DATA SCIENCE PROJECT

AN INDUCTIVE LEARNING APPROACH

F.A.N. VERRI

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To my wife, for inspiring and supporting me in writing this book.

Above all, God be praised.

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Foreword

by *Ana Carolina Lorena*

Data is now a ubiquitous presence and is collected every time and everywhere. However, the real challenge lies in harnessing this data to generate actionable insights that guide decision-making and drive innovation. This is the essence of data science, a multidisciplinary field that leverages mathematical, statistical, and computational techniques to analyse data and solve complex problems.

The book "Data Science Project: An Inductive Learning Approach" by F.A.N. Verri provides readers with a structured and insightful exploration of the entire data science pipeline, from the initial stages of data collection to the final step of model deployment. The book effectively balances theory and practice, focusing on the inductive principles underpinning predictive analytics and machine learning.

While other texts focus solely on machine learning algorithms or delve deeply into tool-specific details, this book provides a holistic view of every stage of a data science project. It emphasises the importance of robust data handling, sound statistical learning principles, and meticulous model evaluation. The author thoughtfully integrates the mathematical foundations and practical considerations needed to design and execute successful data science projects.

Beyond the technical mechanics, this book challenges readers to critically evaluate their models' strengths and limitations. It underscores the importance of semantics in data handling, equipping readers with the skills to interpret and transform data meaningfully.

Whether you are a student embarking on your first data science project or a data scientist professional seeking to expand and refine your skills, this book's clarity, rigour, and practical focus make it a guide that will serve you well in tackling the complex challenges of data-driven decision-making. The book will expand your understanding and inspire you to approach data science projects with a commitment to creating responsible and impactful solutions.

Preface

Dear reader,

This book is based on the lecture notes from my course PO-235 Data Science Project, which I teach to graduate students at both the Aeronautics Institute of Technology (ITA) and the Federal University of São Paulo (UNIFESP) in Brazil. I have been teaching this subject since 2021, and I have continually updated the material each year.

Also, I was the coordinator of the Data Science Specialization Program (CEDS) at ITA. That experience, which included a great deal of administrative work, as well as teaching and supervising professionals in the course, has helped me to understand the needs of the market and the students.

Moreover, parts of the project development methodology presented here came from my experience as a lead data scientist in R&D projects for the Brazilian Air Force, which included projects in areas such as image processing, natural language processing, and spatio-temporal data analysis.

Literature provides us with a wide range of excellent theoretical material on machine learning and statistics, and highly regarded practical books on data science tools. However, I missed something that could provide a solid foundation on data science, covering all steps in a data science project, including its software engineering aspects.

My goal is to provide a book that serves as a textbook for a course on data science projects or as a reference for professionals working in the field. I strive to maintain a formal tone while preserving the practical aspects of the subject. I do not focus on a specific tool or programming language, but rather seek to explain the semantics of data science tasks that can be implemented in any programming language.

Also, instead of teaching specific machine learning algorithms, I try to explain why machine learning works, thereby increasing awareness of its pitfalls and limitations. For this purpose, I assume you have a strong mathematical and statistical foundation.

One important 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 rule mining, transductive learning, anomaly detection, time series forecasting, reinforcement learning, etc.

I expect my approach on the subject to provide understanding of all steps in a data science project, including a deeper focus on correct evaluation and validation of data science solutions.

Note that, in this book, I openly express my opinions and beliefs. On several occasions it may sound controversial. I am not trying to be rude or to demean any researcher or practitioner in the field; rather, I aim to be honest and transparent.

I'd rather be bold and straightforward than cower about my beliefs.

I hope you enjoy reading.

I intend to make this book forever free and open-source. You can find the source code at github.com/verri/dsp-book. Derivatives are not allowed, but you can contribute to the book. Contributors will be acknowledged here.

However, if you like this book, consider purchasing the e-book version at leanpub.com/dsp. Any amount you pay will help me keep this book updated and write new books.

If you have suggestions or questions, please open or join a discussion at github.com/verri/dsp-book/discussions. Feel free to ask anything. Theoretical discussions and practical advice are also welcome.

If you want to support me, you can *buy me a coffee* at buymeacoffee.com/verri. I will greatly appreciate it. I have a number of ideas for new books and courses, and financial support will enable me to make them a reality.

Contributors

I would like to thank the following contributors for their help in improving this book:

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- Vitor V. Curtis

All contributors have freely waived their rights to the content they contributed to this book.

1 A 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 regarding the origin of data science. For the sake of contextualization, I separate the topic into 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 for understanding the context of the discipline. Over the years, the term has been employed to label quite different fields of study. Before presenting my view on the term, I present the views of two influential figures in the history of data science: Peter Naur and William Cleveland.

Moreover, studying the key facts and figures in the history of data-driven sciences enables us to comprehend the evolution of the field and hopefully guide us towards evolving it further. Besides, history also teaches us ways to avoid repeating the same mistakes.

Most of the significant theories and methods in data science have been developed simultaneously across 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 milestones 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 context of inductive learning.

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.”
- Recognize the major milestones in the history of data-driven sciences.
- Identify important figures in the field of data-driven sciences.

Takeaways

- 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 sufficient evidence to support data science as a distinct science.

1.1 The term "data science"

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

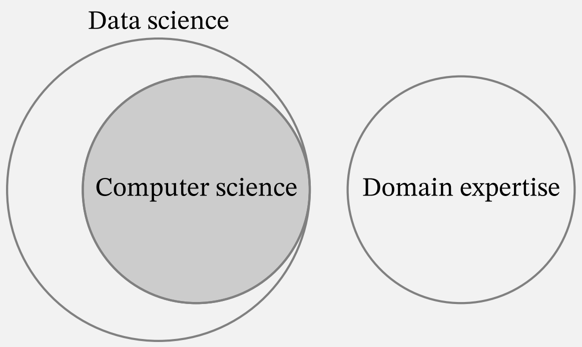
It is interesting to see the central role he gave to data in the field of computer science. His view that the relation of data to what they represent is delegated to other fields and sciences is still debatable today. Some scientists argue that data science should focus on the techniques to deal with 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.

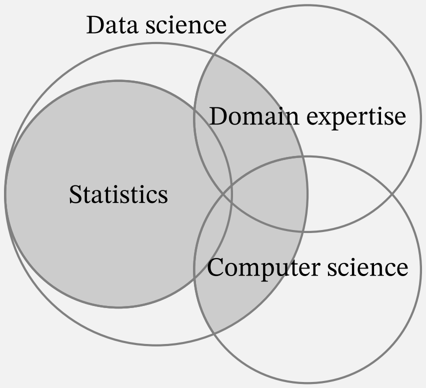
As a result, William Swain Cleveland II is credited with defining data science as it is most used today. He is a highly influential figure in the fields of statistics, machine learning, data visualization, data analysis for multidisciplinary studies, and high performance computing for deep data analysis.

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 an 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 computational

[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.

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 rather an enlarged scope of an existing science. I disagree; the social and economic demand for data-driven solutions has led to an evolution in our understanding of the challenges we are facing. As a result, we see many “data scientists” being hired and many “data science degree” programs emerging.

In chapter 4, 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 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 exceptional remarks from V. N. Vapnik (1999)[8].

I first address data handling — which includes 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.

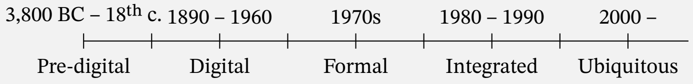


Figure 1.3 illustrates the proposed timeline. Ages have no absolute boundaries, but rather periods where some important events happened. Also, observe that the timescale is not linear. The Pre-digital Age is the longest period, and one could divide it into smaller periods. My choices of ages and their 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 (probably) used to keep track of the passing of time. The Lebombo bone, a baboon fibula with notches, is one of the earliest known mathematical objects. 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

[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.

purpose is unknown. Its 29 notches suggest that it 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 milestone in the history of data collection is the record of demographic data. One of the first known censuses was conducted in 3,800 BC in the Babylonian Empire. It was ordered to assess the population and resources of the empire. Records were stored on clay tiles[10].

Since the early forms of writing, humanity's abilities to register data and events 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. (An Eastern timeline research seems much harder to perform. Unfortunately, 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 a 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. 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-20th 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 does 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 4.2 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 the software Apache Hadoop, proposed both 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 architecture proposed in Hillis (1985)[18] the-

[17]J. Dean and S. Ghemawat (Jan. 2008). "MapReduce: simplified data processing on large clusters". In: *Commun. ACM* 51.1, pp. 107–113. ISSN: 0001-0782. DOI: 10.1145/1327452.1327492.

[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.

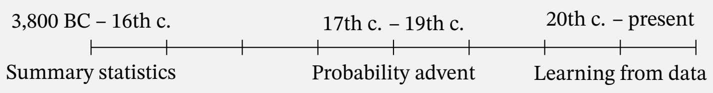


Figure 1.4 illustrates the proposed timeline. I consider changes of ages to be smooth transitions, and not strict boundaries. The theoretical advances are slower than the technological ones — the latter influences more data handling than data analysis —, so not much has changed since the beginning of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

Summary statistics

The earliest known records of systematic data analysis date back to the first censuses. The term *statistics* itself refers 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) and variability (e.g., range).

Probability advent

However, after the 17th century, the foundations of modern probability theory were laid out. Important figures for developing that theory are Blaise Pascal (1623 – 1662), Pierre de Fermat (1601 – 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 — are 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].

The method of least squares marked the beginning of the field of regression analysis. It marked a shift to find the solution of systems of equations — especially, overdetermined systems — using data instead of theoretical models.

Playfair's data visualization Another change in the way we analyze data was the development of data visualization. Data visualization is the graphical representation of information and data.

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 diagrams between the 1780s and 1800s, such as the line, area,

[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.

and bar chart of economic data, and the pie chart and circle graph to show proportions.

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.

This era is characterized by a change of focus from trying to fit data to a theoretical model to trying to extract knowledge from data. The main goal is to develop algorithms that can learn from data with minimal human intervention.

Fisher's discriminant analysis In the 1930s, Sir Ronald A. Fisher (1890 – 1962), a British polymath, developed discriminant analysis[20], which was initially used to find linear functions to solve the problem of separating two or more classes of objects[21].

The method is based on the so-called Fisher discriminant, which is a linear combination of variables. The method can be used not only for classification but also for dimensionality reduction.

Tackling the problem of the importance of the variables for a particular task, Fisher's work increased the understanding of the importance of feature selection in data analysis.

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.

Information theory sees data as a sequence of symbols that can be compressed and transmitted. The theory is used to quantify the amount of information in a data set. It also changed dominant paradigms in

[20]https://digital.library.adelaide.edu.au/dspace/bitstream/2440/15227/1/138.pdf

[21]After Rosenblatt's work, however, it was used to solve inductive inference (classification) as well. For curiosity, Fisher's paper introduced the famous Iris data set.

the field of statistics, such as the use of likelihood functions and the Bayesian approach.

K-Nearest Neighbors In 1951, Evelyn Fix (1904 – 1965) and Joseph L. 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 traditional parametric methods — and purely statistical ones — to non-parametric methods.

It also shows how intuitive models can be used to solve complex problems. The k-nearest neighbors algorithm is based on the idea that objects that are similar are likely to be in the same class.

Rosenblatt's perceptron In the 1960s, a psychologist called 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.

This work was the foundation of the field of artificial neural networks. The "training" of the perceptron was a breakthrough in the field of learning machines, drawing attention to the field of artificial intelligence.

A few years after, the book "Perceptrons: an introduction to computational geometry" by Marvin Minsky and Seymour Papert in 1969 drew attention to the limitations of the perceptron[22]. They showed that a single-layer perceptron was limited to linearly separable problems, a fact that led to a decline in the interest in neural networks. Consult section 6.6.1 for more details about the technique.

This fact contributed to the first AI winter, resulting in funding cuts for neural network research.

Hunt inducing trees In 1966, Hunt, Marin, and Stone's book[23] described a way to induce decision trees from data. The algorithm is based

[22]Although Rosenblatt was aware of the limitations of the perceptron and was probably working on solutions, he died in 1971.

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

on the concept of information entropy and is a precursor of the Quinlan's ID3 algorithm[24] and its variations. These algorithms gave rise to the field of decision trees, which is a popular method for classification and regression.

Trees are intuitive models that can be easily interpreted by humans. They are based on symbolic rules that can be used to explain their internal decision-making process.

Empirical risk minimization principle Although many learning machines were developed until the 1960s, they did not advance significantly the understanding of the general problem of learning from data. Between the 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 fundamental concepts of VC entropy and VC dimension for 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 multi-layer neural network[25]. The method is called backpropagation and is the foundation of the resurgence of neural networks. The technique enabled the training of artificial networks that can solve nonlinearly separable problems.

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 bio-inspired computing and evolutionary computation.

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

[25]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[26] and bagging[27], 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[28], while XGBoost, a gradient boosting method[29], has been extensively used in machine learning competitions.

Support vector machines In 1995, Cortes and V. N. Vapnik (1995)[30] proposed the support vector machine (SVM) algorithm, a learning machine based on the VC theory and the ERM principle. Based on Cover's theorem[31], 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 Although the idea of neural networks with multiple layers was around since the 1960s, only in the late 2000s did the field of deep learning catch 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 conceptual and engineering breakthroughs in the field, winning the 2018 Turing Award[32].

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

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

[28] 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.

[29] 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.

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

[31] 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.

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

LUSI learning theory In the 2010s, the researchers V. N. Vapnik and Izmailov (2015)[33] proposed the learning using statistical inference (LUSI) principle, which is an extension of 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."

[33]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 Fundamental concepts

The simple believes everything,

but the prudent gives thought to his steps.

— Proverbs 14:15 *(ESV)*

A useful starting point for someone studying data science is a definition of the term itself. In this chapter, I discuss some common definitions 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 whose 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 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 be as unproductive as creating a "new math" for each new application. All "sciences" rely on each other in some way

Chapter remarks

Contents

Context

- There is no consensus on the definition of data science.
- Understanding the nature of data is important to extract knowledge from it.
- Structured data are data that are organized in a tabular format.

Objectives

- Define data science.
- Present the main concepts about data theory.

Takeaways

- Data science is a new science that studies the knowledge extraction from measurable phenomena using computational methods.
- Database normalization and tidy data are complementary concepts that interact with each other.

2.1 Data science definition

In literature, we can find many definitions and descriptions of data science.

For Zumel and Mount (2019)[2], *"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 operations research, stating that data science focuses on implementing data-driven decisions and managing consequences of these decisions.

Wickham, Çetinkaya-Rundel, and Grolemund (2023)[3] declare that *"data science is an exciting discipline that allows you to transform raw data into understanding, insight, and knowledge."*

Hayashi (1998)[4] says that data science "is not only a synthetic concept to unify statistics, data analysis, and their related methods, but also comprises its results" and that it "intends to analyze and understand actual phenomena with 'data.'"

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 an 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. The terms "understanding," "insight," and "knowledge" are very important in the context of data science. They are the goals of a data science project.

The third definition brings an important aspect behind the data: the phenomena from which they come. Data science is not only about data, but about understanding the phenomena they represent.

[2]N. Zumel and J. Mount (2019). *Practical Data Science with R*. 2nd ed. Shelter Island, NY, USA: Manning.

[3]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.

[4]C. Hayashi (1998). "What is Data Science? Fundamental Concepts and a Heuristic Example". In: *Data Science, Classification, and Related Methods*. Ed. by C. Hayashi et al. Tokyo, Japan: Springer Japan, pp. 40–51. ISBN: 978-4-431-65950-1.

Note that these definitions do not contradict each other. But, they do not attempt to emphasize the "science" aspect of it. From these ideas, let us define the term.

Definition 2.1: (Data science)

Data science is the study of knowledge extraction from measurable phenomena using computational methods.

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 understand and/or apply to solve problems. *Measurable phenomena* are events or processes where raw data can be quantified in some way[5]. *Raw data* are data collected directly from some source and that have not been subject to any transformation by a software program or a human expert. *Data* is any piece of information that can be digitally stored.

Kelleher and Tierney (2018)[6] summarize very well the challenges of data science: "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 naming contrasts with conventional sciences. Usually, a "science" is named after its object of study. Biology is the study of 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 it to understand a certain phenomenon.

One similar example is "computer science." Computer science is not the study of computers themselves, but the study of computing and computer systems. Similarly, one could state that data science studies knowledge extraction[7] and data systems[8].

Moreover, the conventional scientific paradigm is essentially model-driven: we observe a phenomenon related to the object of study, we rea-

[5]Non-measurable phenomena are related to metaphysics and are not the object of study in data science. They are the object of study in other sciences, such as philosophy, theology, etc. However, many concepts from metaphysics are borrowed to explain data science concepts.

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

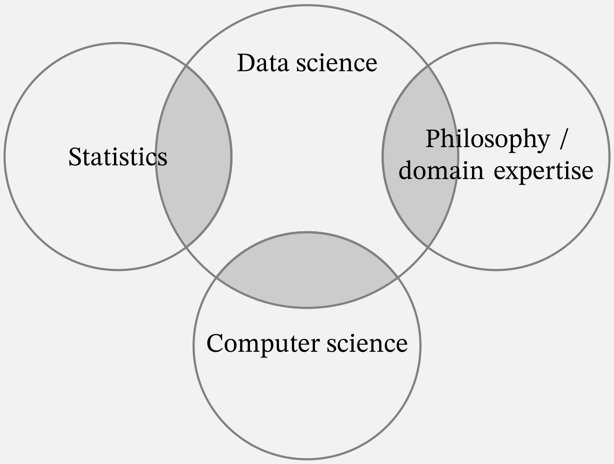
[7]Related to data analysis, see section 1.2.2.

[8]Related to data handling, see section 1.2.1.

son about 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 knowledge directly and primarily from the data. Expert knowledge and reasoning may be taken into account, but we give data the opportunity to surprise us.

Thus, while the objects of study in conventional sciences are the phenomena themselves and the models that can explain them, the objects of study in data science are the means (computational methods and processes) that can extract reliable and ethical knowledge from data acquired from any measurable phenomenon — and, of course, their consequences.

Figure 2.1: My view of data science.



Data science is an entirely 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. Note that I emphasize philosophy over domain expertise because, in terms of scientific knowledge, the former is more general than the latter.

Figure 2.1 shows my view of data science. Data science is an entirely new science that incorporates concepts from other sciences. In the next section, I argue the reasons to understand data science as a new science.

2.2 The data science continuum

In the previous section, I argued that data science is a new science defining its object of study. This is just the first step to establish a new science, especially because the object of study in data science is not new. Computer science, statistics, and other sciences have been studying methods to process data for a long time.

One key aspect of the establishment of a new science is the social demand and the importance of the object of study in our society. Many say that "data is the new oil." This is because the generation, storage, and processing of data has increased exponentially in the last decades. As a consequence, whoever holds the data and can effectively extract knowledge from them has a competitive advantage.

As a consequence of the demand, a set of methods are developed and then experiments are designed to assess their effectiveness. If the methods are effective, they gain credibility, are widely accepted, and become the foundation of a new scientific discipline.

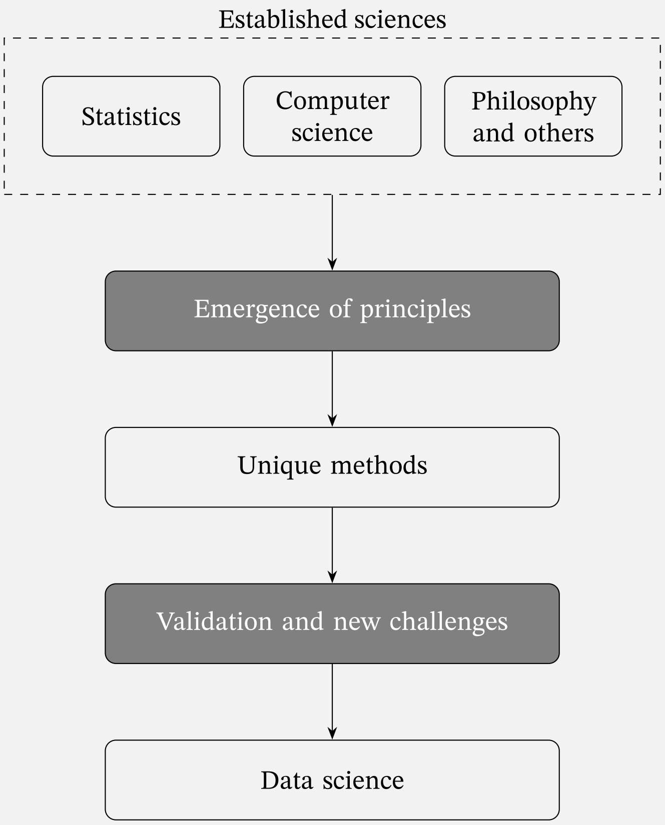
Usually, a practical consequence of academic recognition is the creation of new courses and programs in universities. This is the case of data science. Many universities have created data science programs in the last few years.

Once efforts to develop the subject increase, it is natural that some methodologies and questions not particularly related to any other science evolve. This effect produces what I call the "data science continuum."

In a continuum, the subject is not a new science yet. It is a set of methods and techniques borrowed from other sciences. However, some principles emerge that are connected with more than one already established science. (For instance, a traditional computational method adapted to assume statistical properties of the data.) With time, the premises and hypotheses of new methods become distinctive. The particular properties of the methods lead to the inception of methodologies to validate them. While validating the methods, new questions arise.

The data science continuum is an instance of this process; see fig. 2.2. At first glance, data science seems like just a combination of computer science, statistics, linear algebra, etc. However, the principles and priorities of data science are not the same as those in these disciplines. Simi-

Figure 2.2: The data science continuum.



The data science continuum is the process of development of data science as a new science. It began by borrowing methods and techniques from established sciences. Over time, distinct principles emerged that spanned multiple disciplines. As these principles developed, new methods and their premises became unique. This uniqueness led to the creation of specific methodologies for validating these methods. During the validation process, new questions and challenges arose, further distinguishing data science from its parent disciplines.

larly, the accepted methodologies in data science differ and keep evolving from those in other sciences. New questions arise, such as:

- How can we guarantee that the data we are using is reliable?
- How can we collect data in a way that does not bias our conclusions?
- How can we guarantee that the data we are using is ethical?
- How can we present our results in a way that is understandable to non-experts?

2.3 Fundamental data theory

As I stated, data science is not an isolated science. It incorporates several concepts from other fields and sciences. In this section, I explain the basis of each component of definition 2.1.

2.3.1 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 possible starting point is ontology, which is the study of being, existence, and reality. Ontology studies what exists and how we can classify it. In particular, ontology describes the nature of categories, properties, and relations.

Aristotle (384 – 322 BC) is one of the first philosophers to study ontology. In Κατηγορίαι[9], he proposed a classification of the world into ten categories. Substance, or οὐσία, is the most important one. It is the category of being. The other categories are properties, quantity, quality, relation, place, time, position, state, and action.

Although rudimentary[10], Aristotle's categories served as a basis for the development of logical reasoning and scientific classification, espe-

[9]For Portuguese readers, I suggest Aristotle (2019). *Categorias (Κατηγορίαι)*. Greek and Portuguese. Trans. by J. V. T. da Mata. São Paulo, Brasil: Editora Unesp. ISBN: 978-85-393-0785-2.

[10]Most historians agree that Categories was written before Aristotle's other works. Many concepts are further developed in his later works.

cially in the Western world. The categories are still used in many applications, including computer systems and data systems.

Aristotle marked a rupture with many previous philosophers. While Heraclitus (6th century – 5th century BC) defended that everything is in a constant state of flux and Plato (c. 427 – 348 BC) defended that only the perfect can be known, Aristotle focused on the world we can perceive and understand. His practical view also opposed Antisthenes (c. 446 – 366 BC) view that the predicate determines the object, which leads to the impossibility of negation and consequently contradiction.

What is the importance of ontology for data science? Describing, which is basically reducing the complexity of the world to simple, small pieces, is the first step to understand any phenomenon. Drawing a simplistic parallel, phenomena are like the substance category, and the data we collect are like the other categories, which describe the properties, relations, and states of the substance. A person who can easily organize their thoughts to identify the entities and their properties in a problem is more likely to collect relevant data. Also, the understanding of logical and grammatical limitations — such as univocal and equivocal terms — is important to avoid errors in data science applications[11].

Another important field in Philosophy is epistemology, which is the study of knowledge. Epistemology elaborates on 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.

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.

I further discuss knowledge and reasoning in section 2.3.3.

In the context of a data science project, we usually focus on phenomena from a particular domain of expertise. For example, we may be interested in phenomena related to the stock market, or related to the weather, or related to human health. Thus, we need to understand the nature of the phenomena we are studying.

Fully understanding the phenomena we are tackling requires both general knowledge of epistemology, ontology, and logic, and particular knowledge of the domain of expertise.

[11]It is very common to see data scientists reducing the meaning of the columns in a dataset to a single word. Or even worse, they assume that different columns with the same name have the same meaning. This is a common source of errors in data science projects.

Observe as well that we do not restrict ourselves to the intellectual understanding of philosophy. There are several computational methods that implement 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. An incorrect perception of the phenomena may lead to incorrect data collection, which certainly leads to incorrect conclusions.

2.3.2 Measurements

Similarly to Aristotle's work, data scientists focus on the world we can perceive with our senses (or using external sensors). In a more restrictive way, we focus on the world we can measure[12]. 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 a 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 com-

[12]Some phenomena might be knowable but not measurable. For example, the existence of God is a knowable phenomenon, but it is not measurable.

patible 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.

The fundamental concepts are the same independently of the programming language, hardware architecture, or the relational database management system (RDBMS) we are using. As a consequence, in this book, I focus on the concepts and not on the tools.

2.3.3 Knowledge extraction

Like discussed before, knowledge and reasoning are important aspects of data science. Philosophical and mathematical foundations from epistemology and logic provide us with ways to obtain knowledge from a set of premises and known (and accepted) facts[13].

Deductive reasoning is the process of deriving a conclusion (or new knowledge) from a set of previous knowledge. Deductive reasoning, thus, enables us to infer generalization rules from known general rules.

Important figures that bridged the gap between the subjects of philosophy and mathematics are René Descartes (1596 – 1650) and Gottfried Wilhelm Leibniz (1646 – 1716). Descartes was the first to use algebra to solve knowledge problems, effectively creating methods to mechanize reasoning. Leibniz, after Descartes, envisioned a universal algebraic language that would encompass logical principles and methods. Their work influenced the development of calculus, Boolean algebra, and many other fields.

Once we have collected and stored the data, the next step is to extract knowledge from them. Knowledge extraction is the process of obtaining knowledge from data. The reasoning principle here is inductive reasoning. Inductive reasoning is the process of deriving generalization rules from specific observations. Inductive reasoning and data analysis are closely related. Refer to section 1.2.2 for a timeline of the development of data analysis.

[13]In mathematics, axioms are the premises and accepted facts. Corollaries, lemmas, and theorems are the results of the reasoning process.

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. It is a branch of artificial intelligence.
- Operations research: the study of computational methods to optimize decisions.

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 technique, we may perform data preprocessing[14].

Data preprocessing mainly includes data cleaning, data transformation, and data enhancement. 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 enhancement is the process of adding additional information to the data, usually by integrating data from different sources into a single, unified view.

[14]It is important to highlight that it is expected that some of the method's 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 preprocessing to adjust data as much as possible.

3 Data science project

with contributions from *Johnny C. Marques*

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

— Don Carlton, *Monsters University (2013)*

Once we have established what data science is, we can now discuss how to conduct a data science project. 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 are constructed from data. This means that part of the solution is not designed from the knowledge of the domain expert.

One example of a project is a spam filter that classifies emails into two categories: spam and non-spam. A traditional approach is to design a set of rules that are known to be effective. However, the effectiveness of the filters is limited by the knowledge of the designer and is cumbersome to maintain. A data science approach automatically learns the filters from a set of emails that are already classified as spam or non-spam.

Another important difference in data science projects is that traditional testing methods, such as unit tests, are not sufficient. The solution inferred from the data must be validated considering the stochastic nature of the data.

In this chapter, we discuss common methodologies for data science projects. We also present the concept of agile methodologies and the Scrum framework. We finally propose an extension to Scrum adapted for data science projects.

Chapter remarks

Contents

Context

- A data science project is a software project.
- Data science methodologies focus on the data analysis process.
- The industry demands not only data analysis but also software development.

Objectives

- Explore common methodologies for data science projects.
- Understand agile methodologies and the Scrum framework.
- Propose an extension to Scrum adapted for data science projects.

Takeaways

- Modern data science methodologies take into account the software development aspects of the project.
- Scrum is a good framework for software development, and it can be adapted for data science projects.

3.1 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.

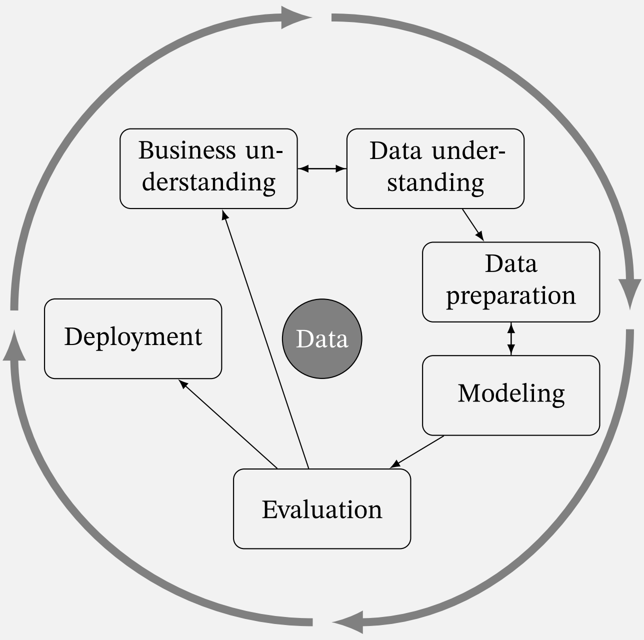
5. Evaluation: this is the phase where the model is evaluated. The model is evaluated using the evaluation data. The phase also includes the definition of the deployment requirements.

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.

CRISP-DM is cyclic and completely focused on the data. However, it does not address the software development aspects of the project. The "product" of the project is both models and findings, not the full software solution. As a result, aspects such as user interface, communication, and integration are not addressed by the methodology.

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

Figure 3.1: 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.

Figure 3.1 shows a diagram of the CRISP-DM process. The double arrow between the business understanding and the data understanding phases represents the iterative nature of these steps. Once we are satisfied with the data understanding, we can proceed to the data preparation phase. The same iteration is possible between the data preparation and the modeling phases, since modeling methods can require different data preparation methods. Finally, an evaluation is performed. If the model is satisfactory, we proceed to the deployment phase. Otherwise, we return to the business understanding phase. The idea is to revisit the project objectives and, if necessary, the project plan.

The CRISP-DM methodology is a good starting point for data science projects. However, it does not mean that it should be followed strictly. The process is flexible, and adaptations are possible at any stage.

3.2 ZM approach

Zumel and Mount (2019)[2] also propose a methodology for data science projects — which we call here the ZM 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.

Requirements of a data science project are dynamic, and we need to perform many exploratory phases. Unlike traditional software projects, we should expect significant changes in the initial requirements and goals of the project.

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.

3.2.1 Roles of the ZM approach

In their approach, they define five roles. The roles are:

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 cannot be the data scientist, but someone who 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

[2]N. Zumel and J. Mount (2019). *Practical Data Science with R*. 2nd ed. Shelter Island, NY, USA: Manning.

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 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 he is not an active participant. He is the one who 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 for defining requirements such as response time, programming language, and the infrastructure to run the software.

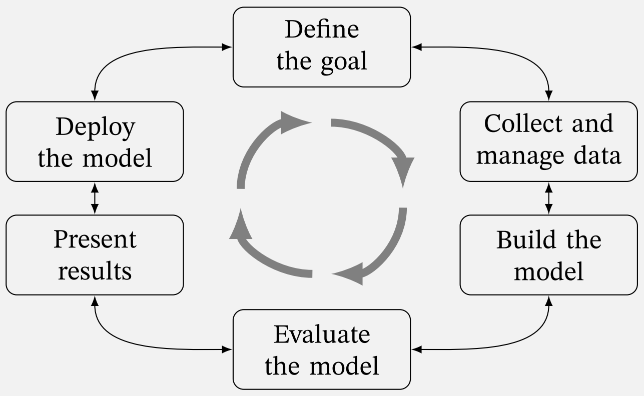
3.2.2 Processes of the ZM approach

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 3.2 shows a diagram of the process. The phases and the answers we are looking for in each phase are:

- Define the goal: what problem are we trying to solve?
- Collect and manage data: what information do we need?
- Build the model: what patterns in the data may solve the problem?
- Evaluate the model: is the model good enough to solve the problem?
- Present results and document: how did we solve the problem?
- Deploy the model: how to use the solution?

The step "Present results and document" is a differentiator from the other approaches, like CRISP-DM. In the ZM approach, result presentation is essential; data scientists must be able to communicate their results effectively to the client/sponsor. This phase is also emphasized in the view of Wickham, Çetinkaya-Rundel, and Grolemund (2023).

Figure 3.2: 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, which can be back-and-forth.

3.2.3 Limitations of the ZM approach

The ZM approach is particularly interesting in consulting projects, as the data scientist is not part of the organization. Note that tasks beyond deployment, such as maintenance and monitoring, are not directly addressed by the methodology but are delegated to the operations role. Like CRISP-DM, the ZM approach does not address the software development aspects of the project.

3.3 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 methodology is based on the four values of the Agile Manifesto[3]:

- Individuals and interactions over processes and tools;

[3]https://agilemanifesto.org/

- Working software over comprehensive documentation;
- Customer collaboration over contract negotiation;
- Responding to change over following a plan.

Note that the manifesto does not discard the items on the right, but rather values the items on the left more. For example, comprehensive documentation is important, but working software is more important.

3.4 Scrum framework

The Scrum framework is one of the most widely adopted agile methodologies. It is an iterative, incremental process that enables teams to deliver high-value products efficiently while adapting to changing requirements. Scrum emphasizes teamwork, accountability, and continuous improvement. Developed by Schwaber and Sutherland (2020)[4] in the early 1990s, Scrum is based on three pillars: transparency, inspection, and adaptation. These principles help teams to navigate complex, adaptive problems and deliver productive outcomes.

Scrum organizes work into cycles called sprints, and involves defined roles, ceremonies, and artifacts that ensure the progress and quality of the product. Key events such as daily stand-ups, retrospectives, and sprint reviews create regular opportunities to inspect and adapt, making Scrum a responsive and resilient framework[5].

3.4.1 Scrum roles

Scrum defines three critical roles: the product owner, the Scrum master, and the development team. Each of these roles has specific responsibilities, and together they ensure that the Scrum process runs smoothly and that the product development aligns with the overall business objectives.

Product owner This role is responsible for defining the product vision and maximizing the value of the work done by the team. The

[4]Latest version of the Scrum Guide available at K. Schwaber and J. Sutherland (2020). *Scrum Guide: The Definitive Guide to Scrum: The Rules of the Game*. Scrum.org. URL: https://scrumguides.org/docs/scrumguide/v2020/2020-Scrum-Guide-US.pdf.

[5]S. Denning (2016). "Why Agile Works: Understanding the Importance of Scrum in Modern Software Development". In: *Forbes*. URL: https://www.forbes.com/sites/stevedenning/2016/08/10/why-agile-works/.

product owner manages the product backlog, ensuring that it is visible, transparent, and prioritized according to business needs. They serve as the main point of contact between stakeholders and the development team[6]. The product owner must constantly balance the requirements of the business and the technical capabilities of the team, ensuring that the highest-value items are worked on first.

Scrum master The Scrum master acts as a facilitator and coach for the Scrum team, ensuring that the team adheres to the Scrum framework and agile principles. Unlike a traditional project manager, the Scrum master is not responsible for managing the team directly but for enabling them to perform optimally by removing impediments and fostering a self-organizing culture[7].

Development team It is a cross-functional group of professionals responsible for delivering potentially shippable product increments at the end of each sprint. The team is self-managing, meaning they decide how to achieve their goals within the sprint. The team is small enough to remain nimble but large enough to complete meaningful work[8]. The development team works collaboratively and takes collective responsibility for the outcome of the sprint.

3.4.2 Sprints and backlog

A sprint is the basic unit of work in Scrum, as presented in fig. 3.3. Sprints are time-boxed iterations, usually lasting between one to four weeks, during which a defined amount of work is completed. The goal is to deliver a potentially shippable product increment at the end of each sprint. Sprints are continuous, with no breaks in between, fostering a regular, predictable rhythm of work.

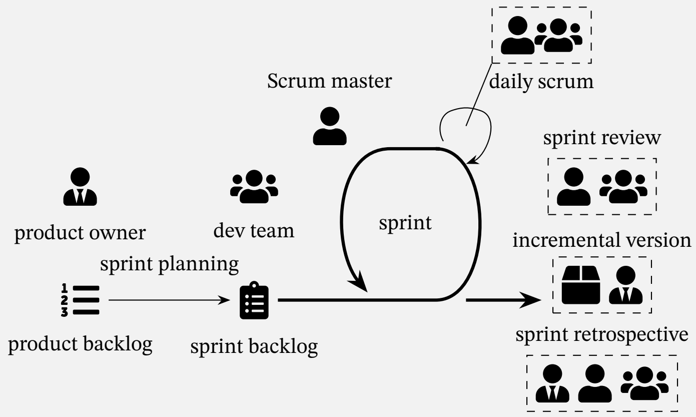
Before a sprint starts, the Scrum team holds a sprint planning meeting to decide what will be worked on. The work for the sprint is selected from the product backlog, which is a prioritized list of features, enhancements, bug fixes, and other deliverables necessary for the product. The product backlog is dynamic and evolves as new requirements

[6]J. Smith (2019). "Understanding Scrum Roles: Product Owner, Scrum Master, and Development Team". In: *Open Agile Journal* 12, pp. 22–28.

[7]C. G. Cobb (2015). *The Project Manager's Guide to Mastering Agile: Principles and Practices for an Adaptive Approach*. John Wiley & Sons.

[8]S. Rubin (2012). "Scrum for Teams: Maximizing Efficiency in Short Iterations". In: *Agile Processes Journal* 8, pp. 45–52.

Figure 3.3: Scrum framework overview.



The development centers around the sprints, which are time-boxed iterations. Roles, other ceremonies, and artifacts support the sprints and ensure the progress and quality of the product.

and changes emerge. The items selected for the sprint become part of the sprint backlog, a subset of the product backlog that the development team commits to completing during the sprint.

At the heart of the Scrum process is the daily scrum (or stand-up meeting), a brief meeting where the team discusses progress toward the sprint goal, any obstacles they are facing, and their plans for the next day. This daily inspection ensures that everyone stays aligned and can quickly adapt to any changes or challenges.

The burn down/up chart is a visual tool used during the sprint to track the Scrum team's progress against the planned tasks. It displays the amount of remaining work (in hours or story points) over time, allowing the team and the product owner to monitor whether the work is on pace to be completed by the end of the sprint. The chart's line decreases as tasks are finished, providing a clear indicator of potential delays or blockers. If progress is falling behind, the team adjusts the approach during the sprint by re-prioritizing tasks or removing impediments. Thus, this chart provides real-time visibility into the team's efficiency and contributes to more agile and proactive work management.

At the end of each sprint, the team holds a sprint review, during which they demonstrate the work completed during the sprint. The sprint review is an opportunity for stakeholders to see progress and provide feedback, which may lead to adjustments in the Product Backlog. Following the review, the team conducts a sprint retrospective to discuss what went well, what did not, and how they can improve their processes moving forward. These continuous improvement cycles are key to Scrum's success, allowing teams to adapt both their work and their working methods iteratively.

The sprint retrospective is a crucial event in the Scrum framework, held at the end of each sprint. Its primary purpose is to provide the Scrum team with an opportunity to reflect on the sprint that just concluded and identify areas for improvement. During the retrospective, the team discusses what went well, what challenges they encountered, and how they can enhance their processes for future sprints. This continuous improvement focus allows the team to adapt their workflow and collaboration methods, fostering a more efficient and effective development cycle. By encouraging open and honest feedback, the retrospective plays a vital role in maintaining team cohesion and driving productivity over time.

3.4.3 Scrum for data science projects

Some 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, data-driven exploratory phases 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[9].

One of my major concerns in the proposal of the extension is that data science projects usually involve "data scientists" who are not primarily developers, but statisticians or domain experts. They usually do

[9]Note that many other adaptations to Scrum have been described in literature. For example, J. Saltz and A. Suthrland (2019). "SKI: An Agile Framework for Data Science". In: *2019 IEEE International Conference on Big Data (Big Data)*, pp. 3468–3476. DOI: 10.1109/BigData47090.2019.9005591; J. Baijens, R. Helms, and D. Iren (2020). "Applying Scrum in Data Science Projects". In: *2020 IEEE 22nd Conference on Business Informatics (CBI)*. vol. 1, pp. 30–38. DOI: 10.1109/CBI49978.2020.00011; N. Kraut and F. Transchel (2022). "On the Application of SCRUM in Data Science Projects". In: *2022 7th International Conference on Big Data Analytics (ICBDA)*, pp. 1–9. DOI: 10.1109/ICBDA55095.2022.9760341.

not possess “hacking-level” skills, and they often do not know good practices of software development.

Scrum is a good starting point for a compromise between the need for autonomy (required in dynamic and exploratory projects) and the need for a detailed plan to guide the project (required to avoid bad practices and low-quality software). A good project methodology is needed to ensure that the project is completed on time and within budget.

3.5 Our approach

The previously mentioned methodologies lack 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 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. For instance, it lacks the exploratory phases of data science projects.

For the sake of this book, we focus on the inductive approach to data science projects. Inductive reasoning is the process of making generalizations based on individual observations. In our case, it means that we develop components (generalization) of the software based on the data (individual observations). Such a component is the model. For a deeper discussion on the inductive approach, refer to section 2.3.3 and chapter 6.

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, with parts constructed from data and other parts constructed like traditional software;
- The solution is usually deployed as a service that must be maintained and monitored;
- Team members not familiar with software development practices must be guided to produce high-quality software.

Moreover, we add two other values besides the Agile Manifesto values. They are:

- Confidence and understanding of the model over 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 being sure that the model behaves as expected (and sometimes why it behaves as expected). It is not uncommon to find models that seem to perform well during evaluation steps[10], 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 consistent and reproducible software solutions. Interactive environments help in the exploratory phases, 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 is not runnable anymore. This is a serious problem, and it is not acceptable for maintaining a software solution.

As in the Agile manifesto, the values on the right are not discarded, but the values on the left are more important. We do not discard the importance of model performance or the convenience of interactive environments, but they are not the most important aspects of the project.

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

3.5.1 The roles of our approach

Although the roles of the ZM approach consider people potentially from different organizations and the roles of Scrum focus on the development team, we can associate the responsibilities between them.

Parts of the responsibilities of the product owner (that represents the stakeholders) in a Scrum project are divided between the sponsor and the client in the ZM approach. The data scientist is the one that leads the project in a similar way as the Scrum master.

In our approach, we consider four roles that cover the responsibilities in a data science project that also involves software development:

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

Table 3.1: Roles and responsibilities of our approach.

Our approach	Scrum	ZM approach
Business spokesman	Stakeholders (customer)	Sponsor and client
Lead data scientist	Product owner	Data scientist
Scrum master	Scrum master	–
Data science team	Development team	Data architect and operations

The roles of Scrum are associated with the roles defined by Zumel and Mount (2019). Note that the association is not exact. In our approach, the data scientist leads the development team and interacts with the business spokesman. The development team includes people with both data science and software engineering expertise.

the business spokesman, the lead data scientist, the Scrum master, and the data science team. An association between the roles of our proposal, Scrum, and the ZM approach is shown in table 3.1.

Business spokesman It is the main stakeholder of the project. He is the one who needs the results of the project and understands the domain of the problem. Like the “client” in the ZM approach, he must be able to translate the business goals into technical requirements. In a sense, the business spokesman evaluates the main functionalities and usability of the software. Like the “sponsor” in the ZM approach, he must be able to express quantitatively the business goals. If possible, his participation in sprint reviews provides valuable feedback and direction to the project.

Lead data scientist The lead data scientist, like the product owner, is the one who represents the interests of the stakeholder. She must be able to understand the application domain and the business goals. We decide to call her “lead data scientist” to make it clear that she also has data science expertise. The reason is that mathematical and statistical expertise is essential to understand the data and the models. Correctly interpreting the results and communicating them to the business spokesman are essential tasks of the lead data scientist. All other responsibilities of the traditional product owner are also delegated to her.

Scrum master No extra responsibilities are added to the Scrum master role, however, some data science expertise may be helpful. For example, the Scrum master must ensure that the data science team is following not only good practices of software development but also data science.

Data science team The data science team is the development team. It includes people with expertise in data science, database management, software engineering, and any other domain-specific expertise that is required for the project.

3.5.2 The principles of our approach

Before describing the functioning of our approach, we present the principles that guide it.

Modularize the solution

Data science projects usually contain four main modules: a front-end, a back-end, a dataset, and a "solution search system." The front-end is the user interface, i.e. the part of the software that the client interacts with. The back-end is the server-side code which usually contains the preprocessor[11] and the model. The dataset is the curated data that is used to train the model. Sometimes, the dataset is not static, but actually scripts and queries that produce a dynamic dataset. The solution search system is the software that employs data preprocessing and machine learning techniques, usually in a hyper-parameter[12] optimization loop, to find the best solution, i.e. the combination of preprocessor and model that best solves the problem.

Version control everything

This includes the code, the data, and the documentation. The most used tool for code version control is Git[13]. For datasets, extensions to Git exist,

[11]Preprocessor is a fitted chain of data handling operations that make the necessary adjustments to the data before it is fed to the model. For more details, consult chapter 7.

[12]Hyper-parameters are parameters that are not fitted or learned from the data, but rather set by the user.

[13]https://git-scm.com/

such as DVC[14]. One important aspect is to version control the solution search code. Interactive environments, such as Jupyter Notebooks or R Markdown, are not suitable for this purpose. They can be used to draft the code, but the final version must be version controlled.

Note that the preprocessors and the models themselves[15] are artifacts that result from a particular version of the dataset and the solution search code. The same occurs with reports generated from exploratory analysis and validation steps. They must be cached for important versions of the dataset and the solution search code.

Continuous integration and continuous deployment

The code should be automatically (or at least semi-automatically) tested and deployed. The back-end and front-end are tested using unit tests. The dataset is not exactly tested, but the exploratory analysis report is updated for each version of the dataset. A human must validate the reports, but the reports must be generated automatically. The solution search code is tested using validation methods such as cross-validation and Bayesian analysis — refer to chapter 8 — on the discovered models.

Usually the solution search code is computationally intensive, and it is not feasible to run it on every commit. Instead, it is usually run periodically, for example once a day. If the cloud infrastructure required to run the solution search code is not available to automate validation and deployment, 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[16] or a similar tool.

Pay attention to the dependencies between the dataset and model training. If the dataset changes significantly, not only the deployed preprocessor and model must be retrained, but the whole model search algorithm may need to be rethought.

Finally, since both the solution search and validation methods are stochastic, one must guarantee that the results are reproducible. Make sure you are using a good framework in which you can set the random seed.

[14]https://dvc.org/

[15]The learned solution that is the result of the application of a learning algorithm to the dataset.

[16]https://www.gnu.org/software/make/manual/make.html

Reports as deliverables

During sprints, the deliverables of phases like exploratory analysis and solution search are not only the source code, but also the reports generated. That is probably the reason why interactive environments are so popular in data science projects. However, the data scientist must guarantee that the reports are version controlled and reproducible. The reports must be generated in a way that is understandable by the business spokesperson.

Setup quantitative goals

Do not fall into the trap of forever improving the model. Instead, set up quantitative goals for the model performance or behavior in general. For example, the model must have a precision of at least 90% and recall of at least 80%. Once you reach the goal, prioritize other tasks.

Measure *exactly* what you want

During model validation, if needed, use custom 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 commonly used in the literature. It is important to know their meanings, properties, and limitations. For example, the accuracy metric is not suitable for imbalanced datasets. They might not be suitable for your project.

Notice that during model training, some methods are limited to the loss functions that they can optimize. However, if possible, choose a method that can optimize the loss function that you want. Otherwise, even if you are not explicitly optimizing the desired metric in the solution search metric, you might find a model that performs well on that metric. This is why a good experimental design is important; so you can identify which strategies are more likely to find a good solution (preprocessor and model).

Report model stability and performance variance

Understanding the limitations and properties of the generated model is more important than the model's performance. For example, if the model's expected performance is high, but the validation results showed instability, it is not suitable for production. Also, in some scenarios, interpretability is more important than performance.

It does not mean that performance is not important. But we only consider optimizing the expected performance once we trust the solution search method. If increasing the average performance of the models generated by the solution search method results in other goals not being met, it is not worth it.

In user interface, mask data-science-specific terminology

Usually, data science software gives the user the option to choose different solutions. For instance, a regressor that predicts the probability of a binary outcome yields different classifiers depending on a threshold. In this scenario, the user must be able to choose the threshold in terms of expected performance of (usually conflicting) metrics of interest.

In order to avoid confusion, the user interface must mask data science terminology, preferring domain-specific terms that are more understandable by the client. This helps non-experts to use the software consciously.

Monitor model performance in production

Good data science products do not finish with the deployment of the model. There should exist means to monitor the model behavior in production. If possible, set up feedback from the user interface. A history of usage is usually kept in a database.

In most cases, the model loses performance over time, usually because of changes in the data distribution. This is called concept drift. If that happens with considerable effect on the model performance, the model must be retrained. The retraining can be automated, but it must be monitored by robust validation methods. Sometimes, the solution must be rethought, restarting the project from the beginning.

Use the appropriate infrastructure

Many data science projects require a significant amount of computational resources during development. The solution search method is usually computationally intensive. The dataset can be large, and the model can be complex. The infrastructure must be able to handle the computational requirements of the project.

Unless the application is known to be challenging, projects should start with the simplest methods and a small dataset. Then, as the project evolves, the complexity of the methods and the size of the dataset can be increased. Nowadays, cloud services are a good option for scalability.

Finally, during development, the requirements of the deployment infrastructure must be considered. The deployment infrastructure must be able to handle the expected usage of the system. For instance, in the back-end, one may need to consider the response time of the system, the programming language, and the infrastructure to run the software. The choice of communication between the front-end and the back-end is also important. For instance, one may choose between a REST API or a WebSocket. A REST API is more suitable for stateless requests, while a WebSocket is more suitable for stateful requests. For example, if the user interface must be updated in real-time, a WebSocket is more suitable. If the user interface is used to submit batch requests, a REST API is more suitable.

3.5.3 Proposed workflow

The proposed workflow is based on the principles described above. Our approach adapts the Scrum framework by establishing three kinds of sprints: data sprints, solution sprints, and application sprints. We also describe where exploratory and reporting phases fit into the workflow.

Product backlog

In the data science methodologies described in this chapter, the problem definition is the first step in a data science project. In our methodology, this task is dealt with in the product backlog. The product backlog is a list of all desired work on the project. The product backlog is dynamic, and it is continuously updated by the lead data scientist.

Each item in the product backlog reflects a requirement or a feature the business spokesperson wants to be implemented. Like in traditional Scrum, the items are ordered by priority. Here, however, they are classified into three types: data tasks, solution search tasks, and application tasks.

Sprints

The sprints are divided into three types: data sprints, solution sprints, and application sprints. Sprints occur sequentially, but it is possible to have multiple sprints of the same type in sequence. Like in traditional Scrum, the sprint review is performed at the end of each sprint. Data sprints comprise only data tasks, solution sprints comprise only solution search tasks, and so on.

Data sprint The *data sprint* is focused on the database-related tasks: collection, integration, tidying, and exploration. Chapter 4 covers the subjects of collection, integration (database normalization and joins) and tidying. Part of data exploration is to semantically describe the variables, especially in terms of data types and their properties; which is also discussed in that chapter. All these tasks aim to prepare a dataset that represents the data that the solution will see in production.

Exploration also refers to *exploratory data analysis*, which is not covered in this book. For a good introduction to exploratory data analysis, which includes both understanding and identifying issues in the data through descriptive statistics and visualization, consult chapter 3 of Zumel and Mount (2019)[17].

The products (deliverables) of the data sprint are the exploratory analysis report and the data itself. The exploratory analysis report is a document that describes the main characteristics of the data, such as the distribution of the variables, the presence of missing values, and the presence of outliers. In our context, this report should be generated automatically, and it should be version controlled. The data is the curated data that is used to train the model. The source code that generates the data — usually scripts and queries that combine data from different places — must be version controlled. At this point of the project, the data scientist must guarantee that the data is of high quality and that it represents the data that the solution will "see" in production. *It is very important that, at this stage, no transformation based on the values of the dataset is performed.* Failing to do so leads to data leakage in the validation phase.

Solution sprint The *solution sprint* is focused on the solution search tasks: data preprocessing, machine learning, and validation. Chapter 7 covers the subjects of data preprocessing — adjustments to the data to be used by specific machine learning models —, chapter 6 covers the subjects of learning machines — methods that can estimate an unknown function based on input and output examples —, and chapter 8 covers the subjects of validation — through evaluation we estimate the ex-

[17]N. Zumel and J. Mount (2019). *Practical Data Science with R*. 2nd ed. Shelter Island, NY, USA: Manning.

Definition 3.1: (Data leakage)

During the validation of the solution, we simulate the production environment by leaving some data out of the training set — consult chapter 8. The remaining dataset, called test set, emulates unseen data. Data leakage is the situation where information from the test set is used to transform the training set in any way or to train the model. As a result, the validation performance of the solution is overestimated. Sometimes, even an excess of data exploration can lead to indirect leakage or bias in the validation phase.

pected performance for unseen data, i.e. the probability distribution of the performance in production.

The products of the solution sprint are the validation report and the solution itself, which is the preprocessor and the model. The validation report is a document that describes the expected performance of the solution in the real-world. The script or program that searches for the best pair of preprocessor and model must be version-controlled. This algorithm is usually computationally intensive, and it should run every time the dataset is updated.

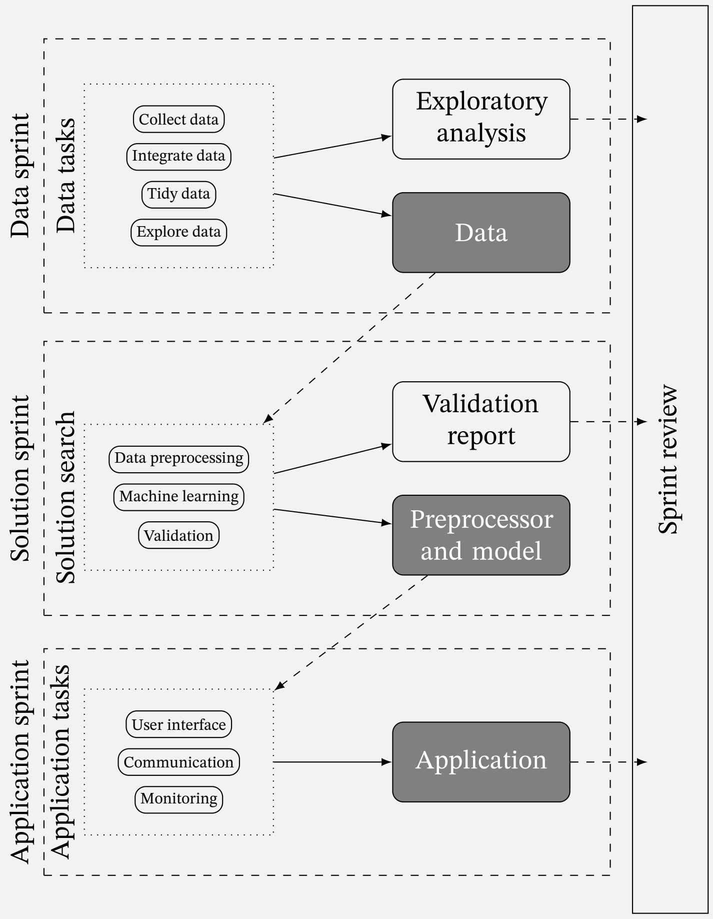
Application sprint The *application sprint* is focused on the application itself. The tasks in this sprint focus on the development of the user interface, the communication between the front-end and the back-end, and the monitoring of the solution in production. Software documentation and unit tests are also part of this sprint.

Figure 3.4 shows the tasks and results for each sprint type and their relationships. Every time a data sprint results in modifications in the dataset, the solution search algorithm must be re-executed. The same occurs when the solution search algorithm is modified: the application must be updated to use the new preprocessor and model.

Choice and order of sprints

Sprints are sequential. Ordinarily, a data sprint is followed by a solution sprint, and a solution sprint is followed by an application sprint. However, it is possible to have multiple sprints of the same type in sequence. Moreover, like the back-and-forth property of the CRISP-DM and ZM

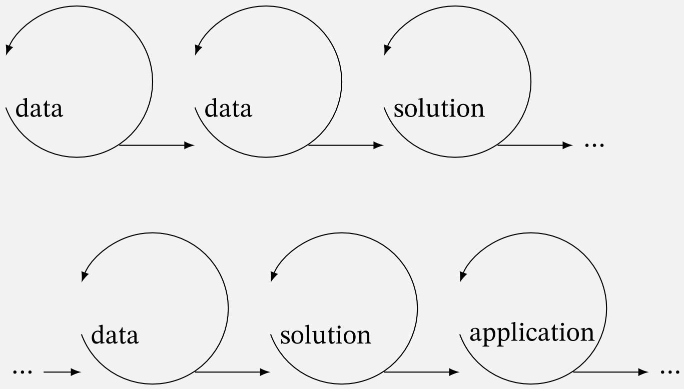
Figure 3.4: Tasks and results for each sprint types and their relationships.



Summary of the tasks and results for each sprint type and their relationships.

approach, it is possible to go back to a previous sprint type, especially when new requirements or problems are identified.

Figure 3.5: Example of sprints of a data science project.



Each loop represents a sprint of a different kind: data sprint, solution sprint, and application sprint. The arrows represent the transitions between the sprints.

Figure 3.5 shows an example of a sequence of sprints of a data science project. The figure shows that the sprints are sequential and their types can appear in any order.

We do not advise having mixed sprints. For instance, a sprint that contains both data and solution tasks. This may lead to a split focus, which may result in the team acting as multiple teams. We argue that, independently of the skill set of the team members, all members must be aware of all parts of the project. This is important to guarantee that the solution is coherent and that the team members can help each other.

Sprint reviews

A proper continuous integration/continuous deployment (CI/CD) pipeline guarantees that by the end of the sprint, exploratory analysis, performance reports, and the working software are ready for review. The sprint review is a meeting where the team presents the results of the sprint to the business spokesman. The business spokesman must approve the results of the sprint. (The lead data scientist approves the results in the absence of the business spokesman.) It is important that the reports use the terminology of the client, and that the software is easy to use for the domain expert.

Relationship with other methodologies

Our approach covers all the phases of the CRISP-DM and the ZM approach. Moreover, it includes aspects of software development that are not covered by the other methodologies. Table 3.2 relates the phases of the CRISP-DM and the ZM approach with the sprint types and other artifacts and ceremonies of our approach.

Table 3.2: Relationship between coverage of other methodologies and our approach.

CRISP-DM	**ZM approach**	**Our approach**
Bus. understanding	Define the goal	Product backlog
Data understanding	Collect/manage data	Data sprint
Data preparation	Collect/manage data	Data/solution sprint
Modeling	Build the model	Solution sprint
Evaluation	Evaluate the model	Solution sprint
	Present results	Sprint reviews
Deployment	Deploy the model	Application sprint

The phases of the CRISP-DM and the ZM approach are compared with the components of our approach. The table shows that our approach covers all the phases of the other methodologies.

One highlight is that we approach CRISP-DM's "data preparation" and ZM's "collect/manage data" tasks more carefully. Data handling operations that are not parametrized by the data values themselves are performed in the data sprint. On the other hand, operations that use statistics/information of a sampling of the data are performed together with modeling — consult chapter 5.

This approach not only improves the reliability of the solution validation, but also improves the maintenance of the solution. (Not surprisingly, frameworks like *scikit-learn* and tidymodels have an object that allows the user to combine data preprocessing and model training.)

4 Structured data

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

— Hadley Wickham, *Tidy 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 are numbers. We can assess English proficiency using an essay test. The resulting data are texts. We can register relationships between proteins and their functions. The resulting data are graphs. Thus, it is essential to understand the nature of the data we are working with.

The most common data format is the *structured data*. Structured data refers to information that is organized in a tabular format. We restrict the kind of information we store in each cell, i.e., the data type of each measurement. The data type restricts the operations we can perform on the data. For example, we can perform arithmetic operations on numbers, but not on text. All cells in the same column must share the same data type.

In this chapter, I discuss the most common data types and the most common data formats. More specifically, we are interested in how the semantics of the data are encoded in the data format. Database normalization and tidy data are two concepts that are crucial for the understanding of structured data.

As a result, the reader will be equipped with the mindset to perform data tasks — collection, integration, tidying, and exploration — well.

Chapter remarks

Contents

Context

- Data comes in many different formats.
- Good data analysis requires understanding the data types and their meanings.

Objectives

- Understand the most common data types and formats.
- Enable the reader to perform data tasks well by associating data format and semantics.

Takeaways

- The choice of the observational unit is not always straightforward.
- Format and types must reflect the information the solution will “see” in production.

4.1 Data types

The most common classification of data types is Stevens' 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.

Table 4.1: Stevens' types.

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

Stevens' types are a classification of data types based on the operations we can perform on them.

Table 4.1 summarizes the allowed operations for each of Stevens' types. All types enable equality comparison. Ordinal data can also be tested in terms of their order, but they do not allow quantitative difference. Interval data, on the other hand, allow addition and subtraction. Finally, the true zero of ratio data enables us to calculate relative differences (multiplication and division).

For example, colors are nominal data. We can classify colors into categories, but we cannot order them. A categorical variable that classifies sizes into small, medium, and large is ordinal data. We can order the sizes, but we cannot say that the difference between small and medium is the same as the difference between medium and large. Temperature in Celsius is interval data. We can order temperatures, and we can say that the difference between 10 and 20 degrees is the same as the difference between 20 and 30 degrees. However, we cannot say that 20 degrees is twice as hot as 10 degrees. Finally, weight is ratio data. We can order weights, we can say that the difference between 10 and 20 kilograms is the same as the difference between 20 and 30 kilograms, and we can say that 20 kilograms is twice as heavy as 10 kilograms.

Nonetheless, Stevens' 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)[1] provide interesting insights about data types. Although I do not agree with all his points, I think it is a good read. In particular, I agree with his criticism of statements that data types are evident from the data independent 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 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 hypotheses 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 and logical foundations and tools for data handling.

4.2 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. The need for database normalization comes from the fact that the same data can be stored in many different ways.

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 database theory and the basic operations in relational algebra.

[1] P. F. Velleman 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.

4.2.1 Relational algebra

Relational algebra is a theory that uses algebraic structures to manipulate relations. Consider the following concepts.

Relation A relation is a table with rows and columns that represent an entity. Each row, or tuple, is assumed to appear only once in the relation. Each column, or attribute, is assumed to have a unique name.

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., $X[A, C]$. The number of rows in the resulting relation might be less than the number of rows in the original relation because of repeated rows.

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, the 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: $\bowtie \{R_1, R_2, \dots, R_n\} = R_1 \bowtie R_2 \bowtie \cdots \bowtie R_n$. 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* $U \rightarrow V$ 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 constrains two sets of attributes in a relation. 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. Note, however, that unlike functional dependencies, multi-valued dependencies are not simple to interpret, so we restrict our discussion to its mathematical properties[2].

[2]In fact, one might naively think that a multi-valued dependency is a functional dependency between many attributes. However, this is not the case.

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

4.2.2 Normal forms

The normal forms are a series of progressive conditions that a relation must satisfy to be considered normalized. The normal forms are cumulative, i.e., a relation that is in n-th normal form is also in $(n-1)$-th normal form. The normal forms are a way to reduce redundancy and improve data integrity.

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 $U \to X,\ \forall X \in V$ and there is no $W \subset U$ such that $W \to X,\ \forall X \in V$.

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 $X \to Y,\ \forall Y \in V$.

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 $U \to V$ in R, the functional dependency $U \to X$ 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[3] if and only if it is in 2NF and the set of key dependencies[4] of R implies each join dependency of R. The PJNF guarantees that the table cannot be decomposed without losing information (except by decompositions based on keys).

The idea behind the definition of BCNF and 4NF is 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 overstrong projection-join normal form[5]. 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.

Simple example Consider the 2NF relation $R[A,B,C,D]$ with functional dependencies $A \rightarrow B$, $B \rightarrow C$, $C \rightarrow D$. 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 $\bowtie \{R_2, R_3, R_4\}$.

Illustrative example of data integrity Consider a relation of students and their grades. The relation contains the attributes "student", "course", "course credits", and "grade". The primary key is the composite of "student" and "course". The functional dependencies are "student" and "course" determine "grade", and "course" determines "course credits". The relation is in 2NF but not 3NF.

[3]Also known as fifth normal form (5NF). The authors themselves prefer the term PJNF because it emphasizes the operations to which the normal form applies.

[4]Key dependency is a functional dependency in the form $K \rightarrow X$, where X encompasses all attributes of the relation.

[5]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.

Table 4.2: Student grade relation.

Student	Course	Course credits	Grade
Alice	Math	4	A
Alice	Physics	3	B
Bob	Math	4	B
Bob	Physics	3	A

An example of a relation of students and their grades in 2NF.

Table 4.2 shows an example of possible values of the relation. If we decide to change the course credits of the course "Math" to 5, we must update the two rows; otherwise, the relation will be inconsistent. A 3NF relation (see table 4.3) would have the attributes "course" and "course credits" in a separate relation, avoiding the possibility of data inconsistency. If needed, the relation would be reconstructed by a join operation.

Table 4.3: Student grade relation in 3NF.

Course	Course credits
Math	4
Physics	3

Student	Course	Grade
Alice	Math	A
Alice	Physics	B
Bob	Math	B
Bob	Physics	A

An example of a relation of students and their grades in 3NF.

Invalid join example Consider the 2NF relation $R[ABC]$[6] 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

[6]Here we abbreviate A,B,C as ABC.

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 $ABC \rightarrow ABC$.) 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 interesting 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.

Important note on PJNF

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.

Valid joins example Consider the 2NF relation $R[A, B, C, D, E]$ with the functional dependencies $A \rightarrow D$, $AB \rightarrow C$, and $B \rightarrow E$. To make it PJNF, we 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[7].

4.3 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 idea is that organized data carries the meaning

[7]I am investigating a formal proof 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: 10.1016/S0304-3975(97)00050-9.

of the data, reducing the time spent on handling the data to get it into the right format for analysis.

Tidy data, proposed by Wickham (2014)[8], 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 a 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 statistical and machine learning methods require a particular data format. Tidy data is a data format that is suitable for those tasks.

In an unrestricted table, the meaning of rows and columns is not fixed. In a tidy table, the meaning of rows and columns is fixed. The semantics are more restrictive than usually required for general tabular data.

Table 4.4: Example of same data in different formats.

	Cases (2019)	**Cases (2020)**
Brazil	100	200
USA		400

	Brazil	**USA**
Cases (2019)	100	
Cases (2020)	200	400

The same data in different formats. Both are considered messy by Wickham.

Table 4.4 shows an example of the same data in different formats. Although they emphasize different aspects (especially for visualization) of the data, both contain the same amount of information. They are considered messy by Wickham because the meaning of the rows and columns is not 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.

[8]H. Wickham (2014). "Tidy Data". In: *Journal of Statistical Software* 59.10, pp. 1–23. DOI: 10.18637/jss.v059.i10.

- Each *variable*, represented by a column, contains all values that measure the same attribute across (observational) units.
- 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, for instance, a person, a day, an experiment.

Table 4.5 summarizes the main concepts.

Table 4.5: Tidy data concepts.

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

Table 4.6: Example of tidy data.

Country	**Year**	**Cases**
Brazil	2019	100
Brazil	2020	200
USA	2019	
USA	2020	400

An example of tidy data from the data in table 4.4.

If we follow this structure, the meaning of the data is implicit in the table. Table 4.6 shows the same data in a tidy format. The table is now longer, but the variables and observations are clear from 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 the observational units in a dataset are[9].

[9]Although Wickham himself implies that there is only one possible way to define the observational units of the 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[10]. 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.

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 understanding. For instance, one usually expects that the first columns are *fixed variables*[11] — i.e., variables that are not the result of a measurement but that describe the experimental design —, 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 usually numerically indexed.

4.3.1 Common messy datasets

Wickham (2014)[12] lists some common problems with messy datasets and how to tidy them. In this subsection, we focus on the problems and the tidy solutions. The data handling operations that enable us to tidy the data are presented in chapter 5. Readers interested in a step-by-step guide for data tidying are encouraged to read Wickham, Çetinkaya-Rundel, and Grolemund (2023)[13].

The problems are summarized in the following.

[10]Observational unit is not the same concept as unit of measurement.

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

[12]H. Wickham (2014). “Tidy Data”. In: *Journal of Statistical Software* 59.10, pp. 1–23. DOI: 10.18637/jss.v059.i10.

[13]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.

Headers are values, not variable names

For example, consider table 4.7. 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 4.7: 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 4.8 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.

Table 4.8: Tidy version of table 4.7 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
...	...	...

Multiple variables are stored in one column

For example, consider the table 4.9. This table is not tidy because the column — interestingly 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 4.9: 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 4.10. 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.

Table 4.10: Tidy version of table 4.9 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	...
...	...	...	...	...	

Variables are stored in both rows and columns

For example, consider the table 4.11. This is the most complicated case of messy data. Usually, one of the columns contains the names of the variables, in this case the column *element*.

Table 4.11: Messy table, adapted from airquality dataset, where variables are stored in both rows and columns.

id	**year**	**mo.**	**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 4.12.

Table 4.12: Partial solution to tidy table 4.11. 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	
...	...	...	...

Afterwards, we widen the table in function of their names. Finally, we remove implicit information, as seen in table 4.13.

Table 4.13: Tidy version of table 4.11 where values are correctly moved.

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

Multiple types of observational units are stored in the same table

For example, consider the table 4.14. It is very common during data collection that many observational units are registered in the same table.

Table 4.14: 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
...	...	...	...	...

To fix this issue, we must ensure that each observation unit is 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 is possible that we have to denormalize them. The two resulting tables are shown in table 4.15 and table 4.16.

Table 4.15: Tidy version of table 4.14 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 4.16: Tidy version of table 4.14 containing the observational unit *rank of the track in a 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 4.17 and 4.18. 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 4.19.

Table 4.17: 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 4.18: 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 4.19: Tidy data where tables 4.17 and 4.18 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	...
...	...	...	...	...

4.4 Bridging normalization, tidiness, 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 (2023)[14] also state that there is only one way to organize the given data.

Wickham (2014)[15] state 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.

Moreover, both of them are related to the philosophical concept of substance (οὐσία) — see section 2.3.1. Entities and observational units are substances while attributes are predicates. Each tuple or observation is a primary substance, i.e., a substance that contrasts with everything else, particular, individual.

We can also understand primary keys and fixed variables as the same concept. They both describe the sample uniquely. They connect the entities/observational units to the remaining attributes. They also should never be fed into a learning machine (more details in chapter 6), since they are individual and thus not appropriate to generalize.

Table 4.20 summarizes the equivalence (or similarity) of terms in different contexts.

4.4.1 Tidy or not tidy?

Consider the following example. We want to study the *phenomenon* of 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 4.21.

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 4.22.

[14]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.

[15]H. Wickham (2014). "Tidy Data". In: *Journal of Statistical Software* 59.10, pp. 1–23. DOI: 10.18637/jss.v059.i10.

Table 4.20: Terms in different contexts.

Relations	Tidy data	Philosophy
Entities	Observational units	Substance
Tuple	Observation	Primary substance
Primary key	Fixed variables	Univocal name
Non-prime attr.	Measured variable	Predicate

Equivalence (or similarity) of data-related terms in different contexts. The ontological understanding of the data influences the way it is organized.

Table 4.21: 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
...	...	...	...

Table 4.22: 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
...	...	...	...	...

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*.

One can state that the first form is more appropriate, since it is flexible enough to add more sensors or sensor-specific attributes (using an extra table). 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. It is just a matter of what ontological view you have of the data.

Table 4.23: Tidy data for measurements of a person's body.

name	**chest**	**waist**	**hip**
Alice	90	70	100
Bob	100	110	110
...	...	...	...

Still, one can argue that the sensors share the same nature and thus only the first form is correct (or can even insist that the more flexible form is the correct one). Consider however the data in table 4.23. The observational unit is the person, and the attributes are the body measurements.

Table 4.24: Another tidy data for measurements of a person's body.

name	**body part**	**measurement**
Alice	chest	90
Alice	waist	70
Alice	hip	100
Bob	chest	100
Bob	waist	110
Bob	hip	110
...	...	...

If we apply the same logic of table 4.21, data in table 4.23 becomes table 4.24. Now, the observational unit is the measurement of a body part of a given person. Now, we can easily include more body parts. Let us say that we want to add the head circumference. We just need to include rows such as “Alice, head, 50” and “Bob, head, 55”. Moreover, what if we want to add the height of the person? Should we create another table (with “name” and “height”) or should we consider “height” as another body part (even though it seems weird to consider the full body a part of the body)?

In the first version of the data (table 4.21), it would be trivial to include head circumference and height. In the second version, the choice becomes inconvenient. This table seems “overly tidy”. If the first fits well for the analysis, it should be preferred.

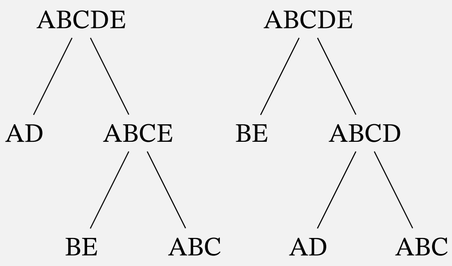
In summary, tidiness is a matter of perspective.

4.4.2 Change of observational unit

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.

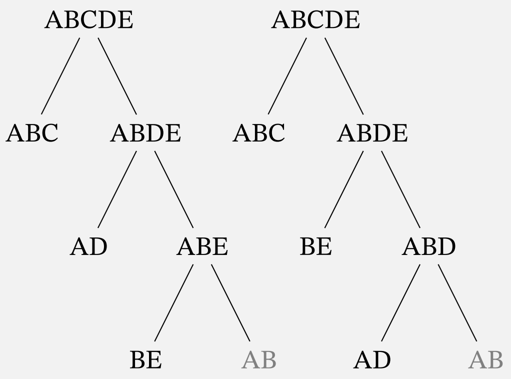
Consider the following example: the relation $R[A, B, C, D, E]$ and the functional dependencies $A \to D$, $B \to E$, and $AB \to C$. The relation can be normalized up to 3NF by following one of the decomposition trees shown in fig. 4.1. Every decomposition tree must take into account that the join of the projections is lossless and dependency preserving.

Figure 4.1: 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 consequence of a functional dependency; see fig. 4.2.

Figure 4.2: Invalid decomposition trees for the relation $R[ABCDE]$.



We consider the functional dependencies $A \rightarrow D$, $B \rightarrow E$, and $AB \rightarrow C$. 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 one we can have.

Observe, however, that transitive dependencies[16] and complex join dependencies restrict even further the joins we are allowed to perform.

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. 4.1 from bottom to top. After each join, a summarization operation is performed on the relation considering the student as the observational unit, i.e., over attribute A. The first join results in relation $R[ABCE]$ and the summarization operation results in a new re-

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

Table 4.25: Example of a dataset where the observational unit is the student.

A (student)	B (course)	C (grade)	E (load)
1	1	7	60
1	2	8	30
2	1	7	60
2	3	9	40
...	...	...	...

A (student)	F (average grade)	G (total load)
1	7.5	90
2	8	100
...	...	...

Relation $R[ABCE]$ becomes $R[AFG]$ after the summarization operation. Now each row represents a student (values in A are unique).

lation $R[AFG]$ where F is the average grade and G is the total course load taken by the student (see table 4.25). They are 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 $A \to DFG$, and it is in 3NF (which is also tidy).

Unfortunately, it is not trivial to calculate all possible decomposition trees for a given dataset. It is up to the data scientist to decide which directions to follow. However, it is important to notice that the order of the joins and summarization operations are crucial to the final result.

4.5 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 the data. For instance, attributes A and B might not be functionally dependent, but they might exist in an unknown $P(A, B)$ that we can estimate from the data. Each observed value of a key can represent an 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 do 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 the 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[17] 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.

4.6 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 one. However, the conversion process is not always straightforward nor lossless. For example, we can convert a text into a structured dataset by

[17]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.

counting the number of occurrences of each word[18]. 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.

[18]This is called a bag-of-words approach.

5 Data handling

† *It's dangerous to go alone! Take this.*

— Unnamed Old Man, *The Legend of Zelda*

In the previous chapter, I discussed the relationship between data format and data semantics. We also saw in chapter 3 that data tasks — specifically integration and tidying — must adjust the available data to reflect the kind of input we expect in production. Data handling consists of operating on this data.

For those tasks, we must be careful with the operations we perform on the data. At the stage of data preparation, for example, we should never parametrize our data handling pipeline in terms of information retrieved[1] by the values of the data. This is because such operations lead to data leakage during evaluation and other biases in our conclusions.

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*.

From a mathematical definition of such tables, we can define a set of operations that can be applied to them. These operations are the building blocks of data handling pipelines: combinations of operations that transform a dataset into another dataset.

Finally, I highlight some important properties of these operations. Especially, the split-invariance property, which ensures that the operations do not add bias to the data due to the way the data was collected.

[1]For instance, imputation by the mean of a column.

Chapter remarks

Contents

Context

- Data handling consists of operating on tables.
- Properties of the operations are important to avoid bias.
- Data handling pipelines are a way to organize these operations.

Objectives

- Define a formal structure for tables.
- Define a set of operations that can be applied to tables.

Takeaways

- Split-invariant operations avoid sampling bias.
- One must understand the properties and premises of the operations.

5.1 Formal structured data

In this section, I present a formal definition of structured data. This definition is compatible with the relational model and tidy data presented in chapter 4. My definition takes into account the index[2] of the table, which is a key concept in data handling. We also consider that values can be missing. Repeated rows are represented by allowing cells to contain sets of values. In this chapter, we consider dataset and table as synonyms.

Definition 5.1: (Indexed table)

An indexed table T is a tuple (K, H, c), where $K = \{K_i : i = 1, \dots, k\}$ is the set of index columns, H is the set of (non-index) columns, and $c : \mathcal{D}(K_1) \times \cdots \times \mathcal{D}(K_k) \times H \to \mathcal{V}$ is the cell function. Here, $\mathcal{V}$ represents the space of all possible tuples of values, which may include missing values ?. Values have arbitrary types, such as integers, real numbers, strings, etc. Each index column K_i has a domain $\mathcal{D}(K_i)$, which is an enumerable set of values.

A possible row r of the table is indexed by a tuple $r = (k_1, \dots, k_k)$, where $k_i \in \mathcal{D}(K_i)$. Each row has a cardinality $\operatorname{card}(r)$, which represents how many times the entity represented by the row is present in the table. A row r with $\operatorname{card}(r) = 0$ is considered to be missing.

A cell is then represented by a row r and a column $h \in H$. The value of the cell, $\mathbf{v} = c(r, h)$ is a tuple of values in the domain $\mathcal{D}(h) \cup \{?\}$, such that $|\mathbf{v}| = \operatorname{card}(r)$. We say that $\mathcal{D}(h)$ is the valid domain of the column h. The order of the elements in the tuple $\mathbf{v}$ is arbitrary but fixed.

We can stack nested rows to form a matrix of values. This matrix is called the value matrix of the row r.

We assume that value matrices — and consequently row cardinalities — are minimal. This means that there are no nested rows

$$v_{i,1}, \dots, v_{i,|H|}$$

in the value matrices such that $v_{i,j} = ?$ for all j.

From these concepts, we can define the basic operations and properties that can be applied to tables.

[2]Also called grouping variables.

Definition 5.2: (Nested row)

A *nested row* consists of a tuple of values that associates different columns with the same repetition of the entity, i.e.

$$\left[v_i^h \,:\, h \in H\right],$$

where $c(r, h) = [v_i^h \,:\, i = 1, \dots, \operatorname{card}(r)]$, assuming an arbitrary fixed order of the columns h.

Definition 5.3: (Value matrix)

The value matrix $V = (v_{i,j})$ of the row r is

$$\left[c(r, h) \,:\, h \in H\right],$$

with dimensions $\operatorname{card}(r) \times |H|$.

5.1.1 Splitting and binding

Split and bind are very basic operations that can be applied to tables. They are inverses of each other and are used to divide and combine tables, respectively. They are important in the data science process because they play a key role in data semantics and validation of solutions.

Definition 5.4: (Split operation)

Given an indicator function $s \,:\, \mathcal{D}(K_1) \times \cdots \times \mathcal{D}(K_k) \to \{0, 1\}$, the split operation creates two tables, T_0 and T_1, that contain only the rows for which $s(r) = 0$ and $s(r) = 1$, respectively.
Mathematically, the split operation is defined as

$$\operatorname{split}(T, s) = (T_0, T_1)\,,$$

where $T = (K, H, c)$, $T_i = (K, H, c_i)$, and

$$c_i(r, h) = \begin{cases} c(r, h) & \text{if } s(r) = i \\ () & \text{otherwise.} \end{cases}$$

Note that, by definition, the split operation never "breaks" a row. So, the indices define the indivisible entities of the table. The resulting tables are disjoint:

Definition 5.5: (Disjoint tables)

Two tables $T_0 = (K, H, c_0)$ and $T_1 = (K, H, c_1)$ are said to be disjoint if $\operatorname{card}(r; c_0) = 0$ whenever $\operatorname{card}(r; c_1) > 0$ for any row r, and vice-versa.

The binding operation is the inverse of the split operation. Given two disjoint tables $T_0 = (K, H, c_0)$ and $T_1 = (K, H, c_1)$, the binding operation creates a new table T that contains all the rows of T_0 and T_1.

Definition 5.6: (Bind operation)

Mathematically, the binding operation is defined as

$$\operatorname{bind}(T_0, T_1) = (K, H, c),$$

where $T_i = (K, H, c_i)$ and

$$c(r, h) = c_0(r, h) + c_1(r, h).$$

The operator $+$ stands for the tuple concatenation operator[a].

[a]The order of the concatenation here is not an issue since we guarantee that at least one of the operands is empty.

Thus, a requirement for the binding operation is that the tables are disjoint in terms of the row entities they have.

Premises in real-world applications One important aspect of these functions is that we assume that the entities represented by the rows are indivisible, and that any binding operation will never occur for tables that share the same entities.

In real-world applications, this is not always true. Many times, we do not know the process someone else has used to collect the data. In these cases, we must be careful about the guarantees we discuss in this chapter. On the other hand, one can consider the premises we use as a guideline to design good data collection processes.

We can see data collection as the result of a splitting operation in the universe set of all possible entities. This is a good way to think about data collection, as we can try to ensure that we collect all possible information about the entities we are interested in.

This, of course, depends on what we define as the index columns of the table. Consider the example of collecting information about grades of students. If we define the student's name and year as the indexes, we must ensure that we collect all the grades of all subjects a student has taken in a year. We do not need, though, to collect information from all students or all years. On the other hand, if we define only the student's name as the index column, we must collect all the grades of all subjects a student has taken in all years.

In summary, the fewer variables we define as index columns, the more information we must collect about each entity. However, in the next sections, we show that assuming many index columns leads to restrictions in the operations we can perform on the table.

This conceptual trade-off is important to understand when structuring the problem we are trying to solve. Neglecting these issues can lead to strong statistical biases and incorrect conclusions.

5.1.2 Split invariance

One property we can study about data handling operations is whether they are distributive over the bind operation. This property is called *split invariance*.

From now on, we will denote

$$T_0 + T_1 = \text{bind}(T_0, T_1),$$

for any tables T_0 and T_1 to simplify the notation.

Definition 5.7: (Split invariance)

An arbitrary data handling operation $f(T)$ is said to be split-invariant if, for any table T and split function s, the following equation holds

$$f(T_0 + T_1) = f(T_0) + f(T_1),$$

where $T_0, T_1 = \text{split}(T; s)$.

Split invariance is a desirable property for data handling operations during the data tasks described in chapter 3: integration and tidying. Even while exploring data, we should take effort to use split-invariant operations.

The reason is that split invariance ensures that the operation does not depend on the split performed (usually unknown to us) to create the table we have in hand. This property is important to avoid data leakage or to bias the results of the analysis.

5.1.3 Illustrative example

Table 5.1: Data table of student grades.

student	subject	year	grade
Alice	Chemistry	2020	6
Alice	Math	2019	8
Alice	Physics	2019	7
Bob	Chemistry	2018	?
Bob	Chemistry	2019	7
Bob	Math	2019	9
Bob	Physics	2019	4
Bob	Physics	2020	8
Carol	Biology	2020	8
Carol	Chemistry	2020	3
Carol	Math	2020	10

Data collected about student grades. All information that is available is presented.

Consider the example of data collected about student grades. Table 5.1 exemplifies all information we can possibly have about the grades of students. A missing value in a cell of that table indicates that, for some reason, the information is not retrievable.

The domains of the variables are:

- $\mathcal{D}(\text{student}) = \{\text{Alice}, \text{Bob}, \text{Carol}\}$;
- $\mathcal{D}(\text{subject}) = \{\text{Biology}, \text{Chemistry}, \text{Math}, \text{Physics}\}$;
- $\mathcal{D}(\text{year}) = \mathbb{Z}$; and

- $\mathcal{D}(\text{grade}) = [0, 10] \cup \{?\}$.

Of course, in practice, we have no guarantee that the data we have is complete nor a clear specification of the domain of the variables. Instead, we must choose good premises about the data we are working with.

Knowing that the data is complete, we can safely assume that:

1. Alice has never taken Biology;
2. Bob passed Physics, although at the second attempt;
3. Carol has only taken classes in 2020.

Table 5.2: Data table of student grades assuming student and subject as indices.

s	student	subject	year	grade
0	Alice	Chemistry	(2020)	(6)
1	Alice	Math	(2019)	(8)
1	Alice	Physics	(2019)	(7)
0	Bob	Chemistry	(2018, 2019)	(?, 7)
0	Bob	Math	(2019)	(9)
1	Bob	Physics	(2019, 2020)	(4, 8)
0	Carol	Biology	(2020)	(8)
0	Carol	Chemistry	(2020)	(3)
1	Carol	Math	(2020)	(10)

Indexed table with data from table 5.1 assuming student and subject as indices. The column s is the split indicator.

Now consider an arbitrary collection mechanism that considers student and subject as the indices of the table. Table 5.2 shows the table we have in hand. The column s is the split indicator. Only rows with $s = 1$ are available to us.

Now, about the statements we made before:

1. There is no way we can know if Alice has taken Biology or not. It could be that the data collection mechanism failed to collect this information or that the information simply does not exist.

2. We can safely assume that Bob has passed Physics in his second attempt, once all information about (Bob, Physics) is assumed to be available.
3. There is no guarantee that Carol has only taken classes in 2020. It could be that some row (Carol, subject) with a year different from 2020 is missing in the table.

Table 5.3: Data table of student grades assuming student as the index.

s	student	subject	year	grade
1	Alice	(Chemistry, Math, Physics)	(2020, 2019, 2019)	(6, 8, 7)
0	Bob	(Chemistry, Chemistry, Math, Physics, Physics)	(2018, 2019, 2019, 2019, 2020)	(?, 7, 9, 4, 8)
1	Carol	(Biology, Chemistry, Math)	(2020, 2020, 2020)	(8, 3, 10)

Indexed table with data from table 5.1 assuming student as index. The column s is the split indicator and only rows with $s = 1$ are available to us.

Now consider an arbitrary collection mechanism that considers student as the index of the table. Imposing this restriction would difficult the data collection process, but it would guarantee that we have all information about each student. Table 5.3 shows the table we have in hand. As before, the column s is the split indicator and only rows with $s = 1$ are available to us.

Our conclusions may change again:

1. We can safely assume that Alice has never taken the Biology class, as Biology $\notin c(\text{Alice}, \text{subject})$.
2. There is no information about Bob's grades, so we can not affirm nor deny anything about his grades.
3. We can safely assume that Carol has only taken classes in 2020, as $c(\text{Carol}, \text{year})$ contains only values with 2020.

It is straightforward to see that the fewer index columns we have, the more information we have about the present entities. Also, it is clear how important the assumptions on the index columns are to the conclusions we can draw from the data. Consequently, split-invariant operations can preserve valid conclusions about the data even when information is missing[3].

5.2 Data handling pipelines

In the literature and in software documentation, you will find a variety of terms used to describe data handling operations[4]. 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[5].

During the preparation of data for our project, we will need to perform a set of operations on possibly multiple datasets. These operations are organized in a pipeline, where the outputs of one operation are the inputs of the next one. Operations are extensively parameterized, for instance, most of them can use predicates to define the groups, arrangements, or conditions under which they should be applied.

In fig. 5.1, we show an example of a data handling pipeline. The pipeline starts with two source datasets, Source 1 and Source 2. The datasets are processed by a set of operations, f_1, f_2, f_3, f_4, f_5, and the output is a single dataset, Data. Our goal at the data tasks — see section 3.5.3 — is to create a dataset that is representative of the observational unit we are interested in. Representative here means that the dataset is tidy[6] and that the priors, i.e. the distribution of the data is faithful to the real distribution of the phenomenon.

A pipeline is more flexible than a chain of operations because it can handle more complex structures, where different branches (forks) of processing occur simultaneously, and then come together (merges) later

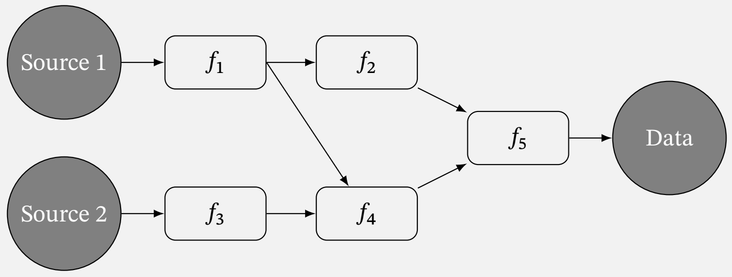
[3]Absence can be due to incomplete data collection or artificial splitting for validation; consult chapter 8.

[4]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" because it seems more generic. Also, it avoids confusion with the term "data manipulation" which has a negative connotation in some contexts.

[5]Which they call *verbs*.

[6]Remember that our definition of tidiness depends on the observational unit. That means, in practice, that if the original data sources are in a observational unit different from the one we are interested in, after joining them, the connecting variables may need to be removed to eliminate transitive dependencies. Consult sections 4.4.1 and 4.4.2.

Figure 5.1: Example of data handling pipeline.



A data handling pipeline is a set of operations that transform a dataset into another dataset. We can have more than one source dataset and the output is a single dataset where each row represents a sample in the observational unit we are interested in.

in the workflow. For instance, the output of f_1 is the input of f_2 and f_4 (fork), and f_5 has as input the outputs of f_2 and f_4 (merge).

Pipelines are great conceptual tools to organize the data handling process. They allow for the separation of concerns, where each operation is responsible for a single task. Also, declaring the whole pipeline at once allows for the optimization of the operations and the use of parallel processing. This is important when dealing with large datasets. The declarative approach, as opposed to the imperative one, makes it easier to reason about and maintain the code[7].

5.3 Split-invariant operations

In this section, I present a set of operations that are split-invariant. One can safely apply these operations to the data without worrying about biasing the dataset.

For each operation, we discuss its application on some tidying issues presented in section 4.3.1. The issues I address here[8]:

- Headers are values, not variable names;

[7]Tidyverse and Polars are examples of libraries that use a declarative approach to data handling.

[8]The issue of multiple types of observational units stored in the same table is better dealt with by database normalization. More on this subject is discussed in section 5.4.1.

- Multiple variables are stored in one column;
- Variables are stored in both rows and columns;
- A single observational unit is stored in multiple tables.

5.3.1 Tagged splitting and binding

We saw that one trivial, yet important, operation is to bind datasets. This is the process of combining two or more datasets into a single dataset. In order to make the operation reversible, we can parametrize it with a split column that indicates the source of each row.

Definition 5.8: (Tagged bind operation)

Given two or more disjoint tables $T_i = (K, H, c_i)$, $i = 0, 1, \dots$, the tagged bind operation creates a new table $T = (K, H \cup \{s\}, c)$ that contains all the rows of tables T_i. The split column s is a new column that indicates the source of each row.
Mathematically, the tagged bind operation is defined as

$$\text{bind}_s(T_0, T_1, \dots) = T,$$

where $c(r, h) = c_0(r, h) + c_1(r, h) + \dots$ if $h \in H$ and

$$c(r, s) = [i]^d,$$

where i is the index of the table T_i that contains the row r, i.e. $d = \text{card}(r; c_i) > 0$.

When binding datasets by rows, the datasets must have the same columns. In practice, one can assume, if a column is missing, that all values in that column are missing.

The indication of the source table usually captures some hidden semantics that has split the tables in the first place. 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. It is important to pay attention to the semantics of the split column, as it can also contain extra information.

Consider table 5.4, which contains monthly gas usage data from US and Brazil residents. From the requirements described in the previous section, we can safely bind these datasets — as they are disjoint. We

Table 5.4: Gas usage datasets.

month	gas	distance
1	48.7	1170
2	36.7	1100
3	37.8	970
...	...	...

month	gas	distance
1	143.7	1470
2	156.7	1700
3	170.8	1870
...	...	...

Monthly gas usage data from US (left) and Brazil (right) residents.

can use as a tag a new column to represent the country. However, an attentive reader will notice that the unit of measurement of the gas usage and distance are different in each table: gallons and miles in the US dataset and liters and kilometers in the Brazil dataset. Ideally, thus, we should create two other columns to represent the units of measurement.

It is straightforward to see that this operation solves the issue of a single observational unit being stored in multiple tables described in section 4.3.1.

The reverse function consists of splitting the dataset using as a predicate the split column.

Definition 5.9: (Tagged split operation)

Let s be a non-index column of a table $T = (K, H \cup \{s\}, c)$ with $\mathcal{D}(s)$ known and finite, and such that $c(r, s)$ contains only unique values. The tagged split operation parametrized by s creates disjoint tables $T_i = (K, H, c_i)$ that contain only the rows r for which $c(r, s) = i$.
Mathematically, the tagged split operation is defined as

$$\text{split}_s(T) = (T_0, T_1, \dots),$$

where $c_i(r, h) = c(r, h)$ if $i \in c(r, s)$ and $c_i(r, h) = ()$ otherwise.

Note that the tagged split is split-invariant by definition, since we assume that the nested rows of the input table T contain only one value for column s for all rows[9]. Failing to meet this assumption can lead to a biased split. Also, in practice, it is good practice to keep the column s in the output tables to preserve information about the source of the rows. In terms of storage, smart strategies can be used to avoid the unnecessary repetition of the same value in column s.

5.3.2 Pivoting

Another important operation is pivoting datasets. There are two types of pivoting: long-to-wide and wide-to-long. These operations are reversible and are the inverse of each other.

Pivoting long-to-wide requires 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. Other than these columns, all remaining columns must be indexes.

Definition 5.10: (Pivot long-to-wide operation)

Let $T = (K \cup \{\text{name}\}, \{\text{value}\}, c)$. The pivot long-to-wide operation is defined as

$$\text{pivot}_{\text{name}}(T) = T',$$

where $T' = (K, \mathcal{D}(\text{name}), c')$ and

$$c'(r, h) = c\left(r + (h),\ \text{value}\right),$$

for all valid row r and $h \in \mathcal{D}(\text{name})$.

Note however that the operation only works if $\text{card}(r + (h); c)$ is constant for all $h \in \mathcal{D}(\text{name})$. If this is not the case, one must aggregate the rows before applying the pivot operation. This is discussed in section 5.3.7.

Pivoting wide-to-long[10] is the reverse operation. One must specify all the columns whose names are the values of the previously called "name column." The values of these columns will be *gathered* into a new column. As before, all remaining columns are indexes.

[9]We consider a slightly different definition of split invariance here, where the binding operation is applied to each element of the output of the split operation.

[10]Also known as unpivot.

Definition 5.11: (Pivot wide-to-long operation)

Let $T = (K, H, c)$ be a table. The pivot wide-to-long operation is defined as

$$\text{pivot}^{-1}(T) = T',$$

where $T' = (K \cup \{\text{name}\}, \{\text{value}\}, c')$, $\mathcal{D}(\text{name}) = H$ and

$$c'((r, h), \text{value}) = c(r, h),$$

for all valid row r and $h \in H$.

In practical applications, where not all remaining columns are indexes, one must aggregate rows or drop extra non-indexed columns beforehand. This is discussed in sections 5.3.4 and 5.3.7.

Table 5.5: Pivoting example.

city	**year**	**qty.**
A	2019	1
A	2020	2
A	2021	3
B	2019	4
B	2020	5
B	2021	6

city	**2019**	**2020**	**2021**
A	1	2	3
B	4	5	6

The left-hand-side table is in the long format and the right-hand-side table is in the wide format.

Table 5.5 shows an example of pivoting. Here, we can consider *city* and *year* as the index columns. The left-hand-side table is in the long format and the right-hand-side table is in the wide format. Using the pivot long-to-wide operation with *year* as the name column and *qty.* as the value column, we can obtain the right-hand-side table. The reverse operation will give us the left-hand-side table.

To show that the pivot operation is split-invariant, one can see that, given $T_0 = (K, H, c_0)$ and $T_1 = (K, H, c_1)$ disjoint tables,

$$\text{pivot}_{\text{name}}(T_0) + \text{pivot}_{\text{name}}(T_1) = (K, \mathcal{D}(\text{name}), c'_0) + (K, \mathcal{D}(\text{name}), c'_1),$$

where $c'_i(r, h) = c_i(r + (h), \text{value})$. However, by the disjoint property of the tables, we have that

$$c_0(r + (h), \text{value}) + c_1(r + (h), \text{value}) = c(r + (h), \text{value}),$$

for the table $T = (K, H, c) = T_0 + T_1$. So,

$$(K, \mathcal{D}(\text{name}), c'_0) + (K, \mathcal{D}(\text{name}), c'_1) = (K, \mathcal{D}(\text{name}), c') = \text{pivot}_{\text{name}}(T),$$

where $c'(r, h) = c(r + (h), \text{value})$.

Similarly, the reverse operation is also split-invariant.

Using the pivot operation, we can solve the issues of headers being values, not variable names and variables being stored in both rows and columns. In the first case, we can pivot the table to have the headers as the domain of a new index (name column). In the second case, we have to pivot both long-to-wide and wide-to-long to solve the issue.

5.3.3 Joining

Joining is the process of combining two datasets into a single dataset based on common columns. This is one of the two fundamental operations in relational algebra. We will see the conditions under which the operation is split invariant. However, the join operation has some other risks you should be aware of; consult section 4.2 for more details.

Adapting the definitions of join in our context, we can define it as follows. For the sake of simplicity, we denote $r[U]$ as the row r restricted to the index columns in U, i.e.

$$r[U] = (k_i : k_i \in \mathcal{D}(K_i) \, \forall K_i \in U).$$

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 index 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.

Note that, like in pivoting long-to-wide, one must ensure that the cardinality of the joined rows is constant for all $h \in H' \cup H''$. If this is not the case, one must aggregate the rows before applying the join operation. This is discussed in section 5.3.7.

Definition 5.12: (Join operation)

Let $T' = (K', H', c')$ and $T'' = (K'', H'', c'')$ be two tables such that $K' \cap K'' \neq \varnothing$ and $H' \cap H'' = \varnothing$. The join operation is defined as

$$\operatorname{join}(T', T'') = T,$$

where $T = (K' \cup K'', H' \cup H'', c)$ and

$$c(r, h) = ()$$

if $\operatorname{card}(r[K']; c') = 0$ or $\operatorname{card}(r[K'']; c'') = 0$, for all h. Otherwise:

$$c(r, h) = \begin{cases} c'(r[K'], h) & \text{if } h \in H', \\ c''(r[K''], h) & \text{if } h \in H''. \end{cases}$$

Before we discuss whether the join operation is split-invariant[11], we can discuss a variation of the join operation: the left join. The left join is the same as the join operation, but if the value of U is missing in the second table, the operation will create a new row with the columns of the first table and missing values for the columns of the second table.

In our context, this operation is a unary operation, where the second table is a fixed parameter.

The left join operation is split-invariant. To see this, consider two disjoint tables $T_0 = (K, H, c_0)$ and $T_1 = (K, H, c_1)$, and a third table $T' = (K', H', c')$ such that $K \cap K' \neq \varnothing$ and $H \cap H' = \varnothing$. We have that

$$\begin{aligned} \operatorname{join}_{T'}(T_0) + \operatorname{join}_{T'}(T_1) = T_0' + T_1' = \\ (K \cup K', H \cup H', c_0') + (K \cup K', H \cup H', c_1'), \end{aligned}$$

where the meaning of each term is clear from the definition 5.13. It is straightforward to see that rows in T_0' and T_1' are disjoint, since at least part of the indices in $K \cup K'$ are different between them.

Moreover,

$$\operatorname{join}_{T'}(T_0 + T_1) = (K \cup K', H \cup H', c')$$

with $c'(r, h) = ()$ only if both $\operatorname{card}(r[K]; c_0) = 0$ and $\operatorname{card}(r[K]; c_1) = 0$. Otherwise, $c'(r, h) = c_0(r[K], h) + c_1(r[K], h)$ if $h \in H$ and $c'(r, h) = c_0(r[K], h)$ if $h \in H'$.

[11]Note that up to this point, we have defined this property only for unary operations.

Definition 5.13: (Left join operation)

Let $T' = (K', H', c')$ and $T'' = (K'', H'', c'')$ be two tables such that $K' \cap K'' \neq \emptyset$ and $H' \cap H'' = \emptyset$. The left join operation is defined as

$$\operatorname{join}(T'; T'') = \operatorname{join}_{T''}(T') = T,$$

where $T = (K' \cup K'', H' \cup H'', c)$ and

$$c(r, h) = ()$$

if $\operatorname{card}(r[K']; c') = 0$ for all h. Otherwise:

$$c(r, h) = \begin{cases} c'(r[K'], h) & \text{if } h \in H', \\ c''(r[K''], h) & \text{if } h \in H''. \end{cases}$$

Thus,

$$\operatorname{join}_{T'}(T_0 + T_1) = \operatorname{join}_{T'}(T_0) + \operatorname{join}_{T'}(T_1).$$

Our conclusion is that the left join operation given a fixed table is split-invariant. So we can safely use it to join tables without worrying about biasing the dataset once we fix the second table.

I conjecture that the (inner) join operation shares similar properties but it is not as safe; nonetheless, a clear definition of split invariance for binary operations is needed. This is left as a thought exercise for the reader. Notice that the traditional join has the ability to "erase" rows from any of the tables involved in the operation. This is a potential source of bias in the data. This further emphasizes the importance of understanding the semantics of the data schema before joining tables — consult section 4.2.

5.3.4 Selecting

Selecting is the process of choosing a subset of non-index columns from a dataset. The remaining columns are discarded. Rows of the table remain unchanged.

Although very simple, the selection operation is useful for removing columns that are not relevant to the analysis. Also, it might be needed before other operations, such as pivoting, to avoid unnecessary columns (wide-to-long) and to keep only the value column (long-to-wide).

Definition 5.14: (Selection operation)

Let $T = (K, H, c)$ be a table and $H' \subseteq H$. The selection operation is defined as

$$\text{select}_{H'}(T) = T',$$

where $T' = (K, H', c)$.

Sometimes, it is useful to select columns based on a function of the column properties. In other words, the selection operation can be parameterized by a predicate. The predicate is a function that returns a logical value given the column.

Definition 5.15: (Predicate selection operation)

Let $T = (K, H, c)$ be a table and $P : H \to \{0, 1\}$ be a predicate. The predicate selection operation is defined as

$$\text{select}_P(T) = T',$$

where $T' = (K, H', c)$ and $H' = \{h \in H : P(h) = 1\}$.

It is trivial to see that, if P does not depend on the values of the columns (i.e., has no access to c), the predicate selection operation is split-invariant. This is because the operation does not change the rows of the table nor does it depend on the values of the rows.

One example of the use of the predicate selection operation is to keep columns whose values are in a specific domain. For instance, to keep only columns that contain real numbers, we choose $P(h) = 1$ if $\mathcal{D}(h) = \mathbb{R}$, and $P(h) = 0$ otherwise.

The case where the predicate depends on the values of the columns is discussed in section 5.4.2.

5.3.5 Filtering

Filtering is the process of selecting a subset of rows from a dataset based on a predicate.

A predicate can be a combination of other predicates using logical operators, such as logical disjunction (or) or logical conjunction (and).

In the general case, predicates need to be robust enough to deal with value matrices of any size and those that contain missing values.

After filtering, the dataset will contain only the rows that satisfy the predicate. Columns remain unchanged.

In its simplest form, we can assume that $\mathrm{card}(r) \leq 1$ for all r and that the predicates are applied to each row independently. In this case, the value matrix $V(r)$ is just a tuple with a single value for each non-index column.

Without loss of generality, we can assume that predicates are combined using logical disjunction (or)[12].

For instance, the predicate `age > 18` will select all rows where the value in the age column is greater than 18. Keeping each row independent, we can also generalize predicates to deal with the values of the indexes as well.

Definition 5.16: (Filtering operation)

Let $T = (K, H, c)$ be a table and $P_1, \dots P_n$ be predicates. The filtering operation is defined as

$$\mathrm{filter}_{P_1,\dots,P_n}(T) = T',$$

where $T' = (K, H, c')$ and

$$c'(r,h) = \begin{cases} c(r,h) & \text{if } \bigvee_{i=1}^{n} P_i(r, V(r)) = 1, \\ () & \text{otherwise,} \end{cases}$$

where predicate

$$P_i : \bigtimes_{K_i} K_i \times \bigtimes_{h \in H} (\mathcal{D}(h) \cup \{?\}) \to \{0,1\}$$

is applied to the value matrix $V(r)$ of the row r.

It is also trivial to see that the filtering operation is split-invariant, even in its generalized form where the value matrix has many rows. This

[12]The reason is that sequential application of filtering is equivalent to combining the predicates using logical conjunction (and).

property comes from the fact that rows are treated independently. More complex cases are discussed in section 5.4.2.

5.3.6 Mutating

Mutating is the process of creating new columns in a table. 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 a function of the rows. The expression is a function that returns a vector of values given the values in the other columns. Similarly to filtering, in its simplest form, we can assume that $\text{card}(r) \leq 1$ for all r and that the predicates are applied to each row independently.

Definition 5.17: (Mutation operation)

Let $T = (K, H, c)$ be a table and f be a transformation function. The mutating operation is defined as

$$\text{mutate}_f(T) = T',$$

where $T' = (K, H \cup \{h'\}, c')$ and

$$c'(r,h) = \begin{cases} c(r,h) & \text{if } h \in H, \\ f(r, V(r)) & \text{if } h = h', \end{cases}$$

where the function

$$f : \bigtimes_{K_i \in K} K_i \times \bigtimes_{h \in H} (\mathcal{D}(h) \cup \{?\}) \to \mathcal{D}(h') \cup \{?\}$$

is applied to the value matrix $V(r)$ of the row r.

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. The `ifelse(a, b, c)` function is a conditional function that returns 1 if the condition is true and 0 otherwise.

This function solves the issue of multiple variables stored in one column described in section 4.3.1.

As with filtering, the mutating operation is split-invariant even if $\text{card}(r) > 1$ for any r[13]. This is because the operation is applied to each row independently. In this general case, an extra requirement is that the function f must return tuples with the same cardinality as the row it is applied to.

5.3.7 Aggregating

Many times, it is easier to reason about the table when all rows have cardinality 1. Aggregation ensures that the table has this property.

Definition 5.18: (Aggregation operation)

Let $T = (K, H, c)$ be a table and f be an aggregation function. The aggregation operation is defined as

$$\text{aggregate}_f(T) = T',$$

where $T' = (K, H, c')$ and

$$c'(r, h) = f(r, V(r))[h],$$

where function f is applied to the value matrix $V(r)$ of the row r and it has an image

$$(\mathcal{D}(h) \cup \{?\} \,:\, h \in H)\,,$$

independently of the input size. The notation $v[h]$ refers to the value corresponding to the column h in the output tuple.

As with mutation, aggregation is split-invariant as it treats each row independently, even if the function f considers order semantics of the values in the matrix.

5.3.8 Ungrouping

We discussed that the fewer index columns a table has — assuming we guarantee that all information about that entity is present — the safer

[13]It just changes the input space of function f.

it is to infer conclusions from the data. Thus, reducing the number of indices must be done very carefully — more on that in section 5.4.1.

On the other hand, sometimes it is useful to increase the number of index columns. For instance, pivoting long-to-wide requires all columns except one to be indexes. The operation that transforms some of the columns in the table into indexes is called ungrouping. The reason for the name is that the operation decreases the cardinality of rows by creating new rows, effectively ungrouping the values.

Definition 5.19: (Ungrouping operation)

Let $T = (K, H, c)$ be a table and $h' \in H$ such that $\mathcal{D}(h')$ is known and finite. The ungrouping operation is defined as

$$\text{ungroup}_{h'}(T) = T',$$

where $T' = (K \cup \{h'\}, H \setminus \{h'\}, c')$, and

$$c'(r + r', h) = (v_{i,h} : i),$$

where r refers to values of the indices in K, r' refers to the value of the new index h', and $v_{i,h}$ is the value of the column h in any i-th nested row of the value matrix $V(r; T)$ in the original table such that

$$v_{i,h'} = r'.$$

Note that the operation requires that the column h' has no missing values.

Table 5.6 shows an example of ungrouping. In the top table, there are two rows, one with cardinality 4 and the other with cardinality 3. The column *year* is ungrouped, creating new rows for each value in the nested row. The bottom table is the result of ungrouping the column *year*. Although there were 7 nested rows in the original table, the bottom table has 6 rows — the number of nested rows is preserved however. The reason is that the row (A, 2020) has cardinality 2.

The ungrouping operation is split-invariant. To see this, consider two disjoint tables $T_0 = (K, H, c_0)$ and $T_1 = (K, H, c_1)$, we have

$$\text{ungroup}_{h'}(T_0) + \text{ungroup}_{h'}(T_1) = \\ (K \cup \{h'\}, H \setminus \{h'\}, c'_0) + (K \cup \{h'\}, H \setminus \{h'\}, c'_1),$$

Table 5.6: Ungrouping example.

city	year	qty.
A	(2019, 2020, 2020, 2021)	(1, 2, 3, 4)
B	(2019, 2020, 2021)	(5, 6, 7)

city	year	qty.
A	2019	1
A	2020	(2, 3)
A	2021	4
B	2019	5
B	2020	6
B	2021	7

The index of the top table is the column *city*. The bottom table is the result of ungrouping the column *year*.

where $c'_j(r + r', h) = (v_{i,h} \ : \ i \text{ such that } v_{i,h'} = r')$. Since the tables are disjoint, the rows of the output tables are also disjoint. In other words, For any r, either $\text{card}(r + r'; c_0) = 0$ or $\text{card}(r + r'; c_1) = 0$ independently of the value of r'. The reason is that there is no possible $v_{i,h'} = r'$ if r is not present in the table.

Then,

$$(K \cup \{h'\}, H \setminus \{h'\}, c'_0) + (K \cup \{h'\}, H \setminus \{h'\}, c'_1) = (K \cup \{h'\}, H \setminus \{h'\}, c'),$$

where $c'(r + r', h) = c'_0(r + r', h) + c'_1(r + r', h)$.

5.4 Other operations

We saw that, under reasonable premises, split-invariant operations are safe to use in the context of tidying and data integration. However, data handling does not happen only in the context of tidying and integrating datasets[14]. It is also used in tasks like data exploration and data preprocessing. In these cases, other operations are needed.

[14]And, sometimes, we may need to use other transformations even for these tasks.

In this section, we discuss some of these operations. Instead of focusing on the mathematical definitions, we will discuss the semantics of the operations and some of their properties.

5.4.1 Projecting or grouping

Projection is one of the two fundamental operations in relational algebra — consult section 4.2 for more details. In database normalization theory, tables — called relations — are slightly different from the tables we are discussing here. The major difference is that they are sets of tuples, which means that each tuple is unique. In our scenario, this is similar to what we call rows represented by the possible values of the index columns of the table.

Adapting the definitions of projection to our context, we can define it as follows.

Definition 5.20: (Projection operation)

Let $T = (K, H, c)$ be a table and $K' \subset K$ a subset of the columns. The projection operation is defined as

$$\text{project}_{K'}(T) = T',$$

where $T' = (K', H \cup (K \setminus K'), c')$ and

$$c'(r,h) = \begin{cases} \sum_{r'} c(r + r', h) & \text{if } h \in H \\ \sum_{k' \in \mathcal{D}(h)} k' & \text{if } h \in K \setminus K', \end{cases}$$

for all valid row r considering the indices K' and for all tuples $r' = (k_i : i)$ such that $k_i \in \mathcal{D}(K_i)$ for all $K_i \in K \setminus K'$.

We can see that projection for our tables is a little more complex than the usual projection in relational algebra. Consider the example we discussed in section 4.2 as well, where we have a table with the columns *student*, *subject*, *year*, and *grade*.

Table 5.7 (top) shows that table adapted for our definitions. Suppose we want to project the table to have only the entity *course*. Now each row (bottom table) represents a course. The column *student* is not an index column anymore, and the values in the column are exhaustive

Table 5.7: Student grade table.

student	**course**	**course credits**	**grade**
Alice	Math	4	A
Alice	Physics	3	B
Bob	Math	4	B
Bob	Physics	3	A
Carol	Math	4	C

course	**student**	**course credits**	**grade**
Math	(Alice, Bob, Carol)	(4, 4, 4)	(A, B, C)
Physics	(Alice, Bob, Carol)	(3, 3, ?)	(B, A, ?)

(Top) An example of a table of students and their grades in courses. The columns *student* and *course* are the index columns. (Bottom) The same table projected into the entity *course*.

and unique, i.e., the whole set $\mathcal{D}$(student) is represented in the column for each row.

Thus, projection is a very useful operation when we want to change the observational unit of the data, particularly to the entity represented by a subset of the index columns. Semantically, projection groups the rows by the values.

It is easy to see that the projection operation is not split-invariant. Consider the following example. If we split the top table in table 5.7 so the first row (Alice, Math) is in one table and the second row (Alice, Physics) is in another, the bind operation between the projection into the entity *student* of these two tables is not allowed. The reason is that the row (Alice) will be present in both tables, violating the disjoint property of the tables.

The consequence is that a poor architecture of the data schema can lead to incorrect conclusions in the face of missing information (due to split). This is one of the reasons why database normalization is so important. The usage of parts of the tables without fully denormalizing them is a bad practice that can lead to spurious information.

5.4.2 Grouped and arranged operations

In practice, when we need more flexibility in the kind of operations we can perform — for instance, in data preprocessing —, we use variations of some operations in section 5.3 that are not split-invariant. These operations are parametrized by the groups and the order of the rows.

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

- **Aggregation function**: a function that returns a single value given a tuple of values; and
- **Window function**: a function that returns a tuple of values given a tuple of values of the same size;

where the order of the values may play a role in the result of the function.

Examples of aggregation functions are `sum` (summation), `mean` (average value), `count` (number of elements), and `first` (first element of the tuple). Examples of window functions are `cumsum` (cumulative sum), `lag` (a tuple with the previous values), and `rank` (the rank of the value in the tuple given some ordering).

Here, we consider that the rows of the table have cardinality equal to one — as discussed before, one can use ungrouping (section 5.3.8) and aggregation (section 5.3.7) to ensure this property. Without loss of generality, we also assume that there is only one index, called row number, such that each row has a unique value for this index[15].

Mutating with groups and order

We can take as an example the operation of creating a new column. To create a new column, we use an expression that depends on the values of the other columns. If the expression depends on an aggregation or window function, one must specify the groups and/or the order of the rows.

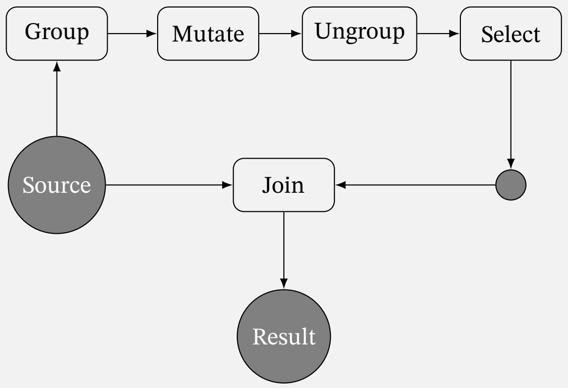
For example, the expression

```
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.

[15]Since the operations we describe here are not split-invariant, we can assume a previous projection of the data, see section 5.4.1.

Figure 5.2: Mutating with groups and order.



The mutating operation with groups and order is implemented as a pipeline.

This operation can be implemented as a pipeline. First, we group (project) the table by the `category` column. Then, we sort all the tuples by the `date` column. Finally, we apply the `cumsum` function to the `x` column and ungroup everything. In the result table, we select only columns `category` and `y`. Going back to the original table, we can left-join the original table with the result table using the `category` column. Now, we have the new column `y` in the original table. This is shown in fig. 5.2.

Note that the trivial group would be the whole table, i.e., a column with a single value. Thus, the grouping is always required, which makes the operation not split-invariant. In practical applications, I suggest being as explicit as possible about the groups and order criteria. This helps to avoid errors and to make the code more readable.

One important aspect about mutating sorted values is that one can use nontrivial strategies — from completing missing values to rolling windows — to deal with implicit missing values. This is a powerful tool to deal with time series data. For example, one can use the `lead` function to create a new column with the next value of the `x` column sorted by `year`.

If data contains both `x = (1, 3)` and `year = (2019, 2021)`, the calculation of the lead will result in

`x = (1, ?, 3)`, `year = (2019, 2020, 2021)`, and
`lead = (?, 3, ?)`,

since the missing value for the year 2020 was implicit.

Filtering with groups and order

It is easy to see that to filter rows of the table taking into account groups and order, we just need to create a new column with the expression that defines the predicate and then filter the rows based on this column. 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.

5.5 An algebra for data handling

In recent years, some researchers have made an effort to create a formal algebra for data transformations. The idea is to define a set of operations that can be combined to create complex transformations and describe their main properties.

Note that statistical data handling differs from relational algebra, because the former focuses on transformations and the latter on information retrieval.

Song, Jagadish, and Alter (2021)[16], 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

[16]J. Song, 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.

between different software, but it is not productive to advance 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. By basic operations, I mean that they are either irreducible — i.e., they cannot be expressed as a sequence of other operations — or they are so common and intuitive that they are worth being considered basic.

In this chapter, I try to shed some light on what could be a start for a formal algebra for general data handling. I present a set of operations and discuss their properties. I also present the novel concept of split invariance, which is a property that I think is important for the operations in the algebra.

For future directions, I suggest that one should try to express completeness in the data handling context. Drawing a parallel with computation theory, one could define a computational model for data handling and try to prove that the operations in the algebra are complete in the sense that they can express any transformation that can be expressed in the model. It would resemble a formal language for data handling that is "Turing complete."

A formal "complete" algebra for data handling would be a powerful tool for the development of new software and the translation of code between different software. It would also benefit performance optimizations and pave the way for semantic analysis of data transformations. It would be a step as significant as C was from assembly language!

6 Learning from data

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

— Florence Nightingale*, her diary*

As we discussed before, in this book, I focus on the problem of inferring a solution for a predictive task from data. In this chapter, we introduce the basic concepts of the statistical learning theory (SLT), a general framework for predictive learning tasks.

More specifically, we discuss the *inductive learning* approach, which involves deriving general rules from specific observations.

We also formally establish the learning problem, and we define the two most common predictive tasks: binary data classification and regression estimation. We discuss the optimal solutions for these tasks in an ideal (although unrealistic) scenario where the distributions of the data are known.

Moreover, we discuss principles that guide the learning process if the distribution of the data is unknown. From those principles, we discuss the properties and limitations of the learning process.

Finally, we realize those concepts for simple linear problems, explaining two basic algorithms for the learning process: the perceptron and the maximal margin classifier.

Chapter remarks

Contents

Context

- Inductive reasoning is the process of deriving general rules from specific observations.

Objectives

- Define the learning problem and the common predictive tasks.
- Understand the main principles that guide the learning process.

Takeaways

- Optimal solutions establish how good a solution can possibly be.
- Reducing error is not enough to guarantee a good solution.
- Controlling model complexity is crucial for generalization.

6.1 Introduction

Several problems can be addressed by techniques that utilize data in some way. Once we focus on one particular problem — inductive learning —, we need to define the scope of the tasks we are interested in. Let us start from the broader fields to the more specific ones.

Artificial intelligence (AI) 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, bio-inspired 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.

A more specific subfield of AI is machine learning (ML), which studies algorithms that enable computers to learn and improve their performance on a task from experience automatically, without being explicitly programmed by a human being.

Programming a computer to play chess is a good example of the difference between traditional AI and ML. In traditional AI, a human programmer would write a program that contains the rules of chess and the strategies to play the game. The algorithm might even "search" among the possible moves to find the best one. In ML, the programmer would write a program that learns to play chess by playing against itself, against other programs, or even from watching games played by humans. The system would learn the rules of chess and the strategies to play the game by itself.

This field is particularly useful when the task is too complex to be solved by traditional programming methods or when we do not know how to solve the task. Among the many tasks that can be addressed by ML, we can specialize even more.

Predictive learning is the ML paradigm that focuses on making predictions about outcomes (sometimes about the future) based on historical data. Predictive tasks involve predicting the value of a target variable based on the values of one or more input variables[1].

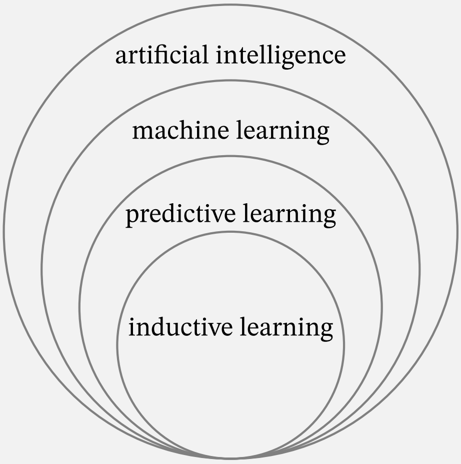
Depending on the reasoning behind the learning algorithms, we can divide the learning field into two main approaches: *inductive learning* and *transductive learning*[2].

[1]Descriptive learning, which is out of the scope of this book, focuses on describing the relationships between variables in the data without the need for a target variable.

[2]Trasduction is the process of obtaining specific knowledge from specific observations, and it is not the focus of this book.

Inductive learning involves deriving general rules from specific observations. The general rules can make predictions about *any* new instances. Such an approach is exactly what we want to apply in the project methodology we described in section 3.5: the solution is the general rule inferred from the data.

Figure 6.1: Organizational chart of the learning field.



Artificial intelligence studies algorithms that exhibit intelligent behavior and the behavior of intelligent systems. Machine learning is a subfield of artificial intelligence that studies algorithms that enable computers to automatically learn from data. Predictive learning, which focuses on making predictions about outcomes given known input data. Inductive learning is a yet more specific type of learning that involves deriving general rules from specific observations.

Figure 6.1 gives 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 book.

Maybe the most general (and useful) framework for predictive learning is SLT. In this chapter, we will introduce the basic concepts of this theory and discuss the properties of the main ML methods.

6.2 The learning problem

Consider the set

$$\{(\mathbf{x}_i, y_i) : i = 1, \dots, n\} \tag{6.1}$$

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, and identically distributed (i.i.d.) observations drawn according to

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

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

This is equivalent to the original SLT setup stated by V. N. Vapnik (1999), where a generator produces 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 4.4). Of course, we assume X, Y are only the measured variables (or non-prime attributes). In practice, it means that we set aside the keys in the learning process.

In terms of the tables defined in section 5.1, any row r in the table $T = (K, H, c)$, in the desired observational unit, such that $\operatorname{card}(r) > 0$, and $h \in H$ the chosen target variable, we have a corresponding target $y = c(r, h)$ and a feature vector $\mathbf{x}$ that corresponds to the tuple

$$\big(c(r, h') : h' \in H \setminus \{h\}\big).$$

Similarly, the variables K that describe each unit are set aside, as it does not make sense to infer general rules from them.

From the statistical point of view, learning problems consist of answering questions about the distribution of the data.

6.2.1 Learning tasks

In terms of predictive learning, given the before-mentioned scenario, we can refine our goals by tackling specific tasks[3].

Consider a *learning machine* capable of generating a set of functions, or *models*, $f(x; \theta) \equiv f_\theta(x)$, for a set of parametrizations $\theta \in \Theta$ and such that $f_\theta : \mathcal{X} \to \mathcal{Y}$. In a learning task, we must choose, among all possible f_θ, the one that predicts the target variable in the best possible way.

[3]I consider tasks as well-defined subproblems of a higher-level problem.

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 learned function.

Then, given the *risk function*

$$R(\theta) = \int \mathcal{L}(y, f_\theta(x))\, d\mathrm{P}(x, y), \tag{6.2}$$

the goal is to find the function f_θ that minimizes $R(\theta)$ where the only available information is the *training set* given by (6.1).

This formulation encompasses many specific tasks. I focus on two of them, which I believe are the most fundamental ones: *binary data classification*[4] and *regression estimation*[5]. (I left aside the density estimation problem, once it is not addressed in the remainder of the book.)

Binary data classification task

In this task, the output y takes on only two possible values, zero or one[6] — called the negative and the positive class, respectively —, and the functions f_θ are indicator functions. Choosing the loss

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

the risk (6.2) becomes the probability of classification error. The function f_θ, in this case, is called a *classifier* and y is called the *label*.

Regression estimation task

In this task, the output y is a real value and the functions f_θ are real-valued functions. The loss function is the squared error

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

In section 6.3, we show that the function that minimizes the risk with such a loss function is the so-called *regression*. The estimator f_θ of the regression, in this case, is called a *regressor*.

[4]In SLT, Vapnik calls it *pattern recognition*.

[5]We are not talking about *regression analysis*; regression estimation is closer to the *scoring* task definition by N. Zumel and J. Mount (2019). *Practical Data Science with R*. 2nd ed. Shelter Island, NY, USA: Manning.

[6]Alternatively, negative class is represented by -1 and positive class by 1.

6.2.2 A few remarks

These two tasks are quite general and can be applied to a wide range of problems. The modeling of the task at hand and choice of the loss function are crucial to the success of the learning process.

About these learning tasks, we can make a few remarks.

Supervised and semisupervised learning In both cases, classification and regression estimation, 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 generates models in a *supervised* manner — i.e., the target is known for all samples in the training set —, there are alternative ways to solve the inductive learning problem, such as the *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 outputs y are unknown.

Generative and discriminative models Any learning machine produces 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 $\mathrm{P}(x, y)$ and can also be used to generate new data. Discriminative models, on the other hand, describe the conditional probability distribution $\mathrm{P}(y \mid x)$ directly and can only be used to make predictions. Generative models are usually much more complex than discriminative models[7], but they hold more information about the data. If you only need to solve the predictive problem, prefer 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 *one-versus-all*, 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.

[7]Since modeling $\mathrm{P}(x, y)$ indirectly models $\mathrm{P}(y \mid x)$ and $\mathrm{P}(x)$.

As one should expect, dealing with more than two classes is more complex than dealing with only two classes. If possible, prefer to deal with binary classification tasks first.

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.

6.3 Optimal solutions

In this section, I show that the optimal solutions for the tasks of binary data classification and regression estimation depend only on $\mathrm{P}(y \mid x)$ (i.e. discriminative models). This is useful to understand how good a solution can possibly be and to derive practical solutions in the next sections.

6.3.1 Bayes classifier

The optimal solution for the binary data classification task is the *Bayes classifier*, which minimizes the probability of classification error. The Bayes classifier is defined as

$$f_{\text{Bayes}}(x) = \arg\max_{y \in \mathcal{Y}} \mathrm{P}(y \mid x).$$

We can easily see that the Bayes classifier is the optimal solution for the binary data classification task. The probability of classification error for an arbitrary classifier f is

$$R(f) = \int \mathbb{1}_{f(x) \neq y} \, d\mathrm{P}(x, y) = \iint \mathbb{1}_{f(x) \neq y} \, d\mathrm{P}(y|x) \, d\mathrm{P}(x),$$

where $\mathbb{1}_{\cdot}$ is the indicator function that returns one if the condition is true and zero otherwise. Let $b(x) = \mathrm{P}(y = 1 \mid x)$; we have that

$$\int \mathbb{1}_{f(x) \neq y} \, d\mathrm{P}(y|x) = b(x)\mathbb{1}_{f(x)=0} + (1 - b(x))\mathbb{1}_{f(x)=1},$$

which means only one of the terms is nonzero for each x. Thus, the risk is minimized by choosing a classifier that $f(x) = 1$ if $b(x) > 1 - b(x)$ and $f(x) = 0$ otherwise. This is the Bayes classifier.

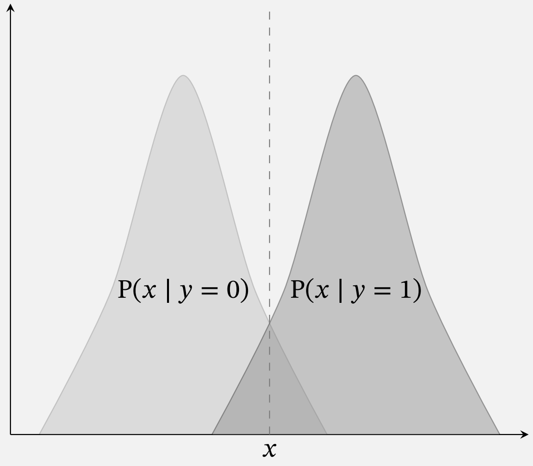
Consequently, the *Bayes error rate*, or irreducible error, is the lowest possible loss for any classifier in a given problem. The Bayes error rate sums the errors of the Bayes classifier for each class:

$$R_{\text{Bayes}} = \int \left[b(x) \mathbb{1}_{f_{\text{Bayes}}(x)=0} + (1 - b(x)) \, \mathbb{1}_{f_{\text{Bayes}}(x)=1} \right] d\mathrm{P}(x).$$

We know that $f_{\text{Bayes}}(x) = 1$ if $b(x) > 0.5$ and $f_{\text{Bayes}}(x) = 0$ otherwise. Thus, the Bayes error rate can be rewritten as

$$R_{\text{Bayes}} = \int \min \{ b(x), 1 - b(x) \} \; d\mathrm{P}(x).$$

Figure 6.2: Bayes classifier illustration.



The Bayes classifier is the line that separates the two classes. The Bayes error is a result of the darker area in which the distributions of the classes intersect.

Figure 6.2 illustrates the Bayes classifier and its error rate. The vertical line represents the Bayes classifier that separates the classes the best way possible in the space of the feature vectors x. Since the distributions $\mathrm{P}(x \mid y = 0)$ and $\mathrm{P}(x \mid y = 1)$ may intersect, there is a region where the Bayes classifier cannot always predict the class correctly.

6.3.2 Regression function

In the regression estimation task, the goal is to approximate the optimal solution, called *regression function*,

$$r(x) = \int y \, d\mathrm{P}(y \mid x), \tag{6.3}$$

that is the expected value of the target variable y given the input x.

It is easy to show that the regression function minimizes the risk (6.2) with loss

$$\mathcal{L}(y, r(x)) = \left(y - r(x)\right)^2.$$

The risk functional for an arbitrary function f is

$$R(f) = \int \left(y - f(x)\right)^2 d\mathrm{P}(x, y) = \\ \int y^2 \, d\mathrm{P}(y) - 2 \int f(x) \left[\int y \, d\mathrm{P}(y \mid x) \right] d\mathrm{P}(x) + \int f(x)^2 \, d\mathrm{P}(x),$$

however we can substitute $r(x)$ for the inner integral and obtain

$$R(f) = \int y^2 \, d\mathrm{P}(y) - 2 \int f(x) r(x) \, d\mathrm{P}(x) + \int f(x)^2 \, d\mathrm{P}(x) = \\ \int y^2 \, d\mathrm{P}(y) + \int \left[f(x)^2 - 2f(x)r(x) \right] d\mathrm{P}(x).$$

Once the first term is a constant, the risk is minimized by minimizing

$$f(x)^2 - 2f(x)r(x).$$

Deriving the last expression with respect to $f(x)$ and setting it to zero, we obtain

$$\frac{d}{df(x)} \left[f(x)^2 - 2f(x)r(x) \right] = 2f(x) - 2r(x) = 0 \Rightarrow f(x) = r(x).$$

Like the Bayes classifier, the stochastic nature of the data leads to an irreducible error in the regression estimation task. We have that

$$R(r) = \int \left(y - r(x)\right)^2 d\mathrm{P}(x, y) = \int y^2 \, d\mathrm{P}(y) - \int r(x)^2 \, d\mathrm{P}(x),$$

where the first term is

$$\mathrm{E}\left[y^2\right] = \mathrm{Var}(y) + \mathrm{E}[y]^2$$

and the second term is

$$\mathrm{E}\left[\mathrm{E}[y \mid x]^2\right] = \mathrm{Var}(\mathrm{E}[y \mid x]) + \mathrm{E}[\mathrm{E}[y \mid x]]^2 = \mathrm{Var}(\mathrm{E}[y \mid x]) + \mathrm{E}[y]^2 .$$

Thus, the irreducible error is

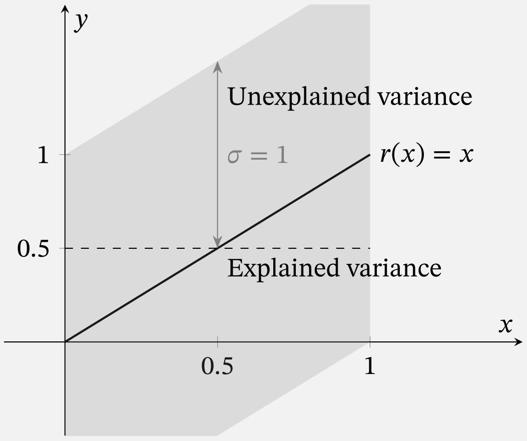
$$R(r) = \mathrm{Var}(y) - \mathrm{Var}(\mathrm{E}[y \mid x]) .$$

The interpretation of the irreducible error comes from the law of the total variance:

$$\mathrm{Var}(y) = \mathrm{E}[\mathrm{Var}(y \mid x)] + \mathrm{Var}(\mathrm{E}[y \mid x]) ,$$

where the first term is known as the unexplained variance and the second term, as the explained variance. The equality $R(r) = \mathrm{E}[\mathrm{Var}(y \mid x)]$ captures the idea that this variance is the intrinsic uncertainty that cannot be further reduced.

Figure 6.3: Unexplained variance is the error of the regression.



Expected error of the regression function for data generated by $\mathrm{P}(y \mid x)\,\mathrm{P}(x)$ such that $\mathrm{P}(y \mid x) = \mathcal{N}(x, 1)$ and $\mathrm{P}(x) = \mathcal{U}(0, 1)$. The regression function is $r(x) = x$.

Figure 6.3 illustrates the irreducible error of the regression function for arbitrary distributions $\mathrm{P}(y \mid x)$ and $\mathrm{P}(x)$. In this case, $\mathrm{E}[\mathrm{Var}(y \mid x)] = 1$, which means that points drawn by $\mathrm{P}(x, y)$ are distributed around the regression function $r(x)$ with a standard deviation of one. The explained variance is the spread of the regression across the x-domain.

6.4 ERM inductive principle

It is very interesting to study the optimal solution for learning tasks, but in the real-world, we do not have access to the distributions $\mathrm{P}(x)$ and $\mathrm{P}(y \mid x)$. We must rely on the training data $(x_1, y_1), \dots, (x_n, y_n)$ to infer a solution.

In the following sections, for the sake of simplicity, let z describe the pair (x, y) and $L(z, \theta)$ be a generic loss function for the model f_θ. Note that the training dataset is thus a set of n i.i.d. samples $z_1, \dots, z_n$.

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

$$R_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} L(z_i, \theta). \tag{6.4}$$

"'

Approximating $R(\theta)$ by the empirical risk functional $R_n(\theta)$ is the so-called empirical risk minimization (ERM) inductive principle. The ERM principle is the basis of the SLT.

Traditional 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.

6.4.1 Consistency of the learning process

One important question about the ERM principle is the consistency of the learning process. Consistency means that, given a sufficient number of samples, the empirical risk functional $R_n(\theta)$ converges to the true risk functional $R(\theta)$ over the hypothesis space Θ.

The consistency of the ERM principle is guaranteed by the uniform (two-sided) convergence[8] of the empirical risk functional $R_n(\theta)$ to the true risk functional $R(\theta)$ over the hypothesis space Θ. The uniform convergence is defined as

$$\lim_{n \to \infty} \mathrm{P}\left(\sup_{\theta \in \Theta} \left| R_n(\theta) - R(\theta) \right| > \epsilon \right) = 0.$$

[8]Actually, only a weaker one-sided uniform convergence is needed; consult a detailed explanation in chapter 2 of V. N. Vapnik (1999). *The nature of statistical learning theory.* 2nd ed. Springer-Verlag New York, Inc. ISBN: 978-1-4419-3160-3. The equivalence is a consequence of the key theorem of learning proved by Vapnik and Chervonenkis in 1989 and later translated to English in V. N. Vapnik and A. Chervonenkis (1991). "The necessary and sufficient conditions for consistency of the method of empirical risk minimization". In: *Pattern Recognition and Image Analysis* 1.3, pp. 284–305.

6.4.2 Rate of convergence

Beyond consistency, it is also useful to understand the rate at which $R_n(\theta)$ converges to $R(\theta)$ as the sample size n increases. It is possible for a learning machine to be consistent but have a slow convergence rate, which means that a large number of samples is needed to achieve a good solution.

The asymptotic rate of convergence of the empirical risk functional $R_n(\theta)$ is fast if, for any $n > n_0$, the exponential bound

$$\mathrm{P}\big(R(\theta_n) - R(\theta) > \epsilon\big) < \exp\big(-cn\epsilon^2\big)$$

holds true, where c is a positive constant.

6.4.3 VC entropy

Let $L(z, \theta)$, $\theta \in \Theta$, be a set of bounded loss functions, i.e.

$$|L(z, \theta)| < M,$$

for some constant M and all z and θ. One can construct n-dimensional vectors

$$l(z_1, \dots, z_n; \theta) = \big[L(z_1, \theta), \dots, L(z_n, \theta)\big].$$

Once the loss functions are bounded, this set of vectors belongs to a n-dimensional cube and has a finite minimal ϵ-net[9].

Consider the quantity $N(z_1, \dots, z_n; \Theta, \epsilon)$ that counts the number of elements of the minimal ϵ-net of that set of vectors. Once the quantity N is a random variable, we can define the VC entropy as

$$H(n; \Theta, \epsilon) = \mathrm{E}[\ln N(z_1, \dots, z_n; \Theta, \epsilon)]\,,$$

where z_i are i.i.d. samples drawn from some $\mathrm{P}(z)$.

If $L(z, \theta)$, $\theta \in \Theta$, is a set of indicator functions (i.e., the loss in a binary classification task), we measure the diversity of this set using the quantity $N(z_1, \dots, z_n; \Theta)$ that counts the number of different separations of the given sample that can be made by the functions. In this case, the minimal ϵ-net for $\epsilon < 1$ does not depend on ϵ and is a subset of the vertices of the unit cube.

A necessary and sufficient condition for uniform convergence is

$$\lim_{n\to\infty} \frac{H(n; \Theta, \epsilon)}{n} = 0, \tag{6.5}$$

[9]An ϵ-net is a set of points that are ϵ-close to any point in the set.

for all $\epsilon > 0$.

The VC entropy measures the complexity of the hypothesis space Θ. The intuition behind the need for a decreasing VC entropy with increasing numbers of observations is related to the nonfalsifiability of the learning machine. For instance, the set of functions that can always separate the training data perfectly (contains all the vertices of the cube) is nonfalsifiable because it implies that the minimum of the empirical risk is zero independently of the value of the true risk.

6.4.4 Growing function and VC dimension

It turns out that we can guarantee both the uniform convergence and the fast rate of convergence independently of P(z). Actually,

$$\lim_{n\to\infty} \frac{G(n;\Theta)}{n} = 0$$

is the necessary and sufficient condition, where

$$G(n;\Theta) = \ln \sup_{z_1,\dots,z_n} N(z_1,\dots,z_n;\Theta),$$

is the *growth function* of the hypothesis space Θ.

V. Vapnik and Chervonenkis (1968)[10] showed that the growth function either satisfies

$$G(n;\Theta) = n\ln 2$$

or is bounded by

$$G(n;\Theta) \le h\left(\ln\frac{n}{h}+1\right),$$

where h is an integer. Thus, the growth function is either linear or logarithmic in n. In the first case, we say that the *VC dimension* of the hypothesis space is infinite, and in the second case, the VC dimension is h.

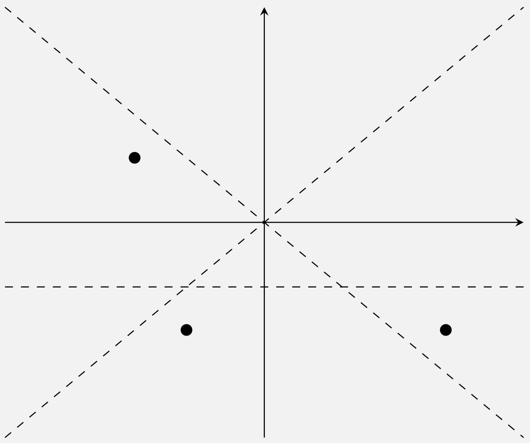
A finite VC dimension is enough to imply both consistency and a fast rate of convergence.

Intuitions about the VC dimension

For a set of indicator functions, the VC dimension is the maximum number of vectors that can be *shattered* by the functions. If, for any n, there

[10]V. Vapnik and A. Chervonenkis (1968). "On the uniform convergence of relative frequencies of events to their probabilities". In: *Doklady Akademii Nauk USSR*. vol. 181. 4, pp. 781–787.

Figure 6.4: VC dimension of a set of lines in the plane.



The VC dimension of the lines in the plane is equal to 3, since a line can shatter 3 points in all 8 possible ways, but not four points.

is a set of n vectors that can be shattered by the functions, the VC dimension is infinite. We say that h vectors can be shattered if they can be separated into two classes in all 2^h possible ways. Figure 6.4 illustrates the VC dimension of a set of lines in the plane.

One misconception about the VC dimension is that it is related to the number of parameters of the model. The VC dimension is actually related to the complexity of the hypothesis space, not to the number of parameters. For instance, the VC dimension of functions

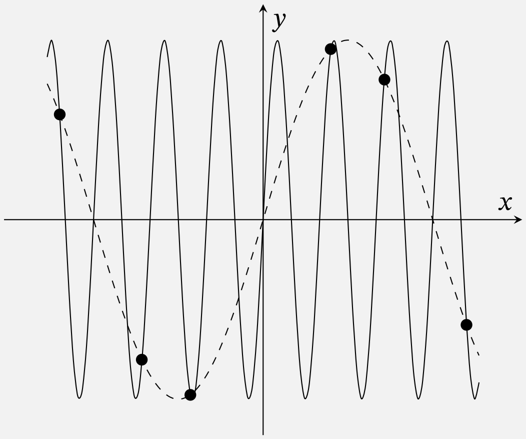
$$f(z; \theta) = \mathbb{1}_{\sin \theta x > 0}$$

is infinite, even though the parameter θ is a scalar. See fig. 6.5. By increasing the frequency θ of the sine wave, the function can approximate any set of points.

This opens remarkable opportunities to find good solutions containing a huge number of parameters[11] but with a finite VC dimension.

[11]Sometimes, like in a linear model, the number of parameters is proportional to the number of dimensions of the feature vector.

Figure 6.5: High-frequency sine wave functions have an infinite VC dimension.



High-frequency sine waves approximate any set of points well, even though they may come from a low-frequency sine wave or any other function.

6.5 SRM inductive principle

The ERM principle is a powerful tool to study the generalization ability of the learning process. By generalization ability, we mean the ability of the learning machine to predict the output of new data that was not seen during the training process. However, it relies on the hypothesis that the number of samples tends to infinity.

In fact, V. N. Vapnik (1999)[12] summarizes the bounds for the generalization ability of learning machines in the following way[13]:

$$R(\theta_n) \leq R_n(\theta_n) + \frac{B\mathcal{E}}{2}\left(1 + \sqrt{1 + \frac{4R_n(\theta_n)}{B\mathcal{E}}}\right), \tag{6.6}$$

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

[13]For the sake of the arguments, we consider only the expression for bounded losses and an hypothesis space with infinite number of functions. Rigorously, the loss function may not be bounded; consult the original work for the complete expressions.

with

$$\mathcal{E} = 4\frac{h\left(\ln\frac{2n}{h}+1\right) - \ln\frac{\eta}{4}}{n},$$

where B is the upper bound of the loss function, h is the VC dimension of the hypothesis space, n is the number of samples. The term η is the confidence level, i.e., the inequality holds with probability $1 - \eta$.

It is easy to see that as the number of samples n increases, the empirical risk $R_n(\theta_n)$ approaches the true risk $R(\theta_n)$. Also, the greater the VC dimension h, the greater the term $\mathcal{E}$, decreasing the generalization ability of the learning machine.

In other words, if n/h is small, a small empirical risk does not guarantee a small value for the actual risk. A consequence is that we need to minimize both terms of the right-hand side of the inequality eq. (6.6) to achieve a good generalization ability.

Table 6.1: Overfitting and underfitting.

Problem	**Empirical risk**	**Confidence interval**
Underfitting	High	Low
Overfitting	Low	High

Two problems that can arise in the learning process are underfitting and overfitting. Underfitting occurs when the model is too simple (low VC dimension) and cannot capture the complexity of the training data (high empirical risk). Overfitting occurs when the model is too complex (high VC dimension increases the confidence interval) and fits the training data almost perfectly (low empirical risk).

Failure to balance the optimization of these terms leads to two problems: underfitting and overfitting. Table 6.1 summarizes the problems.

The structural risk minimization (SRM) principle consists of minimizing both the empirical risk (optimizing the parameters of the model) and the confidence interval (controlling VC dimension).

Let $\Theta_k \subset \Theta$ and

$$S_k = \{L(z, \theta) : \theta \in \Theta_k\}$$

such that

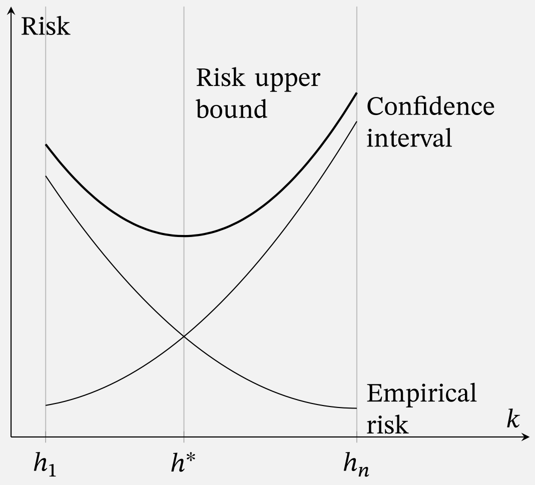
$$S_1 \subset S_2 \subset \cdots \subset S_n \subset \ldots,$$

satisfying

$$h_1 \leq h_2 \leq \cdots \leq h_n \leq \dots,$$

where h_k is the finite VC dimension[14] of each set S_k. This is called an *admissible structure.*

Figure 6.6: SRM trade-off.



The upper bound of the risk is the sum of the empirical risk and the confidence interval. The smallest bound is found for some k^* in the admissible structure.

Given the observations $z_1, \dots, z_n$, the SRM principle chooses a function $L(z, \theta_n^k)$ that minimizes the empirical risk $R_n(\theta_n^k)$ in the subset S_k for which the guaranteed risk — upper bound considering the confidence interval — is minimal. This is a trade-off between the quality of the approximation and the complexity of the approximating function — see fig. 6.6.

[14]Note that the VC dimension considering the whole set Θ might be infinite. Moreover, in the original formulation, the sets S_k also need to satisfy some bounds; read more in chapter 4 of V. N. Vapnik (1999). *The nature of statistical learning theory.* 2nd ed. Springer-Verlag New York, Inc. ISBN: 978-1-4419-3160-3.

6.5.1 Bias invariance trade-off

The trade-off that the SRM principle deals with is the general case of the so-called *bias-variance trade-off*. The bias-variance trade-off is a well-known concept in machine learning that describes the relationship between different kinds of errors a model can have.

The *bias error* comes from failure to capture relevant relationships between features and target outputs. The *variance error* comes from erroneously modeling the random noise in the training data.

The terms bias and variance (and the irreducible error) are clearly illustrated by studying the particular regression estimation task.

Consider a learning machine that produces a function $\hat{f}(x;D)$ based on the training set

$$D = \{(x_1, y_1), \dots, (x_n, y_n)\}$$

such that

$$y_i = f(x_i) + \epsilon,$$

for a fixed function f and a random noise ϵ with zero mean and variance σ^2, where x_i are i.i.d. samples drawn from some distribution $\mathrm{P}(x)$.

Also, consider that $\bar{f}(x)$ is the expected value of the function $\hat{f}(x;D)$ over all possible training sets D, i.e.

$$\bar{f}(x) = \int \hat{f}(x;D)\, d\mathrm{P}(D).$$

(Note that the models themselves are the random variable we are studying here.)

For any model $\hat{f}$, the expected (squared) error for a particular sample (x, y), $\mathrm{E}_D\Big[\big(y - \hat{f}(x;D)\big)^2\Big]$, is

$$\begin{aligned} \int \big(y - \hat{f}(x)\big)^2 d\mathrm{P}(D,\epsilon) &= \int \big(y - f(x) + f(x) - \hat{f}(x)\big)^2 d\mathrm{P}(D,\epsilon) \\ &= \int \big(y - f(x)\big)^2 d\mathrm{P}(D) && (6.7) \\ &+ \int \big(f(x) - \hat{f}(x)\big)^2 d\mathrm{P}(D) && (6.8) \\ &+ 2\int \big(y - f(x)\big)\big(f(x) - \hat{f}(x)\big)\, d\mathrm{P}(D,\epsilon). && (6.9) \end{aligned}$$

The term (6.7) is the irreducible error:

$$\int \left(y - f(x)\right)^2 d\mathrm{P}(D) = \int \left(f(x) + \epsilon - f(x)\right)^2 d\mathrm{P}(D) = \int \epsilon^2\, d\mathrm{P}(D) = \sigma^2. \tag{6.10}$$

As the best solution is f itself, the error that comes from the noise is unavoidable.

The term (6.9) is null:

$$\int \left(y - f(x)\right)\left(f(x) - \hat{f}(x)\right) d\mathrm{P}(D,\epsilon) = \int \epsilon\left(f(x) - \hat{f}(x)\right) d\mathrm{P}(D,\epsilon) =$$

$$\cancelto{0}{\int \epsilon\, d\mathrm{P}(\epsilon)} \int \left(f(x) - \hat{f}(x)\right) d\mathrm{P}(D) = 0,$$

since $\mathrm{P}(D)$ and $\mathrm{P}(\epsilon)$ are independent and $\mathrm{E}[\epsilon] = 0$ by definition.

We can apply a similar strategy to analyze the term (6.8):

$$\begin{aligned}
\int \left(f(x) - \hat{f}(x)\right)^2 d\mathrm{P}(D) &= \int \left(f(x) - \bar{f}(x) + \bar{f}(x) - \hat{f}(x)\right)^2 d\mathrm{P}(D) \\
&= \int \left(f(x) - \bar{f}(x)\right)^2 d\mathrm{P}(D) && (6.11) \\
&+ \int \left(\bar{f}(x) - \hat{f}(x)\right)^2 d\mathrm{P}(D) && (6.12) \\
&+ 2\int \left(f(x) - \bar{f}(x)\right)\left(\bar{f}(x) - \hat{f}(x)\right) d\mathrm{P}(D). && (6.13)
\end{aligned}$$

Now, the term (6.13) is also null:

$$\int \left(f(x) - \bar{f}(x)\right)\left(\bar{f}(x) - \hat{f}(x;D)\right) d\mathrm{P}(D) =$$

$$\left(f(x) - \bar{f}(x)\right) \int \left(\bar{f}(x) - \hat{f}(x;D)\right) d\mathrm{P}(D) =$$

$$\left(f(x) - \bar{f}(x)\right)\left(\cancelto{0}{\bar{f}(x) - \int \hat{f}(x;D)\, d\mathrm{P}(D)}\right) = 0,$$

since $\bar{f}(x)$ is the expected value of $\hat{f}(x;D)$.

The term (6.11) does not depend on the training set, so

$$\int \left(f(x) - \bar{f}(x)\right)^2 d\mathrm{P}(D) = \left(f(x) - \bar{f}(x)\right)^2. \tag{6.14}$$

This term is the square of the bias of the models.

The term (6.12) is the variance of the function $\hat{f}(x; D)$:

$$\int \left(\bar{f}(x) - \hat{f}(x; D)\right)^2 d\mathrm{P}(D) = \\ \mathrm{E}_D\left[\left(\bar{f}(x) - \hat{f}(x; D)\right)^2\right] = \mathrm{Var}_D\left(\hat{f}(x; D)\right). \quad (6.15)$$

Finally, putting all together — i.e. eqs. (6.10), (6.14) and (6.15) —, we have that the expected error for a particular sample (x, y) is

$$\mathrm{E}_D\left[\left(y - \hat{f}(x; D)\right)^2\right] = \sigma^2 + \left(f(x) - \mathrm{E}\left[\hat{f}(x; D)\right]\right)^2 + \mathrm{Var}_D\left(\hat{f}(x; D)\right).$$

The irreducible error is the regression error that cannot be reduced by any model — see section 6.3.2. The bias error is the error that one expects from the model acquired by the learning machine and that we observe in the training data — i.e. the empirical risk. The variance error, which does not depend on the real function f but on the models the learning machine can generate, is the error that comes from how different the models can be from each other — i.e. the confidence interval that comes from the VC dimension.

6.5.2 Regularization

Also related to the SRM principle is the concept of *regularization*. Regularization encourages models to learn robust patterns within the data rather than memorizing it.

Regularization techniques usually modify the loss by adding a penalty term that depends on the complexity of the model. So, instead of minimizing the empirical risk $R_n(\theta)$, the learning machine minimizes the regularized empirical risk

$$R_n(\theta) + \lambda\Omega(\theta),$$

where $\Omega(\theta)$ is the complexity of the model and λ is a hyperparameter that controls the trade-off between the empirical risk and the complexity. Note that the regularization term acts as a proxy for the confidence interval in the SRM principle. However, regularization is often justified by common sense or intuition, rather than by strong theoretical arguments.

Other approaches that indirectly control the complexity of the model — such as early stopping, dropout, ensembles, and pruning — are often called implicit regularization.

6.6 Linear problems

To realize the concepts of the SRM principle in practice, we consider linear classification tasks.

For the examples in the following subsections, we use the datasets for the AND and the XOR problem — see table 6.2. The AND problem is linearly separable, while the XOR problem is not.

Table 6.2: 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 $y = x_1 \oplus x_2$.

We show two learning machines that implement the SRM principle in different ways:

- The perceptron, which fixes the complexity of the model and tries to minimize the empirical risk; and
- The maximal margin classifier, which fixes the empirical risk — in this case, zero – and tries to minimize the confidence interval.

6.6.1 Perceptron

The perceptron is a linear classifier that generates a hyperplane that separates the classes in the feature space. It is a parametric model, and the learning process minimizes the empirical risk by adjusting its fixed set of parameters.

Parametric models are usually simpler and faster to fit, 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 tends to be too complex, too slow to train, and might overfit to the data.

Definition 6.1: (Parametric model)

If the learning machine generates a set of functions f_θ where the number of parameters $|\theta|$ is always fixed, the models are called *parametric*.

Note, however, that the VC dimension and number of parameters are not the same thing — consult section 6.4.4.

The perceptron model (with two inputs) is

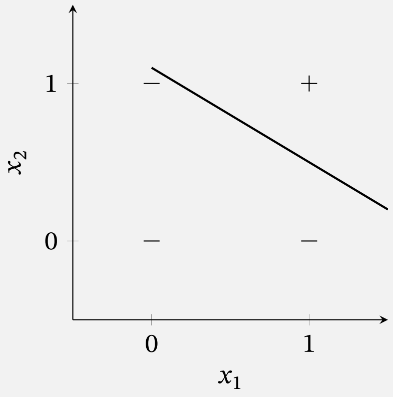
$$f(x_1, x_2; \mathbf{w} = [w_0, w_1, w_2]) = u(w_0 + w_1 x_1 + w_2 x_2),$$

where u is the Heaviside step function

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

The parameters $\theta = \mathbf{w}$ are called the weights of the perceptron. The equation $\mathbf{w} \cdot \mathbf{x} = 0$, where $\mathbf{x} = [1, x_1, x_2]$, is the equation of a hyperplane.

Figure 6.7: Perceptron decision boundaries in the AND dataset.



The perceptron assumes that the classes are linearly separable. The hyperplane that separates the classes comes from the weights of the model. In this case, $w_0 = -1.1$, $w_1 = 0.6$, and $w_2 = 1$.

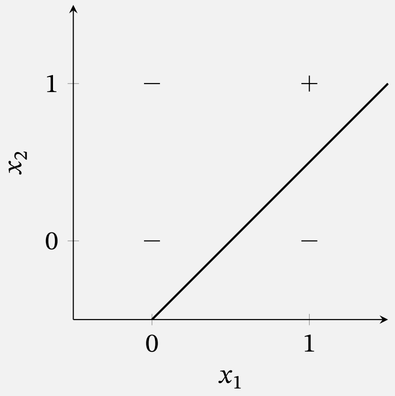
In fig. 6.7, we show the hyperplane (in this case, a line) that the model with weights $\mathbf{w} = [-1.1, 0.6, 1]$ generates in this feature space. As one can see, the classes are linearly separable, and the perceptron model classifies the dataset correctly; see table 6.3.

Table 6.3: Truth table for the predictions of the perceptron in the AND dataset.

x_1	x_2	y	$-1.1 + x_1 + x_2$	$\hat{y}$
0	0	0	-1.1	0
0	1	0	-0.1	0
1	0	0	-0.5	0
1	1	1	0.5	1

The perceptron model with parameters $w_0 = 1.1$, $w_1 = -1$, and $w_2 = -1$ classifies the AND dataset correctly.

Figure 6.8: Perceptron decision boundaries in the XOR dataset.



The XOR dataset is not linearly separable. The hyperplane that separates the classes comes from the weights of the model. In this case, $w_0 = -0.5$, $w_1 = 1$, and $w_2 = -1$. There is no way to classify the XOR dataset correctly with a perceptron.

In fig. 6.8, we show the hyperplane that the model $\mathbf{w} = [-0.5, 1, -1]$ generates for the XOR dataset. As one can see, the perceptron model fails to solve the task since there is no single decision boundary that can classify this data.

Table 6.4: Truth table for the predictions of the perceptron in the XOR dataset.

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.

It is easy to see that there are an infinite number of hyperplanes that can separate the classes in the AND dataset. The training procedure of the perceptron is a simple algorithm that adjusts the weights of the model to find one of these hyperplanes — effectively minimizing the empirical risk. The algorithm updates the weights iteratively for each sample that is misclassified, repeating the samples as many times as necessary. It stops when all samples are correctly classified.

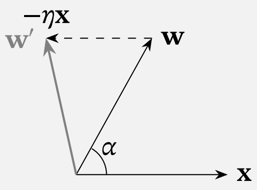
For a binary classification problem and a perceptron with weights $\mathbf{w}$, there are 4 situations for a given sample $\mathbf{x}$ and y:

1. $y = 0$ and $u(\mathbf{w} \cdot \mathbf{x}) = 0$;
2. $y = 0$ and $u(\mathbf{w} \cdot \mathbf{x}) = 1$;
3. $y = 1$ and $u(\mathbf{w} \cdot \mathbf{x}) = 0$;
4. $y = 1$ and $u(\mathbf{w} \cdot \mathbf{x}) = 1$.

By definition, the algorithm must update the weights when situation 2 or 3 occurs. Let $e = y - u(\mathbf{w} \cdot \mathbf{x})$ be the error of the model for a given sample.

In situation 2, we have that $\mathbf{w} \cdot \mathbf{x} > 0$ which means that the angle α between the vectors $\mathbf{w}$ and $\mathbf{x}$ is less than 90°, since $\|\mathbf{w}\|\|\mathbf{x}\| \cos\alpha > 0 \implies \cos\alpha > 0 \implies \alpha < 90°$. To increase the angle between the vectors, we can subtract $\eta\mathbf{x}$ from $\mathbf{w}$, for some small $\eta > 0$ — see fig. 6.9. The error here is $e = -1$.

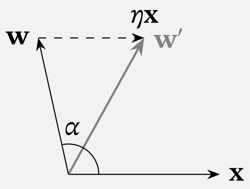
Figure 6.9: Angle between $\mathbf{w}$ and $\mathbf{x}$ in a positive output.



A positive output for the perceptron with weights $\mathbf{w}$ and input $\mathbf{x}$ means that the angle between the vectors is less than 90°. To increase the angle between the vectors, we can subtract $\eta\mathbf{x}$ from $\mathbf{w}$, for some small $\eta > 0$.

In situation 3, we have that $\mathbf{w} \cdot \mathbf{x} < 0$ which means that the angle α between the vectors $\mathbf{w}$ and $\mathbf{x}$ is greater than 90°, since $\|\mathbf{w}\|\|\mathbf{x}\| \cos\alpha < 0 \implies \cos\alpha < 0 \implies \alpha > 90°$. To decrease the angle between the vectors, we can add $\eta\mathbf{x}$ to $\mathbf{w}$, for some small $\eta > 0$ — see fig. 6.10. Now, the error is $e = 1$.

Figure 6.10: Angle between $\mathbf{w}$ and $\mathbf{x}$ in a negative output.



A negative output for the perceptron with weights $\mathbf{w}$ and input $\mathbf{x}$ means that the angle between the vectors is greater than 90°. To decrease the angle between the vectors, we can add $\eta\mathbf{x}$ to $\mathbf{w}$, for some small $\eta > 0$.

From those observations, we can derive a general update rule

$$\mathbf{w}' = \mathbf{w} + \eta e \mathbf{x},$$

where η is a small positive number that controls the step size of the algorithm. Note that this rule works even for cases 1 and 4, where the error is zero.

The algorithm converges given η sufficiently small and the dataset is linearly separable. Note that the algorithm does not make any effort to reduce the confidence interval.

The perceptron is (possibly) the simplest artificial neural network. More complex networks can be built by stacking perceptrons in layers and adding non-linear activation functions. The training strategies for those networks are usually based on reducing the empirical risk using the gradient descent algorithm while controlling the complexity of the model with regularization techniques[15]. Consult appendix B.1.

6.6.2 Maximal margin classifier

We saw that the perceptron tries to minimize the empirical risk, but it makes no effort to reduce the confidence interval. A different approach would be to fix the empirical risk — in our case, assuming that the classes are linearly separable, to fix it to zero — and minimize the confidence interval.

The confidence interval is an increasing function

$$\Omega\left(\frac{h}{n}\right),$$

where h is the VC dimension of the hypothesis space and n is the number of samples. Since the number of training samples n is fixed and finite (sometimes even small), we can minimize the confidence interval by minimizing the VC dimension h.

In the case of the perceptron, since it can generate any hyperplane, the VC dimension is $h = d + 1$, where d is the number of dimensions of the feature space — consult section 6.4.4.

Before we dive into the classifier that minimizes the confidence interval, consider the following property. V. N. Vapnik (1999)[16] state that a Δ-margin separating hyperplane is the hyperplane

$$(\mathbf{w} \cdot \mathbf{x}) - b = 0, \|\mathbf{w}\| = 1,$$

[15]To counterbalance the potential "excess" of neurons, techniques like l_2 regularization "disable" some neurons by pressuring their weights to zero.

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

such that classifies vector $\mathbf{x}$ as

$$y = \begin{cases} 1 & \text{if } (\mathbf{w} \cdot \mathbf{x}) - b \geq \Delta, \\ -1 & \text{if } (\mathbf{w} \cdot \mathbf{x}) - b \leq -\Delta. \end{cases}$$

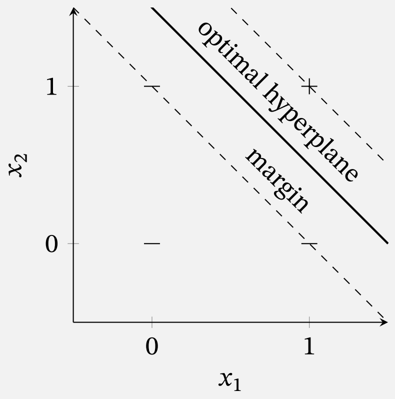
Given that vectors $\mathbf{x} \in \mathbb{R}^d$ belong to a (hyper)sphere of radius R, the VC dimension of the Δ-margin separating hyperplane is

$$h \leq \min\left(\left\lfloor \frac{R^2}{\Delta^2} \right\rfloor, d\right) + 1,$$

which can be less than $d + 1$.

From that property, to minimize the confidence interval, we can maximize the margin Δ of the hyperplane. The *maximal margin classifier* is a learning machine that generates the hyperplane that separates the classes with no error and maximizes the margin between the classes.

Figure 6.11: Maximal margin classifier for the AND dataset.



The maximal margin classifier generates the hyperplane that maximizes the margin between the classes. In this case, the margin is $\Delta = 0.5$.

Thus, given the training set $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$, $\mathbf{x} \in \mathbb{R}^d$ and $y_i \in \{-1, 1\}$, the optimal hyperplane — see fig. 6.11 — is the one that satisfies

$$y_i \left[(\mathbf{w} \cdot \mathbf{x}_i - b)\right] \geq 1,$$

for all $i = 1, \dots, n$ that minimizes $\|\mathbf{w}\|^2$. The intuition of the minimization of the coefficients is that we want only the vectors in the margin to be exactly equal to ± 1. (Consequently, the vectors farther from the margin have values greater than 1 or less than -1.)

Without entering into the details of the optimization process, one interesting property of the maximal margin classifier is that the separating hyperplane is built from the *support vectors* — the vectors that are exactly in the margin. In fig. 6.11, the support vectors are the points $(1, 0)$, $(0, 1)$, and $(1, 1)$.

In other words, maximal margin classifier is

$$f(x) = \operatorname{sign}\left(\sum_{i=1}^{n} y_i a_i (\mathbf{x}_i \cdot x) - b\right),$$

for some b and coefficients $a_i > 0$ for the support vectors ($a_i = 0$ otherwise).

In the case that the classes are not linearly separable, the maximal margin classifier can be extended to the *soft margin classifier*, which sets the empirical risk to a value greater than zero.

Moreover, since the number of parameters of the maximal margin classifier depends on the training data (i.e., the number of support vectors), it is a nonparametric model. Nonparametric models are those in which the number of parameters is not fixed and can grow as needed to fit the data. This property becomes more clear when we consider the kernel trick, which allows the maximal margin classifier to deal with nonlinear problems. Consult V. N. Vapnik (1999)[17] for more details.

6.7 Closing remarks

The SRM principle is a powerful tool to understand the generalization ability of learning machines. The principle not only explains many of the empirical results in ML but also provides a theoretical framework to guide the development of new learning machines.

Many powerful methods have been proposed in the literature — e.g., support vector machines, boosting, and deep learning — that can deal with complex nonlinear problems. I encourage the reader to dive into the literature to learn more about these methods and the theoretical principles behind them. Some comments about a few methods are given in appendix B.

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

7

Data preprocessing

I find your lack of faith disturbing.

— Darth Vader*, Star Wars: Episode IV – A New Hope (1977)*

In this chapter, we discuss the data preprocessing, which is the process of adjusting the data to make it suitable for a particular learning machine or, at the least, to ease the learning process.

Similarly to data handling, data preprocessing is done by applying a series of operations to the data. However, some of the parameters of the operations are not fixed but rather are fit from a data sampling. In the context of inductive learning, the sampling is the training set.

The operations are dependent on the chosen learning method. So, when planning the solution in our project, we must consider the preprocessing tasks that are necessary to make the data suitable for the chosen methods.

I present the most common data preprocessing tasks in three categories: data cleaning, data sampling, and data transformation. For each task, I discuss the behavior of the data preprocessing techniques in terms of fitting, adjustment of the training set, and application of the preprocessor in production.

Finally, I discuss the importance of the default behavior of the model when the preprocessing chain degenerates over a sample, i.e. when the preprocessor decides that it has no strategy to adjust the data to make it suitable for the model.

Chapter remarks

Contents

Context

- Tidy data is not necessarily suitable for modeling.
- Parameters of the preprocessor are fitted rather than being fixed.

Objectives

- Understand the main data preprocessing tasks and techniques.
- Learn the behavior of the preprocessing chain in terms of fitting, adjustment, and application.

Takeaways

- Each learning method requires specific data preprocessing tasks.
- Fitting the preprocessor is crucial to avoid leakage.
- Default behavior of the model when the preprocessing chain degenerates must be specified.

7.1 Introduction

In chapters 4 and 5, we discussed data semantics and the tools to handle data. They provide the grounds for preparation of the data as we described in the data sprint tasks in section 3.5.3. However, the focus is to guarantee that the data is tidy and in the observational unit of interest, not to prepare it for modeling.

As a result, although data might be appropriate for the learning tasks we described in chapter 6 — in the sense that we know what the feature vectors and the target variable are —, they might not be suitable for the machine learning methods we will use.

One simple example is the perceptron (section 6.6.1) that assumes all input variables are real numbers. If the data contains categorical variables, we must convert them to numerical variables before applying the perceptron.

For this reason, the solution sprint tasks in section 3.5.3 include not only the learning tasks but also the *data preprocessing* tasks, which are dependent on the chosen machine learning methods.

Definition 7.1: (Data preprocessing)

The process of adjusting the data to make it suitable for a particular learning machine or, at the least, to ease the learning process.

This is done by applying a series of operations to the data, like in data handling. The difference here is that some of the parameters of the operations are not fixed; rather, they are fit from a data sampling. Once fitted, the operations can be applied to new data, sample by sample.

As a result, a data processing technique acts in three steps:

1. **Fitting**: The parameters of the operation are adjusted to the training data (which has already been integrated and tidied, represents well the phenomenon of interest, and each sample is in the correct observational unit);
2. **Adjustment**: The training data is adjusted according to the fitted parameters, eventually changing the sampling size and distribution;
3. **Applying**: The operation is applied to new data, sample by sample.

Understanding these steps and correctly defining the behavior of each of them is crucial to avoid data leakage and to guarantee that the model will behave as expected in production.

7.1.1 Formal definition

Let $T = (K, H, c)$ be a table that represents the data in the desired observational unit — as defined in section 5.1. In this chapter, without loss of generality — as the keys are not used in the modeling process —, we can consider $K = \{1, 2, \dots\}$ such that $\text{card}(i) = 0$ if, and only if, $i > n$. That means that every row $r \in \{1, \dots, n\}$ is present in the table.

A data preprocessing strategy F is a function that takes a table $T = (K, H, c)$ and returns an adjusted table $T' = (K', H', c')$ and a fitted *preprocessor* $f(z; \phi) \equiv f_\phi(z)$ such that

$$z \in \bigtimes_{h \in H} \mathcal{D}(h) \cup \{?\}$$

and ϕ are the fitted parameters of the operation. Similarly, $z' = f_\phi(z)$, called the preprocessed tuple, satisfies

$$z' \in \bigtimes_{h' \in H'} \mathcal{D}(h') \cup \{?\}.$$

Note that we make no restrictions on the number of rows in the adjusted table, i.e., preprocessing techniques can change the number of rows in the training table.

In practice, strategy F is a chain of dependent preprocessing operations F_1, ..., F_m such that, given $T = T^{(0)}$, each operation F_i is applied to the table $T^{(i-1)}$ to obtain $T^{(i)}$ and the fitted preprocessor f_{ϕ_i}. Thus, $T' = T^{(m)}$ and

$$f(z; \phi = \{\phi_1, \dots, \phi_m\}) = \left(f_{\phi_1} \circ \dots \circ f_{\phi_m}\right)(z),$$

where $\circ$ is the composition operator. I say that they are dependent since none of the operations can be applied to the table without the previous ones.

7.1.2 Degeneration

The objective of the fitted preprocessor is to adjust the data to make it suitable for the model. However, sometimes it cannot achieve this goal for a particular input z. This can happen for many reasons, such as unexpected values, information "too incomplete" to make a prediction, etc.

Formally, we say that the preprocessor f_ϕ degenerates over tuple z if it outputs $z' = f_\phi(z)$ such that $z' = (?, \dots, ?)$. In practice, that means that the preprocessor decided that it has no strategy to adjust the data to make it suitable for the model. For the sake of simplicity, if any step f_{ϕ_i} degenerates over tuple $z^{(i)}$, the whole preprocessing chain degenerates[1] over $z = z^{(0)}$.

Consequently, in the implementation of the solution, the developer must choose a default behavior for the model when the preprocessing chain degenerates over a tuple. It can be as simple as returning a default value or as complex as redirecting the tuple to a different pair of preprocessor and model. Sometimes, the developer can choose to integrate this as an error or warning in the user application.

7.1.3 Data preprocessing tasks

The most common data preprocessing tasks can be divided into three categories:

- Data cleaning;
- Data sampling; and
- Data transformation.

In the next sections, I address some of the most common data preprocessing tasks in each of these categories. I present them in the order they are usually applied in the preprocessing, but note that the order is not fixed and can be changed according to the needs of the problem.

7.2 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 for training and to avoid bias in the learning process. Usually, such errors and inconsistencies make the learning machines "confused" and can lead to poor performance models.

Also, it includes the process of dealing with missing information, which most machine learning methods do not cope with. Solutions

[1]Usually, this is implemented as an exception or similar programming mechanism.

range from the simple removal of the observations with missing data to the creation of new information to encode the missing data.

7.2.1 Treating inconsistent data

There are a few, but important, tasks to be done during data preprocessing in terms of invalid and inconsistent data — note that we assume that most of the issues in terms of the semantics of the data have been solved in the data handling phase. Especially in production, the developer must be aware of the behavior of the model when it faces information that is not supposed to be present in the data.

One of the tasks is to ensure that physical quantities are dealt with standard units. One must 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. A summary of this preprocessing task is presented in table 7.1.

Table 7.1: Unit conversion preprocessing task.

Unit conversion	
Goal	Convert physical quantities into the same unit of measurement.
Fitting	None. User must declare the units to be used and, if appropriate, the conversion factors.
Adjustment	Training set is adjusted sample by sample, independently.
Applying	Preprocessor converts the numerical values and drops the unit of measurement column.

Moreover, if one knows that a variable must follow a specific range of values, we can check whether the values are within this range. If not, one must replace the values with missing data or with the closest valid value. Alternatively, one can discard the observation based on that criterion. Consult table 7.2 for a summary of this operation.

Another common problem in inconsistent information is that the same category might be represented by different strings. This is usually done by creating a dictionary that maps the different names to a single

Table 7.2: Range check preprocessing task.

Range check	
Goal	Check whether the values are within the expected range.
Fitting	None. User must declare the valid range of values.
Adjustment	Training set is adjusted sample by sample, independently. If appropriate, degenerated samples are removed.
Applying	Preprocessor checks whether the value x of a variable is within the range $[a, b]$. If not, it replaces x with: (a) missing value ?, (b) the closest valid value $\max(a, \min(b, x))$, or (c) degenerates (discards the observation).

one, using standardizing lower or upper case, removing special characters, or more advanced fuzzy matching techniques — see table 7.3.

Table 7.3: Category standardization preprocessing task.

Category standardize	
Goal	Create a dictionary and/or function to map different names to a single one.
Fitting	None. User must declare the mapping.
Adjustment	Training set is adjusted sample by sample, independently.
Applying	Preprocessor replaces the categorical variable x with the mapped value $f(x)$ that implements case standardization, special character removal, and/or dictionary fuzzy matching.

Note that these technique parameters are not fitted from the data, but rather are fixed from the problem definition. As a result, they could be done in the data handling phase. The reason we put them here is that the new data in production usually come with the same issues. Having the fixes programmed into the preprocessor makes it easier to guarantee that the model will behave as expected in production.

7.2.2 Outlier detection

Outliers are observations that are significantly different from the other observations. They can be caused by errors or by the presence of different phenomena mixed in the data collection process. In both cases, it is important to deal with outliers before modeling.

The standard way to deal with outliers is to remove them from the dataset. Assuming that the errors or the out-of-distribution data appear randomly and rarely, this is a good strategy.

Another approach is dealing with each variable independently. This way, one can replace the outlier value with missing data. There are many ways to detect outlier values, but the simplest one is probably a heuristic based on the interquartile range (IQR).

Let Q_1 and Q_3 be the first and the third quartiles of the values in a variable, respectively. The IQR is defined as $Q_3 - Q_1$. The values that are less than $Q_1 - 1.5\,\mathrm{IQR}$ or greater than $Q_3 + 1.5\,\mathrm{IQR}$ are considered outliers. See table 7.4.

Table 7.4: Outlier detection using the interquartile range.

Outlier detection using the IQR	
Goal	Detect outliers using the IQR.
Fitting	Store the values of Q_1 and Q_3 for each variable.
Adjustment	Training set is adjusted sample by sample, independently.
Applying	Preprocessor replaces the outlier values with missing data.

More sophisticated methods can be used to detect samples that are outliers, such as using the definition of an outlier in the DBSCAN[2]. But, this is not enough to fit the parameters of the preprocessor. The reason

[2]M. Ester et al. (1996). "A density-based algorithm for discovering clusters in large spatial databases with noise". In: *kdd*. Vol. 96. 34, pp. 226–231.

is that descriptive methods like DBSCAN — in this case, a method for clustering — do not generalize to new data. I suggest using methods like One-Class SVM[3] to fit the parameters of the preprocessor that detects outliers. Thus, any new data point can be classified as an outlier or not.

Like filtering operations in the pipeline, the developer must specify a default behavior for the model when an outlier sample is detected in production. See table 7.5.

Table 7.5: Task of filtering outliers.

Outlier removal	
Goal	Remove the observations that are outliers.
Fitting	Parameters of the outlier classifier.
Adjustment	Training set is adjusted sample by sample, independently, removing degenerated samples.
Applying	Preprocessor degenerates if the sample is classified as an outlier and does nothing, otherwise.

7.2.3 Treating missing data

Since most models cannot handle missing data, it is crucial to deal with it in the data preprocessing.

There are four main strategies to deal with missing data:

- Remove the observations (rows) with missing data;
- Remove the variables (columns) with missing data;
- Just impute the missing data;
- Use an indicator variable to mark the missing data and impute it.

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 "on demand" can artificially change the data distribution, especially when the missing data

[3]B. Schölkopf et al. (2001). "Estimating the support of a high-dimensional distribution". In: *Neural computation* 13.7, pp. 1443–1471.

is not missing at random. Row removal suffers from the same problem as any filtering operations (degeneration) in the preprocessing step; the developer must specify a default behavior for the model when a row is discarded in production. See table 7.6.

Table 7.6: Task of filtering rows based on missing data.

Row removal based on missing data	
Goal	Remove the observations with missing data in any (or some) variables.
Fitting	None. Variables to look for missing data are declared beforehand.
Adjustment	Training set is adjusted sample by sample, independently, removing degenerated samples.
Applying	Preprocessor degenerates over the rows with missing data in the specified variables.

In the case of column removal, the preprocessor just learns to drop the columns that have missing data during fitting. Beware that valuable information might be lost when removing columns for all the samples.

Table 7.7: Task of dropping columns based on missing data.

Column removal based on missing data	
Goal	Remove the variables with missing data.
Fitting	All variables with missing data in the training set are marked to be removed.
Adjustment	Columns marked are dropped from the training set.
Applying	Preprocessor drops the chosen columns in fitting.

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[4]. This is a simple and effective strategy, but it can introduce bias in the data, especially when the number of samples with missing data is large. See table 7.8.

Table 7.8: Task of imputing missing data.

Imputation of missing data	
Goal	Replace the missing data with a statistic of the available values.
Fitting	The statistic is calculated from the available data in the training set.
Adjustment	Training set is adjusted sample by sample, independently.
Applying	Preprocessor replaces the missing values with the chosen statistic. If an indicator variable is required, it is created and filled with the logical value: missing or not missing.

Just imputing data is not suitable when one is not sure whether the missing data is missing because of a systematic error or phenomenon. A model can learn the effect of the underlying reason for missingness for the predictive task. In that 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[5].

Many times the indicator variable is already present in the data. For instance, in a dataset that contains information about pregnancy, let us say the number of days since the last pregnancy. This information will certainly be missing if sex is male or the number of children is zero. In this case, no new indicator variable is needed. See table 7.7.

[4]More sophisticated methods can be used, such as the k-nearest neighbors algorithm, for example, consult O. Troyanskaya et al. (June 2001). "Missing value estimation methods for DNA microarrays". In: *Bioinformatics* 17.6, pp. 520–525. ISSN: 1367-4803. DOI: 10.1093/bioinformatics/17.6.520.

[5]Some kind of imputation is still needed, but we expect the model to deal better with it since it can decide using both the indicator and the original variable.

7.3 Data sampling

Once data is cleaned, the next step is (typically) to sample the data. Sampling is the process of selecting a random subset of the data or creating variations of the original training set.

There are three main tasks that sample the data: subsampling, scope filtering, and class balancing.

7.3.1 Random sampling

Some machine learning methods are computationally expensive, and a smaller dataset might be enough to solve the problem. Random sampling is simply done by selecting a random subset of the training data with a user-defined size.

However, note that the preprocessor for this task *must never do anything with the new data* (or the test set we discuss in chapter 8). See table 7.9.

Table 7.9: Task of random sampling.

Random sampling	
Goal	Select a random subset of the training data.
Fitting	None. User must declare the size of the sample.
Adjustment	Rows of the training set are randomly chosen.
Applying	Pass-through: preprocessor does nothing with the new data.

7.3.2 Scope filtering

Scope filtering is the process of reducing the scope of the phenomenon we want to model. Like the filtering operation in the data handling pipeline (consult section 5.3.5), the data scientists choose a set of predefined rules to filter the data.

Unlike outlier detection, we assume that the rule is fixed and known beforehand. The preprocessor degenerates over the samples that do not satisfy the rule. A summary of the task is presented in table 7.10.

Table 7.10: Task of filtering the scope of the data.

Scope filtering	
Goal	Remove the observations that do not satisfy a predefined rule.
Fitting	None. User must declare the rule.
Adjustment	Training set is adjusted sample by sample, independently, removing degenerated samples.
Applying	Preprocessor degenerates over the samples that do not satisfy the rule.

An interesting variation is the model trees[6]. They are shallow decision trees that are used to filter the data. At each leaf, a different model is trained with the data that satisfies the rules that reach the leaf. This is a good strategy when the phenomenon is complex and can be divided into simpler subproblems. In this case, the preprocessor does not degenerate over the samples, but rather the preprocessing chain branches into different models (and potentially other preprocessing steps).

7.3.3 Class balancing

Some data classification methods are heavily affected by the number of observations in each class. This is especially true for methods that learn the class priors directly from the data, like the naïve Bayes classifier.

Two strategies are often used to balance the classes: oversampling and undersampling. The former is done by creating synthetic observations of the minority class. The latter is done by removing observations of the majority class.

Undersampling can be done by removing observations of the majority class randomly (similarly to random sampling, section 7.3.1). On the other hand, oversampling can be done by creating synthetic observations of the minority class. The most common method is resampling[7], which selects a random subset of the data with replacement. A draw-

[6]F. Stulp and O. Sigaud (2015). "Many regression algorithms, one unified model: A review". In: *Neural Networks* 69, pp. 60–79. ISSN: 0893-6080. DOI: https://doi.org/10.1016/j.neunet.2015.05.005.

[7]Sometimes called bootstrapping.

back of this method is that it produces repeated observations that contain no new information.

In any case, the preprocessor for this task *must never do anything with the new data* (or the test set we discuss in chapter 8). See table 7.11.

Table 7.11: Task of class balancing.

Class balancing	
Goal	Balance the number of observations in each class.
Fitting	None. User must declare the number of samples in each class.
Adjustment	Rows of the training set are randomly chosen.
Applying	Pass-through: preprocessor does nothing with the new data.

More advanced sampling methods exist. For instance, the SMOTE algorithm[8] creates synthetic observations of the minority class without repeating the same observations.

7.4 Data transformation

Another important task in data handling is data transformation. This is the process of adjusting the types of the data and the choice of variables to make it suitable for modeling.

At this point, the data format is acceptable, i.e., each observation is in the correct observational unit, there are no missing values, and the sampling is representative of the phenomenon of interest. Now, 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 to be in a specific range, etc.

[8]N. V. Chawla et al. (2002). "SMOTE: synthetic minority over-sampling technique". In: *Journal of artificial intelligence research* 16, pp. 321–357.

7.4.1 Type conversion

Type conversion is the process of changing the type of the values in the columns. We do so to make the input variables compatible with the machine learning methods we will use.

The most common type conversion is the conversion from categorical to numerical values. Ideally, the possible values of a categorical variable are known beforehand. For instance, given the values $x \in \{a, b, c\}$ in a column, there are two main ways to convert them to numerical values: label encoding and one-hot encoding. If there is a natural order $a < b < c$, label encoding is usually sufficient. Otherwise, one-hot encoding can be used.

Label encoding is the process of replacing the values $x \in \{a, b, c\}$ with the values $x' \in \{1, 2, 3\}$, where $x' = 1$ if $x = a$, $x' = 2$ if $x = b$, and $x' = 3$ if $x = c$. Other numerical values can be assigned depending on the specific problem.

One-hot encoding is the process of creating a new column for each possible value of the categorical variable. The new column is filled with the logical value 1 if the value is present and 0 otherwise.

However, in the second case, the number of categories might be too large or might not be known beforehand. So, the preprocessing step must identify the unique values in the column and create the new columns accordingly. It is common to group the less frequent values into a single column, called the *other* column. See table 7.12.

The other direction is also common: converting numerical values to categorical values. This is usually done by binning the numerical variable, either by frequency or by range. In both cases, the user declares the number of bins. Binning by frequency is done by finding the percentiles of the values and creating the bins accordingly. Binning by range is done by dividing the range of the values into equal parts, given the minimum and maximum values. See table 7.13.

Another common task, although it receives less attention, is the conversion of dates (or other interval variables) to numerical values. Interval variables, like dates, have almost no information in their absolute values. However, the difference between two dates can be very informative. For example, the difference between the date of birth and the date of the last purchase becomes the age of the customer.

Table 7.12: One-hot encoding preprocessing task.

One-hot encoding	
Goal	Create a new column for each possible value of the categorical variable.
Fitting	Store the unique values of the categorical variable. If appropriate, indicate the special category *other*.
Adjustment	Training set is adjusted sample by sample, independently.
Applying	Preprocessor creates a new column for each possible value of the categorical variable. The new column is filled with the logical value 1 if the old value matches the new column and 0 otherwise. If the value is new or among the less frequent values, it is assigned to the *other* column.

Table 7.13: Binning numerical values preprocessing task.

Binning numerical values	
Goal	Create a new categorical column from a numerical one.
Fitting	Store the range of each bin.
Adjustment	Training set is adjusted sample by sample, independently.
Applying	Preprocessor converts each numerical value to a categorical value by checking which bin the value falls into.

7.4.2 Normalization

Normalization is the process of scaling the values in the columns. This is usually done to keep data within a specific range or to make different variables 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 that the values are in a specific range, usually $[0, 1]$ or $[-1, 1]$.

Standardization works well when the values in the column are normally distributed. It not only keeps the values in an expected range but also makes the data distribution comparable with other variables. Given that μ is the mean and σ is the standard deviation of the values in the column, the standardization is done by

$$x' = \frac{x - \mu}{\sigma}. \tag{7.1}$$

See table 7.14.

Table 7.14: Standardization preprocessing task.

	Standardization
Goal	Scale the values in a column.
Fitting	Store the statistics of the variable: the mean and the standard deviation.
Adjustment	Training set is adjusted sample by sample, independently.
Applying	Preprocessor scales the values according to eq. (7.1).

In the case of rescaling, during production, the preprocessor usually clamps[9] the values after rescaling. This is done to avoid the model making predictions that are out of the range of the training data. Given that we want to rescale the values in the column to the range $[a, b]$, and that $x_{\min}$ and $x_{\max}$ are the minimum and maximum values in the column,

[9]The operation $\operatorname{clamp}(x; a, b)$ where a and b are the lower and upper bounds, respectively, is defined as $\max(a, \min(b, x))$.

the rescaling is done by

$$x' = a + (b - a)\frac{x - x_{\min}}{x_{\max} - x_{\min}}. \tag{7.2}$$

See table 7.15.

Table 7.15: Rescaling preprocessing task.

Rescaling	
Goal	Rescale the values in a column.
Fitting	Store the appropriate statistics of the variable: the minimum and the maximum values.
Adjustment	Training set is adjusted sample by sample, independently.
Applying	Preprocessor scales the values according to eq. (7.2).

Related to normalization is the log transformation, which applies the logarithm to the values in the column. This is usually done to make the data distribution more symmetric over the mean or to reduce the effect of outliers.

7.4.3 Dimensionality reduction

Dimensionality reduction is the process of reducing the number of variables in the data. It can identify irrelevant variables and reduce the complexity of the model (since there are fewer variables to deal with).

There are two main types of dimensionality reduction algorithms: feature selection and feature extraction. The former selects a subset of the existing variables that leads to the best models. The latter creates new variables that are combinations of the original ones.

One example of feature selection is ranking the variables by their mutual information with the target variable and selecting the top k variables. Mutual information is a measure of the amount of information that one variable gives about another. So, it is expected that variables with high mutual information with the target variable are more important for the model.

Feature extraction uses either linear methods, such as principal component analysis (PCA), or non-linear methods, such as autoencoders. These methods are able to compress the information in the training data into a smaller number of variables. Thus, the model can learn the solution in a lower-dimensional space. A drawback of this method is that the new variables are hard to interpret, since they are combinations of the original variables.

7.4.4 Data enhancement

The "opposite" of dimensionality reduction is data enhancement. This is the process of bringing to the dataset external information that complements the existing data. For example, imagine that in the tidy data we have a column with the zip code of the customers. We can use this information to join (in this case, always a left join) a dataset with social and economic information about the region of the zip code.

The preprocessor, then, stores the external dataset and the column to join the data. During production, it enhances any new observation with the external information. See table 7.16.

Table 7.16: Data enhancement preprocessing task.

Data enhancement	
Goal	Enhance the dataset with external information.
Fitting	Store the external dataset and the column to join.
Adjustment	Training set is left joined with the external dataset. Because of the properties of the left join, the new dataset has the same number of rows as the original dataset, and it is equivalent to enhancing each row independently.
Applying	Preprocessor enhances the new data with the external information.

7.4.5 Comments on unstructured data

Any unstructured data can be transformed into structured data. We can see this task as a data preprocessing task. Techniques like bag of words, word embeddings, and signal (or image) processing can be seen as preprocessing techniques that transform unstructured data into structured data, which is suitable for modeling.

Also, modern machine learning methods, like convolutional neural networks (CNNs), are simply models that learn both the preprocessing and the model at the same time. This is done by using convolutional layers that learn the features of the data. In digital signal processing, this is called feature extraction. The difference there is that the convolution filters are handcrafted, while in CNNs they are learned from the data.

The study of unstructured data is a vast field and is out of the scope of this book. I recommend Jurafsky and Martin (2008)[10] for a complete introduction to Natural Language Processing and Szeliski (2022)[11] for a comprehensive introduction to Computer Vision.

[10]D. Jurafsky and J. H. Martin (2008). *Speech and Language Processing. An Introduction to Natural Language Processing, Computational Linguistics, and Speech Recognition*. 2nd ed. Hoboken, NJ, USA: Prentice Hall. A new edition is is under preparation and it is available for free: D. Jurafsky and J. H. Martin (2024). *Speech and Language Processing: An Introduction to Natural Language Processing, Computational Linguistics, and Speech Recognition with Language Models*. 3rd ed. Online manuscript released August 20, 2024. URL: https://web.stanford.edu/~jurafsky/slp3/.

[11]R. Szeliski (2022). *Computer vision. Algorithms and applications*. 2nd ed. Springer Nature. URL: https://szeliski.org/Book/.

8 Solution validation

All models are wrong, but some are useful.

— George E. P. Box, *Robustness in Statistics*

Once we have defined what an inductive problem is and the means to solve it, we need to think about how to validate the solution.

In this chapter, we present the experimental planning that 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. This is why we need to run experiments to gather performance data and make inferences from it. The stochastic nature of data and of the learning process makes it more difficult to predict the outcome of a given algorithm on a given dataset. Robust experimental planning is essential to ensure that the results of the experiments are reliable and can be used to make decisions.

Moreover, we need to understand the main metrics that are used to evaluate the performance of a solution — i.e., the pair preprocessor and model. Each learning task has different metrics, and the goals of the project will determine which metrics are more important.

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 for inductive problems.

Chapter remarks

Contents

Context

- Before putting a solution into production, we need to validate it.
- The validation process is experimental.

Objectives

- Understand the importance of experimental planning.
- Learn the main evaluation metrics used in predictive tasks.
- Learn how to design an experimental plan to validate a solution.

Takeaways

- Evaluation metrics should be chosen according to the goals of the project.
- The experimental plan should be designed to gather performance data systematically.
- A hypothesis test can be used to validate the results of the experiments.

8.1 Evaluation

One fundamental step in the validation of a data-driven solution for a task is the *evaluation* of the pair preprocessor and model. This chapter presents strategies to measure performance of classifiers and regressors, and how to interpret the results.

We consider the following setup. Let $T = (K, H, c)$ be a table that represents the data in the desired observational unit — as defined in section 5.1. Without loss of generality — as the keys are not used in the modeling process —, we can consider $K = \{1, 2, \dots\}$ such that $\operatorname{card}(i) = 1$, if $i \in \{1, \dots, n\}$, and $\operatorname{card}(i) = 0$, otherwise. That means that every row $r \in \{1, \dots, n\}$ is present in the table.

The table is split into two sets: a training set, given by indices (or keys) $\mathcal{I}_{\text{training}} \in \{1, \dots, n\}$, and a test set, given by indices $\mathcal{I}_{\text{test}} \in \{1, \dots, n\}$, such that

$$\mathcal{I}_{\text{training}} \cap \mathcal{I}_{\text{test}} = \emptyset$$

and

$$\mathcal{I}_{\text{training}} \cup \mathcal{I}_{\text{test}} = \{1, \dots, n\}.$$

The bridge between the table format (definition 5.1) and the data format used in the learning process (as described in section 6.2) is explained in the following. We say that the pair $(\mathbf{x}_i, y_i)$ contains the feature vector $\mathbf{x}_i$ and the target value y_i of the sample with key i in table T. Mathematically, given target variable $h \in H$, we have that $y_i = c(i, h)$ and $\mathbf{x}_i$ is the tuple

$$\big(c(i, h') : h' \in H \setminus \{h\}\big).$$

For evaluation, we consider a data preprocessing technique F and a learning machine M. The following steps are taken.

Preprocessing Preprocessing technique F is applied to the training set $T_{\text{training}} = (K, H, c_{\text{training}})$ where

$$c_{\text{training}}(i, h) = \begin{cases} c(i, h) & \text{if } i \in \mathcal{I}_{\text{training}}, \\ () & \text{otherwise.} \end{cases}$$

The result is an adjusted training set T'_{training} and a fitted preprocessor $f(\mathbf{x}; \phi) \equiv f_{\phi}(\mathbf{x})$, where $\mathbf{x} \in \mathcal{X}$ for some space $\mathcal{X}$ that does not include (or does not modify) the target variable — consult section 7.1.1. Note that, by definition, the size of the adjusted training set can be different from the original due to sampling or filtering. The hard requirement is that the target variable h is not changed.

Learning The learning machine M is trained on the adjusted training set $D'_{\text{training}} = \{(\mathbf{x}'_i, y'_i)\}$, where pairs $(\mathbf{x}'_i, y'_i)$ come from the table T'_{training}. The result is a model $f(\mathbf{x}'; \theta) \equiv f_\theta(\mathbf{x}')$ — consult chapter 6.

Transformation The preprocessor f_ϕ is applied to the test set $T_{\text{test}} = (K, H, c_{\text{test}})$ where

$$c_{\text{test}}(i, h) = \begin{cases} c(i, h) & \text{if } i \in \mathcal{I}_{\text{test}}, \\ () & \text{otherwise.} \end{cases}$$

The result is a preprocessed test set T'_{test} from which we can obtain the set $D'_{\text{test}} = \{(\mathbf{x}'_i, y_i) : i \in \mathcal{I}_{\text{test}}\}$ such that $\mathbf{x}'_i = f_\phi(\mathbf{x}_i)$. Note that, to avoid data leakage and other issues, the preprocessor has no access to the target values y_i (even if the adjusted training set uses the label somehow).

Prediction The model f_θ is used to make predictions on the preprocessed test set D'_{test} to obtain predicted values $\hat{y}_i = f_\theta(\mathbf{x}'_i)$ for all $i \in \mathcal{I}_{\text{test}}$.

Evaluation By comparing $\hat{y}_i$ with y_i for all $i \in \mathcal{I}_{\text{test}}$, we evaluate how well the choice of ϕ (parameters of the preprocessor) and θ (parameters of the model) is.

8.1.1 Binary classification evaluation

In order to assess the quality of a solution for a binary classification task, 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 metrics in classification tasks.

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

$$\begin{array}{ccc} & & \text{Predicted} \\ & & \begin{array}{cc} 1 & 0 \end{array} \\ \text{Expected} & \begin{array}{c} 1 \\ 0 \end{array} & \begin{pmatrix} \text{TP} & \text{FN} \\ \text{FP} & \text{TN} \end{pmatrix} \end{array}$$

where TP is the number of true positives

$$|\{i \in \mathcal{I}_{\text{test}} : y_i = 1 \land \hat{y}_i = 1\}|,$$

TN is the number of true negatives

$$|\{i \in \mathcal{I}_{\text{test}} : y_i = 0 \land \hat{y}_i = 0\}|,$$

FN is the number of false negatives

$$|\{i \in \mathcal{I}_{\text{test}} : y_i = 1 \land \hat{y}_i = 0\}|,$$

and FP is the number of false positives

$$|\{i \in \mathcal{I}_{\text{test}} : y_i = 0 \land \hat{y}_i = 1\}|.$$

Performance metrics

From the confusion matrix, we can derive several performance metrics. Each of them focuses on different aspects of the classification task, and the choice of the metric depends on the problem at hand. Each metric prioritizes different types of errors and yields a value between 0 and 1, where 1 is the best possible value.

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 metric is simple and easy to interpret: a classifier with an accuracy of 1 is perfect, while a classifier with an accuracy of 0.5 misses half of the predictions. Accuracy assigns the same weight to any kind of error — i.e., false positives and false negatives. As a result, if the proportion of positive and negative samples is imbalanced, the value of accuracy may become misleading. Let π be the ratio of positive samples in the test set — consequently, $1 - \pi$ is the ratio of negative samples —, then a classifier that correctly predicts all positive samples and none of the negative samples will have an accuracy of π. If π is close to 1, the classifier will have a high value of accuracy even if it is not good at predicting the negative class.

This issue is not impeditive for the usage of accuracy in imbalanced datasets, but one needs to be aware that accuracy values lower than $\max(\pi, 1 - \pi)$ are not better than guessing.

Balanced accuracy aims to solve this interpretation issue of the accuracy. It is the average of the true positive rate (TPR) and the true negative rate (TNR), given by

$$\text{Balanced Accuracy} = \frac{\text{TPR} + \text{TNR}}{2},$$

where

$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}},$$

and

$$\text{TNR} = \frac{\text{TN}}{\text{TN} + \text{FP}}.$$

Each term penalizes a different type of error independently: TPR penalizes false negatives, while TNR penalizes false positives. Balanced accuracy is useful when the cost of errors on the minority class is higher than the cost of errors on the majority class. This way, any value greater than 0.5 is better than random guessing.

A limitation of the balanced accuracy is that it “automatically” assigns the weight of errors based on the class proportion, which may not be the best choice for the problem. Other metrics focus only on one of the classes and are more flexible to adjust the weight of errors.

Precision is an asymmetrical metric that focuses on the positive class. It 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 metric is useful when the cost of false alarms 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 (false positive diagnoses). Semantically, precision measures how confident we can be that a positive prediction is actually positive. Note that it measures nothing about the ability of the classifier in terms of the negative predictions.

Recall is another asymmetrical metric that also focuses on the positive class. It is the proportion of true positive predictions over the total number of samples that are actually positive, given by

$$\text{Recall} = \text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}}.$$

This metric is useful when the cost of missing a positive sample is high, as it quantifies the ability of the classifier to avoid false negatives. It can also be interpreted as the "completeness" of the classifier: how many positive samples were correctly retrieved. For example, in a medical diagnosis task, recall is important to avoid missing a diagnosis.

F-score is a way of balancing both kinds of errors, false positives and false negatives, while maintaining the focus on the positive class. It is the weighted harmonic mean of precision and recall given by

$$\text{F-score}(\beta) = \text{F}_\beta\text{-score} = \frac{(1+\beta^2)\cdot\text{Precision}\cdot\text{Recall}}{\beta^2\cdot\text{Precision}+\text{Recall}},$$

where $\beta > 0$ is a parameter that controls the weight of precision in the metric. The most common value for β is 1, which gives the F_1-score. Higher values of β give more weight to precision ($\beta > 1$), while lower values give more weight to recall ($0 < \beta < 1$).

Specificity goes in the opposite direction of recall, focusing on the negative class. It is the proportion of true negative predictions over the total number of samples that are actually negative, given by

$$\text{Specificity} = \text{TNR} = \frac{\text{TN}}{\text{TN}+\text{FP}}.$$

This metric is very common in the medical literature, but less common in other contexts. The probable reason is that it is easier to interpret the metrics that focus on the positive class, as the negative class is usually the majority class — and, thus, less interesting.

Interpretation of metrics

Table 8.1 summarizes the properties of the classification performance metrics. Accuracy and balanced accuracy are good metrics when no particular class is more important than the other. Remember, however, that balanced accuracy gives more weight to errors on the minority class. Precision and recall are useful to evaluate the performance of the solution in terms of the positive class. They are complementary metrics, and looking at only one of them may give a biased view of the performance — more on that below. The F-score is a way to balance precision and recall with a controllable parameter.

Table 8.1: Summary of the properties of data classification performance metrics.

Metric	**Focus**	**Interpretation**
Accuracy	Symmetrical	Penalizes all
Balanced Accuracy	Symmetrical	Penalizes all (weighted)
Recall (TPR)	Positive	Penalizes FN
Precision	Positive	Penalizes FP
F-score	Positive	Penalizes all (weighted)
Specificity (TNR)	Negative	Penalizes FP

A common misconception about the asymmetrical metrics (especially precision) is that they are always robust to class imbalance. Observe table 8.2, which shows the behavior of the classification performance metrics for three (useless) classifiers: one that always predicts the positive class (Guess 1), another that always predicts the negative class (Guess 0), and a classifier that randomly guesses the class independently of the class priors (Random).

Table 8.2: Behavior of classification performance metrics for different classifiers.

Metric	**Guess 1**	**Guess 0**	**Random**
Accuracy†	π	$1-\pi$	0.5
Balanced Accuracy	0.5	0.5	0.5
Recall (TPR)	1	0	0.5
Precision†	π	$0/0=0$	π
F_1-score†	$\frac{2\pi}{1+\pi}$	0	$\frac{2\pi}{1+2\pi}$
Specificity (TNR)	0	1	0.5

Performance of different classifiers in the example of a dataset with ratio π of positive and $1-\pi$ of negative samples. Metrics affected by class imbalance are marked with †.

We can see that, as $\pi \to 1$, i.e. the positive class dominates the dataset, guessing the positive class achieves maximum values for metrics like accuracy, precision, and F_1-score. Even for random guessing the class, precision (and F_1-score) is affected by the class imbalance, yielding 1 (and 2/3) as $\pi \to 1$. As a result, these metrics should be preferred when the positive class is the minority class, so the results are not erroneously inflated — and, consequently, mistakenly interpreted as good. C. K. I. Williams (2021)[1] provides an interesting discussion on that.

Finally, besides accuracy, the other metrics do not behave well when the evaluation set is too small. In this case, the metrics may be too sensitive to the particular samples in the test set or may not be able to be calculated at all.

8.1.2 Regression estimation evaluation

Performance metrics for regression tasks are usually calculated based on the error (also called residual)

$$\epsilon_i = \hat{y}_i - y_i$$

for all $i \in \mathcal{I}_{\text{test}}$ or a scaled version

$$\epsilon_i^{(f)} = f(\hat{y}_i) - f(y_i),$$

for some scaling function f.

Performance metrics

From the errors, we can calculate several performance metrics that give us useful information about the behavior of the model. Specifically, we are interested in understanding what kind of errors the model is making and how large they are. Unlike classification, the higher the value of the metric, the worse the model is.

Mean absolute error is probably the simplest performance metric for regression estimation tasks. It is the average of the absolute values of the errors, given by

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^{n} |\epsilon_i|.$$

[1]C. K. I. Williams (Apr. 2021). "The Effect of Class Imbalance on Precision-Recall Curves". In: *Neural Computation* 33.4, pp. 853–857. ISSN: 0899-7667. DOI: 10.1162/neco_a_01362.

This metric is easy to interpret, is in the same unit as the target variable, and gives an idea of the average error of the model. It ignores the direction of the errors, so it is not useful to understand if the model is systematically overestimating or underestimating the target variable.

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 metric 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 metric is in the same unit as the target variable, which makes it easier to interpret. It keeps the same properties as the mean squared error, such as penalizing large errors more than the mean absolute error.

Both MAE and RMSE (or MSE) work well for positive and negative values of the target variable. However, they might be misleading when the range of the target variable is large.

Mean absolute percentage error is an alternative when the target variable (and the predictions) assume only strictly positive values, i.e., $y_i > 0$ and $\hat{y}_i > 0$. It is the average of the relative errors, given by

$$\text{MAPE} = \frac{1}{n}\sum_{i=1}^{n} \frac{|\epsilon_i|}{y_i}.$$

This metric is useful when the range of the target variable is large, as it gives an idea of the relative error of the model, not the absolute error.

Mean absolute logarithmic error is an alternative for the MAPE under the same premises of the target values. It aims to reduce the influence of outliers in the error calculation, especially when the target variable prior follows a long-tail distribution — many small values and few large values. Distributions like that are common in practice, e.g., in sales, income, and population data. It is given by

$$\text{MALE} = \frac{1}{n}\sum_{i=1}^{n} |\epsilon_i^{(\ln)}| = \frac{1}{n}\sum_{i=1}^{n} |\ln \hat{y}_i - \ln y_i|.$$

Interpretation of metrics

Note that, unlike the classification performance metrics, the scale of the regression performance metrics is not bounded between 0 and 1. This makes it potentially harder to interpret the results, as the values depend on the scale of the target variable.

Absolute error metrics, like MAE and RMSE, are useful for understanding the central tendency of the magnitude of the errors. They are easy to interpret because they are in the same unit as the target variable. However, they tend to be less informative when the target variable has a large range or when the errors are not normally distributed.

In those situations, relative error metrics, like MAPE and MALE, are more useful. For instance, imagine we are predicting house prices. The error of $20,000 for a house that costs $100,000 is more significant than the same error for a house that costs $1,000,000. The absolute error is the same in both cases, but the relative error is different.

In that example, the MAPE would be 20% for the first house and 2% for the second house. Note, however, that MAPE punishes overestimating more than underestimating in multiplicative terms. Consider the example in table 8.3. In the first row, the prediction is ten times larger than the actual value, which results in a MAPE of 900%. In the second row, the prediction is one tenth of the actual value, which results in a MAPE of 90%.

Table 8.3: Comparison of relative error metrics.

$\hat{y}$	y	ϵ	MAPE	exp(MALE)
100	10	90	9.0	10
1	10	9	0.9	10

MAPE and MALE for two predictions. The MAPE punishes overestimating more than underestimating.

If multiplicative factors of the error are important, one should consider using MALE. Observe that $\ln(\hat{y}) - \ln(y) = \ln(\hat{y}/y)$, which is the logarithm of the ratio of the prediction to the actual value. In the case of the absolute value, we have another interesting property:

$$|\ln \hat{y} - \ln y| = |\ln \frac{\hat{y}}{y}| = |\ln \frac{y}{\hat{y}}| = \ln \max\left(\frac{\hat{y}}{y}, \frac{y}{\hat{y}}\right).$$

Tofallis (2015)[2] discuss some of these advantages. To interpret MALE, we can use the exponential function, which gives us a multiplicative factor of the error. In the example in table 8.3, we have that

$$\exp \ln \max\left(\frac{100}{10}, \frac{10}{100}\right) = \max\left(\frac{100}{10}, \frac{10}{100}\right) = 10.$$

Finally, for the experimental plan we propose in this book, we should avoid metrics like coefficient of determination, R^2, as we do not make assumptions about the model — in this case, we do not assume that the model is linear. Similarly to data classification, we should prefer metrics that work well with small test sets.

8.1.3 Probabilistic classification evaluation

A particular case of the regression estimation is when we want to estimate the probability[3] of a sample belonging to the positive class — i.e. $y = 1$. In this case, the output of the model should be a value 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 it is negative, otherwise.

However, the threshold 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

[2]C. Tofallis (2015). "A better measure of relative prediction accuracy for model selection and model estimation". In: *Journal of the Operational Research Society* 66.8, pp. 1352–1362. DOI: 10.1057/jors.2014.103.

[3]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.

τ:

$$f_C(\mathbf{x};\tau) = \begin{cases} 1 & \text{if } f_R(\mathbf{x}) \geq \tau, \\ 0 & \text{otherwise.} \end{cases}$$

Since the task is still a classification task, one should not use regression performance metrics. On the other hand, instead of choosing a particular threshold and measuring the resulting classifier performance, we can summarize the performance of all possible variations of the classifiers using appropriate metrics.

Before diving into the metrics, consider the following error metric. Let false positive rate (FPR) be the proportion of false positive predictions over the total number of samples that are actually negative,

$$\text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}}.$$

It is the complement of the specificity, i.e. $\text{FPR} = 1 - \text{Specificity}$.

Consider the example in table 8.4 of a given test set and the predictions of a regressor. We can see that a threshold of 0.5 would yield a classifier that errors in 3 out of 9 samples. We can adjust the threshold to understand the behavior of the other possible classifiers.

Table 8.4: Illustrative example of probability regressor output.

Expected	**Predicted**
0	0.1
0	0.5
0	0.2
0	0.6
1	0.4
1	0.9
1	0.7
1	0.8
1	0.9

We first sort the samples by the predicted probabilities and then calculate the TPR (recall) and FPR for each threshold. We need to consider only thresholds equal to the predicted values to understand the variations. In this case, TPR values become the cumulative sum of the expected outputs divided by the total number of positive samples, and

FPR values become the cumulative sum of the complement of the expected outputs divided by the total number of negative samples.

Table 8.5: Illustrative example of classifiers derived from different thresholds.

Expected	Threshold	TPR	FPR
-	- / ∞	0/5	0/4
1	0.9	1/5	0/4
1	0.9	2/5	0/4
1	0.8	3/5	0/4
1	0.7	4/5	0/4
0	0.6	4/5	1/4
0	0.5	4/5	2/4
1	0.4	5/5	2/4
0	0.2	5/5	3/4
0	0.1	5/5	4/4

Performance of different classifiers derived from the regressor output in table 8.4. The thresholds are equal to the predicted values.

Note that, from the ordered list of predictions, we can easily see that a threshold of 0.7 would yield a classifier that commits only one error. A way to summarize the performance of all possible classifiers is presented in the following.

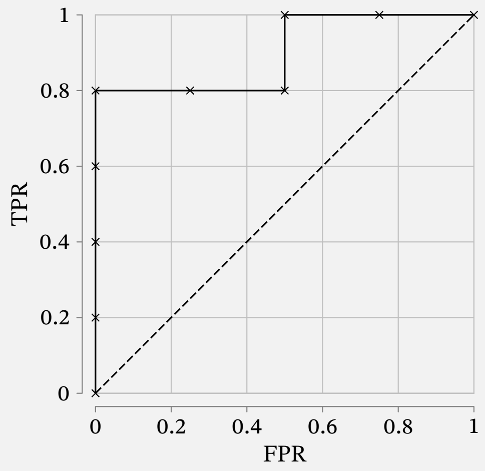
Receiver operating characteristic

The receiver operating characteristic (ROC) curve is a graphical representation of the trade-off between TPR and FPR as the threshold τ is varied. The ROC curve is obtained by plotting the TPR against the FPR for all possible thresholds. Figure 8.1 is the ROC curve for the example in table 8.5.

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 an interesting metric of the performance of the family of classifiers. It ranges between 0 and 1, where 1 is the best possible value. The AUC is scale invariant, which

Figure 8.1: Illustrative example of ROC curve.



ROC curve for the example in table 8.5. The diagonal line represents a random classifier, and points above the diagonal are better than random.

means that it measures how well predictions are ranked, rather than their absolute values. It is also robust to class imbalance, once both recall and specificity are considered. In our example, the AUC is 0.9.

8.2 An experimental plan for data science

Like any other experimental science, data science requires a robust experimental plan to ensure that evaluation results are reliable and can be used to make decisions. Failure to use the resources we have at hand — i.e., the limited amount of data — can lead to incorrect conclusions about the performance of a solution.

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 chapters 2 and 4, we address topics about collecting and organizing data. In chapter 5, we address topics about preparing the data for the experiments.
- **Solution search algorithm**: Techniques that find a solution for the task. We use the term "search" because the chosen algorithm aims at optimizing both the parameters of the preprocessing chain and those of the model. The theoretical basis for these techniques is in chapters 6 and 7.
- **Performance measuring**: The metric that will be used to evaluate the performance of the model. Refer to section 8.1 for the main metrics used in binary classification and regression estimation tasks.

A general example of a description of an experimental plan is "What is the probability that the technique A will 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?"

In the next sections, we consider these two cases: *estimating expected performance* and *comparing algorithms*. Before that, we discuss a strategy to make the best use of the finite amount of data we have available.

8.2.1 Sampling strategy

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 well our solution is expected to be in production.

As we have seen, 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 is that technique 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.

One could argue that we could use a hold-out set to estimate the performance of M — i.e., splitting the dataset into a training set and a test set once. However, this does not solve the problem. The performance p we observe in the test set might be an overestimation or an underestimation of the performance of M in production. This is because the randomly chosen test set might be an “outlier” in the representation of the real world, containing cases that are too easy or too hard to predict.

The correct way to estimate the performance of M is to address performance as a random variable, since both the data and the learning process are stochastic. By doing so, we can study the distribution of the performance, not particular values.

As with 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. Each dataset is further divided into a training set and a test set, which must be disjoint. Each 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.

The most common sampling strategy is the *cross-validation*. It assumes that data are independent and identically distributed (i.i.d.). This sampling strategy 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.

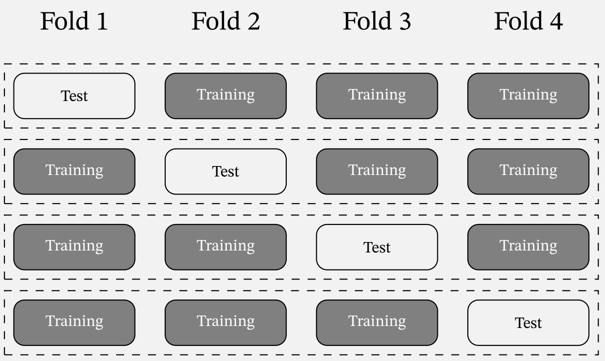
If possible, one should use repeated cross-validation, where this process is repeated many times, each having a different fold partitioning chosen at random. Also, when dealing with classification problems, we should use stratified cross-validation, where the distribution of the classes is preserved in each fold.

8.2.2 Collecting evidence

Once we understand the sampling strategy, we can design the experimental plan to collect evidence about the performance of the solution. The plan involves the following steps.

The solution search algorithm A involves both a given data preprocessing chain 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

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.

parameters ϕ of the data preprocessing step are adjusted — see chapter 7 — and the parameters θ of the machine learning model are adjusted — see chapter 6. These parameters, $[\phi_k, \theta_k]$ are the solution M_k, and must be calculated exclusively using the training set $D_{k,\text{train}}$.

Once the parameters ϕ_k and θ_k 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 $\hat{y}_i = f_{\phi,\theta}(x_i)$. The target value y is called the ground-truth or expected outcome.

Given a performance metric R, for each dataset D_k, we calculate

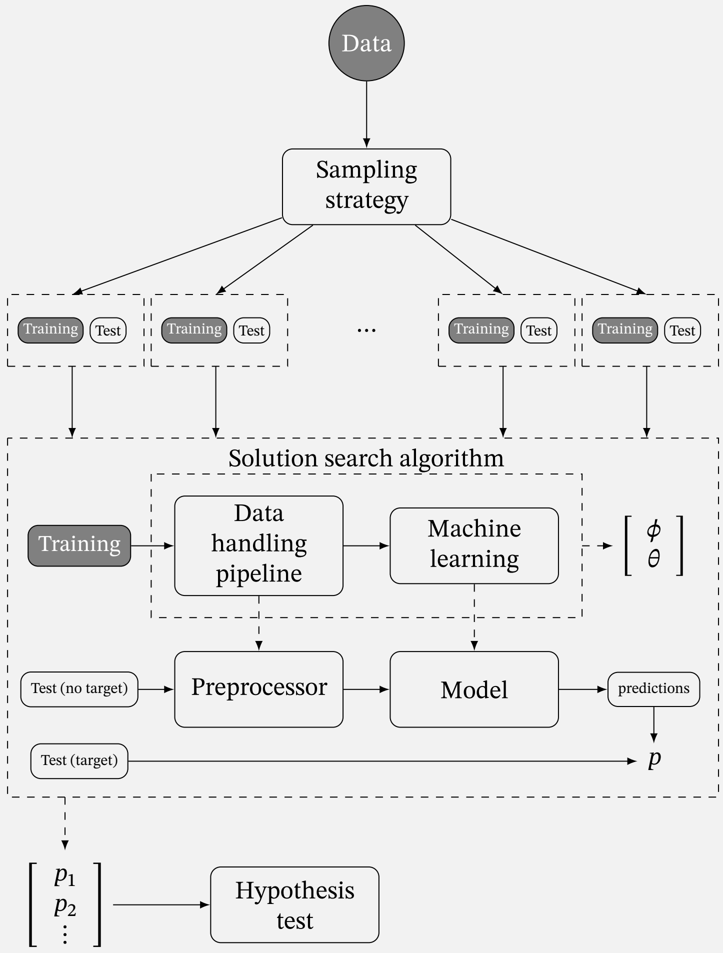
$$p_k = R([y_i \, : \, i], [\hat{y}_i \, : \, i]) \, .$$

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).

For a detailed explanation of this process for each sampling, consult section 8.1. A summary of the experimental plan for estimating expected performance is shown in fig. 8.3.

Finally, we can study the sampled performance values $p_1, p_2, \ldots$ like any other statistical data to prove (or disprove) the hypothesis. This process is called validation.

Figure 8.3: 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.

Definition 8.1: (Validation)

While 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).

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 real-world performance of the solution M.

8.2.3 Estimating expected performance

We have seen that we need a process of interpreting or confirming the meaning of the evaluation results. 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 experiment 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 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)[4] propose an interesting Bayesian test that ac-

[4]A. Benavoli et al. (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.

counts for the overlapping training sets in the cross-validation[5]. 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 $\mathbf{z} = (z_1, z_2, \dots, z_n)$ is the vector of performance gains, $\mathbf{1}$ is a vector of ones, μ is the parameter of interest (the mean performance gain), and $\mathbf{v} \sim \mathrm{MVN}(0, \Sigma)$ 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 $i \neq j \in \{1, 2, \dots, n\}$, where ρ is the correlation (between folds) and σ^2 is the variance. The likelihood model of the data is

$$\mathrm{P}(\mathbf{z} \mid \mu, \Sigma) = \exp\left(-\frac{1}{2}(\mathbf{z} - \mathbf{1}\mu)^T \Sigma^{-1} (\mathbf{z} - \mathbf{1}\mu)\right) \frac{1}{(2\pi)^{n/2}\sqrt{|\Sigma|}}.$$

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. consider the prior

$$\mathrm{P}(\mu, \nu \mid \mu_0, \kappa_0, a, b) = \mathrm{NG}(\mu, \nu; \mu_0, \kappa_0, a, b),$$

which 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

$$\bar{z} = \frac{1}{n}\sum_{i=1}^{n} z_i,$$

[5]This is actually a particular case of the proposal in the paper, where the authors consider the comparison between two performance vectors — which is the case described in section 8.2.4.

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 null hypothesis significance testing, as it allows us to estimate the probability of the hypothesis instead of the probability of observing the data given the hypothesis. Benavoli et al. (2017)[6] thoroughly discuss the subject.

Also, be aware that the choice of the model and the prior distribution can affect the results. Benavoli et al. suggest using 10 repetitions of 10-fold cross-validation to estimate the parameters of the generative model. They also show experimental evidence that their procedure is robust to the choice of the prior distribution. However, one should be aware of the limitations of the model.

8.2.4 Comparing strategies

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[7] 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

[6]A. Benavoli et al. (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.

[7]That includes both data preprocessing and machine learning.

$\mathbf{p}(\lambda)$ are the performance vectors of the baseline and the candidate algorithms, respectively, that are calculated using the same strategy described in section 8.2.3. It is important to note that the same samplings must be used to compare the algorithms — i.e., performance samples must be paired, each one of them coming from the same sampling, and consequently, from the same training and test datasets.

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 $\mathbf{p}(\lambda) - \mathbf{p}(\lambda_0)$. The interpretation of the results is similar; γ is the chosen confidence level and μ is the expected performance gain of the candidate algorithm — or the performance loss, if negative.

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 to whether the probability

$$\mathrm{P}(\mu < 0 \mid \mathbf{z})$$

is too high or not. Always ask yourself if the risk of performance loss is worth it in the real-world scenario.

8.2.5 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 the expected choice of the hyperparameter-optimization technique B is to find the appropriate hyperparameters. Similarly, the choice of the hyperparameters and the parameters that go 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.)

Although nesting experiments usually lead to a general understanding of the performance of the solution, it is not always the best choice.

Nested experiments are computationally expensive, as the possible combinations are multiplied. Also, the size of the dataset in the inner experiment is smaller, which can lead to a less reliable estimate of the performance.

Nonetheless, we can always unnest the search by taking the options as different algorithms two by two, like we described in section 8.2.4. This solves the problem of the size of the dataset in the inner experiment, but it does not solve the problem of the computational cost — often increasing it.

8.3 Final remarks

In this chapter, we presented a framework for experimental planning that can be used in most data science projects for inductive tasks. One major limitation of the framework is that it assumes that the data is i.i.d. This is not always the case, as the data can be dependent on time or space. In these cases, the sampling strategy must be adjusted to account for the dependencies.

Unfortunately, changing the sampling strategy also means that the validation method must be adjusted. That is why tasks like time-series forecasting and spatial data analysis require a different approach to experimental planning.

A Mathematical foundations

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*

Foundations in data science come from a variety of fields, including algebra, statistics, computer science, optimization theory, and information theory. This appendix provides a brief overview of the main computational, algebraic, and statistical concepts in data science.

My 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 a strong programming background and computer scientists with a 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 show 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.

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 of the main definitions and properties of these concepts.
- Consolidate notations and definitions that are used throughout the book.

A.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 for a comprehensive book about algorithms and data structures is Cormen et al. (2022)[1]. An alternative for beginners is Guttag (2021)[2].

A.1.1 Computational complexity

The computational complexity of an algorithm is the total 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, $O(1) < O(\log n) < O(n) < O(n \log n) < O(n^2) < O(2^n) < O(n!)$. Throughout this book, we consider $\log n = \log_2 n$, i.e., whenever the base of the logarithm is not specified, it is assumed to be 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.

[1]T. H. Cormen et al. (2022). *Introduction to Algorithms*. 4th ed. The MIT Press, p. 1312. ISBN: 978-0262046305.

[2]J. V. Guttag (2021). *Introduction to Computation and Programming Using Python. With Application to Computational Modeling and Understanding Data*. 3rd ed. The MIT Press, p. 664. ISBN: 978-0262542364.

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.

A.1.2 Algorithmic 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 A.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
$l \leftarrow 1$;
$r \leftarrow n$;
while $l \leq r$ do
    $m \leftarrow \left\lfloor \frac{l+r}{2} \right\rfloor$;
    if $x = a_m$ then
        return true
    if $x < a_m$ then
        $r \leftarrow m - 1$;
    else
        $l \leftarrow m + 1$;
return false
```

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

Consider as an example the algorithm A.1 that solves the binary search problem. Given an n-element 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.

Algorithm A.2: Recursive binary search algorithm.

```
function bsearch([$a_1, a_2, \dots, a_n$], $x$) is
    if $n = 0$ then
        return false
    $m \leftarrow \left\lfloor \frac{n}{2} \right\rfloor$;
    if $x = a_m$ then
        return true
    if $x < a_m$ then
        return bsearch([$a_1, \dots, a_{m-1}$], $x$)
    else
        return bsearch([$a_{m+1}, \dots, a_n$], $x$)
```

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.

Divide and conquer algorithms can be implemented using recursion. *Recursion* is also an 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 A.2 displays 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 that 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 algorithms are usually very efficient in terms of time complexity — see more in the following.

One example of a 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.

An algorithm that finds a suboptimal solution for the knapsack problem is shown in algorithm A.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.

[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: 978-0262046305 for more details.

Algorithm A.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
Sort the items in decreasing order of value;
$V \leftarrow 0$;
$x_i \leftarrow 0, \forall i$;
for $i \leftarrow 1$ to $n$ do
    if $w_i \leq W$ then
        $x_i \leftarrow 1$;
        $V \leftarrow V + v_i$;
        $W \leftarrow W - w_i$;
return $x_i, \forall i$
```

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

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.

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.

An illustration of backtracking to solve a 4×4 Sudoku puzzle[4] is shown in fig. A.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 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.

A.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].

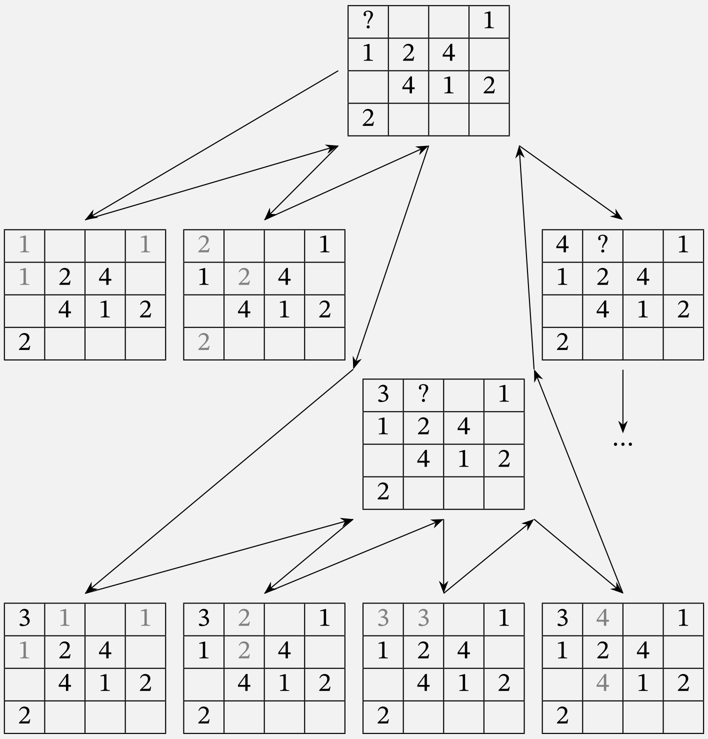
Arrays An array is a homogeneous collection of elements that are accessed by an integer index. The elements are usually stored in contiguous memory locations. In the scope of this book, it is equivalent to a mathematical vector whose elements' type are not necessarily numerical. Thus, a n-elements array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

[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: 978-0262046305.

Figure A.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.

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.

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 $T_l = T_r = \varnothing$.

These properties make 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 $E \subseteq V \times V$ 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 can each node 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.

Figure A.2: A graph with four vertices and five edges.

$$\begin{tikzcd}
4 \arrow[d] & 3 \arrow[l] \\
1 \arrow[r] \arrow[ur] & 2 \arrow[u]
\end{tikzcd}$$

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.

A graphical representation of a directed graph with four vertices and five edges is shown in fig. A.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. A.2 is

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

A.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 $\{\}$.

A.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 $A \subseteq B$.

A.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:

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

A.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 complement 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.

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

A.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

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

and matrices. A common textbook that covers the subject in depth is Strang (2023)[7].

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.

A.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.

[7] G. Strang (2023). *Introduction to Linear Algebra*. 6th ed. Wellesley-Cambridge Press, p. 440. ISBN: 978-1733146678.

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 to be *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 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

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

A.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 $\mathbf{x} = A^{-1}\mathbf{b}$.

A.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

$$A\mathbf{v} = \lambda\mathbf{v}. \tag{A.1}$$

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.

A.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)[8] and Ross (2023)[9].

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

[9]S. M. Ross (2023). *Introduction to Probability Models*. 13th ed. Academic Press, p. 870. ISBN: 978-0443187612.

A.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[10], denoted by Ω, is one, i.e. $\mathrm{P}(\Omega) = 1$; and
3. The probability of the union of disjoint events, $A \cap B = \emptyset$, 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

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

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 $B_1, \dots, B_n$ 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 $\mathrm{P}(A, B) = \mathrm{P}(A) \cdot \mathrm{P}(B)$.

[10]The set of all possible events.

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

$$\mathrm{P}(A \mid B) = \frac{\mathrm{P}(B \mid A) \cdot \mathrm{P}(A)}{\mathrm{P}(B)}. \tag{A.2}$$

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.

A.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

$$\mathrm{P}(X \in A) = \mathrm{P}(\{\omega \in \Omega : X(\omega) \in A\}). \tag{A.3}$$

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

$$p_X(x) = \mathrm{P}(X = x). \tag{A.4}$$

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

$$\mathrm{P}(a \le X \le b) = \int_a^b f_X(x)dx. \tag{A.5}$$

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

$$F_X(x) = \mathrm{P}(X \le x). \tag{A.6}$$

A.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 $\mathrm{Var}(X)$. By definition, it is

$$\mathrm{Var}(X) = \mathrm{E}\left[(X - \mathrm{E}[X])^2\right]. \tag{A.7}$$

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

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

since

$$\begin{aligned}\mathrm{Var}(X) &= \mathrm{E}\left[(X - \mathrm{E}[X])^2\right] \\ &= \mathrm{E}\left[X^2 - 2X\,\mathrm{E}[X] + \mathrm{E}[X]^2\right] \\ &= \mathrm{E}[X^2] - 2\,\mathrm{E}[X]\,\mathrm{E}[X] + \mathrm{E}[X]^2 \\ &= \mathrm{E}[X^2] - \mathrm{E}[X]^2.\end{aligned}$$

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 $X_1, \dots, X_n$ 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 $X_1, \dots, X_n$ 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 $X_1, \dots, X_n$ 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. Otherwise, it is 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 $X_1, \dots, X_n$ 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.

A.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 $\mathrm{Bern}(p)$.

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

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 $\mathrm{Poisson}(\lambda)$.

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

$$p_X(x) = \frac{e^{-\lambda}\lambda^x}{x!}. \tag{A.8}$$

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

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

$$f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right). \tag{A.9}$$

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

Central limit theorem The central limit theorem states that the normalized version of the sample mean converges to a standard normal distribution[11]. Given $X_1, \dots, X_n$ i.i.d. random variables with mean μ and finite variance $\sigma^2 < \infty$,

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

[11]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.

as $n \to \infty$. In other words, for a large enough n, the distribution of the sample mean gets closer[12] 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 $\text{Gamma}(\alpha, \beta)$.

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

$$f_X(x) = \frac{\beta^\alpha x^{\alpha-1} e^{-\beta x}}{\Gamma(\alpha)}, \tag{A.10}$$

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

$$\Gamma(\alpha) = \int_0^\infty t^{\alpha-1} e^{-t} dt. \tag{A.11}$$

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.

[12]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.

A.4.5 Permutations and combinations

For the sake of 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

$$n! = n \cdot (n-1) \cdot \ldots \cdot 2 \cdot 1.$$

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 is also called a choose function, and is read as "n choose k".

B Topics on learning machines

Oh, the depth of the riches and wisdom and knowledge of God! How unsearchable are his judgments and how inscrutable his ways!

— Romans 11:33 *(ESV)*

This appendix is under construction. Topics like the kernel trick, back-propagation, and other machine learning algorithms will be discussed here.

B.1 Multi-layer perceptron

The multilayer perceptron (MLP) is a non-linear classifier that generates a set of hyperplanes that separates the classes. In order to simplify understanding, consider 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 weights $\mathbf{w}^{(1)} = [-0.5, 1, -1]$ (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, a possible solution for the XOR problem is setting $\mathbf{w}^{(3)} = [0, 1, 1]$.

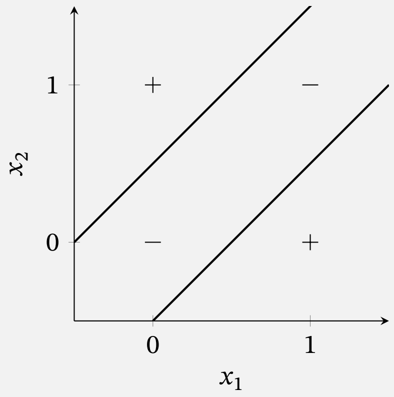
Figure B.1 and table B.1 show the class boundaries and the predictions of the MLP for the XOR problem.

Note that there are many possible solutions for the XOR problem using the MLP. Learning strategies like back-propagation are used to find the optimal parameters for the model and regularization techniques, like l_1 and l_2 regularization, are used to prevent overfitting.

Deep learning is the study of neural networks with many layers. The idea is to use many layers to learn not only the boundaries that separate the classes (or the function that maps inputs and outputs) but also the features that are relevant to the problem. A complete discussion of deep learning can be found in Goodfellow, Bengio, and Courville (2016)[1].

[1] I. Goodfellow, Y. Bengio, and A. Courville (2016). *Deep Learning*. http://www.deeplearningbook.org. MIT Press.

Figure B.1: MLP class boundaries for the XOR problem.



MLP with two neurons in the hidden layer generates two linear hyperplanes that separate the classes, effectively solving the XOR problem.

Table B.1: Truth table for the predictions of the MLP.

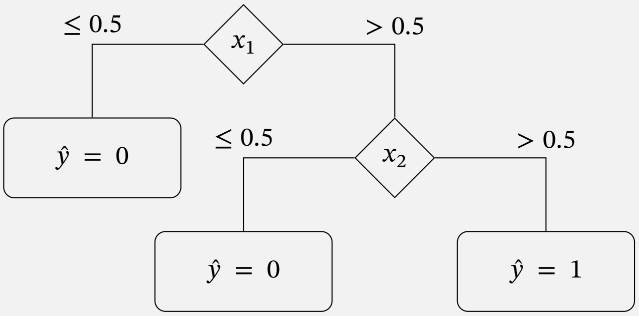
x_1	x_2	y	1st neuron	2nd neuron	$\hat{y}$
0	0	0	0	0	0
0	1	1	0	1	1
1	0	1	1	0	1
1	1	0	0	0	0

Predictions of the MLP for the XOR problem. The output of the 1st and 2nd neurons are hyperplanes that separate the classes in the hidden layer, which are combined by the 3rd neuron to generate the correct output.

B.2 Decision trees

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 fig. B.2.

Figure B.2: Decision tree representation.

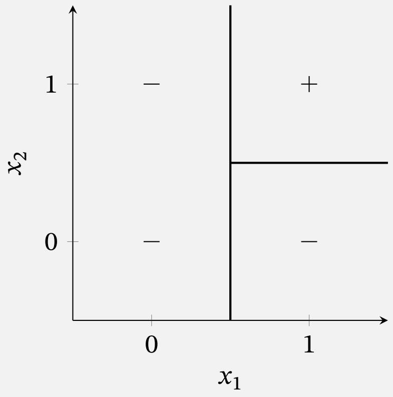


The decision tree that solves the AND problem.

The spatial representation of the decision tree is shown in fig. B.3. Decision trees are a type of classifier that generates a set of hyperplanes orthogonal to the axes.

Decision trees are nonparametric models, one can easily increase the depth of the tree to fit the data, generating as many hyperplanes as necessary to separate the classes. Training a decision tree with a large depth can lead to overfitting, so it is important to use techniques like depth limit and pruning to prevent this from happening.

Figure B.3: Decision tree spatial representation.



Decision trees assume that the classes can be separated with hyperplanes orthogonal to the axes.

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Glossary

AI artificial intelligence 113

BI business intelligence 10

BNF Backus–Naur form 3

CDF cumulative distribution function 202

CI/CD continuous integration/continuous deployment 53

CNN convolutional neural network 160

data leakage A situation where information from the test set is used to transform the training set in any way or to train the model. 50, 51, 81, 87, 144, 164, 178

ERM empirical risk minimization 16, 17, 122, 126

ETL extract, transform, load 9

FIFO first-in-first-out 194

HDFS Hadoop distributed file system 11

IBM International Business Machines Corporation 8

IoT internet of things 12

IQR interquartile range 148

LIFO last-in-first-out 192

LUSI learning using statistical inference 18

ML machine learning 113, 114, 139

MLP multilayer perceptron 210, 211

model A general function that can be used to estimate the relationship between the input and output variables in a dataset. 42

ontology Ontology is the study of being, existence, and reality. In computer science and information science, an ontology is a formal naming and definition of the types, properties, and interrelationships of the entities that really or fundamentally exist for a particular domain. 26

PCA principal component analysis 159

PDF probability density function 202

PMF probability mass function 202

RDBMS relational database management system 9, 29

SLT statistical learning theory 111, 114–116, 122

SQL structured query language 9

SRM structural risk minimization 127–129, 131, 132, 139

SVM support vector machine 17