a relational database to minimize data redundancy and improve data integrity. Section 3.4.1 provides more details on the topic.

His work was a breakthrough in the field of data management. The standardization of relational databases led to the development of Structured Query Language (SQL) in 1974. SQL is a domain-specific language used in programming and designed for managing data held in a Relational Database Management System (RDBMS).

As a result, a new challenge rapidly emerged: how to aggregate data from different sources. Once data is stored in a relational database, it is easy to query and manage it. However, data is usually stored in different databases, and it is not always possible to directly combine them.

Integrated age

The solution to this problem was the development of the Extract, Transform, Load (ETL) process. ETL is a process in data warehousing responsible for extracting data from several sources, transforming it into a format that can be analyzed, and loading it into a data warehouse.

The concept of data warehousing dates back to the late 1980s when IBM researchers Barry Devlin and Paul Murphy developed the "business data warehouse."

Two major figures in the history of ETL are Ralph Kimball (born 1944) and Bill Inmon (born 1945), both American computer scientists.

[15] E. F. Codd (1970). "A Relational Model of Data for Large Shared Data Banks". In: *Commun. ACM* 13.6, pp. 377–387. ISSN: 0001-0782. DOI: 10.1145/362384.362685.

Although they differ in their approaches, they both agree that data warehousing is the foundation for Business Intelligence (BI) and analytics, and that data warehouses should be designed to be easy to understand and fast to query for business users.

A famous debate between Kimball and Inmon is the top-down versus bottom-up approach to data warehousing. Inmon's approach is top-down, where the data warehouse is designed first and then the data marts[16] are created from the data warehouse. Kimball's approach is bottom-up, where the data marts are created first and then the data warehouse is created from the data marts.

One of the earliest and most famous case studies of the implementation of a data warehouse is that of Walmart. In the early 1990s, Walmart faced the challenge of managing and analyzing vast amounts of data from its stores across the United States. The company needed a solution that would enable comprehensive reporting and analysis to support decision-making processes. The solution was to implement a data warehouse that would integrate data from various sources and provide a single source of truth for the organization.

Ubiquitous age

The last and current period of history is the ubiquitous age. It is characterized by the proliferation of data sources.

The ubiquity of data generation and the evolution of data-centric technologies have been made possible by a multitude of figures across various domains.

- Vinton Gray Cerf (born 1943) and Robert Elliot Kahn (born 1938), often referred to as the "Fathers of the Internet," developed the TCP/IP protocols, which are fundamental to internet communication.

- Tim Berners-Lee (born 1955), credited with inventing the World Wide Web, laid the foundation for the massive data flow on the internet.

- Steven Paul Jobs (1955 – 2011) and Stephen Wozniak (born 1950), from Apple Inc., and William Henry Gates III (born 1955), from Microsoft Corporation, were responsible for the introduction of

[16] A data mart is a specialized subset of a data warehouse that is designed to serve the needs of a specific business unit, department, or functional area within an organization.

personal computers, leading to the democratization of data generation.

- Lawrence Edward Page (born 1973) and Sergey Mikhailovich Brin (born 1973), the founders of Google, transformed how we access and search for information.

- Mark Elliot Zuckerberg (born 1984), the co-founder of Facebook, played a crucial role in the rise of social media and the generation of vast amounts of user-generated content.

In terms of data handling, this change of landscape has brought about the development of new technologies and techniques for data storage and processing. Especially the development of NoSQL databases and distributed computing frameworks.

NoSQL databases are non-relational databases that can store and process large volumes of unstructured, semi-structured, and structured data. They are highly scalable and flexible, making them ideal for big data applications.

Some authors argue that the rise of big data is characterized by the five V's of big data: Volume, Velocity, Variety, Veracity, and Value. The amount of data generated is massive, the speed at which data is generated is high, the types of data generated are diverse, the quality of data generated is questionable, and the value of data generated is high.

Once massive amounts of unstructured data became available, the need for new data processing techniques arose. The development of distributed computing frameworks such as Apache Hadoop and Apache Spark enabled the processing of massive amounts of data in a distributed manner.

Douglass Read Cutting and Michael Cafarella, the developers of Apache Hadoop, proposed the Hadoop Distributed File System (HDFS) and MapReduce, which are the cornerstones of the Hadoop framework, in 2006. Hadoop's distributed storage and processing capabilities enabled organizations to handle and analyze massive volumes of data.

Currently, Google holds a patent for MapReduce[17]. However, their framework inherits from the architeture proposed in Hillis (1985)[18] the-

[17] http://static.googleusercontent.com/media/research.google.com/es/us/archive/mapreduce-osdi04.pdf

[18] W. D. Hillis (1985). "The Connection Machine". Hillis, W.D.: The Connection Machine. PhD thesis, MIT (1985). Cambridge, MA, USA: Massachusetts Institute of Technology. URL: http://hdl.handle.net/1721.1/14719.

sis. MapReduce is not particularly novel, but its simplicity and scalability made it popular.

Nowadays, another important topic is Internet of Things (IoT). IoT is a system of interrelated computing devices that communicate with each other over the internet. The devices can be anything from cellphones, coffee makers, washing machines, headphones, lamps, wearable devices, and almost anything else you can think of. The reality of IoT increased the challenges of data handling, especially in terms of data storage and processing.

In summary, we currently live in a world where data is ubiquitous and comes in many different forms. The challenge is to collect, store, and process this data in a way that is meaningful and useful, also respecting privacy and security.

1.2.2 Timeline of data analysis

The way we think about data and knowledge extraction has evolved significantly over the years. In the following, I present some of the most important milestones in the history of data analysis and knowledge extraction.

Figure 1.4: Timeline of the ages of data analysis.

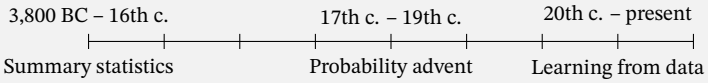


Figure 1.4 illutrates the proposed timeline. I consider changes of ages to be smooth transitions, and not strict boundaries. The theoretical advances are slower than the technological ones — the latter influences more data handling than data analysis —, so not much has changed since the beginning of the 20th century.

Summary statistics

The earliest known records of systematic data analysis date back to the first censuses. The term *statistics* itself refer to the analysis of data *about the state*, including demographics and economics. That early (and simplest) form of statistical analysis is called *summary statistics*, which consists of describing data in terms of its central tendencies (e.g. arithmetic mean) e variability (e.g. range).

Probability advent

However, after the seventeenth century, the foundations of modern probability theory were laid out. Important figures for developing the probability theory are Blaise Pascal (1623 – 1662), Pierre de Fermat (1607 – 1665), Christiaan Huygens (1629 – 1695), and Jacob Bernoulli (1655 – 1705).

The foundation methods brought to life the field of statistical inference. In the following years, important results were achieved.

Bayes' rule Reverend Thomas Bayes (1701 – 1761) was an English statistician, philosopher, and presbyterian minister. He is known for formulating a specific case of the theorem that bears his name: Bayes' theorem. The theorem is used to calculate conditional probabilities using an algorithm (his Proposition 9, published in 1763) that uses evidence to calculate limits on an unknown parameter.

The Bayes' rule is the foundation of learning from evidence, once it allows us to calculate the probability of an event based on prior knowledge of conditions that might be related to the event. Classifiers based on Naïve Bayes — the application of Bayes' theorem with strong independence assumptions between known variables — is likely to have been used since the second half of the eighteenth century.

Gauss' method of least squares Johann Carl Friedrich Gauss (1777 – 1855) was a German mathematician and physicist who made significant contributions to many fields in mathematics and sciences. Circa 1794, he developed the method of least squares for calculating the orbit of Ceres to minimize the impact of measurement error[19].

Playfair's data visualization William Playfair (1759 – 1823) was a secret agent on behalf of Great Britain during its war with France in the 1790s. He invented several types of diagram between 1780s and 1800s, such as the line, area and bar chart of economic data, and the pie chart and circle graph to show proportions.

[19]The method was first published by Adrien-Marie Legendre (1752 – 1833) in 1805, but Gauss claimed in 1809 that he had been using it since circa 1794.

Learning from data

In the twentieth century and beyond, new advances were made in the field of statistics. The development of learning machines enabled the development of new techniques for data analysis.

The recent advances in computation and data storage are crucial for the large-scale application of these techniques.

Fisher's discriminant analysis In the 1930s, Ronald Fisher (1890 – 1962) developed discriminant analysis, which was considered a problem of constructing a decision rule to assign a vector to one of two categories using given probability distribution functions[20].

Shannon's information theory The field, that studies quantification, storage and communication of information, was originally established by the works of Harry Nyquist (1889 – 1976) and Ralph Hartley (1888 – 1970) in the 1920s, and Claude Shannon (1916 – 2001) in the 1940s. Information theory brought many important concepts to the field of data analysis, such as entropy, mutual information, and information gain. This theory is the foundation of several machine learning algorithms.

K-Nearest Neighbors In 1951, Evelyn Fix (1904 – 1965) and Joseph Lawson Hodges Jr. (1922 – 2000) wrote a technical report entitled "Discriminatory Analysis, Nonparametric Discrimination: Consistency Properties." In this paper, they proposed the k-nearest neighbors algorithm, which is a non-parametric method used for classification and regression. The algorithm marks a shift from the traditional parametric methods — and purely statistical — to non-parametric methods.

Rosenblatt's perceptron In the 1960s, Frank Rosenblatt (1928 – 1971) developed the perceptron, the first model of a learning machine. While the idea of a mathematical neuron was not new, he was the first to describe the model as a program, showing the ability of the perceptron to learn simple tasks such as the logical operations AND and OR.

[20] After, Rosenblatt's work, however, it was used to solve inductive inference as well.

Hunt inducing trees In 1966, Hunt, Marin, and Stone's book[21] described a way to induce decision trees from data. The algorithm is based on the concept of information entropy and is a precursor of the Quinlan's ID3 algorithm[22] and its variations. These algorithm gave rise to the field of decision trees, which is a popular method for classification and regression.

Empirical risk minimization principle Although many learning machines where developed until the 1960s, they did not advanced significantly the understanding of the general problem of learning from data. Between 1960s and 1986 — before the backpropagation algorithm was proposed —, the field of practical data analysis was basically stagnant. The main reason for that was the lack of a theoretical framework to support the development of new learning machines.

However, these years were not completely unfruitful. As early as 1968, Vladimir Vapnik (born 1936) and Alexey Chervonenkis (1938 – 2014) developed the foundamental concepts of VC entropy and VC dimension for the data classification problems. As a result, a novel inductive principle was proposed: the Empirical Risk Minimization (ERM) principle. This principle is the foundation of statistical learning theory.

Resurgence of neural networks In 1986, researchers developed independently a method to optimize coefficients of a neural network[23]. The method is called backpropagation and is the foundation of the resurgence of neural networks.

This rebirth of neural networks happened in a scenario very different from the 1960s. The availability of data and computational power fueled a new approach to the problem of learning from data. The new approach preferred the use of simple algorithms and intuitive models over theoretical models, fueling areas such as bioinspired computing and evolutionary computation.

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[21] E. B. Hunt, J. Marin, and P. J. Stone (1966). *Experiments in Induction*. New York, NY, USA: Academic Press.

[22] J. R. Quinlan (1986). "Induction of Decision Trees". In: *Machine Learning* 1, pp. 81–106. URL: https://api.semanticscholar.org/CorpusID:13252401.

[23] Y. Le Cun (1986). "Learning Process in an Asymmetric Threshold Network". In: *Disordered Systems and Biological Organization*. Berlin, Heidelberg: Springer Berlin Heidelberg, pp. 233–240. ISBN: 978-3-642-82657-3; D. E. Rumelhart, G. E. Hinton, and R. J. Williams (1986). "Learning representations by back-propagating errors". In: *Nature* 323.6088, pp. 533–536. DOI: 10.1038/323533a0.

Ensembles Following the new approach, ensemble methods were developed. Based on ideas of boosting[24] and bagging[25], ensemble methods combine multiple learning machines to improve the performance of the individual machines.

The difference between boosting and bagging is the way the ensemble is built. In boosting, the ensemble is built sequentially, where each new model tries to correct the errors of the previous models. In bagging, the ensemble is built in parallel, where each model is trained independently with small changes in the data. The most famous bagging ensemble methods are random forests[26], while XGBoost, a gradient boosting method[27], has been extensively used in machine learning competitions.

Support vector machines In 1995, Cortes and Vapnik[28] proposed the Support Vector Machine (SVM) algorithm, a learning machine based on the VC theory and the ERM principle. Based on Cover's theorem[29], they developed a method that finds the optimal hyperplane that separates two classes of data in a high-dimensional space with the maximum margins. The resulting method led to practical and efficient learning machines.

Deep learning revolution Although the ideia of neural networks with multiple layers were around since the 1960s, only in the late 2000s the field of deep learning caught the attention of the scientific community by achieving state-of-the-art results in computer vision and natural language processing. Yoshua Bengio, Geoffrey Hinton and Yann LeCun are recognized for their for conceptual and engineering breakthroughs in the field, winning the 2018 Turing Award[30].

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[24] R. E. Schapire (1990). "The strength of weak learnability". In: *Machine Learning* 5.2, pp. 197–227. DOI: 10.1007/BF00116037.

[25] L. Breiman (1996). "Bagging predictors". In: *Machine Learning* 24.2, pp. 123–140. DOI: 10.1007/BF00058655.

[26] T. K. Ho (1995). "Random decision forests". In: *Proceedings of 3rd International Conference on Document Analysis and Recognition*. Vol. 1, 278–282 vol.1. DOI: 10.1109/ICDAR.1995.598994.

[27] J. H. Friedman (2001). "Greedy function approximation: A gradient boosting machine." In: *The Annals of Statistics* 29.5, pp. 1189–1232. DOI: 10.1214/aos/1013203451. URL: https://doi.org/10.1214/aos/1013203451.

[28] C. Cortes and V. N. Vapnik (1995). "Support-vector networks". In: *Machine Learning* 20.3, pp. 273–297. DOI: 10.1007/BF00994018.

[29] T. M. Cover (1965). "Geometrical and Statistical Properties of Systems of Linear Inequalities with Applications in Pattern Recognition". In: *IEEE Transactions on Electronic Computers* EC-14.3, pp. 326–334. DOI: 10.1109/PGEC.1965.264137.

[30] https://awards.acm.org/about/2018-turing

Generative deep models Nowadays, generative deep models are a hot topic in machine learning. They are a class of statistical models that can generate new data instances. They are used in unsupervised learning to discover hidden structures in unlabeled data (e.g. clustering), and in supervised learning to generate new synthetic data instances. The most famous generative models are the generative transformers and generative adversarial networks.

LUSI learning theory In 2010s, Vapnik and Izmailov[31] proposed the Learning using Statistical Inference (LUSI) principle, which is an extension of the statistical learning theory. The LUSI theory is based on the concept of statistical invariants, which are properties of the data that are preserved under transformations. The theory is the foundation of the learning from intelligent teachers paradigm. They regard the LUSI theory as the next step in the evolution of learning theory, calling it the "complete statistical theory of learning".

[31] V. N. Vapnik and R. Izmailov (2015). "Learning with Intelligent Teacher: Similarity Control and Knowledge Transfer". In: *Statistical Learning and Data Sciences*. Ed. by A. Gammerman, V. Vovk, and H. Papadopoulos. Cham: Springer International Publishing, pp. 3–32. ISBN: 978-3-319-17091-6.

2

Preliminaries

Maar ik maak steeds wat ik nog niet kan om het te leeren kunnen.

— Vincent van Gogh, *The Complete Letters of Vincent Van Gogh, Volume Three*

Foundamental concepts in data science come from a variety of fields, including mathematics, statistics, computer science, optimization theory, and information theory. This chapter provides a brief overview of the main computational, mathematical and statistical concepts in data science.

The goal is not to provide a comprehensive treatment of these topics, but to consolidate notations and definitions that are used throughout the book. The reader is encouraged to consult the references provided at the end of each topic for a more in-depth treatment. Statisticians with strong programming background and computer scientists with strong statistics background will probably not find much new here.

I first introduce the main concepts in algorithms and data structures, which are the building blocks of computational thinking. Then, I present the basic concepts in set theory and linear algebra, which are important mathematical foundations for data science. Finally, I introduce the main concepts in probability theory, the cornerstone of statistical learning and inference.

If your are familiar with these topics, you can safely skip this chapter. Otherwise, I encourage you to read it carefully, as it will help you understand the rest of the book.

Chapter remarks

Contents

Context

- Data science relies on a variety of mathematical and computational concepts.
- The main concepts are algorithms, data structures, set theory, linear algebra, and probability theory.

Objectives

- Introduce a brief overview of the main computational, mathematical and statistical concepts in data science.
- Remind the reader the main definitions and properties of these concepts.
- Consolidate notations and definitions that are used throughout the book.

2.1 Algorithms and data structures

Algorithms are step-by-step procedures for solving a problem. They are used to manipulate data structures, which are ways of organizing data to solve problems. They are realized in programming languages, which are formal languages that can be used to express algorithms.

My suggestion of a comprehensive book about algorithms and data structures is Cormen et al. (2022)[1].

2.1.1 Computational complexity

The computational complexity of an algorithm is the amount of resources it uses to run as a function of the size of the input. The most common resources are time and space.

Usually, we are interested in the asymptotic complexity of an algorithm, i.e. how the complexity grows as the size of the input grows. The most common notation for asymptotic complexity is the Big-O notation.

Big-O notation Let f and g be functions from the set of natural numbers to the set of real numbers, i.e. $f, g : \mathbb{N} \to \mathbb{R}$. We say that f is $O(g)$ if there exists a constant $c > 0$ such that $f(n) \leq cg(n)$ for all $n \geq n_0$, where n_0 is a natural number. We can order functions by their asymptotic complexity. For example, $O(1) < O(\log n) < O(n) < O(n \log n) < O(n^2) < O(2^n) < O(n!)$[2].

The asymptotic analysis of algorithms is usually done in the worst-case scenario, i.e. the maximum amount of resources the algorithm uses for any input of size n. Thus, it gives us an upper bound on the complexity of the algorithm. In other words, an algorithm with complexity $O(g(n))$ is guaranteed to run in at most $cg(n)$ time for some constant c.

It does not mean, for instance, that an algorithm with time complexity $O(n)$ will always run faster than an algorithm with time complexity $O(n^2)$, but that the former will run faster for a large enough input size.

An important property of the Big-O notation is that

$$O(f) + O(g) = O(\max(f, g)),$$

i.e. if an algorithm has two sequential steps with time complexity $O(f)$ and $O(g)$, the highest complexity is the one that determines the overall complexity.

[1] T. H. Cormen et al. (2022). *Introduction to Algorithms*. 4th ed. The MIT Press, p. 1312. ISBN: 9780262046305.

[2] Throughout this book, we consider $\log n = \log_2 n$.

2.1.2 Algoritmic paradigms

Some programming techniques are used to solve a wide variety of problems. They are called algorithmic paradigms. The most common ones are listed below.

Divide and conquer The problem is divided into smaller subproblems that are solved recursively. The solutions to the subproblems are then combined to give a solution to the original problem. Some example algorithms are merge sort, quick sort, and binary search.

Algorithm 2.1: Binary search algorithm.

Data: A sorted array $\mathbf{a} = [a_1, a_2, \dots, a_n]$ and a key x
Result: True if x is in $\mathbf{a}$, false otherwise

```
1  l ← 1;
2  r ← n;
3  while l ≤ r do
4      m ← ⌊(l+r)/2⌋;
5      if x = a_m then
6          return true
7      if x < a_m then
8          r ← m − 1;
9      else
10         l ← m + 1;
11 return false
```

An iterative algorithm that searches for a key in a sorted array.

Consider as an example the algorithm 2.1 that solves the binary search problem. Given a n-elements sorted array $\mathbf{a} = [a_1, a_2, \dots, a_n]$, $a_1 \leq a_2 \leq \cdots \leq a_n$, and a key x, the algorithm returns true if x is in A and false otherwise. The algorithm works by dividing the array in half at each step and comparing the key with the middle element. Each time the key is not found, the search space is reduced by half.

Divide and conquer algorithms can be implemented using recursion. *Recursion* is also a algorithmic paradigm where a function calls itself to solve smaller instances of the same problem. The recursion stops when the problem is small enough to be solved directly.

Algorithm 2.2: Recursive binary search algorithm.

```
1  function bsearch([a_1, a_2, ..., a_n], x) is
2      if n = 0 then
3          return false
4      m ← ⌊n/2⌋;
5      if x = a_m then
6          return true
7      if x < a_m then
8          return bsearch([a_1, ..., a_{m-1}], x)
9      else
10         return bsearch([a_{m+1}, ..., a_n], x)
```

A recursive algorithm that searches for a key in a sorted array. Note that trivial conditions — $n = 0$ and key found — are handled first, so the recursion stops when the problem is small enough.

Algorithm 2.2 shows a recursive implementation of the binary search algorithm. The smaller instances, or so called *base cases*, are when the array is empty or the key is found in the middle. Other conditions — key is smaller or greater than the middle element — are handled by calling the function recursively with the left or right half of the array.

This solution — both algorithms — has a worst-case time complexity of $O(\log n)$. The search space is halved at each step, thus, in the i-th iteration, the remaining number of elements in the array is $n/2^{i-1}$. In the worst-case, the algorithm stops when the search space has size 1 or smaller, i.e.

$$\frac{n}{2^{i-1}} = 1 \implies i = 1 + \log n.$$

Note this strategy leads to such a low time complexity that we can solve large instances of the problem in a reasonable amount of time. Consider the case of an array with $2^{64} = 18{,}446{,}744{,}073{,}709{,}551{,}616$ elements, the algorithm will find the key in at most 65 steps.

Greedy algorithms The problem is solved with incremental steps, each of which is locally optimal. The overall solution is not guaranteed to (but might) be optimal. Some example algorithms are Dijkstra's algorithm and Prim's algorithm. Greedy algorithm are usually very efficient in terms of time complexity — see more in the following.

One example of suboptimal greedy algorithm is a heuristic solution for the knapsack problem. The *knapsack problem* is a combinatorial optimization problem where the goal is to maximize the value of items in a knapsack without exceeding its capacity. The problem is mathematically defined as

$$\text{maximize} \sum_{i=1}^{n} v_i x_i,$$

$$\text{subject to} \sum_{i=1}^{n} w_i x_i \leq W,$$

where v_i is the value of item i, w_i is the weight of item i, x_i is a binary variable that indicates if item i is in the knapsack, and W is the capacity of the knapsack.

Algorithm 2.3: Heuristic solution for the knapsack problem.

Data: A list of n items, each with a value v_i and a weight w_i, and a capacity W
Result: The binary variable x_i for each item i that maximizes the total value

```
1 Sort the items in decreasing order of value;
2 V ← 0;
3 x_i ← 0, ∀i;
4 for i ← 1 to n do
5     if w_i ≤ W then
6         x_i ← 1;
7         V ← V + v_i;
8         W ← W − w_i;
9 return x_i, ∀i
```

A greedy algorithm that solves suboptimally the knapsack problem. The algorithm iterates over the items in decreasing order of value and puts the item in the knapsack if it fits.

An algorithm that finds a suboptimal solution for the knapsack problem is shown in algorithm 2.3. It iterates over the items in decreasing order of value and puts the item in the knapsack if it fits. The algorithm is suboptimal because there might exist small-value items that, when combined, would fit in the knapsack and yield a higher total value.

The most costly operation in the algorithm is the sorting of the items in decreasing order of value, which has a time complexity[3] of $O(n \log n)$.

Brute force The problem is solved by trying all possible solutions. Most of the time, brute force algorithms have exponential time complexity, leading to impractical solutions for large instances of the problem. On the other hand, brute force algorithms are usually easy to implement and understand, as well as guaranteed to find the optimal solution.

In the previous example, a brute force algorithm for the knapsack problem would try all possible combinations of items and select the one that maximizes the total value without exceeding the capacity. One can easily see that the time complexity of such an algorithm is $O(2^n)$, where n is the number of items, as there are 2^n possible combinations of items. Such an *exhaustive search* is impractical for large n, but it is guaranteed to find the optimal solution.

One should avoid brute force algorithms whenever possible, as they are usually too costly to be practical. However, they are useful for small instances of the problem, for verification of the results of other algorithms, and for educational purposes.

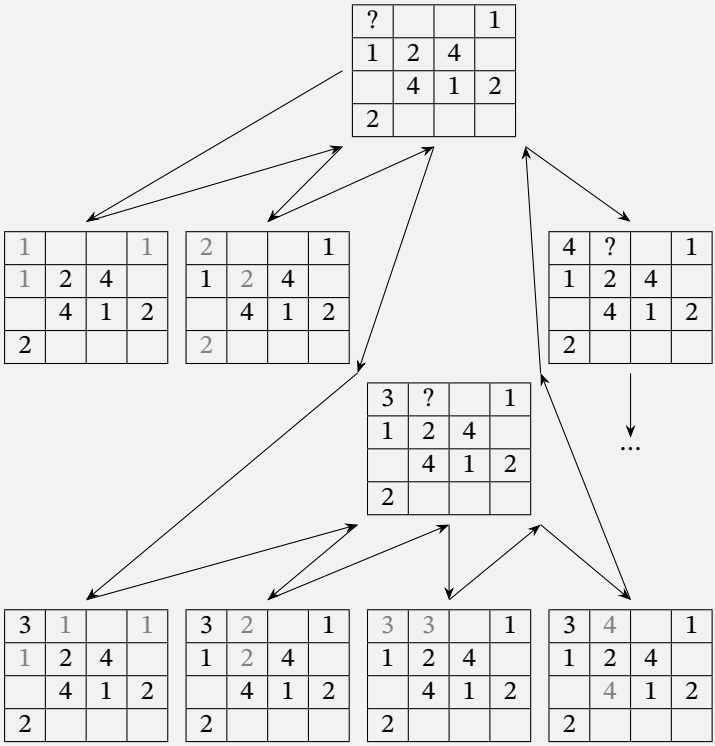
Backtracking The problem is solved incrementally, one piece at a time. If a piece does not fit, it is removed and replaced by another piece. Some example algorithms are the naïve solutions for N-queens problem and for the Sudoku problem. Backtracking, as a special case of brute force, often leads to exponential (or worse) time complexity.

Many times, backtracking algorithms are combined with other techniques to reduce the search space and make the algorithm more efficient. For example, the backtracking algorithm for the Sudoku problem is combined with constraint propagation to reduce the number of possible solutions.

[3]Considering the worst-case time complexity of the sorting algorithm, consult T. H. Cormen et al. (2022). *Introduction to Algorithms*. 4th ed. The MIT Press, p. 1312. ISBN: 9780262046305 for more details.

A Sudoku puzzle consists of an $n \times n$ grid, divided into n subgrids of size $\sqrt{n} \times \sqrt{n}$. The goal is to fill the grid with numbers from 1 to n such that each row, each column, and each subgrid contains all numbers from 1 to n but no repetitions. The most common grid size is 9×9.

Figure 2.1: Backtracking to solve a Sudoku puzzle.



A Sudoku puzzle — in this case, 4×4 — is solved by trying all possible numbers in each cell and backtracking when a number does not fit. The solution is found when all cells are filled and the constraints are satisfied. Arrows indicate the backtracking steps. The question mark indicates an empty cell that needs to be filled at that step. Constraints violation are shown in gray.

An illustration of backtracking to solve a 4×4 Sudoku puzzle[4] is shown in fig. 2.1. The puzzle is solved by trying all possible numbers in each cell and backtracking when a number does not fit. The solution is found when all cells are filled and the constraints are satisfied. Arrows indicate the the steps of the backtracking algorithm. Every time a constraint is violated — indicated in gray —, the algorithm backtracks to the previous cell and tries a different number.

One can easily see that a puzzle with m missing cells has n^m possible solutions. For small values of m and n, the algorithm is practical, but for large values, it becomes too costly.

2.1.3 Data structures

Data structures are ways of organizing data to solve problems. The most common ones are listed below. A comprehensive material about the properties and implementations of data structures can be found in Cormen et al. (2022)[5].

Arrays An array is a homogeneous collection of elements that are accessed by an integer index. The elements are usually stored in contiguous memory locations. In the scope of this book, it is equivalent to a mathematical vector whose element's type are not necessarily numerical. Thus, a n-elements array $\mathbf{a}$ is denoted by $[a_1, a_2, \dots, a_n]$, where the i in a_i is the index of the element.

Stacks A stack is a collection of elements that are accessed in a last-in-first-out (LIFO) order. Elements are added to the top of the stack and removed from the top of the stack. In other words, only two operations are allowed: push (add an element to the top of the stack) and pop (remove the top element). Only the top element is accessible.

Queues A queue is a collection of elements that are accessed in a first-in-first-out (FIFO) order. Elements are added to the back of the queue and removed from the front of the queue. The two operations allowed are enqueue (add an element to the back of the queue) and dequeue (remove the front element). Only the front and back elements are accessible.

[4] Smaller puzzles are more didactic, but the same principles apply to larger puzzles.

[5] T. H. Cormen et al. (2022). *Introduction to Algorithms*. 4th ed. The MIT Press, p. 1312. ISBN: 9780262046305.

Trees A tree is a collection of nodes. Each node contains a value and a list of references to its children. The first node is called the root. A node with no children is called a leaf. No cycles are allowed in a tree, i.e. a child cannot be an ancestor of its parent. The most common type of tree is the binary tree, where each node has at most two children.

Mathematically, a binary tree is a recursive data structure. A binary tree is either empty or consists of a root node and two binary trees, called the left and right children. Thus, a binary tree T is

$$T = \begin{cases} \varnothing & \text{if it is empty, or} \\ (v, T_l, T_r) & \text{if it has a value } v \text{ and two children } T_l \text{ and } T_r. \end{cases}$$

Note that the left and right children are themselves binary trees. If T is a leaf, then $T_l = T_r = \varnothing$.

This properties makes it easy to represent a binary tree using parentheses notation. For example, $(1, (2, \varnothing, \varnothing), (3, \varnothing, \varnothing))$ is a binary tree with root 1, left child 2, and right child 3.

Graphs A graph is also a collection of nodes. Each node contains a value and a list of references to its neighbors; the references are called edges. A graph can be directed or undirected. A graph is directed if the edges have a direction.

Mathematically, a graph is a pair $G = (V, E)$, where V is a set of vertices and $E \in V \times V$ is a set of edges. An edge is a pair of vertices, i.e. $e = (v_i, v_j)$, where $v_i, v_j \in V$. If the graph is directed, the edge is an ordered pair, i.e. $e = (v_i, v_j) \neq (v_j, v_i)$.

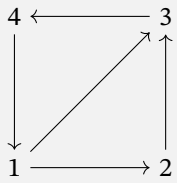
Not only each node can hold a value, but also each edge can have a weight. A weighted graph is a graph where there exists a function $w : E \to \mathbb{R}$ that assigns a real number to each edge.

A graphical representation of a directed graph with four vertices and five edges is shown in fig. 2.2. The vertices are numbered from 1 to 4, and the edges are represented by arrows.

Another common representation of a graph is the adjacency matrix. An adjacency matrix is a square matrix A of size $n \times n$, where n is the number of vertices. The i, j-th entry of the matrix is 1 if there is an edge from vertex i to vertex j, and 0 otherwise. The adjacency matrix of the graph in fig. 2.2 is

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Figure 2.2: A graph with four vertices and five edges.



A graph with four vertices and five edges. Vertices are numbered from 1 to 4, and edges are represented by arrows. The graph is directed, as the edges have a direction.

2.2 Set theory

A set is a collection of elements. The elements of a set can be anything, including other sets. The elements of a set are unordered, and each element is unique. The most common notation for sets is the curly braces notation, e.g. $\{1, 2, 3\}$.

Some special sets are listed below.

Universe set The universe set is the set of all elements in a given context. It is denoted by Ω.

Empty set The empty set is the set with no elements. It is denoted by the symbol $\varnothing$. Depending on the context, it can also be denoted by $\{\}$.

2.2.1 Set operations

The basic operations on sets are union, intersection, difference, and complement.

Union The union of two sets A and B is the set of elements that are in A or B. It is denoted by $A \cup B$. For example, the union of $\{1, 2, 3\}$ and $\{3, 4, 5\}$ is $\{1, 2, 3, 4, 5\}$.

Intersection The intersection of two sets A and B is the set of elements that are in both A and B. It is denoted by $A \cap B$. For example, the intersection of $\{1, 2, 3\}$ and $\{3, 4, 5\}$ is $\{3\}$.

Difference The difference of two sets A and B is the set of elements that are in A but not in B. It is denoted by $A \setminus B$. For example, the difference of $\{1, 2, 3\}$ and $\{3, 4, 5\}$ is $\{1, 2\}$.

Complement The complement of a set A is the set of elements that are not in A. It is denoted by $A^c = \Omega \setminus A$.

Inclusion Inclusion is a relation between sets. A set A is included in a set B if all elements of A are also elements of B. It is denoted by $A \subseteq B$.

2.2.2 Set operations properties

Union and intersection are commutative, associative and distributive. Thus, given sets A, B, and C, the following statements hold:

- *Commutativity:* $A \cup B = B \cup A$ and $A \cap B = B \cap A$;
- *Associativity:* $(A \cup B) \cup C = A \cup (B \cup C)$ and $(A \cap B) \cap C = A \cap (B \cap C)$;
- *Distributivity:* $A \cup (B \cap C) = (A \cup B) \cap (A \cup C)$ and $A \cap (B \cup C) = (A \cap B) \cup (A \cap C)$.

The difference operation can be expressed in terms of union and intersection as

$$A \setminus B = A \cap B^c.$$

The complement of the union of two sets is the intersection of their complements, i.e.

$$(A \cup B)^c = A^c \cap B^c.$$

Similarly, the complement of the intersection of two sets is the union of their complements, i.e.

$$(A \cap B)^c = A^c \cup B^c.$$

This property is known as De Morgan's laws.

In terms of inclusion, given sets A, B, and C, the following statements hold:

- *Reflexity:* $A \subseteq A$;
- *Antisymmetry:* $A \subseteq B$ and $B \subseteq A$ if and only if $A = B$;
- *Transitivity:* $A \subseteq B$ and $B \subseteq C$ implies $A \subseteq C$.

2.2.3 Relation to Boolean algebra

Set operations are closely related to Boolean algebra. In Boolean algebra, the elements of a set are either true or false, many times represented by 1 and 0, respectively. The union operation is equivalent to the logical OR operation, expressed by the symbol $\vee$; and the intersection operation is equivalent to the logical AND operation, expressed by the symbol $\wedge$. The compliment operation is equivalent to the logical NOT operation, expressed by the symbol $\neg$.

The distributive property of set operations is equivalent to the distributive property of Boolean algebra. Important properties like De Morgan's laws also hold in Boolean algebra, i.e. $\neg(A \vee B) = \neg A \wedge \neg B$ and $\neg(A \wedge B) = \neg A \vee \neg B$.

Boolean algebra is the foundation of digital electronics and computer science. The logical operations are implemented in hardware using logic gates, and the logical operations are used in programming languages to control the flow of a program.

Reader interested in more details about Boolean algebra and Discrete Mathematics should consult Rosen (2018)[6].

2.3 Linear algebra

Linear algebra is the branch of mathematics that studies vector spaces and linear transformations. It is a fundamental tool in many areas of science and engineering. The basic objects of linear algebra are vectors and matrices.

Vector A vector is an ordered collection of numbers. It is denoted by a bold lowercase letter, e.g. $\mathbf{v} = [v_i]_{i=1,\ldots,n}$ is a vector of length n.

Matrix A matrix is a rectangular collection of numbers. It is denoted by an uppercase letter, e.g. $A = (a_{ij})_{i=1,\ldots,n;\ j=1,\ldots,m}$ is the matrix with n rows and m columns.

Tensor Tensors are generalizations of vectors and matrices. A tensor of rank k is a multidimensional array with k indices. Scalars are tensors of rank 0, vectors are tensors of rank 1, and matrices are tensors of rank 2. Tensors are commonly used in machine learning and physics.

[6] K. H. Rosen (2018). *Discrete Mathematics and Its Applications*. 8th ed. McGraw Hill, p. 1120. ISBN: 9781259676512.

2.3.1 Operations

The main operations in linear algebra are presented below.

Addition The sum of two vectors $\mathbf{v}$ and $\mathbf{w}$ is the vector $\mathbf{v} + \mathbf{w}$ whose i-th entry is $v_i + w_i$. The sum of two matrices A and B is the matrix $A + B$ whose i, j-th entry is $a_{ij} + b_{ij}$. (The same rules apply to subtraction.)

Scalar multiplication The product of a scalar α and a vector $\mathbf{v}$ is the vector $\alpha\mathbf{v}$ whose i-th entry is αv_i. Similarly, the product of a scalar α and a matrix A is the matrix αA whose i, j-th entry is αa_{ij}.

Dot product The dot product of two vectors $\mathbf{v}$ and $\mathbf{w}$ is the scalar

$$\mathbf{v} \cdot \mathbf{w} = \sum_{i=1}^{n} v_i w_i.$$

The dot product is also called the inner product.

Matrix multiplication The product of two matrices A and B is the matrix $C = AB$ whose i, j-th entry is

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}.$$

The number of columns of A must be equal to the number of rows of B, and the resulting matrix C has the same number of rows as A and the same number of columns as B. Unless otherwise stated, we consider the vector $\mathbf{v}$ with length n as a column matrix, i.e. a matrix with one column and n rows.

Transpose The transpose of a matrix A is the matrix A^T whose i, j-th entry is the j, i-th entry of A. If A is a square matrix, then A^T is the matrix obtained by reflecting A along its main diagonal.

Determinant The determinant of a square matrix A is a scalar that is a measure of the (signed) volume of the parallelepiped spanned by the columns of A. It is denoted by $\det(A)$ or $|A|$.

The determinant is nonzero if and only if the matrix is invertible and the linear map represented by the matrix is an isomorphism – i.e.

it preserves the dimension of the vector space. The determinant of a product of matrices is the product of their determinants.

Particularly, the determinant of a 2×2 matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc.$$

Inverse matrix An $n \times n$ matrix A has an inverse $n \times n$ matrix A^{-1} if

$$AA^{-1} = A^{-1}A = I_n,$$

where I_n is the $n \times n$ identity matrix, i.e. a matrix whose diagonal entries are 1 and all other entries are 0. If such a matrix exists, A is said *invertible*. A square matrix that is not invertible is called singular. A square matrix with entries in a field is singular if and only if its determinant is zero.

To calculate the inverse of a matrix, we can use the formula

$$A^{-1} = \frac{1}{\det(A)} \operatorname{adj}(A),$$

where $\operatorname{adj}(A)$ is the adjugate (or adjoint) of A, i.e. the transpose of the cofactor matrix of A.

The cofactor of the i, j-th entry of a matrix A is the determinant of the matrix obtained by removing the i-th row and the j-th column of A, multiplied by $(-1)^{i+j}$.

In the case of a 2×2 matrix, the inverse is

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}.$$

2.3.2 Systems of linear equations

A system of linear equations is a collection of linear equations that share their unknowns. It is usually written in matrix form as $A\mathbf{x} = \mathbf{b}$, where A is a matrix of constants, $\mathbf{x}$ is a vector of unknowns, and $\mathbf{b}$ is a vector of constants.

The system has a unique solution if and only if the matrix A is invertible. The solution is $\mathbf{x} = A^{-1}\mathbf{b}$.

2.3.3 Eigenvalues and eigenvectors

An eigenvalue of an $n \times n$ square matrix A is a scalar λ such that there exists a non-zero vector $\mathbf{v}$ satisfying

$$A\mathbf{v} = \lambda\mathbf{v}. \tag{2.1}$$

The vector $\mathbf{v}$ is called an eigenvector of A corresponding to λ.

The eigenvalues of a matrix are the roots of its characteristic polynomial, i.e. the roots of the polynomial $\det(A - \lambda I_n) = 0$, where I_n is the $n \times n$ identity matrix.

2.4 Probability

Probability is the branch of mathematics that studies the likelihood of events. It is used to model uncertainty and randomness. The basic objects of probability are events and random variables.

For a comprehensive material about probability theory, the reader is referred to Ross (2018)[7] and Ross (2014)[8].

2.4.1 Axioms of probability and main concepts

The Kolmogorov axioms of probability are the foundation of probability theory. They are

1. The probability of an event A is a non-negative real number, i.e. $\mathrm{P}(A) \geq 0$;
2. The probability of the sample space Ω[9] is one, i.e. $\mathrm{P}(\Omega) = 1$; and
3. The probability of the union of disjoint events, $A \cap B = \varnothing$, is the sum of the probabilities of the events, i.e. $\mathrm{P}(A \cup B) = \mathrm{P}(A) + \mathrm{P}(B)$.

Sum rule A particular consequence of the third axiom is the addition law of probability. If A and B are not disjoint, then

$$\mathrm{P}(A \cup B) = \mathrm{P}(A) + \mathrm{P}(B) - \mathrm{P}(A \cap B).$$

[7] S. M. Ross (2018). *A First Course in Probability*. 10th ed. Pearson, p. 528. ISBN: 978-1292269207.

[8] S. M. Ross (2014). *Introduction to Probability Models*. 11th ed. Academic Press, p. 784. ISBN: 9780124079489.

[9] The set of all possible events.

Joint probability The joint probability of two events A and B is the probability that both events occur. It is denoted by $\mathrm{P}(A, B) = \mathrm{P}(A \cap B)$.

Law of total probability The law of total probability states that if $B_1, \ldots, B_n$ are disjoint events such that $\cup_{i=1}^{n} B_i = \Omega$, then for any event A, we have that

$$\mathrm{P}(A) = \sum_{i=1}^{n} \mathrm{P}(A, B_i).$$

Conditional probability The conditional probability of an event A given an event B is the probability that A occurs given that B occurs. It is denoted by $\mathrm{P}(A \mid B)$.

Independence Two events A and B are independent if the probability of A given B is the same as the probability of A, i.e. $\mathrm{P}(A \mid B) = \mathrm{P}(A)$. It is equivalent to $\mathrm{P}(A, B) = \mathrm{P}(A) \cdot \mathrm{P}(B)$.

Bayes' rule Bayes' rule is a formula that relates the conditional probability of an event A given an event B to the conditional probability of B given A. It is

$$\mathrm{P}(A \mid B) = \frac{\mathrm{P}(B \mid A) \cdot \mathrm{P}(A)}{\mathrm{P}(B)}. \tag{2.2}$$

Bayes' rule is one of the most important formulas in probability theory and is used in many areas of science and engineering. Particularly, for data science, it is used in Bayesian statistics and machine learning.

2.4.2 Random variables

A random variable is a function that maps the sample space Ω to the real numbers. It is denoted by a capital letter, e.g. X.

Formally, let $X : \Omega \to E$ be a random variable. The probability that X takes on a value in a set $A \subseteq E$ is

$$\mathrm{P}(X \in A) = \mathrm{P}(\{\omega \in \Omega : X(\omega) \in A\}). \tag{2.3}$$

If $E = \mathbb{R}$, then X is a continuous random variable. If $E = \mathbb{Z}$, then X is a discrete random variable. The random variable X is said to follow a certain probability distribution P — denoted by $X \sim P$ — given by its probability mass function or probability density function — see below.

Probability mass function The probability mass function (PMF) of a discrete random variable X is the function $p_X : \mathbb{Z} \to [0, 1]$ defined by

$$p_X(x) = \mathrm{P}(X = x). \tag{2.4}$$

Probability density function The probability density function (PDF) of a continuous random variable X is the function $f_X : \mathbb{R} \to [0, \infty)$ defined by

$$\mathrm{P}(a \leq X \leq b) = \int_a^b f_X(x)dx. \tag{2.5}$$

Cumulative distribution function The cumulative distribution function (CDF) of a random variable X is the function $F_X : \mathbb{R} \to [0, 1]$ defined by

$$F_X(x) = \mathrm{P}(X \leq x). \tag{2.6}$$

2.4.3 Expectation and moments

Expectation is a measure of the average value of a random variable. Moments are measures of the shape of a probability distribution.

Expectation The expectation of a random variable X is the average value of X. It is denoted by $\mathrm{E}[X]$. By definition, it is

$$\mathrm{E}[X] = \sum_x x \cdot p_X(x),$$

if X is discrete, or

$$\mathrm{E}[X] = \int_{-\infty}^{\infty} x \cdot f_X(x)dx,$$

if X is continuous.

The main properties of expectation are listed below.

The expectation operator is linear. Given two random variables X and Y and a real number c, we have

$$\mathrm{E}[cX] = c\,\mathrm{E}[X],$$

$$\mathrm{E}[X + c] = \mathrm{E}[X] + c,$$

and

$$\mathrm{E}[X + Y] = \mathrm{E}[X] + \mathrm{E}[Y].$$

Under a more general setting, given a function $g : \mathbb{R} \to \mathbb{R}$, the expectation of $g(X)$ is

$$\mathrm{E}[g(X)] = \sum_x g(x) \cdot p_X(x),$$

if X is discrete, or

$$\mathrm{E}[g(X)] = \int_{-\infty}^{\infty} g(x) \cdot f_X(x) dx,$$

if X is continuous.

Variance The variance of a random variable X is a measure of how spread out the values of X are. It is denoted by $\mathrm{V}(X)$. By definition, it is

$$\mathrm{V}(X) = \mathrm{E}\Big[(X - \mathrm{E}[X])^2\Big]. \tag{2.7}$$

Note that, as a consequence, the expectation of X^2 — called second moment — is

$$\mathrm{E}[X^2] = \mathrm{V}(X) + \mathrm{E}[X]^2,$$

since

$$\begin{aligned}
\mathrm{V}(X) &= \mathrm{E}\Big[(X - \mathrm{E}[X])^2\Big] \\
&= \mathrm{E}\big[X^2 - 2X\,\mathrm{E}[X] + \mathrm{E}[X]^2\big] \\
&= \mathrm{E}[X^2] - 2\,\mathrm{E}[X]\,\mathrm{E}[X] + \mathrm{E}[X]^2 \\
&= \mathrm{E}[X^2] - \mathrm{E}[X]^2.
\end{aligned}$$

Higher moments are defined similarly. The k-th moment of X is

$$\mathrm{E}[X^k] = \sum_x x^k \cdot p_X(x),$$

if X is discrete, or

$$\mathrm{E}[X^k] = \int_{-\infty}^{\infty} x^k \cdot f_X(x) dx,$$

if X is continuous.

Sample mean The sample mean is the average of a sample of random variables. Given a sample $X_1, \ldots, X_n$ such that $X_i \sim X$ for all i, the sample mean is

$$\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i.$$

Law of large numbers The law of large numbers states that the average of a large number of independent and identically distributed (i.i.d.) random variables converges to the expectation of the random variable. Mathematically,

$$\lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n} X_i = \mathrm{E}[X],$$

given $X_i \sim X$ for all i.

Sample variance The sample variance is a measure of how spread out the values of a sample are. Given a sample $X_1, \ldots, X_n$ such that $X_i \sim X$ for all i, the sample variance is

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2.$$

Note that the denominator is $n-1$ instead of n to correct the bias of the sample variance.

Sample standard deviation The sample standard deviation is the square root of the sample variance, i.e. $S = \sqrt{S^2}$.

Sample skewness The skewness is a measure of the asymmetry of a probability distribution. The sample skewness is based on the third moment of the sample. Given a sample $X_1, \ldots, X_n$ such that $X_i \sim X$ for all i, the sample skewness is

$$\text{Skewness} = \frac{\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^3}{S^3}.$$

Skewness is zero for a symmetric distribution, positive for a right-skewed distribution, and negative for a left-skewed distribution.

Sample kurtosis The kurtosis is a measure of the tailedness of a probability distribution. The sample kurtosis is based on the fourth moment of the sample. Given a sample $X_1, \ldots, X_n$ such that $X_i \sim X$ for all i, the sample kurtosis is

$$\text{Kurtosis} = \frac{\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^4}{S^4} - 3.$$

Kurtosis is positive if the tails are heavier than a normal distribution, and negative if the tails are lighter.

2.4.4 Common probability distributions

Several phenomena in nature and society can be modeled as random variables. Some distributions are frequently used to model these phenomena. The main ones are listed below.

Bernoulli distribution The Bernoulli distribution is a discrete distribution with two possible outcomes, usually called success and failure. It is parametrized by a single parameter $p \in [0, 1]$, which is the probability of success. It is denoted by $\text{Bern}(p)$.

The expected value of $X \sim \text{Bern}(p)$ is $\text{E}[X] = p$, and the variance is $\text{V}(X) = p(1 - p)$.

Poisson distribution The Poisson distribution is a discrete distribution that models the number of events occurring in a fixed interval of time or space. It is parametrized by a single parameter $\lambda > 0$, which is the average number of events in the interval. It is denoted by $\text{Poisson}(\lambda)$.

The probability mass function of $X \sim \text{Poisson}(\lambda)$ is

$$p_X(x) = \frac{e^{-\lambda}\lambda^x}{x!}. \tag{2.8}$$

The expected value of $X \sim \text{Poisson}(\lambda)$ is $\text{E}[X] = \lambda$, and the variance is $\text{V}(X) = \lambda$.

Normal distribution The normal distribution is a continuous distribution with a bell-shaped density. It is parametrized by two parameters, the mean $\mu \in \mathbb{R}$ and the standard deviation $\sigma > 0$. It is denoted by $\mathcal{N}(\mu, \sigma^2)$.

The special case where $\mu = 0$ and $\sigma = 1$ is called the standard normal distribution. It is denoted by $\mathcal{N}(0, 1)$.

The probability density function of $X \sim \mathcal{N}(\mu, \sigma^2)$ is

$$f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right). \tag{2.9}$$

The expected value of $X \sim \mathcal{N}(\mu, \sigma^2)$ is $\text{E}[X] = \mu$, and the variance is $\text{V}(X) = \sigma^2$.

Central limit theorem The central limit theorem states that the normalized version of the sample mean converges to a standard normal distribution[10]. Given $X_1, \dots, X_n$ i.i.d. random variables with mean μ and finite variance $\sigma^2 < \infty$,

$$\sqrt{n}(\bar{X} - \mu) \sim \mathcal{N}(0, \sigma^2),$$

as $n \to \infty$. In other words, for a large enough n, the distribution of the sample mean gets closer[11] to a normal distribution with mean μ and variance σ^2/n.

The central limit theorem is one of the most important results in probability theory and statistics. Its implications are fundamental in many areas of science and engineering.

T distribution The T distribution is a continuous distribution with a bell-shaped density. It is parametrized by a single parameter $\nu > 0$, called the degrees of freedom. It is denoted by $\mathcal{T}(\nu)$.

The T distribution generalizes to the three parameter location-scale t distribution $\mathcal{T}(\mu, \sigma^2, \nu)$, where μ is the location parameter and σ is the scale parameter. Thus, given $X \sim \mathcal{T}(\nu)$, we have that $\mu + \sigma X \sim \mathcal{T}(\mu, \sigma^2, \nu)$.

Note that

$$\lim_{\nu \to \infty} \mathcal{T}(\nu) = \mathcal{N}(0, 1).$$

Thus, the T distribution converges to the standard normal distribution as the degrees of freedom go to infinity.

Gamma distribution The Gamma distribution is a continuous distribution with a right-skewed density. It is parametrized by two parameters, the shape parameter $\alpha > 0$ and the rate parameter $\beta > 0$. It is denoted by Gamma(α, β).

The probability density function of $X \sim \text{Gamma}(\alpha, \beta)$ is

$$f_X(x) = \frac{\beta^\alpha x^{\alpha-1} e^{-\beta x}}{\Gamma(\alpha)}, \tag{2.10}$$

[10] This statement of the central limit theorem is known as the Lindeberg-Levy CLT. There are other versions of the central limit theorem, some more general and some more restrictive.

[11] Formally, this is called convergence in distribution, refer to P. Billingsley (1995). *Probability and Measure*. 3rd ed. John Wiley & Sons. ISBN: 0-471-00710-2 for more details.

where $\Gamma(\alpha)$ is the gamma function, defined by

$$\Gamma(\alpha) = \int_0^\infty t^{\alpha-1} e^{-t} dt. \tag{2.11}$$

In Bayesian analysis, the gamma distribution is commonly used as a conjugate prior. A conjugate prior is a prior distribution that, when combined with the likelihood, results in a posterior distribution that is of the same family as the prior.

2.4.5 Permutations and combinations

For the sake of the reference, we present some definitions and formulas from combinatorics. Combinatorics is the branch of mathematics that studies the counting of objects.

Factorial The factorial of a non-negative integer n is the product of all positive integers up to n. It is denoted by $n!$. By definition, $0! = 1$.

Permutation A permutation is an arrangement of a set of elements. The number of permutations of n elements is $n!$. Permutations are used in combinatorics to count the number of ways to arrange a set of elements.

Combination A combination is a selection of a subset of elements from a set. The number of combinations of k elements from a set of n elements is

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}.$$

Combinations are used in combinatorics to count the number of ways to select a subset of elements from a set. The binomial coefficient $\binom{n}{k}$ is also called a choose function.

3

Fundamental data concepts

The simple believes everything,

but the prudent gives thought to his steps.

— Proverbs 14:15 *(ESV)*

A useful start point for someone studying data science is a definition of the term itself. In this chapter, I discuss some definitions in literature and provide a definition of my own. As discussed in chapter 1, there is no consensus on the definition of data science. However, they all agree that data science is cross-disciplinary and a very important field of study.

Another important discussion is the evidence that data science is actually a new science. I argue that a "new science" is not a subject that its basis is built from the ground up[1], but a subject that has a particular object of study and that meets some criteria.

Once we establish that data science is a new science, we need to understand one core concept: data. In this book, I focus on structured data, which are data that are organized in a tabular format. I discuss the importance of understanding the nature of the data we are working with and how we represent them.

Finally, I discuss two important concepts in data science: database normalization and tidy data. Database normalization is mainly focused on the data storage. Tidy data is mainly focused on the requirements of data for analysis. Both concepts interact with each other and have their mathematical foundations. I bridge the gap between the two concepts by discussing their common mathematical foundations.

[1] As it would as improductive as creating a "new math" for each new application. All "sciences" rely on each other in some way

Chapter remarks

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3.1 Data science definition

For Zumel and Mount (2019), *"data science is a cross-disciplinary practice that draws on methods from data engineering, descriptive statistics, data mining, machine learning, and predictive analytics."* They compare the area with the operations research, stating that data science focuses on implementing data-driven decisions and managing their consequences.

Wickham, Çetinkaya-Rundel, and Grolemund (2023) state that *"data science is an exciting discipline that allows you to transform raw data into understanding, insight, and knowledge."*

I find the first definition too restrictive once new methods and techniques are always under development. We never know when new "data-related" methods will become obsolete or a trend. Also, Zumel and Mount's view gives the impression that data science is a operations research subfield. Although I do not try to prove otherwise, I think it is much more useful to see it as an independent field of study. Obviously, there are many intersections between both areas (and many other areas as well). Because of such intersections, I try my best to keep definitions and terms standardized throughout chapters, sometimes avoiding popular terms that may generate ambiguities or confusion.

The second one is not really a definition. However, it states clearly *what* data science enables us to do. From these thoughts, let's define the term.

Definition 3.1

Data science is the study of computational methods to extract knowledge from measurable phenomena.

I want to highlight the meaning of some terms in this definition. *Computational methods* means that data science methods use computers to handle data and perform the calculations. *Knowledge* means information that humans can easily understand or apply to solve problems. *Measurable phenomena* are events or processes where raw data can be quantified in some way[2]. *Raw data* are data collected directly from some source and that have not been subject to any other transformation by a software program or a human expert. *Data* is any piece of information that can be digitally stored.

[2]TODO: talk about non-measurable phenomena

Kelleher and Tierney (2018) summarize very well the challenges data science takes up: "extracting non-obvious and useful patterns from large data sets [...]; capturing, cleaning, and transforming [...] data; [storing and processing] big [...] data sets; and questions related to data ethics and regulation."

Data science contrasts with conventional sciences. Usually, a "science" is named after its object of study. Biology is the study of the life, Earth science studies the planet Earth, and so on. I argue that data science does not study data itself, but how we can use them to understand a phenomenon.

Besides, the conventional scientific paradigm is essentially model-driven: we observe a phenomenon related to the object of study, we reason the possible explanation (the model or hypothesis), and we validate our hypothesis (most of the time using data, though). In data science, however, we extract the knowledge directly and primarily from the data. The expert knowledge and reasoning may be taken into account, but we give data the opportunity to surprise us.

Thus, the objects of the study in data science are the computational methods and processes that can extract reliable and ethical knowledge from huge amounts of data.

3.2 The data science continuum

From which point a subject becomes a new science?

3.3 Fundamental data theory

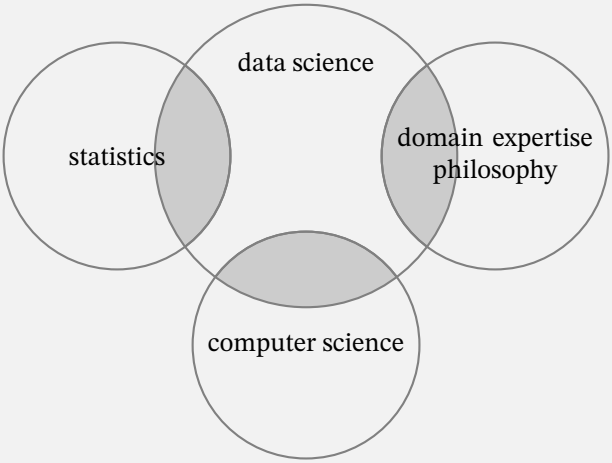
As expected, data science is not a isolated science. It incorporates several concepts from other fields and sciences. In this section, I explain the basis of each component of the provided definition.

3.3.1 Phenomena

Phenomenon is a term used to describe any observable event or process. They are the source we use to understand the world around us. In general, we use our senses to perceive phenomena. To make sense of them, we use our knowledge and reasoning.

Philosophy is the study of knowledge and reasoning. It is a very broad field of study that has been divided into many subfields. One of them is epistemology, which is the study of knowledge. Epistemology is

Figure 3.1: My view of data science.



Data science is an entire new science. Being a new science does not mean that its basis is built from the ground up. Most of the subjects in data science come from other sciences, but its object of study (computational methods to extract knowledge from measurable phenomena) is particular enough to unfold new scientific questions – such as data ethics, data collection, etc.

the field of philosophy that studies how we can acquire knowledge and how we can distinguish between knowledge and opinion. In particular, epistemology studies the nature of knowledge, justification, and the rationality of belief.

Another important subfield in philosophy is ontology, which is the study of being. It studies the nature of being, existence, or reality. Ontology is the field of philosophy that studies what exists and how we can classify it. In particular, ontology studies the nature of categories, properties, and relations.

Finally, logic is the study of reasoning. It studies the nature of reasoning and argumentation. In particular, logic studies the nature of inference, validity, and fallacies.

In the context of data science, we usually focus on phenomena from particular domain of expertise. For example, we may be interested in

the phenomena related to the stock market, the phenomena related to the weather, or the phenomena related to the human health. Thus, we need to understand the nature of the phenomena we are studying.

Thus, fully understading the phenomena we are tackling requires both a general knowledge of epistemology, ontology, and logic, and a particular knowledge of the domain of expertise.

Observe as well that we do not restrict ourselves to the "qualitative" understanding of philosophy. There are several computational methods that implements the concepts of epistemology, ontology, and logic. For example, we can use a computer to perform deductive reasoning, to classify objects, or to validate an argument. Also, we have strong mathematical foundations and computational tools to organize categories, relations, and properties.

The reason we need to understand the nature of the phenomena we are studying is that we need to guarantee that the data we are collecting are relevant to the problem we are trying to solve. Incorrectly perception of the phenomena may lead to incorrect data collection, which may lead to incorrect conclusions.

3.3.2 Measurements

In data science, we are interested in measurable phenomena. Measurable phenomena are those that we can quantify in some way. For example, the temperature of a room is a measurable phenomenon because we can measure it using a thermometer. The number of people in a room is also a measurable phenomenon because we can count them.

When we quantify a phenomenon, we perform data collection. Data collection is the process of gathering data on targeted phenomenon in an established systematic way. Systematic means that we have a plan to collect the data and we understand the consequences of the plan, including the sampling bias. Sampling bias is the influence that the method of collecting the data has on the conclusions we can draw from them. Once we have collected the data, we need to store them. Data storage is the process of storing data in a computer.

To perform those tasks, we need to understand the nature of data. Data are any piece of information that can be digitally stored. Data can be stored in many different formats. For example, we can store data in a spreadsheet, in a database, or in a text file. We can also store data in many different types. For example, we can store data as numbers, strings, or dates.

In data science, studying data types is important because they need to correctly reflect the nature of the source phenomenon and be compatible with the computational methods we are using. Data types also restrict the operations we can perform on the data.

The foundation and tools to understand data types come from computer science. Among the subfields, I highlight:

- Algorithms and data structures: the study of data types and the computational methods to manipulate them.
- Databases: the study of storing and retrieving data.

3.3.3 Knowledge extraction

Once we have collected and stored the data, we need to extract knowledge from them. In data science, we use computational methods to extract knowledge from data. These computational methods may come from many different fields. In particular, I highlight:

- Statistics: the study of data collection, organization, analysis, interpretation, and presentation.
- Machine learning: the study of computational methods that can automatically learn from data.
- Artificial intelligence: the study of computational methods that can mimic human intelligence.

Also, many other fields contribute to the development of domain-specific computational methods to extract knowledge from data. For example, in the field of biology, we have bioinformatics, which is the study of computational methods to analyze biological data. Earth sciences have geoinformatics, which is the study of computational methods to analyze geographical data. And so on.

Each method has its own assumptions and limitations. Thus, we need to understand the nature of the methods we are using. In particular, we need to understand the expected input and output of them. Whenever the available data do not match the requirements of the method, we may perform data handling[3].

[3] It is important to highlight that it is expected that some of the methods assumptions are not fully met. These methods are usually robust enough to extract valuable knowledge even when data contain imperfections, errors and noise. However, it is still useful to perform data handling to adjust data as much as possible.

Data handling mainly includes data cleaning, data transformation, and data integration. Data cleaning is the process of detecting and correcting (or removing) corrupt or inaccurate pieces of data. Data transformation is the process of converting data from one format or type to another. Data integration is the process of combining data from different sources into a single, unified view.

3.4 Structured data

As one expects, when we measure a phenomenon, the resulting data come in many different formats. For example, we can measure the temperature of a room using a thermometer. The resulting data is a number. We can assess English proficiency using an essay test. The resulting data is a text. We can register relationships between proteins and their functions. The resulting data is a graph.

Thus, it is important to understand the nature of the data we are working with.

The most common data format is the *structured data*. Structured data are data that are organized in a tabular format. Each row in the table represents a single observation and each column represents a variable that describes the observation.

We restrict the kind of information we store in each cell, i.e. the data type of each measurement. Each column has a data type. The data type restrict the operations we can perform on the data. For example, we can perform arithmetic operations on numbers, but not on text.

The most common classification of data types is Stevens's types: nominal, ordinal, interval, and ratio. Nominal data are data that can be classified into categories. Ordinal data are data that can be classified into categories and ordered. Interval data are data that can be classified into categories, ordered, and measured in fixed units. Ratio data are data that can be classified into categories, ordered, measured in fixed units, and have a true zero. In practice, they differ on the logical and arithmetic operations we can perform on them.

However, Stevens's types do not exhaust all possibilities for data types. For example, probabilities are bounded at both ends, and thus do not tolerate arbitrary scale shifts. Velleman and Wilkinson (1993) provide interesting insights about data types. Although I do not agree with all his points, I think it is a good reading. In particular, I agree with his criticism of statements that data types are evident from the data inde-

Table 3.1: Stevens's types.

Data type	Operations
Nominal	$=$
Ordinal	$=, <$
Interval	$=, <, +, -$
Ratio	$=, <, +, -, \times, \div$

pendent of the questions asked. The same data can be interpreted in different ways depending on the context and the goals of the analysis.

However, I do not agree with the idea that good data analysis does not assume data types. I think that data scientists should be aware of the data types they are working with and how they affect the analysis. With no bias, there is no learning. There is no such a thing as a "bias-free" analysis, the amount of possible combinations of assumptions easily grows out of control. The data scientist must take responsibility for the consequences of their assumptions. Good assumptions and hypothesis are a key part of the data science methodology.

When we work with structured data, two concepts are very important: database normalization and tidy data. Database normalization is mainly focused on the data storage. Tidy data is mainly focused on the requirements of data for analysis. Both concepts have their mathematical foundations and tools for data handling.

3.4.1 Database normalization

Database normalization is the process of organizing the columns and tables of a relational database to minimize data redundancy and improve data integrity.

Normal form is a state of a database that is free of certain types of data redundancy. Before studying normal forms, we need to understand basic concepts in the database theory and the basic operations in relational algebra.

Relational database theory

Projection The projection of a relation is the operation that returns a relation with only the columns specified in the projection. For example,

if we have a relation $X[A, B, C]$ and we perform the projection $\pi_{A,C}(X)$, we get a relation with only the columns A and C, i.e. $X[A, C]$.

Join The (natural) join of two relations is the operation that returns a relation with the columns of both relations. For example, if we have two relations $S[U \cup V]$ and $T[U \cup W]$, where U is the common set of attributes, join $S \bowtie T$ of S and T is the relation with tuples (u, v, w) such that $(u, v) \in S$ and $(u, w) \in T$. The generalized join is built up out of binary joins: $\bowtie \{R_1, R_2, \ldots, R_n\} = R_1 \bowtie R_2 \bowtie \cdots \bowtie R_n$. Since the join operation is associative and commutative, we can parenthesize however we want.

Functional dependency A functional dependency is a constraint between two sets of attributes in a relation. It is a statement that if two tuples agree on certain attributes, then they must agree on another attribute. Specifically, the *functional dependency* $U \to V$ holds in R if and only if for every pair of tuples t_1 and t_2 in R such that $t_1[U] = t_2[U]$, it is also true that $t_1[V] = t_2[V]$.

Multi-valued dependency A multi-valued dependency is a constraint between two sets of attributes in a relation. It is a statement that if two tuples agree on certain attributes, then they must agree on another set of attributes. Specifically, the *multi-valued dependency* $U \twoheadrightarrow V$ holds in R if and only if $R = R[UV] \bowtie R[UW]$, where W are the remaining attributes.

Join dependency A join dependency is a constraint between subsets of attributes (not necessarily disjoint) in a relation. R obeys the join dependency $*\{X_1, X_2, \ldots, X_n\}$ if $R = \bowtie \{R[X_1], R[X_2], \ldots, R[X_n]\}$.

Normal forms

First normal form (1NF) A relation is in 1NF if and only if all attributes are atomic. An attribute is atomic if it is not a set of attributes. For example, the relation $R[A, B, C]$ is in 1NF if and only if A, B, and C are atomic.

Second normal form (2NF) A relation is in 2NF if and only if it is in 1NF and every non-prime attribute is fully functionally dependent on the primary key. A non-prime attribute is an attribute that is not part

of the primary key. A primary key is a set of attributes that uniquely identifies a tuple. A non-prime attribute is fully functionally dependent on the primary key if it is functionally dependent on the primary key and not on any subset of the primary key. For example, the relation $R[U \cup V]$ is in 2NF if and only if $U \rightarrow X$, $\forall X \in V$ and there is no $W \subset U$ such that $W \rightarrow X$, $\forall X \in V$.

Third normal form (3NF) A relation is in 3NF if and only if it is in 2NF and every non-prime attribute is non-transitively dependent on the primary key. A non-prime attribute is non-transitively dependent on the primary key if it is not functionally dependent on another non-prime attribute. For example, the relation $R[U \cup V]$ is in 3NF if and only if U is the primary key and there is no $X \in V$ such that $X \rightarrow Y$, $\forall Y \in V$.

Boyce-Codd normal form (BCNF) A relation R with attributes X is in BCNF if and only if it is in 2NF and for each nontrivial functional dependency $U \rightarrow V$ in R, the functional dependency $U \rightarrow X$ is in R. In other words, a relation is in BCNF if and only if every functional dependency is the result of keys.

Fourth normal form (4NF) A relation R with attributes X is in 4NF if and only if it is in 2NF and for each nontrivial multi-valued dependency $U \twoheadrightarrow V$ in R, the functional dependency $U \rightarrow X$ is in R. In other words, a relation is in 4NF if and only if every multi-valued dependency is the result of keys.

Projection join normal form (PJNF) A relation R with attributes X is in PJNF[4] if and only if it is in 2NF and the set of key dependencies[5] of R impllies each join dependency of R. The PJNF guarantees that the table cannot be decomposed without losing information (except by decompositions based on keys).

Note that the ideia behind the definition of BCNF and 4NF are slightly different from the PJNF. In fact, if we consider that for each key dependency implies a join dependency, the relation is in the so-called over-

[4] Also known as fifth normal form (5NF).

[5] Key dependency is a functional dependency in the form $K \rightarrow X$.

strong projection-join normal form[6]. Such a level of normalization does not improve data storage or eliminate inconsistencies. In practice, it means that if a relation is in PJNF, careless joins — i.e. those that violate a join dependency — produce inconsistent results.

Example 1 Consider the 2NF relation $R[A, B, C, D]$ with the functional dependencies $A \to B$, $B \to C$, $C \to D$. The relation is not in 3NF because C is transitively dependent on A. To normalize it, we can decompose it into the relations $R_1[A, B, C]$ and $R_2[C, D]$. Now, R_2 is in 3NF and R_1 is in 2NF, but not in 3NF. We can decompose R_1 into the relations $R_3[A, B]$ and $R_4[B, C]$. The original relation can be reconstructed by $\bowtie \{R_2, R_3, R_4\}$.

Example 2 Consider the 2NF relation $R[ABC]$[7] such that the primary key is the composite of A, B, and C. The relation is thus in the 4NF, as no column is a determinant of another column. Suppose, however, the following constraint: if (a, b, c'), (a, b', c), and (a', b, c) are in R, then (a, b, c) is also in R. This can be illustrated if we consider A as a agent, B as a product, and C as a company. If an agent a represents companies c and c', and product b is in his portfolio, then assuming both companies make b, a must offer b from both companies.

The relation is not in PJNF, as the join dependency $*\{AB, AC, BC\}$ is not implied by the primary key. (In fact, the only functional dependency is the trivial $ABC \to ABC$.) In this case, to avoid redundancies and inconsistencies, we must split the relation into the relations $R_1[AB]$, $R_2[AC]$, and $R_3[BC]$.

It is iteresting to notice that in this case, the relation $R_1 \bowtie R_2$ might contain tuples that do not make sense in the context of the original relation. For example, if R_1 contains (a, b) and R_2 contains (a, c'), the join contains (a, b, c'), which might not be a valid tuple in the original relation if (b, c') is not in R_3. *This is very important to notice, as it is a common mistake to assume that the join of the decomposed relations always contains valid tuples.*

Example 3 Consider the 2NF relation $R[A, B, C, D, E]$ with the functional dependencies $A \to D$, $AB \to C$, and $B \to E$. To make it PJNF, we

[6] R. Fagin (1979). "Normal forms and relational database operators". In: *Proceedings of the 1979 ACM SIGMOD International Conference on Management of Data*. SIGMOD '79. Boston, Massachusetts: Association for Computing Machinery, pp. 153–160. ISBN: 089791001X. DOI: 10.1145/582095.582120. URL: https://doi.org/10.1145/582095.582120.

[7] Here we abreviate A, B, C as ABC.

can decompose it into the relations $R_1[A, D]$, $R_2[A, B, C]$, and $R_3[B, E]$. The original relation can be reconstructed by $\bowtie \{R_1, R_2, R_3\}$. However, unlike the previous example, the join of the decomposed relations always contains valid tuples — excluding degenerate joins, where there are no common attributes. The reason is that all join dependencies implied by the key dependencies are trivial when reduced[8].

3.4.2 Tidy data

It is estimated that 80% of the time spent on data analysis is spent on data preparation. Usually, the same process is repeated many times in different datasets. The ideia is that organized data carries the meaning of the data, reducing the time spent on handling the data to get it into the right format for analysis.

Tidy data is a data format that provides a standardized way to organize data values within a dataset. The main advantage of tidy data is that it provides clear semantics with focus on only one view of the data.

Many data formats might be ideal for particular tasks, such as raw data, dense tensors, or normalized databases. However, most of the statitiscal and machine learning methods require a particular data format. Tidy data is a data format that is appropriate to those tasks.

Wickham's thoughts on tidy data

Like families, tidy datasets are all alike but every messy dataset is messy in its own way.

In an unrestricted table, the meaning of rows and columns are not fixed. In a tidy table, the meaning of rows and columns are fixed.

It is based on the idea that a dataset is a collection of values, where:

- Each *value* belongs to a variable and an observation.
- Each *variable*, represented by a column, contains all values that measure the same attribute across (observational) units.

[8] A proof in under development based on M. W. Vincent (1997). "A corrected 5NF definition for relational database design". In: *Theoretical Computer Science* 185.2. Theoretical Computer Science in Australia and New Zealand, pp. 379–391. ISSN: 0304-3975. DOI: https://doi.org/10.1016/S0304-3975(97)00050-9. URL: https://www.sciencedirect.com/science/article/pii/S0304397597000509.

- Each *observation*, represented by a row, contains all values measured on the same unit across attributes.
- *Attributes* are the characteristics of the units, e.g. height, temperature, duration.
- *Observational units* are the individual entities being measured, e.g. a person, a day, an experiment.

Table 3.2 summarizes the main concepts.

Table 3.2: Tidy data concepts.

Concept	Structure	Contains	Across
Variable	Column	Same attribute	Units
Observation	Row	Same unit	Attributes

If we follow this structure, the meaning of data is implicit in the table itself. However, it is not always trivial to organize data in a tidy format. Usually, we have more than one level of observational units, each one represented by a table. Moreover, there might exist more than one way to define what are the observational units in a dataset.

To organize data in a tidy format, one can consider that:

- Attributes are functionally related among themselves — e.g. Z is a linear combination of X and Y, or X and Y are correlated, or $P(X, Y)$ follows some joint distribution.
- Units can be grouped or compared — e.g. person A is taller than person B, or the temperature in day 1 is higher than in day 2.

A particular point that tidy data do not address is that values in a column might not be in the same scale or unit of measurement[9]. For example, a column might contain the temperature in an experiment, and another column might contain the unit of measurement that was used to measure the temperature. This is a common problem in databases, and it must be addressed for machine learning and statistical methods to work properly.

[9] Attention: observational unit is not unit of measurement.

Note that the order of the rows and columns is not important. However, it might be convenient to sort data in a particular way to facilitate the understanding. For instance, one usually expects that the first columns are *fixed variables*[10], i.e. variables that are not the result of a measurement, and the last columns are *measured variables*. Also, arranging rows by some variable might highlight some pattern in the data.

Usually, columns are named — the collection of all column names is called the header, while rows are numerically indexed.

Common messy datasets

Wickham (2014) lists some common problems with messy datasets and how to tidy them[11]. The problems are summarized below.

Headers are values, not variable names For example, consider table 3.3. This table is not tidy because the column headers are values, not variable names. This format is frequently used in presentations since it is more compact. It is also useful to perform matrix operations. However, it is not appropriate for general analysis.

Table 3.3: Messy table, from Pew Forum dataset, where headers are values, not variable names.

Religion	<$10k	$10-20k	$20-30k	...
Agnostic	27	34	60	...
Atheist	12	27	37	...
Buddhist	27	21	30	...
...	...	...	...	...

To make it tidy, we can transform it into the table 3.4 by explicitly introducing variables *Income* and *Frequency*. Note that the table is now longer, but it is also narrower. This is a common pattern when fixing this kind of issue. The table is now tidy because the column headers are variable names, not values.

Multiple variables are stored in one column For example, consider the table 3.5. This table is not tidy because the column — interestly

[10] Closely related (and potentially the same as) key in database theory.

[11] Operations are presented in chapter 6.

Table 3.4: Tidy version of table 3.3 where values are correctly moved.

Religion	Income	Frequency
Agnostic	<$10k	27
Agnostic	$10-20k	34
Agnostic	$20-30k	60
...	...	...
Atheist	<$10k	12
Atheist	$10-20k	27
Atheist	$20-30k	37
...	...	...

called *column* —, contains multiple variables. This format is frequent, and sometimes the column name contains the names of the variables. Sometimes it is very hard to separate the variables.

Table 3.5: Messy table, from TB dataset, where multiple variables are stored in one column.

country	year	column	cases	...
AD	2000	m014	0	...
AD	2000	m1524	0	...
AD	2000	m2534	1	...
AD	2000	m3544	0	...
...	...	...	...	

To make it tidy, we can transform it into the table 3.6. Two columns are created to contain the variables *Sex* and *Age*, and the old column is removed. The table keeps the same number of rows, but it is now wider. This is a common pattern when fixing this kind of issue. The new version usually fixes the issue of correctly calculating ratios and frequency.

Variables are stored in both rows and columns For example, consider the table 3.7. This is the most complicated case of messy data.

Table 3.6: Tidy version of table 3.5 where values are correctly moved.

country	year	sex	age	cases	...
AD	2000	m	0–14	0	...
AD	2000	m	15–24	0	...
AD	2000	m	25–34	1	...
AD	2000	m	35–44	0	...
...	...	...	...	...	

Usually, one of the columns contains the names of the variables, in this case the column *element*.

Table 3.7: Messy table, adapted from airquality dataset, where variables are stored in both rows and columns.

id	year	month	element	d1	d2	...	d31
MX17004	2010	1	tmax		24	...	27
MX17004	2010	1	tmin	14		...	
MX17004	2010	2	tmax	27	24	...	27
MX17004	2010	2	tmin	14		...	13
...	...	...	...	...	...	...	...

To fix this issue, we must first decide which column contains the names of the variables. Then, we must lengthen the table in function of the variables (and potentially their names), as seen in table 3.8. Aftwards, we widen the table in function of their names. Finally, we remove implicit information, as seen in table 3.9.

Multiple types of observational units are stored in the same table For example, consider the table 3.10. It is very common during data collection that many observational units are registered in the same table.

To fix this issue, we must each observation unit must be moved to a different table. Sometimes, it is useful to create unique identifiers for each observation. The separation avoids several types of potential inconsistencies. However, take into account that during data analysis, it

Table 3.8: Partial solution to tidy table 3.7. Note that the table is now longer.

id	date	element	value
MX17004	2010-01-01	tmax	
MX17004	2010-01-01	tmin	14
MX17004	2010-01-02	tmax	24
MX17004	2010-01-02	tmin	
...	...	...	...

Table 3.9: Tidy version of table 3.7 where values are correctly moved.

id	date	tmin	tmax
MX17004	2010-01-01	14	
MX17004	2010-01-02		24
...	...	...	...

Table 3.10: Messy table, adapted from billboard dataset, where multiple types of observational units are stored in the same table.

year	artist	track	date	rank
2000	2 Pac	Baby Don't Cry	2000-02-26	87
2000	2 Pac	Baby Don't Cry	2000-03-04	82
2000	2 Pac	Baby Don't Cry	2000-03-11	72
2000	2 Pac	Baby Don't Cry	2000-03-18	77
...	...	...	...	...
2000	2Ge+her	The Hardest...	2000-09-02	91
2000	2Ge+her	The Hardest...	2000-09-09	87
2000	2Ge+her	The Hardest...	2000-09-16	92
...	...	...	...	...

is possible that we have to denormalize them. The two resulting tables are shown in table 3.11 and table 3.12.

Table 3.11: Tidy version of table 3.10 containing the observational unit *track*.

track id	artist	track
1	2 Pac	Baby Don't Cry
2	2Ge+her	The Hardest Part Of Breaking Up
...	...	...

Table 3.12: Tidy version of table 3.10 containing the observational unit *rank of the track in certain week*.

track id	date	rank
1	2000-02-26	87
1	2000-03-04	82
1	2000-03-11	72
1	2000-03-18	77
...	...	...
2	2000-09-02	91
2	2000-09-09	87
2	2000-09-16	92
...	...	...

A single observational unit is stored in multiple tables For example, consider tables 3.13 and 3.14. It is very common during data collection that a single observational unit is stored in multiple tables. Usually, the table (or file) itself represents the value of a variable. When columns are compatible, it is straightforward to combine the tables.

To fix this issue, we must first make the columns compatible. Then, we can combine the tables adding a new column that identifies the origin of the data. The resulting table is shown in table 3.15.

Table 3.13: Messy tables, adapted from nycflights13 dataset, where a single observational unit is stored in multiple tables. Assume that the origin filename is called `2013.csv`.

month	day	time	...
1	1	517	...
1	1	533	...
1	1	542	...
1	1	544	...
...	...	...	...

Table 3.14: Messy tables, adapted from nycflights13 dataset, where a single observational unit is stored in multiple tables. Assume that the origin filename is called `2014.csv`.

month	day	time	...
1	1	830	...
1	1	850	...
1	1	923	...
1	1	1004	...
...	...	...	...

Table 3.15: Tidy data where tables 3.13 and 3.14 are combined.

year	month	day	time	...
2013	1	1	517	...
2013	1	1	533	...
2013	1	1	542	...
2013	1	1	544	...
...	...	...	...	...
2014	1	1	830	...
2014	1	1	850	...
2014	1	1	923	...
2014	1	1	1004	...
...	...	...	...	...

3.4.3 Bridging normalization, tidyness, and data theory

First and foremost, both concepts, normalization and tidy data, are not in conflict.

In data normalization, given a set of functional, multivalued and join dependencies, there exists a normal form that is free of redundancy. In tidy data, Wickham, Çetinkaya-Rundel, and Grolemund also state that there is only one way to organize the given data.

Wickham (2014) states that tidy data is 3NF. However, he does not provide a formal proof. Since tidy data focuses on data analysis and not on data storage, I argue that there is more than one way to organize the data in a tidy format. It actually depends on what you define as the observational unit.

Consider the following example. We want to study the *phenomenon* temperature in a certain city. We fix three sensors in different locations to measure the temperature. We collect data three times a day. If we consider as the observational unit the event of measuring the temperature, we can organize the data in a tidy format as shown in table 3.16.

Table 3.16: Tidy data where the observational unit is the event of measuring the temperature.

date	time	sensor	temperature
2023-01-01	00:00	1	20
2023-01-01	00:00	2	21
2023-01-01	00:00	3	22
2023-01-01	08:00	1	21
2023-01-01	08:00	2	22
2023-01-01	08:00	3	23
...	...	...	...

However, since the sensors are fixed, we can consider the observational unit as the *temperature at some time*. In this case, we can organize the data in a tidy format as shown in table 3.17.

In both cases, one can argue that the data is also normalized. In the first case, the primary key is the composite of the columns *date*, *time*, and *sensor*. In the second case, the primary key is the composite of the columns *date* and *time*.

Table 3.17: Tidy data where the observational unit is the temperature at some time.

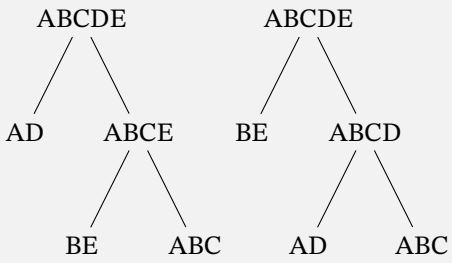
date	time	temp. 1	temp. 2	temp. 3
2023-01-01	00:00	20	21	22
2023-01-01	08:00	21	22	23
...	...	...	...	...

One can state that the first form is more appropriate, since it is flexible to add more sensors. However, the second form is very natural for machine learning and statistical methods. Given the definition of tidy data, I believe both forms are correct.

Another very interesting conjecture is whether we can formalize the eventual *change of observational unit* in terms of the order that joins and grouping operations are performed.

Example Consider the following example: the relation $R[A, B, C, D, E]$ and the functional dependencies $A \to D, B \to E$, and $AB \to C$. The relation can be normalized up to 3NF by following one of the decomposition trees shown in fig. 3.2. Every decomposition tree must take into account that the join of the projections are lossless and dependency preserving.

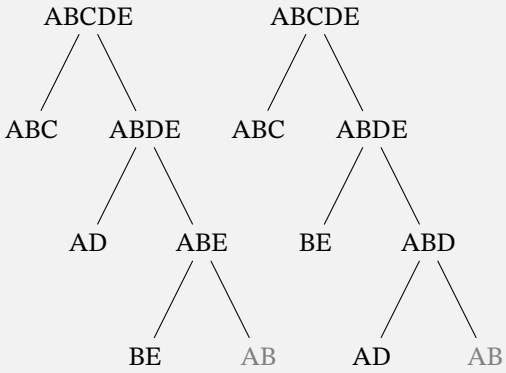
Figure 3.2: Decomposition trees for the relation $R[ABCDE]$ and the functional dependencies $A \to D$, $B \to E$, and $AB \to C$ to reach 3NF.



Note that the decomposition that splits first $R[ABC]$ is not valid, since the resulting relation $R[AB]$ is not a consequences of a functional

dependency, see fig. 3.3.

Figure 3.3: Invalid decomposition trees for the relation $R[ABCDE]$.



We consider the functional dependencies $A \to D$, $B \to E$, and $AB \to C$. Note that $R[AB]$ is not a consequence of a functional dependency.

In this kind of relation schema, we have a set of key attributes, here $\mathcal{K} = AB$, and a set of non-prime attributes, here $\mathcal{N} = CDE$. Note that the case $\mathcal{K} \cap \mathcal{N} = \varnothing$ is the simplest we can have.

Observe, however, that transitive dependencies[12] and complex join dependencies restrict even further the joins we are allowed to perform. Further formalization and study is under progress.

Now, consider a very common case: in our dataset, keys are unknown. Let A be a student id, B be the course id, D be the student age, E be the course load, and C be the student grade at the course. If only CDE is known, the table $R[CDE]$ is already tidy — and the observational unit is the enrollment — once there is no key to perform any kind of normalization. This happens in many cases where privacy is a concern.

But we can also consider that the observational unit is the student. In this case, we must perform joins traversing the leftmost decomposition tree in fig. 3.2 from bottom to top. After each join, a summarization operation is performed on the relation considering the student as

[12] Actually, when an attribute is both key and non-prime, some joins may generate invalid tables.

the observational unit, i.e. over attribute A. The first join results in relation $R[ABCE]$ and the summarization operation results in a new relation $R[AFG]$ where F is the average grade and G is the total course load taken by the student. They all calculated based on the rows that are grouped in function of A. It is important to notice that, after the summarization operation, all observations must contain a different value of A. The second join results in relation $R[ADFG] = R[AD] \bowtie R[AFG]$. This relation has functional dependency $A \rightarrow DFG$, and it is in 3NF (which is also tidy).

Unfortunately, it is not trivial to calculate all possible decomposition trees for a given dataset. Further formalization and study is under progress.

3.4.4 Data semantics and interpretation

In the rest of the book, we focus on a statistical view of the data. Besides the functional dependencies, we also consider the statistical dependencies of data. For instance, attributes A and B might not be functionally dependent, but they might exits unknown $P(A, B)$ that we can estimate from the data. Each observed value of a key can represent a instance of a random variable, and the other attributes can represent measured attributes or calculated properties.

For data analysis, it is very important to understand the relationships between the observations. For example, we might want to know if the observations are independent, if they are identically distributed, or if there is a known selection bias. We might also want to know if the observations are dependent on time, and if there are hidden variables that affect the observations.

Following wrong assumptions can lead to wrong conclusions. For example, if we assume that the observations are independent, but they are not, we might underestimate the variance of the estimators.

Although we not focus on time series, we must consider the temporal dependence of the observations. For example, we might want to know how the observation x_t is affected by x_{t-1}, x_{t-2}, and so on. We might also want to know if Markov property holds, and if there is periodicity and seasonality in the data.

For the sake of the scope of this book, we suggest that any prediction on temporal data should be done in the state space, where it is safer to assume that observations are independent and identically distributed. This is a common practice in reinforcement learning and deep

learning. Takens' theorem[13] allows you to reconstruct the state space of a dynamical system using time-delay embedding. Given a single observed time series, you can create a multidimensional representation of the underlying dynamical system by embedding the time series in a higher-dimensional space. This embedding can reveal the underlying dynamics and structure of the system.

3.5 Unstructured data

Unstructured data are data that do not have a predefined data model or are not organized in a predefined manner. For example, text, images, and videos are unstructured data.

Every unstructured dataset can be converted into a structured dataset. However, the conversion process is not always straightforward nor lossless. For example, we can convert a text into a structured dataset by counting the number of occurrences of each word. However, we lose the order of the words in the text.

The study of unstructured data is, for the moment, out of the scope of this book.

[13] F. Takens (2006). "Detecting strange attractors in turbulence". In: *Dynamical Systems and Turbulence, Warwick 1980: proceedings of a symposium held at the University of Warwick 1979/80*. Springer, pp. 366–381.

4

Data science project

Figured I could throw myself a pity party or go back to school and learn the computers.

— Don Carlton, *Monsters University (2013)*

First of all, a data science project is a software project. The difference between a data science software and a traditional software is that some components of the former is constructed from data. This means that part of the solution cannot be designed from the knowledge of the domain expert, but must be learned from the data. (Alternatively, the cost of designing the solution is too high, and it is more efficient to learn it from the data.)

One good example of a data science project is a spam filter. The spam filter is a software that classifies emails into two categories: spam and non-spam. The software is trained using a set of emails that are already classified as spam or non-spam. The software is then used to classify new emails. The software is a data science software because the classification algorithm is learned from the data, i.e. the filters are not designed "by hand".

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4.1 CRISP-DM

CRISP-DM[1] is a methodology for data mining projects. It is an acronym for Cross Industry Standard Process for Data Mining. It is a methodology that was developed in the 1990s by IBM, and it is still widely used today.

CRISP-DM is a cyclic process. The process is composed of six phases:

1. Business understanding: this is the phase where the project objectives are defined. The objectives must be defined in a way that is measurable. The phase also includes the definition of the project plan.

2. Data understanding: this is the phase where the data is collected and explored. The data is collected from the data sources, and it is explored to understand its characteristics. The phase also includes the definition of the data quality requirements.

3. Data preparation: this is the phase where the data is prepared for the modeling phase. The data is cleaned, transformed, and aggregated. The phase also includes the definition of the modeling requirements.

4. Modeling: this is the phase where the model is trained and validated. The model is trained using the prepared data, and it is validated using the validation data. The phase also includes the definition of the evaluation requirements.

5. Evaluation: this is the phase where the model is evaluated. The model is evaluated using the evaluation data. The phase also includes the definition of the deployment requirements.

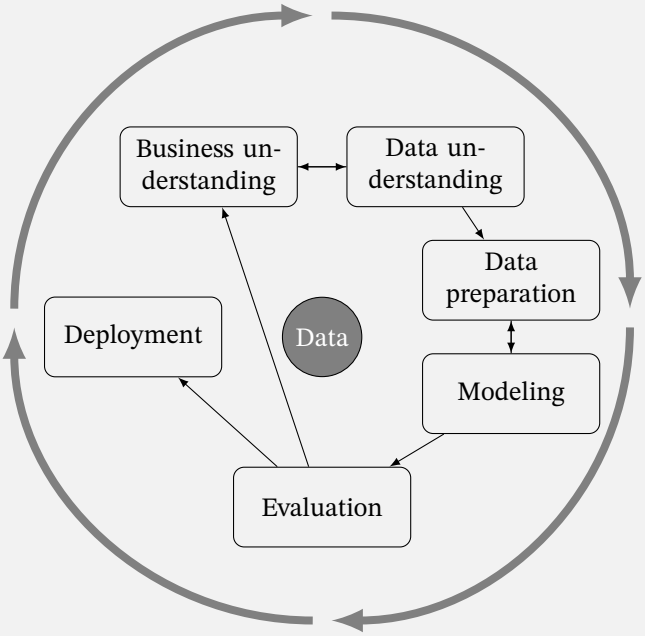
6. Deployment: this is the phase where the model is deployed. The model is deployed using the deployment requirements. The phase also includes the definition of the monitoring requirements.

Figure 4.1 shows a diagram of the CRISP-DM process. Note that the process is cyclic and completly focused on the data. The process do not address the software development aspects of the project.

The CRISP-DM methodology is a good starting point for data science projects. However, it does not mean that should be followed strictly. The

[1] Official guide available at https://www.ibm.com/docs/it/SS3RA7_18.3.0/pdf/ModelerCRISPDM.pdf.

Figure 4.1: Diagram of the CRISP-DM process.



Each block represents a phase of the CRISP-DM process. Data is the central element of the process. Arrows represent the transitions between the phases.

process is cyclic and flexible, and adaptations are possible at any stage of the process.

4.2 ZN approach

Zumel and Mount (2019) also propose a methodology for data science projects — which we call the ZN approach. Besides describing each step in a data science project, they further address the roles of each individual involved in the project. They state that data science projects are always collaborative, as they require domain expertise, data expertise, and software expertise. The requirements are dynamic, and the project has many exploratory phases. Usually, projects based on data are urgent,

and they must be completed in a short time — not only due to the business requirements, but also because the data changes over time. The authors state that agile methodologies are suitable (and necessary) for data science projects.

4.2.1 Roles of the ZN approach

In their approach, five roles are defined.

Project sponsor It is the main stakeholder of the project, the one that needs the results of the project. He represents the business interests and champions the project. The project is considered successful if the sponsor is satisfied. Note that, ideally, the sponsor can not be the data scientist, but someone that is not involved in the development of the project. However, he needs to be able to express *quantitatively* the business goals and participate actively in the project.

Client The client is the domain expert. He represents the end users' interests. In a small project, he is usually the sponsor. He translates the daily activities of the business into the technical requirements of the software.

Data scientist The data scientist is the one that sets and executes the analytic strategy. He is the one that communicates with the sponsor and the client, effectively connecting all the roles. In small projects, he can also act as the developer of the software. However, in large projects, he is usually the project manager. Although it is not required to be a domain expert, the data scientist must be able to understand the domain of the problem. He must be able to understand the business goals and the client's requirements. Most importantly, he must be able to define and to solve the right tasks.

Data architect The data architect is the one that manages data and data storage. He usually is involved in more than one project, so it is not an active participant. He that receives instructions to adapt the data storage and means to collect data.

Operations The operations role is the one that manages infrastructure and deploys final project results. He is responsible to define re-

quirements such as response time, programming language, and the infrastructure to run the software.

4.2.2 Processes of the ZN approach

Zumel and Mount's model is similar to CRISP-DM, but emphasizes that back-and-forth is possible at any stage of the process. Figure 4.2 shows a diagram of the process. The phases are:

- Define the goal: what problem are we trying to solve?
- Collect and manage data: what information do we need?
- Build the model: find patterns in the data that may solve the problem.
- Evaluate the model: is the model good enough to solve the problem?
- Present results and document: establish that we can solve the problem and how we did it. (This step is a differentiator from CRISP-DM. In ZN approach, result presentation is essential; data scientists must be able to communicate their results effectively to the client/sponsor.)
- Deploy the model: make the model available to the end users.

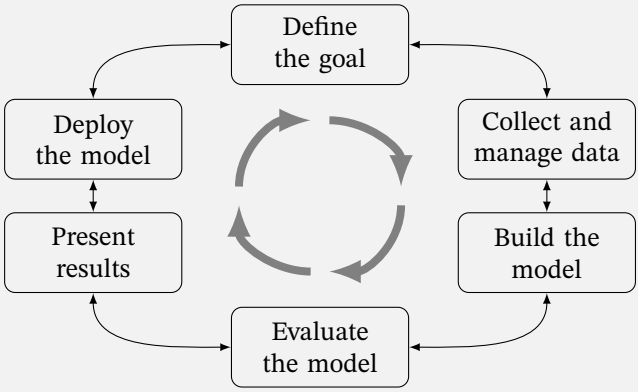
4.3 Agile methodology

Agile is a methodology for software development. It is an alternative to the waterfall methodology. The waterfall methodology is a sequential design where each phase must be completed before the next phase can begin.

The four values of agile manifesto are:

- Individuals and interactions over processes and tools;
- Working software over comprehensive documentation;
- Customer collaboration over contract negotiation;
- Responding to change over following a plan.

Figure 4.2: Diagram of the data science process proposed by Zumel and Mount (2019).



Each block represents a phase of the data science process. The emphasis is on the cyclic nature of the process. Arrows represent the transitions between the phases, that can be back-and-forth.

4.4 SCRUM framework

SCRUM is an agile framework for software development. It is a process framework for managing complex projects. It is a lightweight, which means that it provides just enough guidance to be effective.

Many consider that SCRUM is not adequate for data science projects. The main reason is that SCRUM is designed for projects where the requirements are known in advance. Also, that data science projects have exploratory phases, which are not well supported by SCRUM.

I argue that this view is wrong. SCRUM is a framework, and it is designed to be adapted to the needs of the project. SCRUM is not a rigid process. In the following, I propose an extension to SCRUM that makes it suitable for data science projects.

(In real-world, most developers do not have hacking-level skills. They are not autonomous enough to work without a plan. This is especially true for "data scientists," who are often not even developers. SCRUM is a good compromise between the need for autonomy and the need for a detailed plan. Project methodology is needed to ensure that the project is completed in time and within budget.)

4.5 Our approach

The previously mentioned methodologies lack the focus on the software development aspects of the data science project. For instance, CRISP-DM defines the stages only of the data mining process, i.e. it does not explicitly address user interface or data collection. Zumel and Mount's approach addresses data collection and presentation of results, but delegates the software development to the operations role, barely mentioning it. SCRUM is a good framework for software development, but it is not designed for data science projects. It lacks the exploratory phases of data science projects.

Thus, we propose an extension to SCRUM that makes it suitable for data science projects. The extension is based on the following observations:

- Data science projects have exploratory phases;
- Data itself is a component of the solution;
- The solution is usually modularized, parts of it are constructed from data while the other parts are constructed like traditional software;
- The solution is usually deployed as a service, that must be maintained and monitored.

Moreover, we add two other values besides the agile manifesto values. They are:

- Model confidence/understanding over model performance;
- Code version control over interactive environments.

The first value is based on the observation that the model performance is not the most important aspect of the model. The most important aspect is the being sure that the model behaves as expected (and sometimes why it behaves as expected). It is not uncommon to find models that seems to perform well during evaluation steps[2], but that are not suitable for production.

The second value is based on the observation that interactive environments are not suitable for the development of the model search code, for instance. Interactive environments auxiliate the exploratory phases,

[2] Of course, when evaluation is not performed correctly.

but the final version of the code must be version controlled. Often, we hear stories that models cannot be reproduced because the code that generated them are not runnable anymore. This is a serious problem, and it is not acceptable for maintaining a software solution.

These observations and values are the basis of our approach. The roles and principles of our approach are described in the following sections.

4.5.1 The roles of our approach

Combine SCRUM roles with the roles defined by Zumel and Mount (2019).

Table 4.1: Roles of our approach.

Our approach	SCRUM	ZM
Sponsor	Product owner	Project sponsor
Client	Stakeholder	Client
Data scientist	Scrum master	Data scientist
Dev Team		Data architect/operations

The roles of SCRUM are associated with the roles defined by Zumel and Mount (2019). In our approach, the data scientist leads the development team and interacts with the sponsor and the client. The development team includes people with both database and software engineering expertise.

4.5.2 The principles of our approach

1. Modularize the solution. Usually, in four main modules: frontend, backend, dataset, and model search. The frontend is the user interface. The backend is the server-side code. The dataset is the data that is used to train the model. The model search is the code that searches for the best model.

2. Version control everything. This includes the code, the data, and the documentation. The most used tool for code version control

is Git. For datasets, extensions to Git exist, such as DVC[3]. One important aspect is to version control the model search code. Interactive environments such as Jupyter notebooks are not suitable for this purpose. They can be used to draft the code, but the final version must be version controlled.

3. Continuous integration and continuous deployment. This means that the code is automatically (or at least semi-automatically) tested and deployed. The backend and frontend code is tested using unit tests. The model search code is tested using validation methods such as cross-validation and Bayesian analysis on the discovered models. Usually the model search code is very computationally intensive, and it is not feasible to run it on every commit. Instead, it is run periodically, for example once a day. If the clould infrastructure required to run the model search code is not available to automate validation and deploymen, at least make sure that the code is easily runnable. This means that the code must be well documented, and that the required infrastructure must be well documented. Also aggregate commands using a Makefile or a similar tool. Pay attention on the dependences between dataset and the model training. If the dataset changes significantly, not only the deployed model must be retrained, but the model search algorithm may need to be rethought.

4. Reports as deliverables. During sprints, the deliverables of data exploration are reports. The reports must be version controlled and must be reproducible. The reports must be generated in a way that is understandable by the client and the sponsor.

5. Setup quantitative goals. Do not fall on the trap of forever improving the model. Instead, setup quantitative goals for the model performance. For example, the model must have a precision of at least 90%. Once you reach the goal, prioritize other tasks.

6. Measure *exactly* what you want. During model validation, use your own metrics based on the project goals. Usually, more than one metric is needed, and they might be conflicting. Use strategies to balance the metrics, such as Pareto optimization. Beware of the metrics that are most used in the literature. They might not be suitable for your project. Notice that during model training, some methods are limited to the loss functions that they can

[3] https://dvc.org/

optimize. If possible, choose a method that can optimize the loss function that you want. Even if you are not explicitly optimizing the wanted metric, you might find a model that performs well on that metric. That is a reason validation is important.

7. Report model stability and performance variance. Understanding the limitations and characteristics of the model is more important than the model performance. For example, if the model performance is high, but the model is unstable, it is not suitable for production. Also, in some scenarios, interpretability is more important than performance.

8. In user interface, mask data-science-specific terminology. Usually, data science software gives the user the option to choose the model. In order to avoid confusion, the user interface must mask the data-science-specific terminology. This helps non experts to use the software consciously.

9. Monitor model performance in production. If possible setup feedback from the user interface. Avoid automation of model releases because concept drift usually requires exploratory analysis.

10. Use the appropriate backend. REST API vs websocket. The choice depends on the requirements of the project. REST API is more suitable for stateless requests, while websocket is more suitable for stateful requests. For example, if the user interface must be updated in real-time, websocket is more suitable. If the user interface is used to submit batch requests, REST API is more suitable.

4.5.3 Solution search framework

TODO Move part of the chapter 8 here, dropping the sampling strategy but bringing the main defitions.

5

Statistical learning theory

To understand God's thoughts we must study statistics, for these are the measure of His purpose.

— Florence Nightingale, *her diary*

We can address several kinds of problems using algorithms that learn from data. However, we focus on the problem of *inductive learning*. Before we go further, let us define some terms.

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Definition 5.1: Artificial intelligence

The field that studies algorithms that exhibit intelligent behavior.

Artificial intelligence is a very broad field, including not only the study of algorithms that exhibit intelligent behavior, but also the study of the behavior of intelligent systems. For instance, it encompasses the study of optimization methods, bioinspired algorithms, robotics, philosophy of mind, and many other topics. We are interested in the subfield of artificial intelligence that studies algorithms that exhibit some form of intelligent behavior.

Definition 5.2: Machine learning

The subfield of artificial intelligence that studies algorithms that enable computers to automatically learn from data.

Machine learning is the subfield of artificial intelligence that studies algorithms that enable computers to automatically learn and improve their performance on a task from experience, without being explicitly programmed by a human being.

Definition 5.3: Predictive learning

The machine learning paradigm that studies the problem of making predictions given known input data.

The machine learning paradigm that focuses on making predictions about outcomes (sometimes about the future) based on historical data. Depending on the reasoning behind the learning algorithms, the main predictive algorithms are classified in either inductive or transductive.

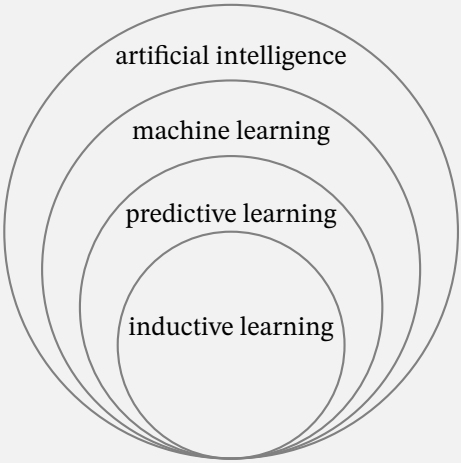
Definition 5.4: Inductive learning

The machine learning approach that involves deriving general rules from specific observations.

Induction a type of reasoning that goes from specific instances to more general principles. Inductive learning is the machine learning approach that studies algorithms that, given data representing the set of specific instances, derive general rules that can make predictions about *any* new instances.

Figure 5.1 give us a hierarchical view of the learning field. Alternatives — such as descriptive learning in opposition to predictive learning, or transductive learning in opposition to inductive learning — are out of the scope of this course.

Figure 5.1: Organizational chart of the learning field.



Maybe the most general (and useful) framework for predictive learning is Statistical Learning Theory. In this chapter, we will introduce the basic concepts of this theory.

5.1 Hypothesis and setup

Consider the set

$$\{(\mathbf{x}_i, y_i) : i = 1, \dots, n\} \tag{5.1}$$

where each sample i is associated with a feature vector $\mathbf{x}_i \in \mathcal{X}$ and a target variable $y_i \in \mathcal{Y}$. We assume that samples are random independent identically distributed (i.i.d.) observations drawn according to

$$\mathrm{P}(x, y) = \mathrm{P}(y \mid x)\,\mathrm{P}(x).$$

Both $\mathrm{P}(x)$ and $\mathrm{P}(y \mid x)$ are fixed but unknown.

This is equivalent to the original learning problem stated by Vapnik (1999), where a generator produce random vectors $\mathbf{x}$ according to a fixed but unknown probability distribution $\mathrm{P}(x)$ and a supervisor returns an output value y for every input vector x according to a conditional distribution function $\mathrm{P}(y \mid x)$, also fixed but unknown.

Moreover, note that this setup is compatible with the idea of tidy data and 3NF (see section 3.4.3). Of course, we assume X, Y are only the measured variables (or non-prime attributes). In practice, it means that we left aside the keys in the learning process.

5.2 The learning problem

Consider a *learning machine* capable of generating a set of functions $f(x;\theta) \equiv f_\theta(x)$, $\theta \in \Theta$ and $f_\theta : \mathcal{X} \to \mathcal{Y}$. The problem of learning is that of choosing, among all possible f_θ, the one that predicts the target variable the best possible way.

In order to learn, we must first define the *loss* (or discrepancy) $\mathcal{L}$ between the response y to a given input x, drawn from $\mathrm{P}(x, y)$, and the response provided by the learning machine.

Then, given the *risk function*

$$R(\theta) = \int \mathcal{L}(y, f_\theta(x))\, d\,\mathrm{P}(x, y), \tag{5.2}$$

the goal is to find the function f_θ that minimizes $R(\theta)$ where the only available information is the *training set* (5.1). This is the *empirical risk minimization* (ERM) problem.

This formulation encompasses many specific problems. I focus on the two of them which I believe are the most fundamental ones: *binary data classification*[1] and *regression estimation*[2]. I left aside the density estimation problem, once it is not addressed in the remaining of the book.

Binary data classification task. In this task, the output y take on only two possible values, zero or one — called classes —, and the func-

[1] Vapnik calls it *pattern recognition*.

[2] We are not talking about *regression analysis*, it is closer to the *scoring* task definition by Zumel and Mount (2019).

tions f_θ are indicator functions. For the loss

$$\mathcal{L}(y, f_\theta(x)) = \begin{cases} 0 & \text{if } y = f_\theta(x) \\ 1 & \text{if } y \neq f_\theta(x), \end{cases}$$

we aim at minimizing the risk (5.2) which becomes the probability of classification error. The function f, in this case, is called *classifier*.

Regression estimation task. Let the outcome y be a real value and the *regression* r be

$$r(x) = \int y \, d\,\mathrm{P}(y|x).$$

The regression function is the function $r = f_\theta$ that minimizes the risk function (5.2) with the loss

$$\mathcal{L}(y, f_\theta(x)) = \big(y - f_\theta(x)\big)^2.$$

If $r \notin \{f_\theta : \theta \in \Theta\}$, the function $f_{\theta'}$ that minimizes the risk function is the closest to the regression function in the metric l_2, i.e. we look for θ' such that

$$\theta' = \arg\min_{\theta \in \Theta} \sqrt{\int \big(r(x) - f_\theta(x)\big)^2 \, d\,\mathrm{P}(x)}.$$

The function f, in this case, is called *regressor*.

5.2.1 A few remarks and definitions

Supervised and semisupervised learning In both cases, classification and regression, the learning task is to find the function that maps the input data to the output data in the best possible way. Although the learning machine described generate models in a *supervised* manner, there are alternative ways to solve the inductive learning problem, such as *semisupervised* approach, where the model can be trained with a small subset of labeled data and a large subset of unlabeled data — that is, data whose labels y are unknown.

Mislabeled data Another important premise is that all given labels are correct. This is a strong assumption, but it is necessary to ensure the learning process. In practice, it is possible to have mislabeled data, but it is a different problem that must be addressed before the learning process. Some works address the robustness of learning machines in cases of mislabeled data (Silva and Zhao 2013).

Generative and discriminative models Any learning machine generates a model that describes the relationship between the input and output data. This model can be generative or discriminative. Generative models describe the joint probability distribution $P(x, y)$ and can be used to generate new data. Discriminative models, on the other hand, describe the conditional probability distribution $P(y \mid x)$ and are used to make predictions. Generative models are usually much more complex than discriminative models, but they hold more information about the data, solving indirectly the conditional probability. As a general rule, if you only need to solve the predictive problem, use a discriminative model.

Multiclass classification In the binary classification task, the output y is a binary variable. However, it is possible to have a multiclass classification task, where y can take on more than two possible values. Although some learning methods can address directly the multiclass classification task, it is possible to transform the problem into a binary classification task. The most common method is the *one-versus-all* method where we train l binary classifiers, one for each class, and the class with the highest score is the predicted class. Another method is the *one-versus-one* method, where we train $l(l-1)/2$ binary classifiers, one for each pair of classes, and the class with the most votes is the predicted class.

Number of inputs and outputs Note that the definition of the learning problem does not restrict the number of inputs and outputs. The input data can be a scalar, a vector, a matrix, or a tensor, and the output as well. The learning machine must be able to handle the input and output data according to the problem.

Parametric vs nonparametric models The learning machine generates a set of functions f_θ where $|\theta|$ can be fixed or not. If $|\theta|$ is always fixed, the model is called *parametric*. If $|\theta|$ is not fixed beforehand, the model is called *nonparametric*. Parametric models are usually simpler and faster, but they are less flexible. In other words, it is up to the researcher to choose the best model "size" for the problem. If the model is too small, it will not be able to capture the complexity of the data. If the model is too large, it will be too complex, too slow to train and might overfit to the data. Non parametric models are more flexible, but they usually require more data to be trained.

5.3 ERM inductive principle

In the following sections, z describes the pair (x, y) and $L(z, \theta)$ a generic loss function. The training dataset is thus a set of n i.i.d. samples $z_1, \dots, z_n$.

Since the distribution $P(z)$ is unknown, the risk functional $R(\theta)$ is replaced by the *empirical risk functional*

$$R_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} L(z_i, \theta). \tag{5.3}$$

Approximating $R(\theta)$ by the empirical risk functional $R_n(\theta)$ is the so called ERM inductive principle. The ERM principle is the basis of the statistical learning theory.

Classical methods, such as least-squares, maximum likelihood, and maximum a posteriori are all realizations of the ERM principle for specific loss functions and hypothesis spaces.

In the following sections, we address the four main questions of learning theory. We summarize them in table 5.1.

Table 5.1: The four main questions of learning theory.

Part	Question
Consistency	What are the necessary and sufficient conditions for consistency of a learning process?
Rate of convergence	How fast is the rate of convergence of the learning process?
Generalization	How can one controle the generalization ability of the learning process?
Construction	How can one construct a learning machine that satisfies the conditions of consistency and generalization?

5.4 Consistency of learning processes

Addressing consistency of a learning process means that we are interested in the convergence of the empirical risk functional $R_n(\theta)$ to the

risk functional $R(\theta)$ as $n \to \infty$. In other words, it is an asymptotic theory about the behavior of the empirical risk functional as the sample size n goes to infinity.

The necessary and sufficient conditions for consistency give us guarantees that the learning process is general and cannot be improved given our premises. The most important topic in this section is the Vapnik-Chervonenkis (VC) entropy.

5.4.1 Definition of consistency

An ERM method is consistent if it produces a sequence of functions f_{θ_n}, for $n = 1, 2, \ldots$, for which both the expected risk and the empirical risk converge to the their minimum values.

Definition 5.5: Consistency of a learning process

Let θ_n be the solution of

$$\theta_n = \arg\min_{\theta \in \Theta} R_n(\theta).$$

An ERM method is consistent for the set of functions $\{L(z, \theta) : \theta \in \Theta\}$ and the probability distribution $P(z)$ if

$$\lim_{n \to \infty} R(\theta_n) = \inf_{\theta \in \Theta} R(\theta),$$
$$\lim_{n \to \infty} R_n(\theta_n) = \inf_{\theta \in \Theta} R(\theta).$$

This definition means that one can estimate the risk functional $R(\theta)$ by the empirical risk functional $R_n(\theta)$, while the values of achieved risks converge to the minimum value of the risk functional. See fig. 5.2.

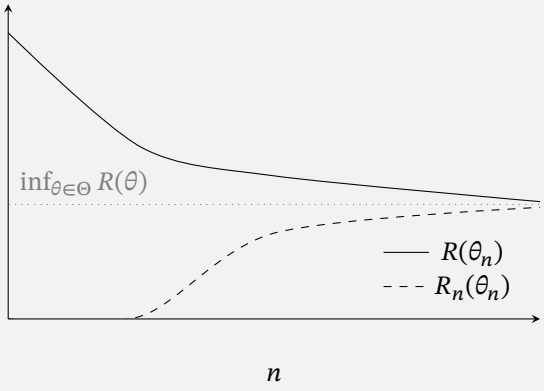
However, since this definition of consistency includes cases of trivial consistency, there is no way to obtain such conditions.

Consider the following example. Suppose we have found a set of functions $\{f_\theta : \theta \in \Theta\}$ such that the ERM method is not consistent. Let's add one more function $\phi(z)$ to the set, such that

$$\inf_{\theta \in \Theta} L(z, \theta) > \phi(z), \ \forall z.$$

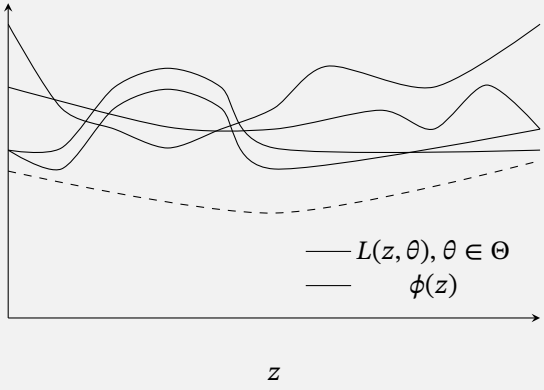
It is straightforward to see that the ERM method is consistent for the new set of functions $\{L(z, \theta) : \theta \in \Theta\} \cup \{\phi\}$ and the probability distribution $P(z)$. In this case, the function $\phi(z)$ gives both the minimum

Figure 5.2: Convergence of the empirical and expected risk functionals.



value of the risk functional and the empirical risk functional. This is illustrated in fig. 5.3.

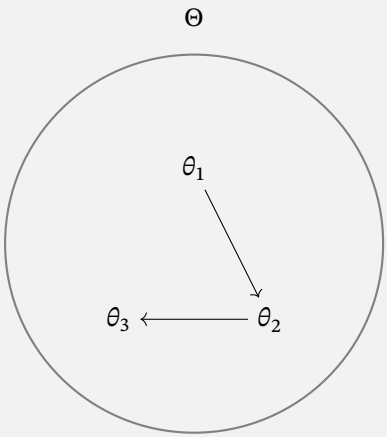
Figure 5.3: An illustrative case of trivial consistency.



5.8 Learning bias

Learning bias, or *inductive bias*, is the set of assumptions that the learning machine uses to generate the set of functions $\{f_\theta : \theta \in \Theta\}$ — see fig. 5.4. Vapnik shows that the learning bias is the key to the generalization ability of the learning process: the smaller the learning bias, the better the generalization ability (Vapnik 1999). In an illustrative thought experiment, one can see that "no bias means no learning," since the learning machine would generate all possible functions, which is impossible, including the function that perfectly fits the training data but fails to generalize.

Figure 5.4: Learning bias illustration.



A learning machine searches for the best parameter θ in the space Θ. The learning bias is the set of assumptions that the learning machine uses to control how and where to search for the best parameter.

It is important to understand the learning bias of the main machine-learning methods. Let's consider the binary classification task, which is more intuitive. Some common learning methods are the perceptron, the multi-layer perceptron, the decision tree, and the k-nearest neighbors.

For the examples in the following subsections, we consider the datasets for the AND and the XOR problem — see table 5.3.

Table 5.2: Learning machines paradigms and characteristics.

Method	Paradigm	Characteristics
Perceptron	Functional (parametric)	The perceptron is a linear classifier that generates a hyperplane that separates the classes.
MLP	Functional (parametric)	The multi-layer perceptron is a non-linear classifier that generates a set of hyperplanes that separates the classes.
DT	Symbolic (nonparametric)	The decision tree is a classifier that comprises a set of rules that separate the classes.
k-NN	Instance-based (non-parametric)	The k-nearest neighbors is a classifier that classifies the data based on the majority of the k-nearest neighbors.

Table 5.3: AND and XOR datasets.

x_1	x_2	$y = x_1 \wedge x_2$
0	0	0
0	1	0
1	0	0
1	1	1

x_1	x_2	$y = x_1 \oplus x_2$
0	0	0
0	1	1
1	0	1
1	1	0

The AND and XOR datasets are binary classification datasets where the output y is the "logical AND" and the "exclusive OR" of the inputs x_1 and x_2, i.e. $y = x_1 \wedge x_2$ and $y = x_1 \oplus x_2$.

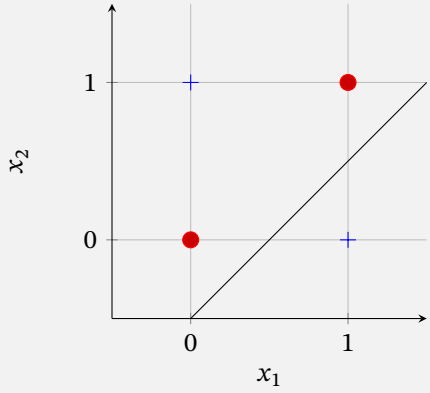
5.8.1 Perceptron learning bias

The perceptron is a linear classifier that generates a hyperplane that separates the classes. The model for our example is

$$f(x_1, x_2; \theta = \mathbf{w} = [w_0, w_1, w_2]) = \begin{cases} 1 & \text{if } w_0 + w_1 x_1 + w_2 x_2 > 0 \\ 0 & \text{otherwise.} \end{cases}$$

As one can see, the perceptron learning bias is the assumption that the classes are linearly separable. The equation $\mathbf{w} \cdot \mathbf{x} = 0$, where $\mathbf{x} = [1, x_1, x_2]$, is the equation of a hyperplane.

Figure 5.5: Perceptron learning bias.



The perceptron learning bias is the assumption that the classes are linearly separable. The hyperplane that separates the classes is the learning machine model. In this case, $w_0 = -0.5$, $w_1 = 1$, and $w_2 = -1$.

In fig. 5.5, we show the hyperplane that the model $\mathbf{w} = [-0.5, 1, -1]$ generates for the XOR dataset. As one can see, the classes are not linearly separable, and the perceptron model fails to classify the dataset correctly, see table 5.4.

5.8.2 Multi-layer perceptron learning bias

The multi-layer perceptron (MLP) is a non-linear classifier that generates a set of hyperplanes that separates the classes. In order to simplify

Table 5.4: Truth table for the predictions of the perceptron.

x_1	x_2	y	$-0.5 + x_1 - x_2$	$\hat{y}$
0	0	0	-0.5	0
0	1	1	-1.5	0
1	0	1	0.5	1
1	1	0	-0.5	0

The perceptron model with parameters $w_0 = -0.5$, $w_1 = 1$, and $w_2 = -1$ fails to classify the XOR dataset correctly — as any other perceptron would do.

Think about...

What happens if we remove w_0 from the model?

the understanding, consider the that the activation function of the hidden layer is the discrete step function

$$\sigma(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise.} \end{cases}$$

A model with two neurons in the hidden layer (effectively the combination of three perceptrons) is

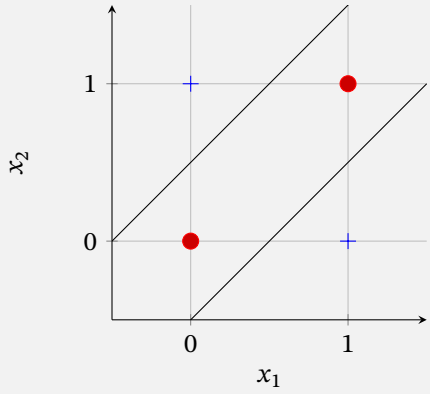
$$f(x_1, x_2; \theta = \{\mathbf{w}^{(1)}, \mathbf{w}^{(2)}, \mathbf{w}^{(3)}\}) = \\ \sigma\left(\mathbf{w}^{(3)} \cdot \left[1, \sigma(\mathbf{w}^{(1)} \cdot \mathbf{x}), \sigma(\mathbf{w}^{(2)} \cdot \mathbf{x})\right]\right).$$

The parameters $\mathbf{w}^{(1)}$ and $\mathbf{w}^{(2)}$ represent the hyperplanes that separate the classes in the hidden layer, and $\mathbf{w}^{(3)}$ represents how the hyperplanes are combined to generate the output. If we set $\mathbf{w}^{(1)} = [-0.5, 1, -1]$ (like the perceptron in the previous example) and $\mathbf{w}^{(2)} = [-0.5, -1, 1]$, we use the third neuron to combine the results of the first two neurons. This way, solution for the XOR problem is setting $\mathbf{w}^{(3)} = [0, 1, 1]$.

5.8.3 Decision tree learning bias

The decision tree is a non-linear classifier that generates a set of hyperplanes that are orthogonal to the axes. Consider the decision tree in

Figure 5.6: MLP learning bias.



...

Table 5.5: Truth table for the predictions of the MLP.

x_1	x_2	y	1st neuron	2nd neuron	$\hat{y}$
0	0	0	0	0	0
0	1	1	0	1	1
1	0	1	1	0	1
1	1	0	0	0	0

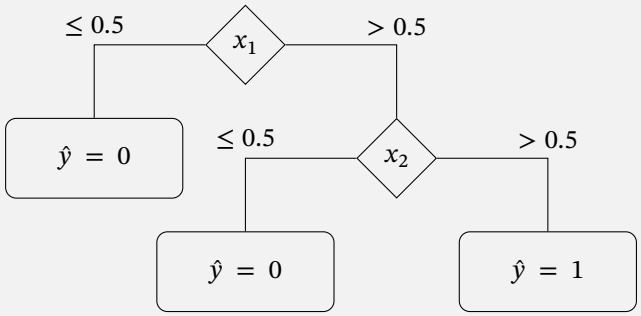
...

Think about...

Note that there are many possible solutions for the XOR problem using the MLP.

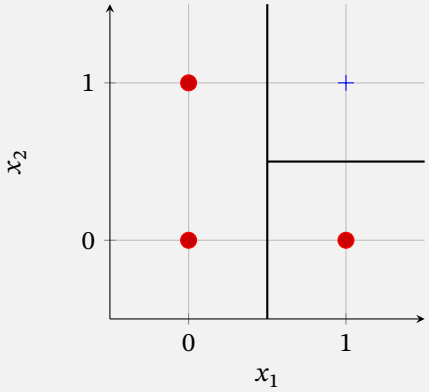
fig. 5.7.

Figure 5.7: Decision tree representation.



The decision tree that separates the AND dataset.

Figure 5.8: Decision tree learning bias.



The decision tree learning bias is the assumption that the classes can be separated with hyperplanes orthogonal to the axes.

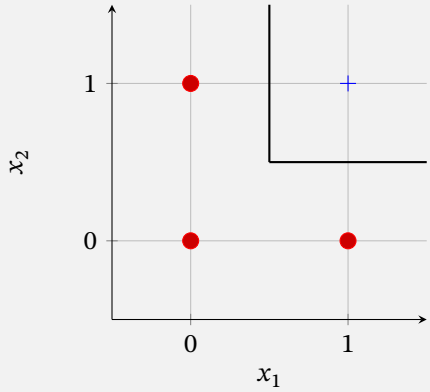
Think about...

Decision tree are nonparametric models, one can easily increase the depth of the tree to fit the data.

5.8.4 k-nearest neighbors learning bias

The k-nearest neighbors (k-NN) is a non-linear nonparametric classifier that generate arbitrarily complex decision boundaries by "memoring" the training data. The behavior of the boundaries depends on the value of k and the distance metric one uses to find the nearest neighbors of a point.

Figure 5.9: 1-NN learning bias.



In this particular case, the 1-NN boundaries match the decision tree boundaries.

As k increases the boundaries become smoother: example.
See illustration: here.

6

Data handling

> *Tidy datasets are all alike, but every messy dataset is messy in its own way.*
>
> — Hadley Wickham, *Tidy Data*

Data handling is the process of adjusting data to make it suitable for analysis. It involves three main tasks: data transformation, data cleaning, and data integration.

In this chapter, we consider that tables are rectangular data structures in which values of the same column share the same properties (i.e. the same type, same restrictions, etc.) and each column has a name. Moreover, we assume that any value is possibly *missing*.

Chapter remarks

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6.1 Data handling operators

In the literature and in software documentation, you will find a variety of terms used to describe data handling operations[1]. They often refer to the same or similar operations, but the terminology can be confusing. In this section, I present a summary of these operations mostly based on Wickham, Çetinkaya-Rundel, and Grolemund (2023) definitions[2].

These operations are the building blocks of the data handling tasks we will discuss in the next sections. They can also be extensively parametrized and combined to create more elaborate data handling pipelines. For instance, most of them can use predicates to define the groups, arrangements, or conditions under which they should be applied.

We use the following terminology to refer to the data handling parameters:

- **Predicate**: a function that returns a logical value, used to filter rows/columns or to define the groups of rows/columns to be processed;
- **Aggregation function**: a function that returns a single value given a vector of values (in which, the order of the values may be important);
- **Window function**: a function that returns a vector of values given a vector of values in which, the order of the values is important;
- **Expression**: a function that returns a vector of values elementwise, used to create new columns or to modify existing ones.

Operators are also vectorized, meaning that they can be applied to multiple columns or rows at once. This is a key feature of data handling operations, as it allows for expressive and efficient data manipulation.

Many of them are also reversible, meaning that they can be undone. This is important because it allows for reproducibility and traceability of the data handling process.

They operate on a dataset (or more than one) given as input and return a new dataset as output. This is important because it allows for the

[1]The terminology "data handling" itself is not universal. Some authors and libraries call it "data manipulation", "data wrangling", "data shaping", or "data engineering". I use the term "data handling" to avoid confusion with the term "data manipulation" which has a negative connotation in some contexts.

[2]Which are called *verbs*.

creation of data handling pipelines, where the output of one operation is the input of the next one. Parameters like column names, predicates, aggregation functions, and expressions can be passed to these operations to customize their behavior.

Unlike traditional procedural programming, where conditional statements and loops are used to manipulate data, data handling operations are declarative. This means that they are expressed in terms of what should be done, not how it should be done. This is a powerful abstraction that allows for the creation of complex pipelines with a few lines of code.

6.1.1 Filtering rows

Filtering is the process of selecting a subset of rows from a dataset based on a predicate. If more than a single predicate is used, they are combined using a logical operator, such as `AND` or `OR`.

After filtering, the dataset will contain only the rows that satisfy the predicate. Columns remain unchanged. This operation is potentially irreversible, as the removed rows are lost.

In the basic form, each row is treated independently. For instance, the predicate `age > 18` will select all rows where the value in the `age` column is greater than 18.

However, if the predicate depends on an aggregation or window function, one must specify the groups and/or the order of the rows. For instance, the predicate `age > mean(age) group by country` will select the rows where the value in the `age` column is greater than the mean of the `age` for each `country`. Another example is the predicate `cumsum(price) < 100 sort by date`, which selects the rows that satisfy the condition that the cumulative sum of the `price` column is less than 100 given the order of the rows defined by the `date` column.

The trivial group is the entire dataset, so it is usually not necessary to specify it explicitly. However, it is usually not sensible to not specify the order of the rows.

When dealing with real values, be aware of floating-point precision issues. In other words, do not use the equality operator to compare real numbers. Most of libraries provide operators to compare real numbers within a given tolerance.

Practical tips

- Use filtering to remove rows that are not relevant to your analysis;
- Use predicates to define the conditions under which rows should be removed;
- When aggregation functions are needed to define the predicate, specify the groups and the order of the rows;
- Be aware of floating-point precision issues when comparing real numbers.

6.1.2 Selecting columns

Selecting is the process of choosing a subset of columns from a dataset. The remaining columns are discarded. This operation is not reversible, as the discarded columns are lost. Rows remain unchanged.

There are two main ways to select columns: by name or by predicate. The former is the most common and is used to select a fixed set of columns. The latter is used to select columns that satisfy a given condition, i.e., the values in the columns are used to determine which columns should be selected.

When selecting columns by name, one can use a list of column names or a regular expression[3]. The latter is useful when the column names follow a pattern that reflects the semantics of the columns. For instance, one can use the regular expression `col[0-9]+` to select all columns whose names start with `col` followed by one or more digits.

When selecting columns by predicate, one can use a function that returns a logical value to define the condition under which a column should be selected. For instance, one can use the predicate `isnumeric` to select all columns that contain numeric values. Notice, however, that the predicate is applied to each column independently and returns a single logical value for each column.

Like filtering, selecting predicates might contain aggregation functions. Although it is theorically possible to consider the order of the values in the columns, it is not common to do so. (Especially because

[3]Regular expressions are very general and powerful, but they are also complex and error-prone. An alternative is to use some form of hierarchical naming, such as `type.column` to express groups of columns.

one would need to assume that the rows are previously sorted by some criterion.) Groups, however, never make sense in this context, once the predicate is applied to each column independently.

Depending on the context, it may be useful to "drop" columns instead of selecting them. This is the same as selecting all columns except the ones specified. This is useful when the number of columns to be dropped is small compared to the total number of columns. Strictly speaking, we just need to negate the predicate or the regular expression used to select the columns.

Finally, it is very common to find libraries and framework in which the order of the columns is important. As a result, columns can be selected by position as well. I find this practice error-prone and I recommend avoiding it whenever possible.

Practical tips

- Use selecting to remove columns that are not relevant to your analysis;
- Use column names or regular expressions (or hierarchical names) to select columns;
- Use predicates (many to one, with no aggregation functions) to define the conditions under which columns should be selected;
- Avoid depending on the order of the columns.

6.1.3 Mutating columns

Mutating is the process of creating new columns. The operation is reversible, as the original columns are kept. The new columns are added to the dataset.

The values in the new column are determined by an expression. The expression is a function that returns a vector of values given the values in the other columns. The expression can be a simple function, such as `y = x + 1`, or a more complex function, such as `y = ifelse(x > 0, 1, 0)`. Here, `x` and `y` are the names of an existing and the new column, respectively.

One may also use an aggregation and window function in the expression. This is particularly useful when performing mutation considering a group. In this case, the returned value is repeated (aggregation function) for each row of the same group. Like in filtering, the more explicit you can be about order and groups, the better.

For example, the expression `y = cumsum(x) group by category sort by date` will create a new column `y` with the cumulative sum of the `x` column for each `category` given the order of the rows defined by the `date` column.

Sometimes, the same expression can be used to create multiple columns. This is useful when the new columns are related. To do so, one first specifies the columns in the same way as when selecting columns. Then, one needs to specify a rule to name the new columns. For instance, `x_new = x + 1 across x matches ^col[0-9]+$`.

Practically speaking, mutation can overwrite existing columns. This is useful when the new column is a replacement for the old one. Formally, overwriting is just a sequence of mutation and selection operations.

Practical tips

- Use mutating to create new columns that are relevant to your analysis;
- Use expressions to define the values of the new columns;
- Use aggregation and window functions in the expression to create new columns based on groups and order;
- Use the same expression to create multiple columns when the new columns are related.

6.1.4 Aggregating rows

We can aggregate the rows of a dataset to create a new dataset with fewer rows. The operation is not reversible, as the discarded rows are lost. The columns are also lost, only the new aggregate columns remain.

The values in the new columns are determined by an aggregation function. Like filtering and mutation, the aggregation function can be parametrized by specifying a group and/or an order.

The resulting dataset will contain one row for each group. The values in the new columns are determined by the aggregation function applied to the values in the other columns. All columns that define the groups are usually kept in the resulting dataset. In this case, as expected, values of such columns are equal for all rows in the same group.

For instance, the aggregation function `mean(x) group by category` will create a new dataset with one row for each different value of `category` and a new column with the mean of the `x` column for each group.

Practical tips

- Use aggregation to summarize the data in a dataset;
- Use aggregation functions to define the values of the new columns;
- Other columns are lost;
- Use the group and order parameters to define the groups and the behavior of the aggregation function.

6.1.5 Binding datasets

One trivial, yet important, operation is to bind datasets. This is the process of combining two or more datasets into a single dataset. The operation is reversible, as the original datasets are kept. The new dataset contains all the rows and columns of the original datasets.

There are two ways to bind datasets: by rows or by columns. The former is used to combine datasets that have exactly the same columns but represent different parts of the same dataset. The latter is used to combine datasets that comprise the same observations (rows) but captures different aspects of the same dataset.

When binding datasets by rows, the datasets must have the same columns[4]. The resulting dataset will contain all the rows of the original datasets. The columns remain unchanged. It is a good practice to create a new column that represents the source of each row. For instance, if each table represents data collected in a different year, one can create a new column `year` that contains the year of the data.

[4]In practice, it is usually required that they share the same order of the columns as well. This is not a theoretical requirement, but a common limitation of most libraries.

When binding datasets by columns, the datasets must have the same number of rows. Each matching row represent the same observation[5]. The resulting dataset will contain all the columns of the original datasets. The rows remain unchanged.

Practical tips

- Use binding to combine datasets that represent different parts of the same dataset;
- Use binding by rows to combine datasets that have the same columns — in this case, create a new column that represents the source of each row;
- Use binding by columns to combine datasets that have the same number of rows.

Talk about splitting as the reverse function, and the reason why missing columns may be a problem. Example of the unit of measurement.

6.1.6 Joining datasets

Joining is the process of combining two datasets into a single dataset based on common columns. The operation may not be reversible, consult section 3.4.1 for more details.

The join of two tables is the operation that returns a new table with the columns of both tables. Let `U` be the common set of columns. For each occurring value of `U` in the first table, the operation will look for the same value in the second table. If it finds it, it will create a new row with the columns of both tables. If it does not find it, no row will be created. This operation assumes that values in `U` are unique in each table.

The variation described above is usually called natural or inner join. Three other variations are possible.

- Left join: for each occurring value of `U` in the first table, the operation will look for the same value in the second table. If it finds it, it will create a new row with the columns of both tables. If it does not find it, it will create a new row with the columns of the first table and missing values for the columns of the second table.

[5] Practically speaking, either the order of the rows or a key column is used to match the rows of the datasets. In both situations, this is equivalent to a join operation by the row number or the key column; assuming that both datasets contains the same observations.

- Right join: the same as the left join, but the roles of the tables are reversed.
- Outer join: for each different value of `U` in both tables, the operation will create a new row with the columns of both tables. If a value is missing in one table, it will be filled with a missing value.

Practical tips

- Use joining to integrate datasets;
- Be aware of the risks of joining datasets (section 3.4.1), for example, that some joins may create invalid rows;
- Use the appropriate variation of the join operation in applications.

6.1.7 Pivoting and unpivoting

Another important operation is to pivot and unpivot datasets. These are the processes of transforming a dataset from a long format to a wide format and vice versa. The operations are reversible and they are the inverse of each other.

Pivoting requires to specify a name column — whose discrete and finite possible values will become the names of the new columns — and a value column — whose values will be spread across the rows. All remaining columns are considered to be keys, uniquely identifying each row of new the dataset.

Unpivoting[6] is the reverse operation. One must specify all the columns whose names are the values of the before called name column. The values of these columns will be gathered into a new column. As before, all remaining columns are considered to be keys.

In practical applications, where not all remaining columns are keys, one must aggregate rows beforehand.

Table 6.1 shows an example of pivoting. The left table is in the long format and the right table is in the wide format. The name column is `year`, the value column is `value`, and the remaining column is `name` which is an unique identifier of the rows in the wide format.

[6] Which Wickham, Çetinkaya-Rundel, and Grolemund call pivot longer.

Table 6.1: Pivoting example.

name	year	value
A	2019	1
A	2020	2
A	2021	3
B	2019	4
B	2020	5
B	2021	6

name	2019	2020	2021
A	1	2	3
B	4	5	6

The left table is in the long format and the right table is in the wide format. The name column is `year` and the value column is `value`.

Practical tips

- Use pivoting to transform datasets from a long format to a wide format;
- Use unpivoting to transform datasets from a wide format to a long format;
- Be aware of the need to aggregate rows before unpivoting.

6.1.8 An algebra for statistical transformations

In recent years, some researchers made an effort to create a formal algebra for statistical transformations. The idea is to create a set of operations that can be combined to create complex statistical transformations. This is similar to the idea of relational algebra, which is a set of operations that can be combined to create complex queries.

The difference between relational algebra and a formal algebra for statistical transformations is that the latter is more complex. This is because statistical transformations are more complex than queries. For instance, the concept of missing data is not present in relational algebra, but it is in statistical transformations.

Song, Jagadish, and Alter (2021), for example, propose a formal paradigm for statistical data transformation. They present a data model,

an algebra, and a formal language. Their goal is to create a standard for statistical data transformation that can be used by different statistical software.

However, in my opinion, the major deficiency of their work is that they mostly try to "reverse engineer" the operations that are commonly used in statistical software. This is useful for the translation of code between different software, but it is not productive to advance in the theoretical understanding of statistical transformations.

If one ought to tackle the challenge of formally expressing statistical transformations, I think one should start from the basic operations. Basic operations mean that they are irreducible, i.e., they cannot be expressed as a sequence of other operations.

Some thoughts about it:

- Binding columns can be expressed as a join operation, thus it is not a basic operation.

- Some software provide features that can be better expressed in other (often simpler) ways. Row naming is an example. It is useful to keep track of the origin of each row, but names can be just another column. I argue for excluding row naming in a formal algebra.

- Some operations are very useful and recurring, even if they are not basic. Such operations must be omitted from the formal algebra for the sake of simplicity. However, any software that implements a language for the formal algebra can provide syntax sugar for these operations.

- Not defining your algebra in terms of a specific programming language is a good practice. This is because the algebra is a theoretical concept and should be independent of any implementation. It also gives opportunities to rethink the things that commonly done in a specific way. This can lead to new insights and correct error-prone practices.

- Pivoting seems to be "different" enough to the other operations to be considered in the set of basic operations. However, it is not hard to see that they can be rewritten as combinations with the meta tables containing the possible values of the attributes (or some sort of aggregation function).

6.2 Data handling pipeline

Before we study the data handling tasks, we need to understand that a data handling pipeline is a sequence of operations that *does* depend on the input data. This might seem obvious, but the implications are not.

A common error in data handling is to perform operations ad hoc, usually leading to data leakage. For instance, one might impute missing values before splitting the data into training and testing sets. This is a mistake because the imputation is based on the entire dataset, including the testing set.

To avoid this kind of error, one must declare[7] the operations that will be performed on the data before applying them. This is usually done by creating the full data handling pipeline beforehand.

The pipeline, like a model, must be "fitted" to the data. This means that parameters of the operations are not fixed until the first data is given as input. Subsequent data fed to the pipeline will be handled keeping the first "learned" parameters.

Consider the following example. Suppose we have a dataset with missing values for variable `A`. We want to impute the missing values and then standardize `A`. The pipeline is created as follows: `D -> impute_zero(A) -> standardize(A)`.

The operation `impute_zero(A)` is parametrized by the value 0, which, in this case, is fixed. However, the operation `standardize(A)` is parametrized by the mean and the standard deviation of the values in `A`. These values are not fixed until the first data is given as input.

A note about fixed parameters

Even if your data handling pipeline contains operations that have fixed parameters and can be safely applied to data before the model search, *I strongly recommend* that you declare the pipeline as a whole. This is because it is easier to maintain and reproduce the data handling process, especially in deployment. Performing ad hoc handling in your data is a source of errors and important transformations can be forgotten when receiving new data.

In a practical scenario, the source code of the *model search* method includes not only strategies for the model, but also the data handling

[7] This is the declarative nature of data handling operations.

pipeline. Moreover, the deployment of the model includes the data handling pipeline as well. In other words, it does not matter which model is used, in the example above, the mean and the standard deviation of the values in `A` should be stored and used in deployed models.

In terms of reproducibility and validation, having a single consolidated pipeline is crucial.

A note about "filtering" operations

Some operations may conditionally remove rows from the dataset. For instance, after observing that there exists few missing values in an important column, one might decide to remove rows with missing values in it. In production, this means that some new observations might be discarded before reaching the model itself. However, the user still expects an answer from the model. In this case, one must define either a default value for the answer or a default behavior to handle discarded examples.

XXX: maybe state that before reaching the pipeline data is already tidy, this way simple integration (not enhancement), pivoting and aggregating are kept outside the pipeline. These operations must depend only on variable names and not variable values.

6.3 Data transformation

The first task in data handling is data transformation. This is the process of adjusting the format and the types of the data to make it suitable for analysis.

Usually, the starting point of data transformation is to make the data tidy, i.e., to have each variable in a column and each observation in a row. Remember that, depending on the problem definition, we target a particular observational unit. Having a clear picture of the observational unit is important to define the columns and the rows of the dataset.

Then, when the data format is acceptable, we can perform a series of operations to make the column's types and values suitable for modeling. The reason for this is that most machine learning methods require the input variables to follow some restrictions. For instance, some methods require the input variables to be real numbers, others require the input variables are in a specific range, etc.

6.3.1 Reshaping

TODO: pipeline exceptions: like pivoting and aggregating are kept outside the pipeline.

Reshaping is the process of changing the format of the data. The most common reshaping operations are pivoting and unpivoting, which we have already discussed. However, there are other reshaping operations that are useful in practice.

For instance, one can reshape a dataset by splitting a column into multiple columns. This is useful when a column contains multiple values that should be separated. This can be done with mutation with appropriate expressions. Some frameworks might provide special functions to do this, usually called splitting functions.

We can also consider reshaping the operations of filtering, selecting, and aggregating. Filtering is usually done to reduce the scope of the data, given some conditions on the variables. Selecting is usually done to remove irrelevant variables or highly correlated ones. Aggregating in a reshaping task is usually applied together with pivoting to change the observational unit of the dataset.

6.3.2 Type conversion

Type conversion is the process of changing the type of the values in the columns. This is usually done to make the data suitable for modeling. For instance, some machine learning methods require the input variables to be real numbers.

The most common type conversions are from categorical to numerical and from numerical to categorical. The former is usually done by creating dummy variables, i.e., a new column for each possible value of the categorical variable. This transformation is also known as one-hot encoding. The latter is usually done by binning (discretizing) the numerical variable, either by frequency or by range.

6.3.3 Normalization

Normalization is the process of scaling the values in the columns. This is usually done to keep data in a specific range or to make the data comparable. For instance, some machine learning methods require the input variables to be in the range $[0, 1]$.

The most common normalization methods are standardization and rescaling. The former is done by subtracting the mean and dividing by

the standard deviation of the values in the column. The latter is performed so the values are in a specific range, usually $[0, 1]$ or $[-1, 1]$.

Clamping after rescaling

In production, it is common to clamp the values after rescaling. This is done to avoid the model to make predictions that are out of the range of the training data.

Related to normalization is the log transformation. This is usually done to make the data more symmetric or to reduce the effect of outliers. The log transformation is the process of taking the logarithm of the values in the column.

6.3.4 Sampling

Sampling is the process of selecting a random subset of the data. This is usually done to reduce the size of the data or to create a balanced dataset. For instance, some machine learning methods are heavily affected by the number of observations in each class. Also, some methods are computationally expensive and a smaller dataset might be enough to solve the problem.

The most common sampling methods are random sampling and resampling[8]. The former is done by selecting a random subset of the data. The latter is done by selecting a random subset of the data with replacement.

While random sampling is useful to reduce the size of the data, resampling can be used to increase the size of the data. (Although this has some caveats.) Moreover, resampling can also create variations of the original dataset with the same distribution of the values.

6.3.5 Dimensionality reduction

Dimensionality reduction is the process of reducing the number of variables in the data. This is usually done to reduce the complexity of the model or to identify irrelevant variables. The so-called *curse of dimensionality* is a common problem in machine learning, where the number of variables is much larger than the number of observations.

[8] Resampling is the process of sampling with replacement, sometimes called bootstrapping.

There are two main types of dimensionality reduction algorithms: feature selection and feature extraction. The former is done by selecting a subset of the variables that leads to the best models. The latter is done by creating new variables that are combinations of the original ones.

Feature selection can be performed before modeling (filter), together with the model search (wrapper), or as a part of the model itself (embedded).

Feature extraction is usually done by linear methods, such as principal component analysis (PCA), or by non-linear methods, such as autoencoders. These methods are able to compress the information in the data into a smaller number of variables.

Practice!

Can you identify which data transformation operations are used to make datasets presented in chapter 3 tidy?

6.4 Data cleaning

Data cleaning is the process of removing errors and inconsistencies from the data. This is usually done to make the data more reliable and to avoid bias in the analysis.

6.4.1 Dealing with missing data

Since most models do not cope with missing data, it is crucial to deal with it in the data handling pipelines.

There are four main strategies to deal with missing data:

- Remove the rows with missing data;
- Remove the columns with missing data;
- Impute the missing data;
- Use an indicator variable to mark the missing data.

Removing rows and columns are commonly used when the number of missing data is small compared to the total number of rows or columns. However, be aware that removing rows can artificially change

data distribution, especially when the missing data is not missing at random.

Imputing the missing data is usually done by replacing the missing values with some statistic of the available values in the column, such as the mean, the median, or the mode. This is a simple and effective strategy, but it can introduce bias in the data. Also, it is not suitable when one is not sure whether the missing data is missing because of a systematic error or phenomenon.

For this case, creating an indicator variable is a good strategy. This is done by creating a new column that contains a logical value indicating whether the data is missing or not[9]. By doing so, the model can learn the importance of the missing data[10].

6.4.2 Dealing with invalid and inconsistent information

Sometimes, during data collection, information is recorded using special codes. For instance, the value 9999 might be used to indicate that the data is missing. Such codes must be replaced with more appropriate values before modeling.

Another common problem is inconsistent information. For instance, the same category might be represented by different names. This is usually done by creating a dictionary that maps the different names to a single one.

It is also useful to check whether all columns that store physical quantities have the same unit of measurement. If not, one must convert the values to the same unit.

If one knows that a variable has a specific range of values, it is useful to check whether the values are within this range. If not, one must replace the values wit missing data or with the closest valid value.

6.4.3 Outliers

Outliers are observations that are significantly different from the other observations. They can be caused by errors in the data collection process or by the presence of a different phenomenon. In both cases, it is important to deal with outliers before modeling.

There are many outliers detection methods, consult TODO.

[9] Some kind of imputation is still needed, but we expect the model to deal better with it

[10] Sometimes the indicator variable is already present: pregnancy and sex example.

6.5 Data integration

Data integration is the process of combining data from different sources into a single dataset. This is usually done to create a more complete dataset or to create a dataset with a different observational unit.

To perform integration, consider the discussions in sections 3.4.1 and 3.4.3.

Additionally, one must consider the following points:

- Sometimes the same column may have different names in different datasets. Redundant columns must be removed.
- Separate datasets that share the same variables usually happen because there is a hidden variable that is not present in the datasets. During integration, the new variable must be created.

Hard to incorporate in the pipeline when joins only, but data enhancement works better inside the pipeline.

7

Model evaluation

It's dangerous to go alone! Take this.

— Unnamed Old Man, *The Legend of Zelda*

One fundamental step in the development of a data driven solution for a task is the evaluation of the model. This chapter presents strategies to measure performance of classifiers and regressors, and how to interpret the results.

We consider the following setup. Let $D = \{(\mathbf{x}_i, y_i)\}_{i=1,\dots,n}$ be the dataset, where $\mathbf{x}_i$ is a feature vector and y_i is the target value. We assume that the dataset is split into a training set, given by indices $\mathcal{I}_{\text{training}}$, and a test set, given by indices $\mathcal{I}_{\text{test}}$, where $\mathcal{I}_{\text{training}} \cap \mathcal{I}_{\text{test}} = \varnothing$ and $\mathcal{I}_{\text{training}} \cup \mathcal{I}_{\text{test}} = \{1, \dots, n\}$.

For evaluation, we assume that the model has been trained on the training set and that predictions are made on the test set. We denote the predicted values as $\hat{y}_i$ for $i \in \mathcal{I}_{\text{test}}$, such that

$$\hat{y}_i = f_\theta(\mathbf{x}_i),$$

where θ is the solution found by the learning algorithm from the training set, see eq. (5.2).

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7.1 Binary classification evaluation

In order to assess the quality of a binary classification model, we need to know which samples in the test set were classified into which classes. This information is summarized in the *confusion matrix*, which is the basis for performance measures in classification tasks.

7.1.1 Confusion matrix

The confusion matrix is a table where the rows represent the true classes and the columns represent the predicted classes. The diagonal of the matrix represents the correct classifications, while the off-diagonal elements represent errors. For binary classification, the confusion matrix is given by

$$\begin{array}{cc} & \text{Predicted} \\ & \begin{array}{cc} 1 & 0 \end{array} \\ \text{Expected} \begin{array}{c} 1 \\ 0 \end{array} & \begin{pmatrix} \text{TP} & \text{FN} \\ \text{FP} & \text{TN} \end{pmatrix} \end{array}$$

where

- FP is the number of false positives $|\{i \in \mathcal{I}_{\text{test}} \mid y_i = 0 \wedge \hat{y}_i = 1\}|$,
- FN is the number of false negatives $|\{i \in \mathcal{I}_{\text{test}} \mid y_i = 1 \wedge \hat{y}_i = 0\}|$,
- TP is the number of true positives $|\{i \in \mathcal{I}_{\text{test}} \mid y_i = 1 \wedge \hat{y}_i = 1\}|$, and
- TN is the number of true negatives $|\{i \in \mathcal{I}_{\text{test}} \mid y_i = 0 \wedge \hat{y}_i = 0\}|$.

7.1.2 Performance measures

From the confusion matrix, we can derive several performance measures. The most common ones are the accuracy, precision, recall, and F-score.

Accuracy is the proportion of correct predictions over the total number of samples in the test set, given by

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}.$$

This measure is simple and easy to interpret, but it can be misleading when the classes are imbalanced — i.e. when the number of samples in

each class is very different. Consider the case where the dataset has 90% of samples in class 0 and 10% in class 1; a classifier that always predicts class 0 will have an accuracy of 90%, but it is not useful for the task.

Specificity is the proportion of true negative predictions over the total number of samples that are actually negative, given by

$$\text{Specificity} = \frac{\text{TN}}{\text{TN} + \text{FP}}.$$

This measure is useful when the cost of false positives is high, as it quantifies the ability of the classifier to avoid false positives. A test with a higher specificity has a lower type I error rate. In terms of a medical diagnosis, a type I error corresponds to diagnosing a patient as sick[1] when they are healthy. A classifier that always predicts class 1 will have a specificity of 0% in the example above. On the other hand, a classifier that always predicts class 0 will have a specificity of 100%.

Precision is the proportion of true positive predictions over the total number of samples predicted as positive, given by

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}.$$

This measure is useful when the cost of false positives is high, as it quantifies the ability of the classifier to avoid false positives. For example, in a medical diagnosis task, precision is important to avoid unnecessary treatments. However, precision does not consider false negatives, which can be problematic in other scenarios. For instance, in fraud detection, a false negative means that a fraudulent transaction was not detected. A classifier that always predicts class 1 will have a precision of 10% in the example above. On the other hand, a classifier that always predicts class 0 will have a precision of 0% — consider $0/0 = 0$.

Recall is the proportion of true positive predictions over the total number of samples that are actually positive, given by

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}.$$

This measure is useful when the cost of false negatives is high, as it quantifies the ability of the classifier to avoid false negatives. It can also be

[1] Sick is the positive class

interpreted as the "completeness" of the classifier: how many positive samples were correctly identified. For example, in a medical diagnosis task, recall is important to avoid missing a diagnosis. A classifier that always predicts class 1 will have a recall of 100% in the example above. On the other hand, a classifier that always predicts class 0 will have a recall of 0%.

F-score is the weighted harmonic mean of precision and recall given by

$$\text{F-score}(\beta) = \frac{(1+\beta^2) \cdot \text{Precision} \cdot \text{Recall}}{\beta^2 \cdot \text{Precision} + \text{Recall}},$$

where β is a parameter that controls the weight of precision in the measure. The most common value for β is 1, which gives the F_1-score. The F-score is useful when we want to balance precision and recall, as it considers both false positives and false negatives. For instance, a classifier that always predicts class 1 will have an F_1-score of 0.18 in the example above. On the other hand, a classifier that always predicts class 0 will have an F_1-score of 0. Note that, although guessing 1 is better than guessing 0 in terms of F_1-score, this measure is much better than accuracy to evaluate the performance of the classifier in imbalanced problems.

7.2 Regression estimation evaluation

Performance measures for regression tasks are usally calculated based on the error or residual $\epsilon_i = \hat{y}_i - y_i$ for all $i \in \mathcal{I}_{\text{test}}$. The most common measures are the mean absolute error, mean squared error.

Mean absolute error is the average of the absolute values of the residuals, given by

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n} |\epsilon_i|.$$

This measure is easy to interpret and gives an idea of the average error of the model.

Mean squared error is the average of the squared residuals, given by

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n} \epsilon_i^2.$$

This measure penalizes large errors more than the mean absolute error, as the squared residuals are summed.

Root mean squared error is the square root of the mean squared error, given by

$$\text{RMSE} = \sqrt{\text{MSE}}.$$

This measure is in the same unit as the target variable, which makes it easier to interpret.

7.3 Probabilistic classification evaluation

A particular case of the regression estimation is when we want to estimate the probability[2] of a sample belonging to the positive class — i.e. $y = 1$. In this case, the output of the model should be a probability in the interval $[0, 1]$. We can use a threshold τ to convert the probabilities into binary predictions. The default threshold is usually $\tau = 0.5$ — a sample is positive if the probability is greater than or equal to 0.5 and negative otherwise —, but it can be adjusted to change the trade-off between recall and specificity. A low threshold, $\tau \approx 0$, will increase recall at the expense of specificity, while a high threshold, $\tau \approx 1$, will increase specificity at the expense of recall.

Thus, any regressor $f_R : \mathcal{X} \to [0, 1]$ can be converted into a binary classifier $f_C : \mathcal{X} \to \{0, 1\}$ by comparing the output with the threshold τ:

$$f_C(\mathbf{x}) = \begin{cases} 1 & \text{if } f_R(\mathbf{x}) \geq \tau, \\ 0 & \text{otherwise.} \end{cases}$$

Before we discuss the performance measures for probabilistic classifiers, let us define some rates that are used in the evaluation. The true positive rate (TPR) is the proportion of true positive predictions over the total number of samples that are actually positive,

$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}},$$

and the false positive rate (FPR) is the proportion of false positive predictions over the total number of samples that are actually negative,

$$\text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}}.$$

[2] Although the term probability is used, the output of the regressor does not need to be a probability in the strict sense. It is a confidence level in the interval $[0, 1]$ that can be interpreted as a probability.

The performance of the possible variations of the classifiers can be evaluated using appropriate measures. Consider the example below of a given test set and the predictions of a regressor. We first sort the samples by the predicted probabilities and then calculate the true positive rate and false positive rate for each threshold. We need to consider only thresholds equal to the unique predicted values to understand the variations.

Table 7.1: Illustrative example of probability .

Predicted/Threshold	Expected	TPR	FPR
- / ∞	-	0/5	0/5
0.98	1	1/5	0/5
0.97	1	2/5	0/5
0.80	0	2/5	1/5
0.72	1	3/5	1/5
0.70	1	4/5	1/5
0.66	0	4/5	2/5
0.52	0	4/5	3/5
0.40	1	5/5	3/5
0.25	0	5/5	4/5
0.10	0	5/5	5/5

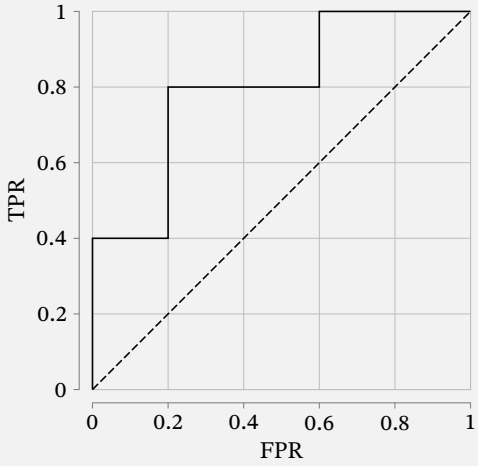
From this table, we can calculate the performance measures that are useful for probabilistic classifiers.

7.3.1 Receiver operating characteristic

The receiver operating characteristic (ROC) curve is a graphical representation of the trade-off between the true positive rate and the false positive rate as the threshold τ is varied. The ROC curve is obtained by plotting the TPR against the FPR for all possible thresholds. Figure 7.1 is the ROC curve for the example in table 7.1.

The ROC curve is useful to explore the trade-off between recall and specificity. The diagonal line represents a random classifier, and points above the diagonal are better than random. The area under the ROC curve (AUC) is a possible measure of the performance of the classifier. The AUC is scale invariant, which means that it measures how well pre-

Figure 7.1: Illustrative example of ROC curve.



ROC curve for the example in table 7.1. The diagonal line represents a random classifier, and points above the diagonal are better than random.

dictions are ranked, rather than their absolute values. In our example, the AUC is 0.8.

7.3.2 Detection error trade-off

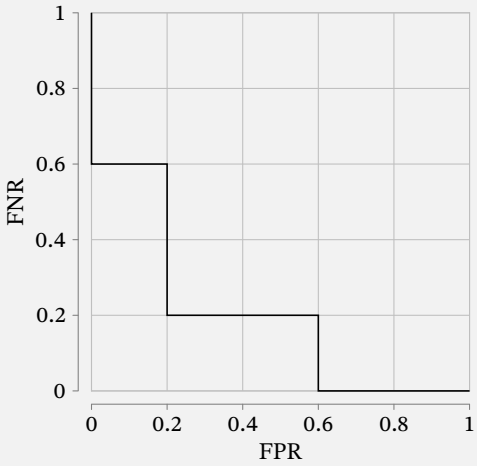
The detection error trade-off (DET) curve is a graphical representation of the trade-off between the false positive rate and the false negative rate (FNR),

$$\mathrm{FNR} = \frac{\mathrm{FN}}{\mathrm{TP} + \mathrm{FN}} = 1 - \mathrm{TPR}.$$

The DET curve is similar to the ROC curve, but by plotting only the FPR and FNR, it gives a better view of the "cost" (errors) of different thresholds. The DET curve is especially useful when the cost of false positives and false negatives is different. The DET curve of our example is shown in fig. 7.2.

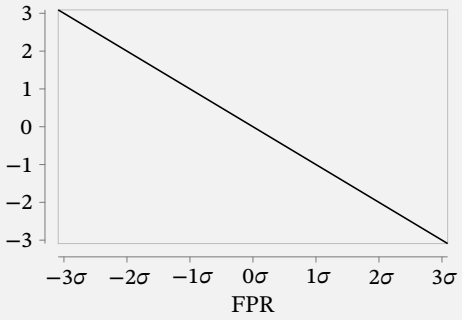
Usually, the DET curve is plotted in a normal deviate scale (Martin et al. 1997). In this scale, the axes are transformed to show the error rates in a more linear way.

Figure 7.2: Illustrative example of DET curve.



DET curve for the example in table 7.1. The diagonal line represents a random classifier, and points below the diagonal are better than random.

Figure 7.3: Illustrative example of DET curve (normal deviate scale).



7.4 Other variations

Some other points:

- measures for classification are asymmetric;
- prefer measures that work well with averaging;
- multiclass how to evaluate?
- customize to address the real problem.

8

Validation and experimental planning

All models are wrong, but some are useful.

— George E. P. Box, *Robustness in Statistics*

Once we have defined what an inductive problem is, we can start to think about how to solve it in practical terms.

In this chapter, we present the experimental planning one can use in the data-driven parts of a data science project. *Experimental planning* in the context of data science involves designing and organizing experiments to gather performance data systematically in order to reach specific goals or test hypotheses.

The reason we need to plan experiments is that data science is experimental, i.e. we usually lack a theoretical model that can predict the outcome of a given algorithm on a given dataset — in other words, the quality of the solution given a certain approach. This is why we need to run experiments to gather data and make inferences from it.

There is not a single way to plan experiments, but there are some common steps that can be followed to design a good experimental plan. In this chapter, we present a framework for experimental planning that can be used in most data science projects.

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8.1 Elements of an experimental plan

There are important elements that should be considered when designing an experimental plan. These elements are:

- **Hypothesis**: The main question that the experiment aims to validate. In this chapter, we address common questions in data science projects and how to validate them.
- **Data**: The dataset that will be used in the experiment. In chapter 3, we address topics about collecting and organizing data.
- **Solution search algorithm**[1]: Techniques that find a solution for the task. For us, a task includes both adjusting the appropriate data-handling pipeline and learning the model. The theoretical basis for these techniques is in chapter 5, and the practical aspects are in chapter 6 and **??**.
- **Performance measure**: The metric that will be used to evaluate the performance of the model. Refer to chapter 7 for more information.

A general example of a description of an experimental plan is "What is the probability of the technique A to find a model that reaches a performance X in terms of metric Y in the real-world given dataset Z as training set (assuming Z is a representative dataset)?"

Another example is "Is technique A better than technique B for finding a model that predicts the output with D as a training set in terms of metric E?"

We consider these two cases: *estimating expected performance* and *comparing algorithms*.

8.2 Estimating expected performance

When dealing with a data-driven solution, the available data is a representation of the real world. So, we have to make the best use of the data we have to estimate how good our solution is expected to be in production.

[1] We use the term "search" because, the chosen algorithm aim at optimizing both the parameters of the data handling pipeline and the ones of the model

Obviously, the more data we use to search for a solution, the better the solution is expected to be. Thus, we use the whole dataset for deploying a solution. But, what method for preprocessing and learning should we use? How well that technique is expected to perform in the real world?

Let us say we fix a certain technique, let us call it A. Let M be the solution found by A using the whole dataset D. If we assess M using the whole dataset D, the performance p we get is optimistic. This is because M has been trained and tested on the same data.

Hold out does not solve the problem.

To estimate better the expected performance of M in production, we can use the following experimental plan.

Sampling strategy As any statistical evaluation, we need to generate samples of the performance of the possible solutions that A is able to obtain. To do so, we use a sampling strategy to generate datasets $D_1, D_2, \ldots$ from D. Since we assume the dataset D is a representative sample of the real world, we must ensure that each sampled dataset has similar characteristics. So handling operators like balancing the dataset should be applied only afterwards. Each dataset is further divided into a training set and a test set, which must be disjoint. The training set is thus used to find a solution — $M_1, M_2, \ldots$ for each training set — and the test set is used to evaluate the performance — $p_1, p_2, \ldots$ for each test set — of the solution. The test set emulates the real-world scenario, where the model is used to make predictions on new data.

Solution search algorithm The solution search algorithm A involves both a given data handling pipeline and a machine learning method. Both of them generate a different result for each dataset D_k used as an input. In other words, the parameters ϕ of the data handling operators are adjusted — see chapter 6 — and the parameters θ of the machine learning model are adjusted — see chapter 5. These parameters, $[\phi_k, \theta_k]$ are the solution M_i, and must be calculated exclusively using the training set $D_{k,\text{train}}$.

Prediction Once the parameters ϕ and θ are fixed, we apply them in the test set $D_{k,\text{test}}$. For each sample $(x_i, y_i) \in D_{k,\text{test}}$, we calculate the prediction $\hat{y} = f_{\phi,\theta}(x_i)$. The target value y is called the ground-truth or expected outcome.

Performance assessment Given a performance metric R, for each dataset D_k, we calculate

$$p_k = R\big([y_i]_i, [\hat{y}_i]_i\big).$$

Note that, by definition, p_k is free of data leakage, as $[\phi_k, \theta_k]$ are found without the use of the data in $D_{k,\text{test}}$ and to calculate $\hat{y}_i$ we use only x_i (with no target y_i).

Analysing the results Finally, we study the sampled performance values $p_1, p_2, \ldots$ like any other statistical data. We can calculate summary statistics, like the mean, median, variance, and standard deviation, or visualization techniques, like box plots or other distribution-based plots. We can also use hypothesis tests to calculate the probability of the performance of the solution being better than a certain threshold.

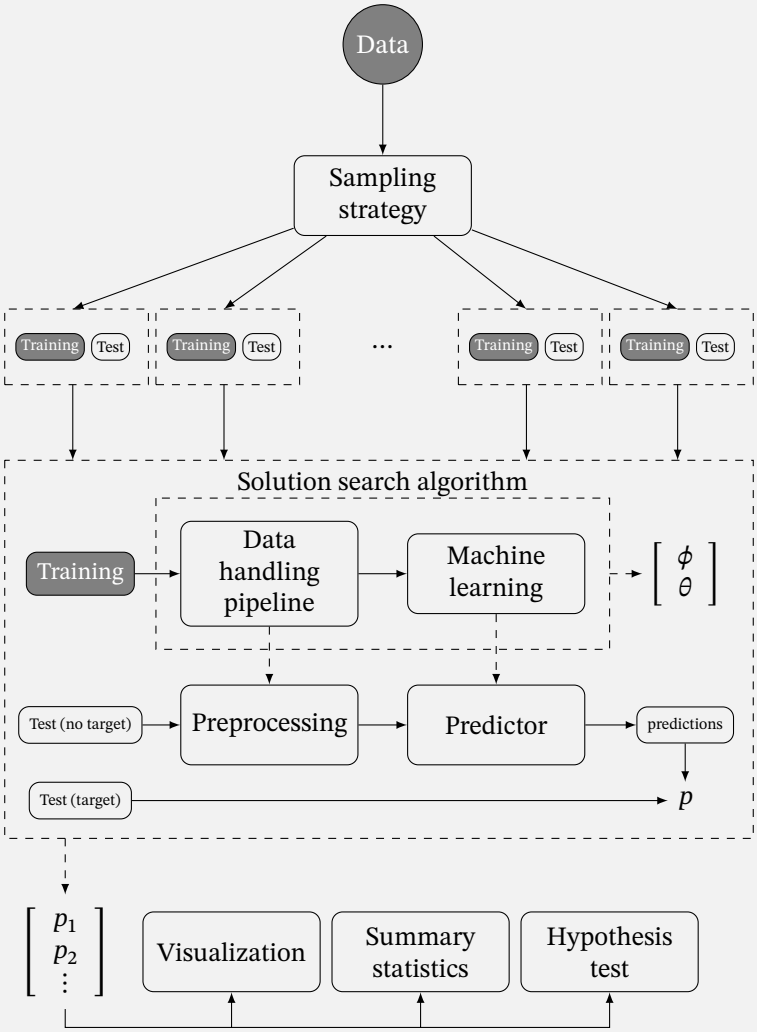
Evaluation *vs.* validation

We call evaluation the process of assessing the performance of a solution using a test set. Validation, on the other hand, is the process of interpreting or confirming the meaning of the evaluation results. Validation is the process of determining the degree to which the evaluation results support the intended use of the solution (unseen data).

Interpretation The results are not the "real" performance of the solution M in the real world, as that would require new data to be collected. However, we can safely interpret the performance samples as being sampled from the same distribution as the performance of the solution M.

A summary of the experimental plan for estimating expected performance is shown in fig. 8.1.

Figure 8.1: Experimental plan for estimating expected performance of a solution.

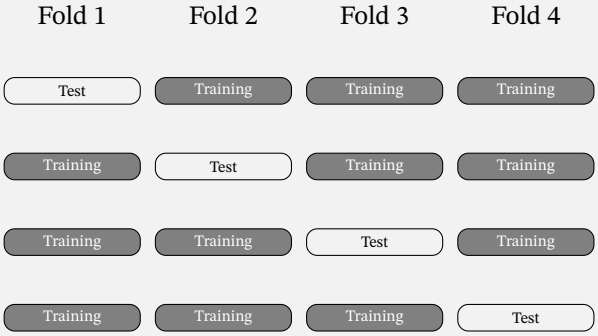


The experimental plan for estimating the expected performance of a solution involves sampling the data, training and testing the solution, evaluating the performance, and validating the results.

8.2.1 Cross validation

The most common sampling strategy is the *cross-validation*. It assumes that data is independent and identically distributed (i.i.d.). The cross-validation technique divides the dataset into r folds randomly, with the same size. Each part (fold) is used as a test set once and as a training set $r-1$ times. So, first we use as training set folds $2, 3, \ldots, r$ and as test set fold 1. Then, we use as training set folds $1, 3, \ldots, r$ and as test set fold 2. And so on. (See fig. 8.2.)

Figure 8.2: Cross-validation



Cross-validation is a technique to sample training and test sets. It divides the dataset into r folds, using $r-1$ folds as a training set and the remaining fold as a test set.

If possible, one should use repeated cross-validation, where this process is repeated many times. Also, when dealing with classification problems, we should use stratified cross-validation, where the distribution of the classes is preserved in each fold.

Also, the application of a single cross-validation sampling enables us to create a predicted vector for the whole dataset. This is done by concatenating the predictions for each fold. (Note however that the predictions are not totally independent, as they share some training data. This dependency should be taken into account when analyzing the results.) This vector can be used to perform hypothesis tests — like McNemar's test, see section 8.3 — or to plot ROC (Receiver Operating Characteristic) curves or DET (Detection Error Tradeoff) curves — see chapter 7.

8.2.2 Validation methods

Validation is the process of interpreting or confirming the meaning of the evaluation results. It is the process of determining the degree to which the evaluation results support the intended use of the solution.

Sometimes, it is as simple as calculating the mean and standard deviation of the performance samples. Other times, we need to use more sophisticated techniques, like hypothesis tests or Bayesian analysis.

Let us say our goal is to reach a certain performance threshold p_0. After an experiments done with 10 repeated 10-fold cross-validation, we have the average performance $\bar{p}$ and the standard deviation σ. If $\bar{p} - \sigma \gg p_0$, it is very likely that the solution will reach the threshold in production. Although this is not a formal validation, it is a good and likely enough indication.

Also, it is common to use visualization techniques to analyze the results. Box plots are a good way to see the distribution of the performance samples.

A more sophisticated technique is to use Bayesian analysis. In this case, we use the performance samples to estimate the probability distribution of the performance of the algorithm. This distribution can be used to calculate the probability of the performance being better than a certain threshold.

Benavoli et al. (2017) propose an interesting Bayesian test that accounts for the overlapping training sets in the cross-validation[2]. Let $z_k = p_k - p^*$ be the difference between the performance of the k-th fold and the performance goal p^*, a generative model for the data is

$$\mathbf{z} = \mathbf{1}\mu + \mathbf{v},$$

where $\mathbf{z} = (z_1, z_2, \ldots, z_n)$ is the vector performance gains, $\mathbf{1}$ is a vector of ones, μ is the parameter of interest (the mean performance gain), and $\mathbf{v} \sim \text{MVN}(0, \Sigma)$ is a multivariate normal noise with zero mean and covariance matrix Σ. The covariance matrix Σ is characterized as

$$\Sigma_{ii} = \sigma^2, \quad \Sigma_{ij} = \sigma^2\rho,$$

for all $i \neq j \in \{1, 2, \ldots, n\}$, where ρ is the correlation (between folds) and σ^2 is the variance. The likelihood model of the data is

$$\text{P}(\mathbf{z} \mid \mu, \Sigma) = \exp\left(-\frac{1}{2}(\mathbf{z} - \mathbf{1}\mu)^T\Sigma^{-1}(\mathbf{z} - \mathbf{1}\mu)\right)\frac{1}{(2\pi)^{n/2}\sqrt{|\Sigma|}}.$$

[2]This is actually a particular case of the proposal in the paper, where the authors consider the comparison between two performance vector — which is the case described in section 8.3.

According to them, such likelihood does not allow to estimate the correlation from data, as the maximum likelihood estimate of ρ is zero regardless of the observations. Since ρ is not identifiable, the authors suggest using the heuristic where ρ is the ratio between the number of folds and the total number of performance samples.

To estimate the probability of the performance of the solution being greater than the threshold, we first estimate the parameters μ and $\nu = \sigma^{-2}$ of the generative model. Benavoli et al. (2017) consider the prior

$$\mathrm{P}(\mu, \nu \mid \mu_0, \kappa_0, a, b) = \mathrm{NG}(\mu, \nu; \mu_0, \kappa_0, a, b),$$

that is a Normal-Gamma distribution with parameters (μ_0, κ_0, a, b). This is a conjugate prior to the likelihood model. Choosing the prior parameters $\mu_0 = 0$, $\kappa_0 \to \infty$, $a = -1/2$, and $b = 0$, the posterior distribution of μ is a location-scale Student distribution. Mathematically, we have

$$\mathrm{P}(\mu \mid \mathbf{z}, \mu_0, \kappa_0, a, b) = \mathrm{St}(\mu; n-1, \bar{z}, \left(\frac{1}{n} + \frac{\rho}{1-\rho}\right) s^2),$$

where

$$\bar{z} = \frac{1}{n} \sum_{i=1}^{n} z_i,$$

and

$$s^2 = \frac{1}{n-1} \sum_{i=1}^{n-1} (z_i - \bar{z})^2.$$

Thus, validating that the solution obtained by the algorithm in production will surpass the threshold p^* consists of calculating the probability

$$\mathrm{P}(\mu > 0 \mid \mathbf{z}) > \gamma,$$

where γ is the confidence level.

Note that the Bayesian analysis is a more sophisticated technique than the null hypothesis significance testing, as it allows us to estimate the probability of the performance of the solution being better than a certain threshold.

Also, be aware that the choice of the model and the prior distribution can affect the results. Benavoli et al. (2017) suggest using 10 repetitions of 10-fold cross-validation to estimate the parameters of the generative model. They also show experimental evidence that their choices are robust to the choice of the prior distribution. However, one should be aware of the limitations of the model.

8.3 Comparing strategies

Talk about paired dataset samples.

When we have two or more strategies to solve a problem, we need to compare them to see which one is better. This is a common situation in data science projects, as we usually have many techniques to solve a problem.

One way to look at this problem is to consider that the algorithm[3] A has *hyperparameters* $\lambda \in \Lambda$. A hyperparameter here is a parameter that is not learned by the algorithm, but is set by the user. For example, the number of neighbors in a k-NN algorithm is a hyperparameter. For the sake of generality, we can consider that the hyperparameters may also include different learning algorithms or data handling pipelines.

Let us say we have a baseline algorithm $A(\lambda_0)$ — for instance, something that is in production, the result of the last sprint or a well-known algorithm — and a new candidate algorithm $A(\lambda)$. Suppose $\mathbf{p}(\lambda_0)$ and $\mathbf{p}(\lambda)$ are the performance vectors of the baseline and the candidate algorithms, respectively, that are calculated using the same strategy described in section 8.2. We can validate whether the candidate is better than the baseline by

$$\mathrm{P}(\mu > 0 \mid \mathbf{z}) > \gamma,$$

where $\mathbf{z}$ is now $\mathbf{p}(\lambda) - \mathbf{p}(\lambda_0)$ and γ is the confidence level. Also, the expected performance gain of the candidate algorithm is μ — if negative, the performance loss.

This strategy can be applied iteratively to compare many algorithms. For example, we can compare $A(\lambda_1)$ with $A(\lambda_0)$, $A(\lambda_2)$ with $A(\lambda_1)$, and so on, keeping the best algorithm found so far as the baseline. In the cases where the confidence level is not reached, but the expected performance gain is positive, we can consider additional characteristics of the algorithms, like the interpretability of the model, the computational cost, or the ease of implementation, to decide which one is better. However, one should pay attention whether the probability

$$\mathrm{P}(\mu < 0 \mid \mathbf{z})$$

is too high or not. Always ask yourself if the risk of the performance loss is worth in the real-world scenario.

[3] That includes both data handling and machine learning.

8.3.1 About nesting experiments

Mathematically speaking, there is no difference between assessing the choice of $[\phi, \theta]$ and the choice of λ. Thus, some techniques — like grid search — can be used to find the best hyperparameters using a nested experimental plan.

The idea is the same, we assess how good is the expected choice of the hyperparameter-optimization technique B to find the appropriate hyperparameters. Similarly, the choice of the hyperparameters and the parameters that goes to production is the application of B to the whole dataset. However, never use the choices of the hyperparameters in the experimental plan to make decisions about what goes to production. (The same is true for the parameters $[\phi, \theta]$ in the traditional case.)

We can unnest the search by interpreting the options as different algorithms two by two.

8.4 Grouping

TODO Grouped cross validation.

9

Ethical, privacy and legal issues

It's a trap!

— Admiral Ackbar, *Star Wars Episode VI: Return of the Jedi*

A few comments on the ethical, privacy and legal issues that data scientists should be aware of.

Chapter remarks

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9.1 Ethical and moral values

9.2 Privacy and data protection

9.2.1 Homomorphic encryption

9.2.2 Federated learning

9.3 Major legal frameworks

9.3.1 General Data Protection Regulation (GDPR)

9.3.2 California Consumer Privacy Act (CCPA)

Bibliography

Beaumont, P. B. and R. G. Bednarik (2013). In: *Rock Art Research* 30.1, pp. 33–54. URL: https://search.informit.org/doi/10.3316/informit.488018706238392 (cit. on p. 7).

Benavoli, A., G. Corani, J. Demšar, and M. Zaffalon (2017). "Time for a Change: a Tutorial for Comparing Multiple Classifiers Through Bayesian Analysis". In: *Journal of Machine Learning Research* 18.77, pp. 1–36. URL: http://jmlr.org/papers/v18/16-305.html (cit. on pp. 136, 137).

Billingsley, P. (1995). *Probability and Measure*. 3rd ed. John Wiley & Sons. ISBN: 0-471-00710-2 (cit. on p. 40).

Breiman, L. (1996). "Bagging predictors". In: *Machine Learning* 24.2, pp. 123–140. DOI: 10.1007/BF00058655 (cit. on p. 16).

Cleveland, W. S. (2001). "Data Science: An Action Plan for Expanding the Technical Areas of the Field of Statistics". In: *ISI Review*. Vol. 69, pp. 21–26 (cit. on p. 4).

Codd, E. F. (1970). "A Relational Model of Data for Large Shared Data Banks". In: *Commun. ACM* 13.6, pp. 377–387. ISSN: 0001-0782. DOI: 10.1145/362384.362685 (cit. on p. 9).

Cormen, T. H., C. E. Leiserson, R. L. Rivest, and C. Stein (2022). *Introduction to Algorithms*. 4th ed. The MIT Press, p. 1312. ISBN: 9780262046305 (cit. on pp. 21, 25, 27).

Cortes, C. and V. N. Vapnik (1995). "Support-vector networks". In: *Machine Learning* 20.3, pp. 273–297. DOI: 10.1007/BF00994018 (cit. on p. 16).

Cover, T. M. (1965). "Geometrical and Statistical Properties of Systems of Linear Inequalities with Applications in Pattern Recognition". In: *IEEE Transactions on Electronic Computers* EC-14.3, pp. 326–334. DOI: 10.1109/PGEC.1965.264137 (cit. on p. 16).

Fagin, R. (1979). "Normal forms and relational database operators". In: *Proceedings of the 1979 ACM SIGMOD International Conference on Management of Data*. SIGMOD '79. Boston, Massachusetts: Association for Computing Machinery, pp. 153–160. ISBN: 089791001X. DOI: 10.1145/582095.582120. URL: https://doi.org/10.1145/582095.582120 (cit. on p. 54).

Friedman, J. H. (2001). "Greedy function approximation: A gradient boosting machine." In: *The Annals of Statistics* 29.5, pp. 1189–1232. DOI: 10.1214/aos/1013203451. URL: https://doi.org/10.1214/aos/1013203451 (cit. on p. 16).

Grajalez, C. G., E. Magnello, R. Woods, and J. Champkin (2013). "Great moments in statistics". In: *Significance* 10.6, pp. 21–28. DOI: 10.1111/j.1740-9713.2013.00706.x (cit. on p. 7).

Hillis, W. D. (1985). "The Connection Machine". Hillis, W.D.: The Connection Machine. PhD thesis, MIT (1985). Cambridge, MA, USA: Massachusetts Institute of Technology. URL: http://hdl.handle.net/1721.1/14719 (cit. on p. 11).

Ho, T. K. (1995). "Random decision forests". In: *Proceedings of 3rd International Conference on Document Analysis and Recognition*. Vol. 1, 278–282 vol.1. DOI: 10.1109/ICDAR.1995.598994 (cit. on p. 16).

Hunt, E. B., J. Marin, and P. J. Stone (1966). *Experiments in Induction*. New York, NY, USA: Academic Press (cit. on p. 15).

Ifrah, G. (1998). *The Universal History of Numbers, from Prehistory to the Invention of the Computer*. First published in French, 1994. London: Harvill. ISBN: 1 86046 324 x (cit. on p. 7).

Kelleher, J. D. and B. Tierney (2018). *Data science*. The MIT Press (cit. on pp. xiii, xvi, 6, 46).

Le Cun, Y. (1986). "Learning Process in an Asymmetric Threshold Network". In: *Disordered Systems and Biological Organization*. Berlin, Heidelberg: Springer Berlin Heidelberg, pp. 233–240. ISBN: 978-3-642-82657-3 (cit. on p. 15).

Martin, A. F., G. R. Doddington, T. Kamm, M. Ordowski, and M. A. Przybocki (1997). "The DET curve in assessment of detection task performance." In: *EUROSPEECH*. Ed. by G. Kokkinakis, N. Fako-

takis, and E. Dermatas. ISCA, pp. 1895–1898. URL: http://dblp.uni-trier.de/db/conf/interspeech/eurospeech1997.html#MartinDKOP97 (cit. on p. 126).

Naur, P. (1974). *Concise Survey of Computer Methods*. Lund, Sweden: Studentlitteratur. ISBN: 91-44-07881-1. URL: http://www.naur.com/Conc.Surv.html (cit. on p. 3).

Quinlan, J. R. (1986). "Induction of Decision Trees". In: *Machine Learning* 1, pp. 81–106. URL: https://api.semanticscholar.org/CorpusID:13252401 (cit. on p. 15).

Rosen, K. H. (2018). *Discrete Mathematics and Its Applications*. 8th ed. McGraw Hill, p. 1120. ISBN: 9781259676512 (cit. on p. 31).

Ross, S. M. (2014). *Introduction to Probability Models*. 11th ed. Academic Press, p. 784. ISBN: 9780124079489 (cit. on p. 34).

— (2018). *A First Course in Probability*. 10th ed. Pearson, p. 528. ISBN: 978-1292269207 (cit. on p. 34).

Rumelhart, D. E., G. E. Hinton, and R. J. Williams (1986). "Learning representations by back-propagating errors". In: *Nature* 323.6088, pp. 533–536. DOI: 10.1038/323533a0 (cit. on p. 15).

Schapire, R. E. (1990). "The strength of weak learnability". In: *Machine Learning* 5.2, pp. 197–227. DOI: 10.1007/BF00116037 (cit. on p. 16).

Silva, T. C. and L. Zhao (2013). "Detecting and preventing error propagation via competitive learning". In: *Neural Networks* 41. Special Issue on Autonomous Learning, pp. 70–84. ISSN: 0893-6080. DOI: https://doi.org/10.1016/j.neunet.2012.11.001. URL: https://www.sciencedirect.com/science/article/pii/S0893608012002778 (cit. on p. 86).

Song, J., H. V. Jagadish, and G. Alter (2021). "SDTA: An Algebra for Statistical Data Transformation". In: *Proc. of 33rd International Conference on Scientific and Statistical Database Management (SSDBM 2021)*. Tampa, FL, USA: Association for Computing Machinery, p. 12. DOI: 10.1145/3468791.3468811 (cit. on p. 109).

Takens, F. (2006). "Detecting strange attractors in turbulence". In: *Dynamical Systems and Turbulence, Warwick 1980: proceedings of a symposium held at the University of Warwick 1979/80*. Springer, pp. 366–381 (cit. on p. 67).

Vapnik, V. N. (1999). *The nature of statistical learning theory*. 2nd ed. Springer-Verlag New York, Inc. ISBN: 978-1-4419-3160-3 (cit. on pp. 6, 85, 92).

Vapnik, V. N. and R. Izmailov (2015). "Learning with Intelligent Teacher: Similarity Control and Knowledge Transfer". In: *Statistical Learning and Data Sciences*. Ed. by A. Gammerman, V. Vovk, and H. Pa-

padopoulos. Cham: Springer International Publishing, pp. 3–32. ISBN: 978-3-319-17091-6 (cit. on p. 17).

Velleman, P. F. and L. Wilkinson (1993). "Nominal, Ordinal, Interval, and Ratio Typologies are Misleading". In: *The American Statistician* 47.1, pp. 65–72. DOI: 10.1080/00031305.1993.10475938 (cit. on p. 50).

Vincent, M. W. (1997). "A corrected 5NF definition for relational database design". In: *Theoretical Computer Science* 185.2. Theoretical Computer Science in Australia and New Zealand, pp. 379–391. ISSN: 0304-3975. DOI: https://doi.org/10.1016/S0304-3975(97)00050-9. URL: https://www.sciencedirect.com/science/article/pii/S0304397597000509 (cit. on p. 55).

Wickham, H. (2014). "Tidy Data". In: *Journal of Statistical Software* 59.10, pp. 1–23. DOI: 10.18637/jss.v059.i10. URL: https://www.jstatsoft.org/index.php/jss/article/view/v059i10 (cit. on pp. 57, 63).

Wickham, H., M. Çetinkaya-Rundel, and G. Grolemund (2023). *R for Data Science: Import, Tidy, Transform, Visualize, and Model Data*. 2nd ed. O'Reilly Media (cit. on pp. xiii, xvi, 45, 63, 101, 108).

Zumel, N. and J. Mount (2019). *Practical Data Science with R*. 2nd ed. Manning (cit. on pp. xiii, xvi, 45, 72, 74–77, 85).

Glossary

BI Business Intelligence 10

BNF Backus–Naur form 3

CDF cumulative distribution function 36

ERM Empirical Risk Minimization 15, 16

ETL Extract, Transform, Load 9

FIFO first-in-first-out 27

HDFS Hadoop Distributed File System 11

IBM International Business Machines Corporation 8

IoT Internet of Things 12

LIFO last-in-first-out 27

LUSI Learning using Statistical Inference 17

PDF probability density function 36

PMF probability mass function 36

RDBMS Relational Database Management System 9

SQL Structured Query Language 9

SVM Support Vector Machine 16