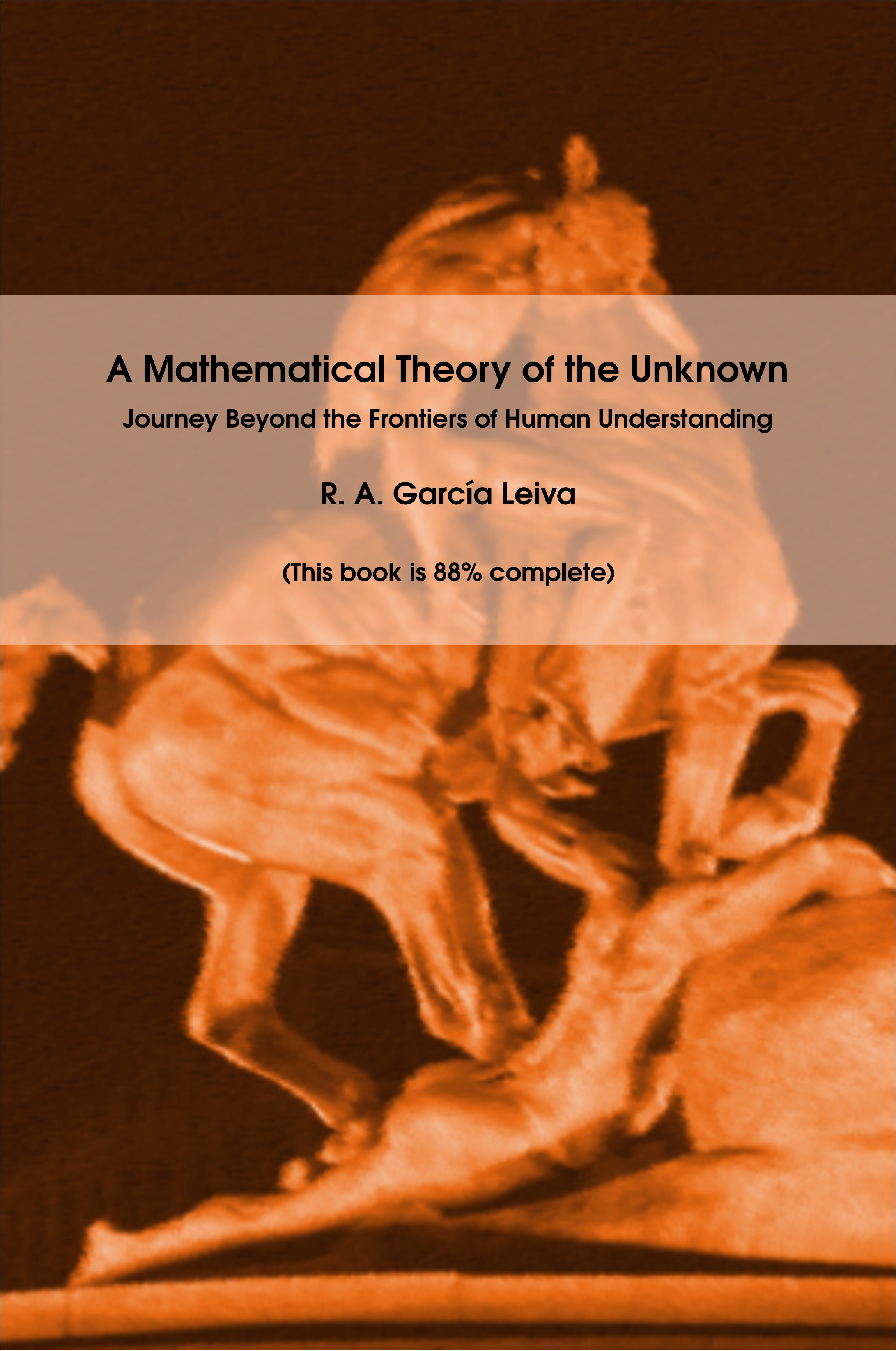

A Mathematical Theory of the Unknown

Journey Beyond the Frontiers of Human Understanding

R. A. García Leiva

(This book is 88% complete)

PUBLISHED BY THE AUTHOR

To my wife Justi, my son Daniel,
and my two daughters Teresa and Lucía.

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Preface

Perfection is achieved not when there is nothing more to add,
but when there is nothing left to take away.
Antoine de Saint-Exupéry

We live in an era that places a high value on knowledge and celebrates scientific advancement. The development of vaccines in record time, the detection of gravitational waves, and the use of artificial intelligence to model protein structures are just a few examples of the extraordinary progress science has made in recent years. However, this celebration of progress should not obscure the structural limitations within the scientific enterprise itself. Despite its accomplishments, science is constrained by the methodological and conceptual frameworks it employs. For example, the "publish or perish" culture in academia often results in a flood of low-quality publications, which can dilute the impact of meaningful scientific work. Another major constraint lies in the allocation of research funding, which often fails to prioritize investigations with the highest potential societal return.

This book is driven by a central aspiration: to overcome the methodological constraints of science in order to challenge established knowledge, explore the unknown, and progress towards the limits of scientific understanding. Our aim is to investigate not only well-known unsolved problems but also those that remain outside our current awareness, the known unknowns and the unknown unknowns. But this pursuit is not merely an academic curiosity; it is a practical necessity. Rather than developing a purely theoretical framework, our goal is to create an approach that can be applied in real-world scientific contexts.

Our assumption is that to explore and ultimately reduce what we do not yet know, we need a structured framework for understanding ignorance itself. To this end, we propose a rigorous mathematical theory, named the Theory of Nescience, grounded in the principles of computability, randomness, and artificial intelligence. The theory builds upon a striking insight: perfect knowledge implies randomness. Although this may initially appear counterintuitive, given that science is traditionally associated with structure, order, and explanation, it becomes clearer when we consider the process of theory refinement. As scientific understanding improves, our descriptions of phenomena become more concise. Eventually, a theory becomes so concise that it cannot be simplified any further. Its representation becomes incompressible, which aligns with the mathematical definition of a random string.

Randomness sets the ultimate limit to our knowledge, since a random description cannot be refined any further and, assuming the theory is accurate, our understanding must be perfect. Far from being a handicap, the constraints that randomness imposes on knowledge pave the way for new possibilities in science and technology. By comprehending these limitations, we can address the most challenging open problems and discover completely new research topics.

From this theoretical foundation emerges a new mathematical framework for understanding nescience, or human ignorance, and the processes by which knowledge is acquired, organized, and refined. Some fo the contributions of this book are:

- A mathematical theory to quantify our lack of scientific knowledge, based on computability and randomness, and on the assumption that measuring how much we do not know is easier than measuring how much we do know.
- A new collection of metrics to measure how much we do not know, whether about individual research topics or broader research areas, and how new research contributions either reduce or fail to reduce that ignorance.
- A practical framework to address some of the most relevant challenges in science, such as defining what constitutes perfect knowledge, identifying the limits of science, and discovering new, previously unknown, research topics.

- A software library that combines the Theory of Nescience with principles of artificial intelligence to automatically derive new knowledge and make predictions based on data.

The Theory of Nescience challenges us to rethink the aims of scientific inquiry. Instead of striving to maximize what we know, it encourages us to minimize what we do not know. By shifting our focus from accumulation to reduction, we open the door to more meaningful measures of scientific progress. The chapters that follow lay the theoretical groundwork for this new approach, one that begins with ignorance and ends in knowledge.

Research Agenda

In this section, we present a focused list of research questions aimed at addressing important gaps in our current understanding of science and the scientific method. Our goal is to stimulate thoughtful investigation by drawing from a variety of academic perspectives. By pursuing these questions, we hope to push the boundaries of human knowledge and inspire innovative solutions that can benefit both scientific inquiry and society more broadly.

Can we provide a quantitative characterization of our ignorance regarding a research topic? Developing such a metric would give us a way to measure not just what we know, but how much we are still missing. This would be especially useful for evaluating scientific contributions, as we could measure how much each new idea or publication actually improves our understanding. By combining this with relevance metrics, we would gain a powerful tool for assessing the true value of scientific work.

Can we compare the extent of our ignorance across disparate scientific fields? If this is possible, we could evaluate and prioritize research based on how much there is left to understand, regardless of the field. This approach could help distribute scientific attention and funding more effectively, highlighting areas of science that are in greater need of exploration while still valuing fundamental research.

Can we establish a systematic procedure to enhance our knowledge? While the scientific method has long served as the cornerstone of research, it varies significantly across disciplines and often lacks clear, measurable criteria for success. Developing a unified and precise approach could improve the consistency and efficiency of scientific discovery. If successful, it would allow us to evaluate and refine how knowledge is generated, leading to more reliable and accelerated progress across all areas of inquiry.

Can we devise a method for discovering new, previously unknown, and intriguing research entities and problems? Many major discoveries arise from questions we had not thought to ask. If we could build a systematic way to identify these unknown unknowns, we could unlock entirely new areas of research and significantly accelerate scientific progress.

What constitutes perfect knowledge? Understanding what it means to know something completely is essential to defining the limits of science. If we could precisely define and recognize perfect knowledge, we would know when a field is complete and when it is time to shift our focus elsewhere. Clarifying whether such completeness is always possible would also help set realistic goals for scientific inquiry.

What effort is required to fully comprehend an unfamiliar subject? Measuring the cost of understanding could fundamentally change how we plan and fund research. For example, knowing the minimal effort needed to improve our grasp of cancer treatment by a small percentage would help us allocate resources more wisely. Even an estimate would be useful for setting priorities and managing expectations.

Do some research topics inherently possess a higher degree of complexity than others? This question addresses a long-standing debate about intellectual differences across disciplines. If we could objectively measure topic complexity, we might dispel myths of superiority and develop more targeted educational strategies. It would also help explain why some areas advance faster than others.

Are there research topics beyond the scope of human comprehension? Human cognition has limits, and it is possible that some problems are fundamentally beyond our capacity to solve. Acknowledging these limits could help us better delegate scientific exploration to machines where appropriate, especially as artificial intelligence becomes more capable of original thought.

How can we differentiate between science and pseudo-science? Many fields present themselves as scientific but lack rigorous foundations. A mathematically grounded method for identifying what qualifies as science would have major implications for public policy, education, and research funding. It would also help protect scientific integrity by distinguishing valid inquiry from unsupported speculation.

Each chapter in this book engages with these questions from both theoretical and practical standpoints. Some offer detailed responses, while others lay the groundwork for future research. This openness is by design. The Theory of Nescience is not a closed doctrine but a platform for further exploration—an invitation to investigate the limits of science and to imagine new pathways of understanding. In this light, the book is not merely a treatise, but a research agenda, a provocation to conventional thinking, and a call to those who are driven to explore the boundaries of knowledge itself.

Origins of the Theory of Nescience

It was in 1991, when I was eighteen years old, that I first encountered the statement, *"Computers are useless, they can only give you answers."* This quote, attributed to Pablo Picasso, struck me as profoundly true. Of course, Picasso was referring to the early calculators of his time, not modern computers. But the underlying idea remains relevant: machines are designed to process predefined tasks, not to generate new and meaningful questions on their own. That realization stayed with me for years. However, it wasn't until 2014—more than two decades later—that I began to explore the implications of Picasso's observation from a practical and computational perspective.

The core ideas behind the Theory of Nescience came together during one particularly restless night. Concepts such as nescience, relevance, and the unknown unknown suddenly aligned. In hindsight, my long-standing interests in information theory and Kolmogorov complexity had likely prepared me for this moment. These disciplines proved essential in articulating the mathematical foundation for a theory that had first emerged as a series of intuitive insights.

Over the following weeks, I conducted a series of computer experiments to test these concepts. The results were promising, but the theory needed time, several years, to develop into a rigorous mathematical framework. Initially, my goal was quite focused: to devise a method for identifying interesting and underexplored scientific questions. But as I examined how ignorance, or nescience, changes over time within scientific disciplines, my scope expanded. I began to wonder whether it was possible to define perfect knowledge and to determine whether such a state could be formally described.

This line of inquiry led to an unexpected and striking insight: perfect knowledge could be expressed in terms of randomness. Specifically, when a theory's description cannot be compressed further, when it becomes algorithmically random, it may indicate that the theory is as complete as possible. This realization broadened my original focus into a general framework for studying the structure of ignorance, the development of understanding, and the mechanisms that drive scientific progress.

Encouraging early feedback from colleagues and researchers helped me refine the theory and explore new applications, particularly in data science and machine learning. Its potential to shed light on long-standing questions in the philosophy of science was especially motivating. For instance, it offered new ways to compare our understanding across fields like mathematics and sociology, and to examine why some research areas appear intrinsically more difficult than others.

Still, something was missing. Although the theory provided compelling explanations, it initially lacked the ability to make testable predictions. To remedy this, I developed a predictive model: a function describing how nescience diminishes as research effort increases. This allowed me to estimate the expected gain in knowledge based on the resources devoted to studying a topic.

Yet even this was not enough. I sought a surprising prediction, one that could reshape how we think about inquiry. Continued mathematical development eventually led to such a discovery: in certain types of topics, additional research can actually increase our ignorance. In these cases, there may exist a critical threshold beyond which further investigation does not improve understanding, but instead introduces greater uncertainty.

This deepened my belief that grappling with ignorance is as fundamental as pursuing knowledge. The Theory of Nescience represents my response to Picasso's challenge: not merely to construct systems that answer questions, but to build frameworks capable of identifying which questions are most worth asking.

These developments and insights have shaped what has become a comprehensive and mature theory. One that I hope will not only reframe how we understand knowledge, but also inspire readers to question more deeply, think more broadly, and search more boldly. The chapters that follow present this journey in both its theoretical depth and practical implications.

About the Book

The Theory of Nescience draws on concepts from multiple academic disciplines, including computability, complexity theory, artificial intelligence, and the philosophy of science. Despite the breadth of its foundations, this book is designed to be self-contained. Readers are expected to have only a basic understanding of first-year calculus and some experience with programming. The content is crafted to serve a wide technical audience, including mathematicians, computer scientists, engineers, and other scientifically inclined readers. The mathematical level is suitable for graduate students and advanced undergraduates.

The book is organized into three main parts: Foundations, Applications, and Mathematical Prerequisites. Readers who already have a background in the mathematics covered in the Mathematical Prerequisites may wish to begin directly with the Foundations. However, we recommend at least a brief review of the notation and key concepts introduced in those chapters. Once readers are familiar with the core ideas presented in the Foundations, they can proceed to the Applications. A detailed understanding of the underlying formalism is not essential; a general grasp of the main concepts and results is sufficient to engage with the practical examples and insights explored in that part of the book.

- *Chapter 1 Introduction* provides a gentle entry point to the theory of nescience, presenting a brief overview of its main concepts and results. While it avoids the use of advanced mathematics, the ideas are introduced in a semi-formal manner. Although it is not recommended as a substitute for the full theoretical exposition, readers who find the mathematics challenging may choose to read only this chapter before proceeding directly to the Applications.

PART I Foundations presents a comprehensive account of the theory of nescience, including formal definitions of its core concepts and proofs of key theoretical results. This section forms the core of the book. Readers with prior knowledge in computability, complexity, information theory, probability, and artificial intelligence may choose to begin here directly.

- *Chapter 2 Fundamental Elements* includes the initial step toward quantifying our lack of knowledge, which involves the precise identification of the research entities under examination, determining how to represent them as strings of symbols, and identifying suitable models to explain them. The chapter introduces these fundamental components of the theory of nescience: entities, representations, and descriptions. It examines their properties and the relationships among them. The chapter also discusses how various representations and descriptions can be combined, how background knowledge influences research, and explores the link between perfect knowledge and randomness. It concludes by proposing a novel concept of a research area.
- *Chapter 3 Miscoding* explores the challenge of representing both abstract and concrete research entities as strings of symbols for research purposes. It formally introduces the concept of miscoding and examines its theoretical properties. Miscoding serves as a measure of the error introduced by inaccurate or inappropriate encodings of the entities being studied. The chapter also discusses strategies for minimizing the errors introduced by poor representations, thereby improving the accuracy and utility of symbolic encodings in research. Furthermore, it investigates issues associated with targetless representations, cases where a symbolic encoding exists without a clear or well-defined entity it aims to represent.
- *Chapter 4 Inaccuracy* presents a new interpretation of the classical concept of error, specifically how accurately a description reflects an entity. The concept is generalized to apply to a wide range of topics, including abstract ones. The chapter also introduces joint and conditional variants of inaccuracy and examines their theoretical

properties. It investigates techniques to reduce inaccuracy and explores how miscoding (errors resulting from poor representations) influences the degree of inaccuracy observed.

- *Chapter 5 Surfeit* investigates the redundancy present in a description, specifically how many unnecessary elements it contains. Surfeit serves as an indicator of how well we currently understand research topics and areas, since our lack of knowledge about the entity is typically reflected in the length of our prevailing description. The chapter also introduces joint and conditional variants of surfeit and derives a practical approximation that can be applied in real-world scenarios. Finally, it examines the relationship between miscoding, inaccuracy, and surfeit, and how these three components can be minimized simultaneously.
- *Chapter 6 Nescience* serves as the core of the book, presenting the mathematical foundations of the theory. It defines science as a non-linear multiobjective optimization problem in which the conflicting metrics of miscoding, inaccuracy, and surfeit are minimized simultaneously. A new metric, nescience, is introduced as a function of these three components. The chapter also explores key properties of this metric, including its evolution over time, the concept of perfect knowledge (zero nescience), and methods for identifying our current best model. In addition, it introduces a definition for the frontier of human knowledge and offers a characterization of what lies beyond that boundary.
- *Chapter 7 Interesting Questions* presents a methodology for identifying new research ideas, based on combinatorics and computational creativity, and focusing on how to address challenging open problems. It introduces two new metrics to measure a topic's relevance and its applicability to existing problems, and examines the properties of these metrics. The chapter also outlines a systematic approach to uncovering what lies hidden in the unknown unknown, illustrating how previously unrecognized research directions may be revealed.

PART II Applications presents a collection of practical uses of the concept of nescience in areas such as machine learning, the philosophy of science, and the discovery of new research topics. The included examples have been selected to illustrate the broad applicability of the theory, spanning from abstract research questions to more tangible problems grounded in datasets.

- *Chapter 8 Machine Learning* explores how the concept of nescience can be applied to entities represented by collections of measured samples. We introduce mnplib, a software library that can be used to analyze datasets, select relevant features, identify optimal model hyperparameters, and compute the errors of trained models. In addition, the chapter presents novel machine learning algorithms, including an innovative method for deriving optimal decision trees and for the automated construction of machine learning models.

- *Chapter 9 Analysis of Science* investigates how well we understand current research topics by applying the proposed metrics. Our aim is to assess the degree of understanding across different areas of science. To this end, we compare research topics within the same academic discipline, as well as across multiple disciplines. The chapter also addresses major open questions in the philosophy of science, including the demarcation problem (how to distinguish science from pseudoscience) and the nature of scientific progress.
- *Chapter 10 The Discovery of the Unknown* demonstrates the practical application of the theory of nescience for identifying promising research questions. Specifically, we show how nescience can be leveraged to generate new research ideas aimed at solving the most difficult open problems. We also propose a methodology for identifying new research topics—that is, for uncovering what lies hidden in the unknown unknown. Multiple examples of such research questions and novel research areas are provided.

PART III Mathematical Prerequisites introduces the mathematical foundations necessary to quantify our lack of knowledge about a research topic and to assess the randomness of a string. Its primary aim is to establish consistent notation, formally define key concepts, and present important theoretical results. While no prior expertise is required to follow the material, readers are encouraged to consult the standard references provided at the end of each chapter for deeper understanding. Additional mathematical elements are discussed in the appendices.

- *Chapter A Discrete Mathematics* offers a summary of the fundamentals of discrete mathematics needed to understand the more advanced topics discussed in the book. This chapter serves as a quick review of these concepts without providing formal definitions or proofs. Topics covered include sets, relations, strings, graphs, and counting methods. A section on linear algebra (matrices and vectors) is also included.
- *Chapter B Discrete Probability* introduces the foundational concepts of probability related to discrete events. Topics covered include conditional probability, random variables, distribution characterization, common distributions, and large random samples. This chapter aims to equip readers with the necessary background in probability to understand the more advanced statistical learning discussed later in the

book.

- *Chapter C Computability* presents a formal definition of the concept of algorithm. It introduces the idea of a universal Turing machine and shows that certain well-defined mathematical problems cannot be solved by computers. The chapter also examines the essential tools of oracle Turing machines and Turing reducibility. Key results in computational complexity, relevant to later chapters, are briefly reviewed.
- *Chapter D Coding* explores how codes function and how they enable us to compress text by eliminating redundant patterns without losing essential information. It shows that there is a limit to how much text can be compressed using this technique, and that this limit is determined by the entropy of the source. The relationship between optimal codes and discrete probabilities is also discussed.
- *Chapter E Complexity* introduces an absolute metric known as Kolmogorov complexity, which measures the amount of information contained in a string by calculating the length of the shortest computer program that can produce it. The chapter studies the properties of this metric in detail and explores the relationship between string complexity and randomness.
- *Chapter F Learning* offers a concise overview of the field of statistical learning, presenting key results from statistical inference and machine learning. It also examines the relationship between codes and probabilities, focusing on practical approaches that apply the concept of minimum string length. Additionally, the chapter introduces the concepts and notation associated with nonlinear multiobjective optimization problems.
- *Chapter G Philosophy of Science* provides a brief introduction to the field from a philosophical perspective. It reviews key concepts such as scientific representations, models, and theories, and identifies the essential components that any formal theory of science should include. The chapter also offers an overview of the current state of the scientific method.

Finally, the Appendices provide additional information that complements the content of the book.

- *Appendix* **??** *Research Agenda* contains a collection of all those elements of the theory of nescience that are still under heavy development. Some of these elements are more advanced than others, but all of them are insufficilently mature to be included in the main corpus of this book. They are also presented here as an invitation to those interested readers to contribute to their development.

- *Appendix* **??** *Advanced Mathematics* offers a set of in-depth analyses that support the results presented in the preceding chapters. While these analyses are necessary to validate our findings, their inclusion in the main text would have disrupted the flow of the narrative. For this reason, they have been grouped together in this appendix.

  Finally, *Appendix H About the Photos* explains the origin and intended meaning of the carefully selected photographs featured at the beginning of each chapter.

Acknowledgements

I would like to express my gratitude to everyone who has contributed their comments and ideas to the development of the theory of nescience. In particular, I am grateful to Antonio Fernández, Vincenzo Mancuso, and Paolo Casari, who believed in and supported this project from its very beginning when it was merely a far-fetched idea (although it may still be). Others who have provided contributions and valuable feedback include Héctor Cordobés, Luis F. Chiroque, Agustín Santos, Marco Ajmone, Pablo Rojo, Manuel Cebrián, Andrés Ortega, Emilio Amaya, Mattis Choummanivong, Alexander Lynch, Andrés Carrillo, and Simon Bihoreau. The `mnplib` library described in Chapter 8 has been partially funded by the IMDEA Networks Institute, the European Union's Horizon 2020 research and innovation programme under grant agreement No 732667 RECAP, and Nokia Spain through the project NetPredict.

I would like to express my sincere gratitude to the open source community. This book would not have been possible without the extensive use of open source tools, which provided both the technical foundation and the flexibility required throughout its development. From the writing process, carried out using TeX and LaTeX, to the data analysis and machine learning experiments—powered by libraries such as `scikit-learn`, `statsmodels`, `pandas`, `NumPy`, and `Matplotlib`, the contributions of countless developers and researchers who share their work openly have been indispensable. Their dedication to building and maintaining high-quality, freely available software is a testament to the collaborative spirit of scientific progress.

I would also like to acknowledge the role of ChatGPT in the preparation of this book. As an AI assistant, ChatGPT provided valuable support throughout the writing process, helping to refine ideas, clarify language, structure arguments, and review technical content[1]. While all decisions and

[1]The following prompts have been used in the review process:

- Review the English and clarity of the following text.

final content were ultimately my own, the ability to engage in thoughtful dialogue, receive constructive feedback, and explore alternative phrasings and formulations greatly enhanced the clarity and coherence of the work. I am grateful for this tool, which has proven to be both efficient and intellectually stimulating.

Finally, I am grateful to my parents, who gave me the opportunities they never had in life, and to my wife and three children, who give ultimate meaning to my existence.

Disclaimer

I would like to clarify that the vast majority of the ideas presented in this book are not my own. The inspiration comes from the brilliant minds of history—thinkers such as Occam, Llull, Leibniz, and Newton, as well as philosophers like Plato, Popper, Feyerabend, and Wittgenstein. I have also built upon the mathematical foundations laid by Turing, Church, Post, Shannon, Solomonoff, Chaitin, Kolmogorov, and many others. My original contribution, if any, lies in connecting some of these ideas and offering what I hope is a compelling reinterpretation of established concepts. The References section at the end of each chapter contains brief descriptions of the sources that have influenced my thinking.

Throughout the text, I use the passive voice ("it is defined") when referring to concepts whose origins I recognize, and the active voice ("we define") when I am unaware of any prior formulation.

- Clarify the following paragraph.
- Propose an example to clarify the following concept.
- Provide a draft proof for the following proposition.
- Review the following section and find logical inconsistencies and mathematical errors.
- Draw a figure in Tikz.

1. Introduction

If presented with a choice between indifferent alternatives,
then one ought to select the simplest one.
Occam's razor principle

We find ourselves in an age where knowledge has become one of our most valued resources, driving both economic progress and societal well-being. Science continually provides us with deeper insights and practical solutions, shaping our daily lives through innovations ranging from advanced medical therapies to transformative digital technologies. However, the path of scientific exploration is neither straightforward nor free from significant barriers. Despite remarkable progress, our current scientific methodologies remain bounded by inherent limitations that restrict our ability to fully understand and address complex issues.

These limitations manifest in various ways, including fragmented research efforts, rigid disciplinary boundaries, and an often narrow approach to funding allocation, which tends to overlook bold, high-risk projects with transformative potential. Moreover, the conventional metrics of scientific success frequently incentivize incremental progress rather than genuinely groundbreaking discoveries, limiting innovation's pace and scope.

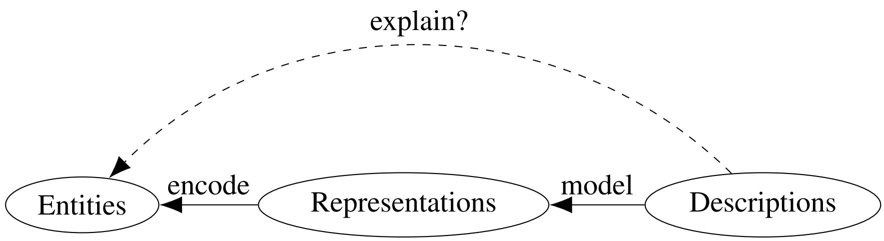


Figure 1.1: The Problem of Understanding

The theory of nescience emerges from the critical recognition of these challenges and the profound need to overcome them. It advocates a renewed approach to exploring the unknown, driven by curiosity and the willingness to question accepted knowledge rigorously. By systematically addressing the limitations inherent in contemporary scientific practice, our objective is to provide robust frameworks that significantly enhance our capability to solve real-world problems and catalyze meaningful advancements across diverse fields.

1.1 Scientific Knowledge

The pursuit of knowledge begins with identifying the *entities* we seek to understand, entities that are often extraordinarily diverse. Mathematicians focus on abstract concepts, biologists on living organisms, and engineers on machines. Our quest for understanding is fundamentally driven by our need to predict outcomes, solve problems, and navigate the complexities of the world around us. For instance, we know that applying sufficient heat to wood will ignite a fire, or that a fever may indicate a viral infection. Practical problem-solving, therefore, hinges crucially on our ability to recognize patterns and create simplified models of these entities. These models empower us to interact beneficially with the world.

Yet, while ideally, we strive to build precise *descriptions* capable of fully reconstructing the entities we study, in reality, such perfection often eludes us, particularly with abstract entities. Consequently, we rely on *representations*, texts or datasets capturing essential details of these entities. Physicists might represent an entity through experimental results; computer scientists through measured data; sociologists through observed facts. Figure 1.1 illustrates this critical interplay: although we aim to directly describe entities, practically, our descriptions are based on constructed representations.

Understanding the effectiveness of our descriptions involves examining potential errors deeply. Firstly, encoding methods can introduce errors, what we call *miscoding*. Secondly, our descriptions themselves may fail to precisely recreate the encoded representations, resulting in *inaccuracy*. Lastly, due to human cognitive limitations, descriptions should not become unnecessarily complex, introducing *surfeit*.

Collectively, miscoding, inaccuracy, and surfeit hinder our quest for clear understanding and reliable predictions. By amalgamating these three error types into a single measure, known as *nescience*, we quantify our lack of knowledge, providing an essential tool for systematically addressing and reducing our ignorance.

1.2 Entities

At the core of our theory of nescience is the recognition that science is, at its essence, a quest to understand the world around us. Throughout history, scientists have examined an extraordinary variety of things (planets, particles, languages, ecosystems, human societies, and much more) in an effort to uncover patterns, formulate explanations, and make predictions. These things we seek to understand, which we refer to as *entities*, form the basis of all scientific activity. An entity might be a tangible object, such as a chemical compound or a cell, or something more abstract, like a mathematical function or a cultural practice.

The scope of what science might investigate is vast and continually evolving. New technologies, shifting societal needs, and fresh philosophical insights regularly bring new entities into view. What unifies this effort is a foundational belief: that some of these entities can be understood through science. That is, we hold that at least part of the unknown is ultimately knowable (see Section G.2). This belief fuels the scientific drive to bring clarity to what was once obscure, to shed light on complexity, and to convert speculation into knowledge. Understanding how we fall short of this ideal, how ignorance persists and why, is the starting point for the theory of nescience.

One important conceptual difficulty we face is that the set of all entities under consideration, what we refer to symbolically as $\mathcal{E}$, cannot be rigorously defined in mathematical terms, except to say that it must be non-empty. This may seem like a minor point, but it carries deep implications.

In mathematics, the idea of a "set of everything" is fraught with contradictions. For instance, if we tried to construct a set that included absolutely all things (physical objects, abstract ideas, ...) we would quickly encounter logical problems. This is why we deliberately avoid the notion of a universal set in the theory of nescience. A key reason for this caution lies in Cantor's theorem, which we discuss further in Section 2.1. Cantor's result shows that for any set, the collection of all its subsets is strictly larger in size than the set itself. As a consequence, it becomes impossible to form a set that includes everything without running into contradictions. Similarly, we steer clear of problematic constructions that lead to paradoxes, such as Russell's paradox, another example covered in Section 2.1, which illustrates how self-referential sets can collapse logical consistency.

These mathematical constraints are not mere formalities; they serve a vital purpose. By enforcing clear boundaries around the sets of entities we analyze, we ensure that the theory we are building remains coherent, consistent, and applicable. It allows us to focus our attention on meaningful, well-defined domains where real progress in understanding can be made.

In practice, we will work with well-defined sets, each associated with a specific domain of inquiry and its unique goals. These sets provide a practical framework for applying our theory to real-world contexts. For example, in mathematics, such a set might include different classes of abstract structures such as groups, functions, or topological spaces. In biology, it could encompass the vast diversity of living organisms, from microscopic bacteria to complex multicellular animals. In the realm of social sciences, the entities might include human behaviors, social systems, or economic models. And in computer science, we may focus on algorithms, data structures, and executable programs.

By tailoring our analysis to these different sets, we are able to apply a unified theoretical framework to a wide variety of disciplines. This adaptability is one of the strengths of our approach: it allows us to measure and reduce human ignorance, or nescience, in fields with very different kinds of entities. Our goal is not only to improve our theoretical understanding of these domains but also to contribute practical tools that can support deeper insights, better decision-making, and more effective problem-solving across the sciences and beyond.

1.3 Representations

In many instances, entities cannot be directly scrutinized through scientific analysis, particularly if they are abstract. As a result, we are compelled to rely on representations, i.e., symbolic encodings that stand in for the entities we aim to understand. We designate the collection of strings that encode the entities of $\mathcal{E}$ as $\mathcal{R}_{\mathcal{E}}$. These strings, referred to as *representations*, may differ depending on the application of the theory of nescience. In certain scenarios, entities may inherently be string-based (e.g., computer programs), while others might be abstract objects that require encoding into string format (e.g., human needs). It is not uncommon for a single entity

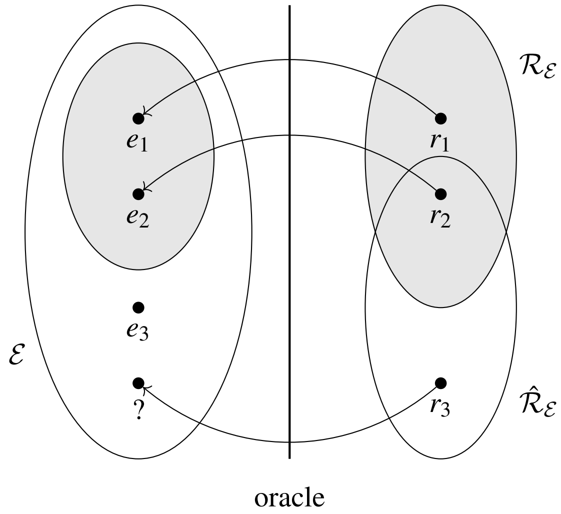


Figure 1.2: Entities and Representations.

$e \in \mathcal{E}$ to have multiple valid representations within $\mathcal{R}_{\mathcal{E}}$, for example, a text-based description, a diagram saved as a computer file, or a collection of empirical measurements. Each representation emphasizes different aspects of the entity and may be better suited to particular investigative goals or scientific approaches. Transforming abstract entities into symbol strings in a manner that faithfully captures their complexities and subtleties remains a formidable and unresolved challenge. Consequently, the exact composition of $\mathcal{R}_{\mathcal{E}}$ often eludes us.

In a world where understanding depends on symbolic surrogates, the idea of constructing an encoding function $f : \mathcal{E} \to \mathcal{R}_{\mathcal{E}}$ becomes not only attractive but essential. The function f represents an idealized encoding process: it assigns to each entity $e \in \mathcal{E}$ one of its symbolic representations $r \in \mathcal{R}_{\mathcal{E}}$. In essence, this function models the act of transforming something we wish to understand (like a physical object, a biological system, or an abstract concept) into a format that can be studied, manipulated, or stored using symbols, typically as strings. In practice, such a function would allow us to systematically move from the domain of real-world or conceptual entities to their formal encodings, which are necessary for analysis in science, computation, and communication. However, defining such a function is no trivial task, precisely because $\mathcal{E}$ itself is not well defined. The boundaries of what should or should not be included in $\mathcal{E}$ are inherently blurred. For example, we still lack a precise and universally accepted definition of what constitutes a human need.

To grapple with this indeterminacy, one may resort to theoretical constructs such as the *oracle Turing machine* (see Chapter C). While a standard *Turing machine* serves as a mathematical model of computation, the oracle variant introduces a conceptual leap: it simulates a computer with access to an external source of information. The oracle Turing machine can be imagined as a theoretical computer connected not to the actual internet of today, but to an idealized version, an omniscient information source containing perfect knowledge about everything that exists or could exist. This imaginary machine is allowed to submit string-based queries to this vast external database. For instance, it might ask whether a given string r encodes any entity in $\mathcal{E}$. Unfortunately, formulating the question "does r represent e?" would require expressing e itself as a string of symbols. And since we do not know how to encode e in advance, we cannot construct such a query. This irony captures the very dilemma we aim to address, the tension between what can be queried, what can be known, and the inherent limitations of representation in scientific inquiry.

From a practical perspective, we typically approximate the set $\mathcal{R}_{\mathcal{E}}$ with another set $\hat{\mathcal{R}}_{\mathcal{E}}$ of strings, which we consider to be adequate representations of the entities of $\mathcal{E}$. In scientific practice, these representations have traditionally taken the form of illustrations or images (e.g., in biology), collections of factual data (e.g., in sociology), or experimental results (e.g., in physics). With recent significant advancements in the capability of computers to gather and store data, a novel and potent method for encoding entities has emerged: using vast data sets as representations. It's essential to note that in the encoding process, our objective is not to find the shortest possible representation of the entities but to seek out high-quality representations.

It's crucial to acknowledge that in numerous practical scenarios, the chosen representations of abstract entities may not fully encapsulate all nuances of the original objects. This means we are grappling with simplified abstractions of reality, which could potentially curtail our capacity to make sweeping assertions about nature (see Chapter 3).

■ **Example 1.1** If we're studying animals (the set $\mathcal{E}$), we could use a binary encoding of their DNA (the set $\mathcal{R}_{\mathcal{E}}$) as representations. While our current technology doesn't allow us to bring a creature to life solely from its DNA, theoretically, it could be feasible. However, DNA alone doesn't fully replicate the original animal, as it doesn't include life experiences. For instance, how would we represent a cat that only has three legs due to an accident? That detail is not recorded in its DNA. If our goal is to study the traits of certain species, working with the DNA of a representative sample of individuals within each species would be adequate. However, if we're studying specific individuals within a species, we would also need a way to encode each animal's history or the details not encapsulated by the DNA. ■

Working with strings as representations (the set $\mathcal{R}_{\mathcal{E}}$) inevitably results in certain entities lacking any corresponding encoding (see the gray areas in Figure 1.2; specifically, entity e_3 has no representation). This limitation becomes particularly evident when the set of entities is uncountable. For example, if $\mathcal{E}$ is the set of real numbers, many elements cannot be represented, since we restrict representations to finite binary strings. Real numbers that require infinite precision (such as most irrational numbers) cannot be fully encoded. This mismatch reveals a deeper asymmetry: in many domains of knowledge, the space of conceivable problems or entities far exceeds the space of valid, encodable representations. Intuitively, this suggests that in such domains, the quantity of problems may exceed the number of solutions.

Using approximations of representations (the set $\hat{\mathcal{R}}_{\mathcal{E}}$) can also result in some representations encoding the wrong entities, as illustrated by representation r_3 in Figure 1.2. This occurs because our knowledge about the entities in $\mathcal{E}$ is often incomplete or imprecise, which can lead us to construct representations that appear valid but fail to correspond to the intended entity.

Another issue with incomplete knowledge is the possibility of having unknown entities whose existence we are unaware of. For instance, representation r_1 in Figure 1.2 is not part of the set $\hat{\mathcal{R}}_{\mathcal{E}}$ and is therefore overlooked by researchers despite being the representation of a knowable entity e_1. One of the objectives of this book is to provide a procedure to uncover new, previously unknown, research entities from the set $\mathcal{R}_{\mathcal{E}}$ (refer to Section **??** and Chapter 10).

1.4 Descriptions

Upon identifying the set $\mathcal{R}$ of potential representations, we are faced with the deeper motivation that drives much of scientific inquiry: the desire to bring order to the complexity of the world. To do this, we must devise appropriate methods to describe these representations, an endeavor that underlies our attempt to form theories or models that articulate how the world operates. Our limited cognitive capacities as humans compel us to work with simplified, yet insightful, models of nature. These abstractions help us interpret phenomena and forecast the consequences of our actions. Descriptions also change over time, as our understanding of the entities studied improves.

■ **Example 1.2** To anchor these ideas in the concrete, consider the evolving effort to describe the macroscopic behavior of the physical universe (the entity e). The sequence of proposed descriptions includes Aristotelian physics, Cartesian mechanics, Newtonian laws, Einstein's relativity, and, potentially, superstring theory. Each successive model attempts to refine our grasp of reality. Among these, Einstein's theory currently stands as the most complete, given that alternatives like superstring theory still await experimental corroboration. ■

Defining a valid description for an entity is not merely a technical challenge; it embodies a fundamental limitation of knowledge. The Berry paradox serves as a compelling reminder of these philosophical intricacies. A phrase like "the smallest positive integer not definable in less than twelve words" becomes paradoxical by succeeding in doing just that within eleven words. To avoid such pitfalls, the theory of nescience imposes stricter demands: a valid description must be a finite symbol string that allows us to effectively and completely reconstruct a possible representation of the original entity. By "effectively," we mean that this reconstruction can be performed by a machine, or computer, without human intervention.

From Newton's formulation of classical mechanics to today's explorations, the scientific journey has been shaped by the pursuit of mathematical models. The theory of nescience follows this lineage but extends it by demanding that models be computable, i.e. executable by computers. This requirement of computability of descriptions allows us to remove many of the paradoxes traditionally associated with the concept of description. In this light, science becomes not only a quest for understanding but also a computable-driven endeavor to approximate reality.

Descriptions are typically divided into two components: a Turing machine TM (a computer program) that encapsulates all the regularities found in the entity's representation (the compressible part), and an input string a that contains a literal description of the remaining elements (the non-compressible part). This dualistic nature of descriptions parallels traditional distinctions in science, such as theories and assumptions, theories and initial conditions, problems and specific problem instances, species and individuals, and so on. For instance, a description might consist of a system-modeling set of differential equations (the compressible part), accompanied by a compilation of initial conditions (the non-compressible part). The precise interpretation of the pair TM, a relies on the specific characteristics of the entity set to which the theory is applied.

Figure 1.3 illustrates the relationship between entities, representations, and descriptions. The set of all potential descriptions is denoted by $\mathcal{D}$. However, not all strings qualify as valid descriptions: each must be grounded in a Turing machine, ensuring that it is computationally meaningful. Furthermore, not every valid description corresponds to a legitimate representation. Since representations r can be described in multiple ways, the overarching scientific goal emerges as the search for the shortest possible description d

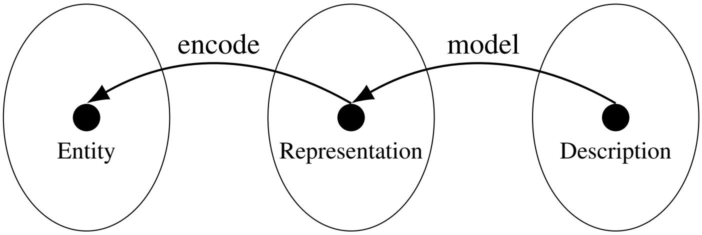


Figure 1.3: Entities, representations and descriptions.

that faithfully reconstructs the observed data.

However, a fundamental obstacle lies in the incomputability of this task. As discussed in Chapter E, there exists no general procedure to determine the shortest program that outputs a given string. This impossibility extends to representations, rendering the pursuit of optimal scientific models as a challenge beyond computer capabilities. As a result, science must rely on heuristic strategies to approximate ideal solutions. Collectively, these heuristics define what we call the *scientific method*.

The theory of nescience is driven by the desire to understand, and ultimately quantify, the various errors that arise in the process of scientific discovery. Figure 1.3 provides the conceptual framework for this endeavor. In Sections 1.5, 1.6, and 1.7, we introduce metrics designed to capture distinct sources of error. These components are then synthesized in Section 1.8 into a single, unified measure: nescience. Although inherently uncomputable, this measure formally expresses the extent to which a given research entity remains poorly understood. It highlights not only the boundaries of current knowledge but also the areas most deserving of scientific attention.

1.5 Miscoding

As we've observed, in many scientific disciplines, the effort to understand the world often begins with an elusive challenge: the entities we wish to study, denoted as the set $\mathcal{E}$, do not always lend themselves to clear or complete representations. Some of these entities are too abstract, others too complex, and many remain partially known. This mismatch between the reality we wish to grasp and the means we have to represent it is not merely a technical limitation, it reflects the very heart of scientific inquiry.

The scientist's journey, then, often starts in uncertainty. We make do with approximations, crafting descriptions that we hope capture enough truth to be useful. Yet, we are aware that these representations carry errors. Our goal becomes not just to encode entities, but to quantify the error introduced by using these inaccurate representations.

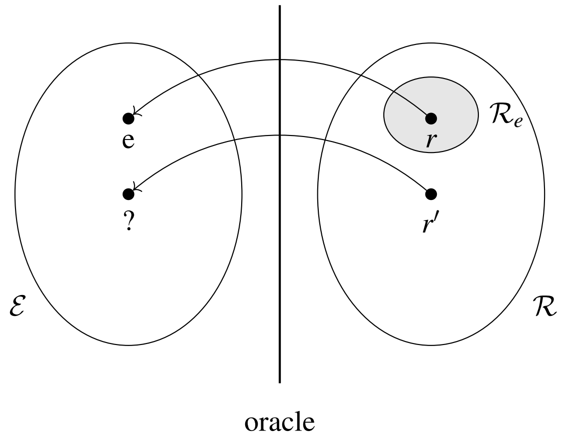


Figure 1.4: Miscoding of topics.

We propose to measure the *miscoding* of an inaccurate representation r' by assessing how difficult it is to transform this flawed representation into a correct one. In more technical terms, this difficulty is expressed as the length of the shortest computer program that, when given r' as input, is able to produce the accurate representation r. Figure 1.4 provides a visual depiction of this process. The set $\mathcal{R}_e$ consists of all the strings that are considered accurate representations of the entity e. If falls outside this set, it means our understanding is flawed. Miscoding represents the cost of bridging that gap. Importantly, this cost is not about computational time or speed. It is about descriptional complexity, how much must be said, or programmed, to repair the mistakes. If r' contains inaccuracies, the required program must identify these deviations and correct them. If instead r' lacks key information altogether, the missing content must be embedded within the program itself. In this way, miscoding becomes a reflection of our ignorance: the larger the program needed, the more knowledge we have to include to arrive at the truth. Miscoding measures how much we still need to learn before our representations truly encode the entities we seek to understand.

However, the previous method of measuring miscoding does not fully capture our intuitive understanding of what it means for a representation to be flawed. There is a deeper issue that emerges when a representation includes more than what is necessary. In other words, it may not only be inaccurate by omission but also by addition. Consider a situation where the representation r' contains extra information that is irrelevant or unrelated to the entity e we are trying to understand. This surplus information is not just noise, it actively distorts the description by forcing any model based on e to account for elements that have no bearing on the actual entity. The result is a bloated and misleading representation. The description becomes longer not because the entity itself is more complex, but because our flawed representation includes unnecessary baggage. This problem is not just theoretical. In real-world scientific practice, we frequently encounter such scenarios. Imagine an experiment where multiple variables are being recorded, but only a few of them actually influence the outcome. If we do not yet know which variables are relevant, our current models might treat all recorded features as potentially significant. This lack of understanding can lead us to build explanations and predictors around elements that are, in reality, unrelated to the entity or phenomenon of interest.

To account for this kind of misrepresentation, we must expand our definition of miscoding. We need to ask not only how much effort is required to fix an inaccurate representation, but also how much effort it would take to reconstruct that flawed version from the correct one r. The higher this effort, the worse the representation is, as it suggests that the inaccurate description deviates significantly from what is accurate. This leads us to introduce the a second measure, as the length of the shortest computer program that can output the incorrect description r' given the accurate one r. Only by considering both directions, how difficult it is to go from r' to r, and how difficult it is to go from r to r', can we fully assess the degree of miscoding. We therefore define miscoding as the maximum of these two values. This revised definition acknowledges that misinformation can come in multiple forms. It captures both the missing and the misleading, recognizing that a poor representation might not only fail to say what is necessary, but might also say unnecessary things. In this way, miscoding becomes a more complete reflection of the divergence between what we currently believe and what truly is.

Nevertheless, this latest definition still poses practical challenges. In many cases, the same entity can be described in multiple, equally valid ways. This multiplicity creates a dilemma: what should we do when our inaccurate representation r' is far from one correct representation r_1, but quite close to another valid one r_2? Judging solely by its distance to r_1 could unfairly suggest a high level of miscoding, when in fact r_2 may be a legitimate approximation of e.

The core issue here is that correctness is not always unique. Scientific and mathematical entities often admit many forms of expression—each highlighting different properties, or suited for different contexts. Penalizing a representation for not being similar to just one of these correct forms would ignore the richness and flexibility of representation.

■ **Example 1.3** Consider e as the abstract entity known as the "Pi constant", the ratio of a circle's circumference to its diameter. Let r be the Wallis product, expressed as $2(\frac{2}{1} \cdot \frac{2}{3} \cdot \frac{4}{3} \cdot \frac{4}{5} \cdot \frac{6}{5} \cdot \ldots)$, a well-known infinite product that converges to π. Suppose r' is the infinite series $4(1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \ldots)$ which corresponds to the Leibniz series. Although r' is structurally very different from r, it also accurately represents the same entity e. To declare r' as highly miscoded with respect to r would be misleading, because r' is not an error, it's an alternative, equally correct expression. ■

As example 1.3 indicates, defining miscoding poses challenges because the set $\mathcal{R}_e$ of valid representations for the entity e is generally unknown. Theoretically, we could rely again on the oracle Turing machine to solve this problem. However, as observed, we can't ask the oracle if the string r is a valid representation of our interested entity e (the set $\mathcal{R}_e$), since that would require us to provide a valid encoding of e as a string of symbols, which typically can't be done. Perhaps, all we can do is ask this oracle how close a given string r is to being a valid description of some entity in the entire set of entities $\mathcal{R}_\mathcal{E}$.

With this constraint in mind, we have to define the miscoding of a representation as the smallest possible discrepancy, as judged by the oracle, between our given string and any valid representation of any entity. In this way, we allow the oracle to search through the universe of all correct representations, looking for the one that is most similar to our candidate. This definition enables us to talk about miscoding even in the absence of a known ground truth.

But there is one final complication we must confront. Because this definition of miscoding does not rely on knowing the actual entity being represented, it opens the door to a subtle yet critical problem: we might not be representing what we think we are. In other words, our descriptions might be well-formed and internally consistent, yet point to an entirely different entity than we had intended. This kind of mistaken identity is not just a philosophical curiosity, it has occurred repeatedly in the history of science. Researchers have often believed they were investigating one phenomenon, only to later discover that their results pertained to something entirely different.

■ **Example 1.4** In the late eighteenth century, chemist Joseph Priestley believed he was studying a substance called "phlogiston", which was thought to be a fire-like element released during combustion. All of his experiments and representations were constructed around this idea. However, in reality, Priestley was observing the properties of a completely different entity: oxygen. Though his descriptions were coherent and reproducible, they were ultimately anchored to the wrong conceptual foundation. ■

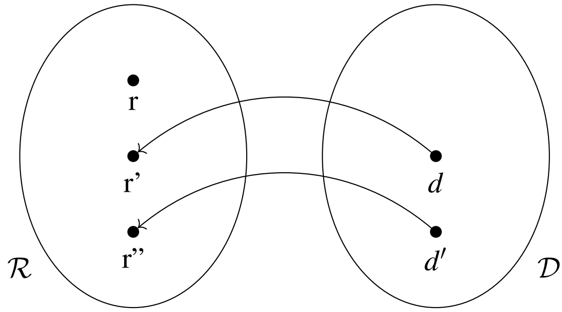


Figure 1.5: Inaccuracy of a description.

According to the theory of nescience, our role as researchers goes beyond the mere identification of correct representations for the entities we wish to understand. It also involves a deeper and more ambitious task: uncovering the principles by which an idealized oracle machine would reconstruct the original entities given their representations. In other words, it is not enough to arrive at accurate representations, we must also strive to understand why these representations are accurate, what makes them effective, and how they reflect the intrinsic structure of the underlying entities, by understanding how this hypothetical abstract oracle would work. This shift in perspective moves us from a practice of isolated trial and error to a more reflective inquiry into the nature of scientific representation itself. Our goal is not just to find a representation that works, but to understand the encoding process more deeply.

1.6 Inaccuracy

In the preceding section, we explored how ignorance may arise when the representation r' we use to encode an entity e does not match the actual entity's correct representation r. That was the problem addressed by miscoding. Now, we turn to another, equally important source of ignorance, what we call *inaccuracy*, which emerges not from selecting the wrong representation, but from failing to describe it adequately.

In an ideal scenario, we would have a description d, that is, a computer program, capable of fully reconstructing the representation r', even if the true representation r remains unknown. However, this level of precision is rarely attainable in practice. More commonly, we rely on an approximate description d', which produces a string r'' that resembles r', but is not exactly the same. In such cases, we refer to d' as an *inaccurate* description of the representation r' (see Figure 1.5).

If a description is inaccurate for a representation, it is useful to have a quantitative measure of how much we deviate from accurately modeling the representation. A viable method to define this measure could be calculating the effort needed to rectify the output of our inaccurate description. In this context, the inaccuracy could be determined by the length of the shortest computer program that can generate the correct representation when fed with the incorrect one produced by the description. However, similar to the case with miscoding, to have a holistic understanding of the error associated with the description d, we must also calculate the difficulty of generating the inaccurate representation given the correct one. It's possible that our description d models elements unrelated to the representation r', and merely ignoring these elements won't solve the problem.

In other words, the inaccuracy measures how difficult it is to convert the output of the description into the intended representation, or the other way around, how difficult is to convert the representation in the output of our description. The larger the maximum of these two values, the more the description deviates from accurately capturing the intended representation.

We deliberately prefer the term *inaccuracy* over the term *error*. In the language of continuous systems, error includes both precision and accuracy. But in our discrete framework, where descriptions are finite symbol strings, precision loses its relevance. What matters here is how well the structure of the description aligns with the structure of the representation.

In practice, calculating the inaccuracy associated with the description of a representation is a challenging task. As previously mentioned, determining the length of the shortest computer program that can print a string is a non-computable problem. If the original entities are texts themselves, we could approximate the inaccuracy using compression algorithms. Here, the string complexity is approximated by the length of the compressed text using a compressor. If the topics are abstract entities, such as mathematical concepts, their descriptions could be derived from the result of an experiment. Hence, the inaccuracy could be based on the model's error (for instance, by calculating the length of additional information required to thoroughly describe the experiment's results given the model). In this regard, our definition of inaccuracy is a generalization of the concept of error. It can be applied to various types of entities, not only those that can be encoded as datasets.

■ **Example 1.5** Consider Newton's second law of motion, $F = ma$. Suppose we construct a dataset by applying known forces to objects of varying masses and measuring their resulting accelerations. If our goal is to study gravitational acceleration, the force and mass terms cancel, isolating acceleration as the variable of interest. Encoding this dataset in full would require a significant number of bits. Yet, recall that our objective with representations is not to minimize string length but to ensure that the encoding captures the richness and structure of the underlying phenomenon.

In this example, we draw on a historical experiment conducted by the National Bureau of Standards in Washington D.C. between May 1934 and July 1935. The dataset includes 81 measurements of acceleration in centimeters per second squared, for instance, a value like 980,078. Using a uniform 20-bit encoding per measurement, the full dataset requires 1,620 bits. Suppose a model predicts a gravitational acceleration of $980,000 cm/s^2$ plus noise. If encoding the dataset using this model only requires 453 bits, the model's inaccuracy is estimated as:

$$\frac{453}{1,620} = 0.27$$

This tells us how much information must be added to the model to fully account for the empirical data. It quantifies the gap between representation and reality. ■

What this example illustrates is a profound ambiguity: when our models and our data disagree, we cannot determine, in general, whether the failure lies in the experiment (miscoding) or in the model (inaccuracy). This ambiguity is not a flaw of the framework, it is a reflection of the inherent uncertainty we face when attempting to describe the world. And it is precisely this uncertainty that the theory of nescience seeks to explore, quantify, and ultimately reduce.

1.7 Surfeit

In our pursuit of understanding, we often encounter a paradox: the more complex and verbose our explanations, the less confident we should be in the depth of our knowledge. Complexity, when unnecessary, signals confusion. When we struggle to explain a concept concisely, it is likely because our grasp of it remains partial. This observation reveals a deeper motivation behind scientific inquiry: the drive to eliminate what is superfluous, to strip our models down to their essential structure. By doing so, we gain clarity not only in explanation but also in prediction and control.

Science depends on descriptions, most often in the form of mathematical models, to interpret the past, predict the future, trace the connections between cause and effect, and engineer solutions to practical problems. But these models, to serve us effectively, must remain within the limits of our cognitive capacities. As scientists and engineers, we are compelled to seek out models that are not only correct but also minimal. This minimality is not an aesthetic preference; it is a cognitive and computational necessity. Even if, in the

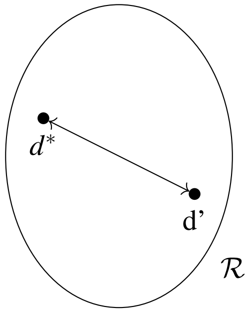


Figure 1.6: Surfeit of a model.

future, machines take over the work of scientific reasoning, and our concern for human comprehensibility fades, the idea of minimizing unnecessary complexity will remain a conceptual cornerstone, albeit perhaps relegated to a more theoretical realm.

The theoretical limit of our knowledge about a representation, denoted as its perfect description d^*, is given by the shortest possible computer program that can reconstruct that representation. In practice, we rarely achieve this ideal. The excess or surfeit of a description d' can be calculated by comparing the length of this specific description to the length of the shortest possible description d^* for that representation (refer to Figure 1.6). In other words, *surfeit* measures how much longer a description is compared to the most concise description we could ideally achieve. Regrettably, due to our incomplete knowledge, we generally do not know the shortest description of a representation, hence, surfeit is a value that must be estimated in practice.

This definition leads us to a profound insight: perfect knowledge implies randomness. If a description were perfect, it would be incompressible, any pattern or regularity would suggest redundancy that could be eliminated. According to the theory of computation, incompressible strings are indistinguishable from random sequences (see Section E.6). Thus, within the framework of our theory, a perfect description of a phenomenon must be random.

This conclusion might seem counterintuitive. Traditionally, randomness has been associated with disorder and the absence of meaning. But in our context, a random description is not meaningless, it is simply maximally informative, packing as much content as possible into the smallest possible space. Still, not all random descriptions are perfect. A theory might become increasingly compressed and eventually appear random, only for a new representation to emerge, perhaps based on a different encoding, that offers a shorter and more insightful description.

Understanding randomness in this way reshapes the boundaries of what we consider knowable. Rather than seeing randomness as a wall, we see it as a marker of how far we've progressed. It signals the frontier of comprehension, a point where additional refinement is no longer possible unless we reconceptualize the problem. And crucially, this perspective doesn't just limit us to analyzing what we already know; it provides a strategy for identifying gaps in knowledge and pointing toward new avenues of discovery.

With our definition of surfeit, in which lengthier explanations are deemed inferior, we aren't implying that textbooks should always strive for utmost brevity. Contrarily, in certain situations, we anticipate textbooks to be highly redundant. A concise book contains an abundance of information in a very condensed space, making it challenging for humans to assimilate (understand) that information. However, a redundant textbook (such as this one) presents the same amount of information but in a larger space, hence, its content is easier to comprehend. Moreover, in fields outside of science, redundancy may be desirable. For instance, in law, redundancy aids lawyers in memorizing legal texts, and in music, repetition can contribute positively to harmony, as exemplified in a canon.

1.8 Nescience

Nescience is an old-fashioned English word meaning "lack of knowledge or awareness." At first glance, it appears to be synonymous with the word "ignorance." However, there is a subtle but important distinction: ignorance refers to the absence of knowledge when such knowledge exists and could be acquired (for instance, by reading a book), whereas nescience refers to the absence of knowledge when that knowledge does not yet exist, when it is unknown to everyone. The theory of nescience has been developed to quantitatively measure how much we do not know in situations where knowledge is not yet available, aiming to capture the extent of our collective ignorance as a species.

Intuitively, the extent of what we do not know about a research entity can be assessed through the metrics of miscoding, inaccuracy, and surfeit associated with a given representation and description. These three metrics capture the main types of errors we might make. Miscoding reflects how well the representation encodes the original entity under investigation; inaccuracy indicates how effectively the description models that representation; and surfeit measures the quality of the description itself in terms of unnecessary complexity or verbosity. The best combinations of representations and descriptions are those that exhibit low miscoding, low inaccuracy, and low surfeit.

However, these factors are often in tension with one another. Improving one dimension can inadvertently worsen another, making the process of refining knowledge inherently complex. For example, increasing the complexity of a description might improve its accuracy, bringing the output closer to the intended representation, but this gain may come at the cost of clarity and simplicity, thereby increasing surfeit. Similarly, modifying a representation to better match the original entity, thus reducing miscoding, can lead to an increase in the inaccuracy of the description, which may no longer align well with the new representation. In scientific research, such trade-offs are frequently encountered. More accurate models often require additional parameters, more sophisticated computations, or richer structures, which can obscure understanding, hinder reproducibility, or limit practical applicability. Recognizing these tensions helps researchers make more informed decisions about model selection, balancing the competing goals of simplicity, fidelity, and succinctness. The theory of nescience makes these trade-offs explicit, providing a structured way to analyze and optimize them.

A pair (d, r), composed of a description and a representation, is said to be Pareto optimal if there is no other pair (d', r') that improves at least one of the three components of nescience—miscoding, inaccuracy, or surfeit—without worsening another. In this sense, a Pareto optimal pair represents a balance point where any improvement in one dimension would result in a degradation in another. This notion helps us identify a set of candidate (d, r) pairs that offer the best possible trade-offs and jointly provide strong explanatory value for an entity e.

However, in scientific practice, we typically aim to select a single description to serve as the model for a research entity. To make this selection, we must define a utility function that enables us to classify and rank the candidate descriptions. The exact form of this utility function depends on the field in which the theory of nescience is being applied. For instance, in machine learning, where entities are represented as datasets, a reasonable utility function might be the average of the three components of nescience: miscoding, inaccuracy, and surfeit. This provides a simple and effective way to evaluate and choose the most suitable description.

In traditional scientific approaches, it is common to fix a particular representation of the entity under investigation and then focus on selecting or developing a model that minimizes inaccuracy, and possibly surfeit. While this methodology is often effective within well-established domains, it risks overlooking better alternatives that arise from reconsidering the representation itself. The theory of nescience emphasizes that miscoding, inaccuracy, and surfeit must be minimized simultaneously. This holistic approach avoids the danger of settling into a local minimum—where a model seems optimal given a fixed representation, but a better explanation might exist elsewhere in the space of possible (representation, description) pairs. By jointly considering and optimizing both the representation and description, the theory enables a more comprehensive and flexible exploration of scientific models.

1.9 Perfect Knowledge

In this book, we assume that the final objective of science is to achieve perfect knowledge, understood as the state in which our understanding of an entity is both accurate and efficient. This is equivalent to discovering pairs of descriptions and representations with the lowest possible nescience. Scientific progress, from this perspective, is inherently iterative: over time, new candidate pairs of descriptions and representations are proposed, each intended to bring us closer to this ideal state by reducing nescience.

There are two fundamental strategies for decreasing nescience. One is to develop new descriptions, these could stem from the formulation of novel theories, improvements upon existing explanations, or the elimination of unnecessary assumptions. The second is to discover better representations, ways of encoding or framing the entity under study that more faithfully reflect its essential properties. Both avenues are crucial and complementary, as a poor representation can obscure the merits of an otherwise sound description, and vice versa. Thus, progress in science involves the dynamic refinement of both how we represent and how we describe reality.

When the nescience of a pair composed of a representation and a description is equal to zero, we say that *perfect knowledge* about an entity has been achieved. This state corresponds to the simultaneous minimization of the three components of nescience: miscoding, inaccuracy, and surfeit. Miscoding being zero means the representation perfectly encodes the intended entity; inaccuracy being zero means the description fully and faithfully reconstructs the representation; and surfeit being zero means the description contains no redundancy, it is as concise as possible. In this ideal scenario, our understanding of the entity is complete, exact, and optimally efficient.

As previously described, representations aim for completeness: they must encapsulate all relevant aspects of an entity, even at the cost of introducing redundancy. This ensures that nothing essential is omitted and that the representation is faithful to the entity as it exists. In contrast, descriptions are governed by a strict economy of expression. Brevity is essential and is formally measured by surfeit. The ideal description is one that conveys the maximum possible information using the fewest possible symbols. In fact, perfect knowledge requires descriptions that are random in the algorithmic sense, meaning they are incompressible and contain no patterns that would allow them to be expressed more succinctly. Such descriptions are optimally efficient: they cannot be improved upon. However, it is a mistake to assume that any random-looking description necessarily corresponds to perfect knowledge. Randomness alone does not guarantee that miscoding and inaccuracy are zero; a random string may still be describing the wrong representation or doing so poorly.

More critically, if a description is already random, if it is the shortest and most accurate possible for a given representation, then any attempt to replace it with an alternative will necessarily result in increased nescience. Continuing to search for new descriptions in such a case, without recognizing that the current one is already optimal, leads to a regression in understanding. We may introduce inaccuracy or redundancy, thereby increasing our ignorance rather than reducing it. This underlines the importance of knowing when to stop: in some cases, further research into new descriptions can obscure rather than clarify.

It is important to recognize that there may not be a single ultimate theory or uniquely optimal pair. Multiple combinations of representations and descriptions may yield a nescience of zero. The most suitable combination in any given context often depends on the intended practical application. Different applications may favor different aspects of a representation or description, such as interpretability, computational efficiency, or generalizability, leading to different but equally valid realizations of perfect knowledge.

If performed properly, the nescience of an entity should exhibit a strictly decreasing trend as new descriptions and representations are introduced. This principle relies on the notion that a newly proposed pair should only be accepted if it demonstrates a genuine improvement, namely, a reduction in overall nescience compared to the existing best-known alternative. It is possible that a new description may increase one component of nescience (miscoding, inaccuracy, or surfeit), but this increase must be compensated by a larger decrease in one of the others, so that total nescience does not rise. A simultaneous increase in all of them would clearly indicate regression.

Nevertheless, reality is more complicated. Our current measurements of miscoding, inaccuracy, and surfeit are merely estimations, approximations that are themselves subject to error and limited by our tools and understanding. Consequently, it is not always evident whether a particular refinement is truly superior. From a practical standpoint, we therefore relax the requirement of strict monotonic decrease and instead accept the weaker condition that nescience should decrease on average over time. Temporary setbacks or local increases are tolerable, as long as the general trajectory is toward a deeper and more refined understanding of the entity under study.

We can use this property of the reduction of nescience as a criterion to distinguish between valid scientific disciplines and those that fall outside the scope of science, a challenge known as the *demarcation problem* in the philosophy of science. In scientific fields, successive refinements in descriptions and representations tend to yield a measurable decrease in nescience, signifying genuine progress in understanding. In contrast, non-scientific theories, including pseudosciences, typically do not exhibit this pattern. Despite the introduction of new descriptions or representations, there is no meaningful reduction in nescience over time. This implies that such disciplines fail to produce cumulative knowledge or deeper insights. In pseudoscientific domains, further research often leads to reinterpretations, embellishments, or rhetorical shifts, rather than the kind of substantive progress that characterizes scientific inquiry. As a result, these areas remain stagnant, unable to break new ground or approach perfect knowledge.

1.10 Unknown Unknown

We have previously discussed the existence of an *unknown unknown* area, comprising problems for which we not only lack solutions but whose very existence escapes our awareness. Within the framework of the theory of nescience, our goal is to develop a systematic procedure to identify and explore potential research entities hidden in this region. One approach could involve randomly generating binary strings and querying an oracle to assess whether any of them closely approximate the representation of a (hopefully unknown) entity. This conceptually embraces the idea of discovering new knowledge by pure chance. However, the sheer magnitude of the space of possible strings makes this brute-force strategy computationally impractical. Consequently, we must seek more efficient and guided methods for navigating this uncharted domain.

To discover what lies hidden in the unknown unknown, we must first delineate the area that encompasses everything already known. This known region comprises two types of topics. The first are the known knowns—topics that are well understood, where our descriptions are accurate, concise, and reliable. The second group includes the known unknowns, problems we are aware of but for which we still lack complete or satisfactory explanations. The boundary separating this region of known topics from what lies beyond is what we refer to as the *knowledge frontier*. It represents the outer limit of our current understanding, a conceptual demarcation where the known ends and the unexplored begins. Any entity that exists beyond this frontier—one that has not yet been identified or studied,constitutes a *new research entity*, residing in the domain of the unknown unknown.

Yet, identifying in practice the exact list of already known topics is far from straightforward. The main challenge lies in determining which topics have already been studied and formally documented through published research. Scientific knowledge is dispersed across countless articles, journals, and disciplines, and there is no single, unified repository that captures the full extent of human understanding. Moreover, variations in terminology and differences in how topics are categorized further complicate the task. Thus, establishing the scope of the known demands careful analysis of bibliographic data, ontological classifications, and, often, expert consensus.

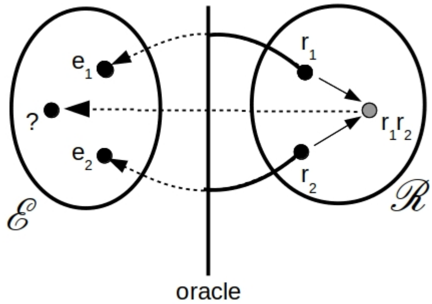


Figure 1.7: Discovering new research entities.

In this book, we explore an alternative strategy for identifying new research directions by combining concepts that are already known. The basic idea is straightforward: by taking two distinct representations, each corresponding to a different known entity, we identify a new entity by joining them into a single representation. To make this approach systematic, we assume that the space of valid representations is closed under such combinations—in other words, that combining any two representations will always yield another valid one. This assumption enables us to construct joint topics in a mechanical way and to explore their potential to uncover novel insights or previously unexamined questions. In practical terms, this involves computing all possible combinations of known entities and selecting those that appear to have the greatest potential to yield new and interesting research directions. However, the precise meaning and significance of any new entity formed in this way must still be determined through further investigation and reflection.

■ **Example 1.6** We could combine compelling topics from the field of theoretical computer science with those from phenomenology to identify promising new research directions. By merging the concepts of "minimum complexity computer programs" and "self-awareness," we arrive at a potential new research topic: "minimum complexity self-aware computers." This would involve investigating the minimum complexity required for a computer program to possess the capacity for self-awareness. ■

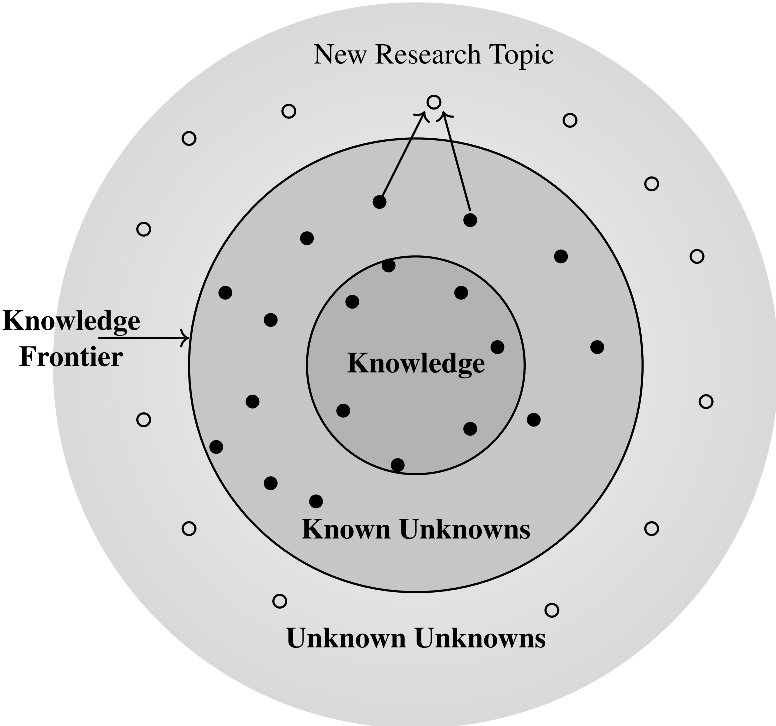


Figure 1.8: The structure of knowledge

As wisely stated by Saint John of the Cross, *to go where we do not know, we must go by a path we do not know*. This insight holds true in scientific discovery: the likelihood that a combination of two already known entities leads to a new entity located in the unknown unknown is greater when the entities being combined are themselves poorly understood. In contrast, combining well-understood entities is more likely to produce a result that remains within the bounds of current knowledge—that is, inside the knowledge frontier (see Figure 1.8). This is because the areas surrounding a well-known entity are often already thoroughly explored, leaving little room for the kind of novelty we are looking for, namely, ideas that lie beyond the current boundaries of knowledge and have the potential to open up entirely new lines of inquiry.

Another approach to increasing the chances of reaching the unknown unknown is by combining topics from two distinct fields of knowledge. The likelihood that such a combination has already been explored is relatively low, primarily because it would require someone with substantial expertise in both areas—a rarity in today's academic landscape, where scientists are increasingly specialized in narrow domains. Interdisciplinary combinations, therefore, offer a fertile ground for novel discoveries, as they may produce connections that have never been examined or even imagined within the confines of a single discipline.

References

The theory of nescience builds upon several well-established foundations across information theory, computability, algorithmic complexity, and the philosophy of science. The following references provide the theoretical background and conceptual tools necessary to understand and contextualize the ideas introduced in this chapter.

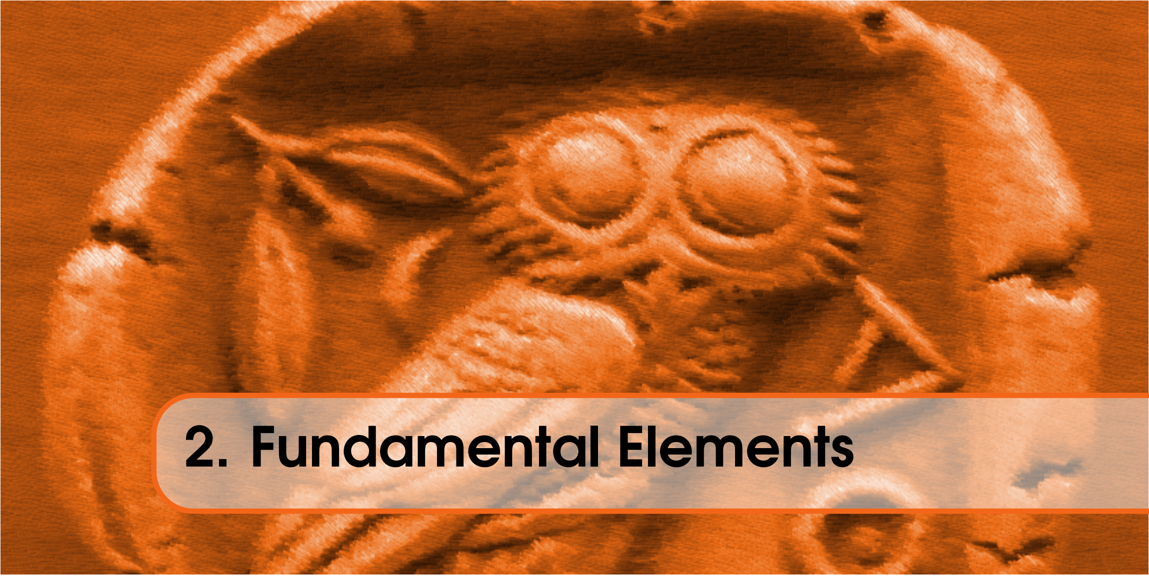
Sipser's book [Sip12] is a widely respected introduction to formal languages, automata, and computability theory. It lays the groundwork for understanding which descriptions are computationally feasible, an essential aspect of the theory of nescience, which assumes that knowledge must be computable to be meaningful.

[LV13] is a comprehensive volume that presents the theory of Kolmogorov complexity, which formalizes the idea of description length using the shortest program capable of generating a given object. The concepts developed by Li and Vitányi are central to the theory of nescience, especially in defining metrics such as inaccuracy, miscoding, and surfeit based on algorithmic information.

Chalmers' book [Cha13] offers a critical and historical introduction to the philosophy of science. It examines the assumptions, limits, and methodologies of scientific practice. This perspective is invaluable for situating the theory of nescience within the broader discourse on how scientific knowledge is constructed, evaluated, and refined over time.

[CT12] is a foundational text in information theory, providing the mathematical framework for understanding concepts such as entropy, mutual information, and data compression. It serves as a rigorous yet accessible introduction to how information can be quantified, transmitted, and encoded, ideas that relate the notions of description length in the theory of nescience.

Part 1: Foundations



2. Fundamental Elements

We are all agreed that your theory is crazy.
The question which divides us is whether it is crazy enough.
Niels Bohr

The first step in quantifying our lack of knowledge involves the precise identification of the research entities of interest. The elements of this collection depend largely on the specific application of the theory of nescience. Each application requires a distinct set of entities, whether mathematical objects, living organisms, human needs, or otherwise. Fortunately, the process of quantifying what we do not know remains consistent across all such domains.

The next step is to devise a procedure for representing the identified entities as strings of symbols. Accurately encoding a research entity is a complex and unresolved epistemological challenge. The solution proposed within the theory of nescience is based on the concept of oracle Turing machine. The practical feasibility of this solution depends largely on the abstractness of the entities being studied. For example, encoding abstract mathematical objects poses significant difficulties and often requires an approximation. In contrast, encoding computer programs is relatively straightforward, as they are already expressed as strings.

Once a suitable method for encoding the original entities into string-based representations has been established, the final step is to produce a description. This description should be both accurate and concise, reflecting our current understanding of the representation. In the theory of nescience, descriptions are required to be computable, meaning that a computer must be able to fully reconstruct the original representation from its description. However, descriptions refer to representations, that is, the way entities are encoded, not to the entities themselves. As a result, how well a description captures knowledge about an entity depends largely on the quality of the representation used.

In this chapter, we will formalize these core concepts: entities, representations, and descriptions, among others. We will also explore what constitutes a perfect description, how to compute the combined representation of multiple entities, and how to describe a representation assuming some prior background knowledge. Additionally, we will examine the concept of a research area and its associated properties.

2.1 Entities

Defining the nature of a research entity is a complex and unresolved philosophical problem. We approach this complexity from a fundamentally pragmatic perspective, rather than a philosophical-otological one. Our theory starts from the premise that there exists a non-empty set of *entities* that we seek to understand.

Notation 2.1. *We represent the set of research entities of interest as $\mathcal{E}$.*

The contents of $\mathcal{E}$ depend on the specific domain in which theory of nescience is employed, and are usually aligned with a specific area of knowledge. Examples of entity sets could include: research components in mathematics (abstract); the kingdom Animalia (living entities); known and unknown human needs (abstract); all potential computer programs (strings), etc. From a formal point of view, $\mathcal{E}$ is not a well-defined set, since there is usually no rule or procedure for deciding which elements comprise this set.

The abstract nature of $\mathcal{E}$ offers certain advantages, but also imposes significant restrictions. The main restriction is that our definition of nescience is, in most cases, a non-computable quantity, which requires the use of approximations in practice. The main advantage is that the new concepts and methods presented in this book can be applied to a wide range of problems, not limited only to the search for new scientific knowledge.

In the theory of nescience, the possibility of using universal sets is excluded; that is, the existence of a set ξ containing everything cannot be assumed. The problem with universal sets is that they contravene Cantor's theorem (see the example 2.1). Cantor's theorem proves that the power set $\mathcal{P}(\xi)$, consisting of all possible subsets of ξ, has more elements than the original set ξ. This contradicts the assumption that ξ includes everything. In the theory of nescience, the set $\mathcal{E}$ must be a specific set.

■ **Example 2.1 — Cantor's theorem.** Cantor's theorem proves that for any set A, $d(A) < d(\mathcal{P}(A))$. Consider $f : A \to \mathcal{P}(A)$, a function that maps each element $x \in A$ to the set $\{x\} \in \mathcal{P}(A)$; evidently, f is injective, implying $d(A) \leq d(\mathcal{P}(A))$. To substantiate that the inequality is strict, let's assume there exists a surjective function $g : A \to \mathcal{P}(A)$ and consider the set $B = \{x \in A : x \notin g(x)\}$. As g is surjective, there must exist a $y \in A$ such that $g(y) = B$. This, however, raises a contradiction, $y \in B \Leftrightarrow y \notin g(y) = B$. Consequently, the function g cannot exist, therefore $d(A) < d(\mathcal{P}(A))$. ■

In the theory of nescience, not all conceivable sets are acceptable, as some may give rise to paradoxes. Take, for example, Russell's paradox, which proposes a set R consisting of all sets that are not members of themselves. The paradox arises when we try to discern whether R is a member of itself (see the example 2.2). To avoid such problems, the theory of nescience is based on the Zermelo-Fraenkel axiom set, along with the Axiom of Choice. The *axiom of separation* (if P is a property with parameter p, then for any set x and parameter p there exists a set $y = \{u \in x : P(u)\}$ that includes all those sets $u \in x$ that have property P) allows the use of this notation only to construct sets that are subsets of already existing sets. A more extensive *axiom of comprehension* (if P is a property, then there exists a set $y = \{u : P(u)\}$) would be required to allow sets like the one proposed by Russell's paradox. Russell's paradox arises from the use of an unrestricted comprehension principle. In the axioms of ZFC, and in the theory of nescience, the axiom of comprehension is considered false.

■ **Example 2.2 — Russell's Paradox.** Suppose R is the set of all sets not members of themselves, such that $R = \{x : x \notin x\}$. The contradiction arises when querying if R is a member of itself. If R is not a member of itself, by its own definition, it should be; conversely, if R is declared to be a member of itself, its definition dictates it should not be. Symbolically, this can be written as $R \in R \Leftrightarrow R \notin R$. ■

In the theory of nescience, we do not address the classic problems of ontology, that is, the classification of entities that exist in the world and can be known. Furthermore, we do not attempt to resolve epistemological questions, such as how scientific knowledge is validated by evidence, or what the nature of that evidence is.

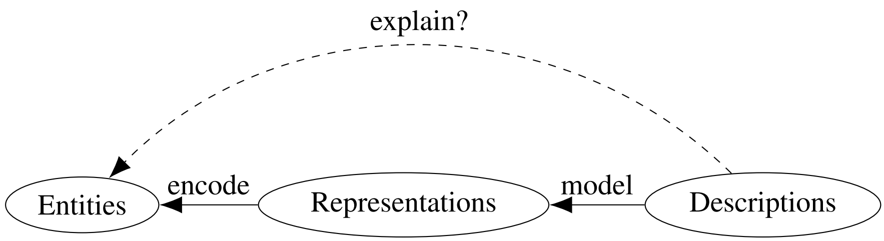


Figure 2.1: The Problem of Understanding

Once a set $\mathcal{E}$ of entities has been selected, the next step is to uniquely encode them as strings of symbols, which will make them easier to describe. A method for doing this encoding efficiently is described in the following section.

2.2 Representations

The representation of the entities that compose the set $\mathcal{E}$, which can be abstract in nature, poses important epistemological challenges that have been the subject of research for more than two millennia (see Section G.4 for a brief overview of the solutions proposed by the scientific community and their limitations). This book describes a possible solution to this complex problem, which has certain advantages, but also disadvantages. Our approach proposes dividing the problem of scientific representation into two interconnected subproblems: the encoding of entities by means of representations, and the modeling of these representations by means of descriptions. Thus, scientific models would explain the entities indirectly through their representations (see Figure 1.1 in the Introduction of the book, reproduced in this section for ease of reference). In this section we will focus on the aspects related to encoding, and in Section 2.5 on the descriptions.

Within the field of Kolmogorov complexity, the representation issue is tackled by presupposing that the set $\mathcal{E}$ is well-defined, countable, and that a total encoding function $f : \mathcal{E} \to \mathbb{N}$ exists, mapping the set of entities to the set of natural numbers (akin to Gödel numbering). The nescience theory similarly embraces this concept of encoding entities via numbers, or, in other words, strings of symbols. However, our approach to the problem of encoding an arbitrary set $\mathcal{E}$ involves an inversion of the problem. This involves defining a partial function $\mathcal{O}_\mathcal{E} : \mathcal{S}^* \to \mathcal{E}$ that maps the well-defined set $\mathcal{S}^*$ (comprising all possible finite strings from an alphabet $\mathcal{S}$) to the potentially non-countable and non-well defined set $\mathcal{E}$ containing the entities of interest.

Our function $\mathcal{O}_\mathcal{E}$, which depends on the set $\mathcal{E}$, operates much like an oracle (taking inspiration from the concept of an oracle Turing machine as per Definition C.5.1). This function has the capacity to entirely reconstruct an entity $\mathcal{O}_{\mathcal{E}}(x) \in \mathcal{E}$ using its encoding string $x \in \mathcal{S}^*$, without the need for additional information. Evidently, this oracle is an abstract concept, and its construction in the real world would be impossible for most sets $\mathcal{E}$. However, the theoretical existence of this oracle assists in the elucidation and verification of key attributes of the scientific discovery process. Due to its oracle nature, $\mathcal{O}_{\mathcal{E}}$ has limitations with respect to the mathematical operations in which it can be used, as will be explained in the subsequent paragraphs.

Our premise is based on the assumption that there exists a single, objective physical world that is independent of observers. In addition, we assume that, for certain collections of entities $\mathcal{E}$, it is logically coherent to postulate the existence of an oracle $\mathcal{O}_{\mathcal{E}}$ (see the discussion of the scientific representation problem in Section G.4).

For the purposes of this book, without any loss of generality, we will exclusively regard binary strings as the means of encoding entities.

Definition 2.2.1 Given $\mathcal{E}$ as a set of entities, a *representation function* is defined as an oracle partial function $\mathcal{O}_{\mathcal{E}} : \mathcal{B}^* \to \mathcal{E}$ that maps elements of the set $\mathcal{B}^*$, which comprises all conceivable finite binary strings, to the elements of the set $\mathcal{E}$, corresponding to the entities under examination.

Within this framework, only the elements of the set $\mathcal{B}^*$, that is, binary strings, are eligible to serve as representations of entities (see problem of ontology in Section G.4). We do not permit other forms of physical models, including drawings, unless they can be transcribed into binary strings. We do not distinguish between scientific representations and other forms of representations (see representational demarcation in Section G.4). The oracle assumes the responsibility of determining which entity is encoded by each representation. It is also pivotal to note that the oracle $\mathcal{O}_{\mathcal{E}}$ is a partial function, meaning not all potential strings represent entities (targetless models are allowed in the theory of nescience, see Section 3.4 and Section G.4).

■ **Example 2.3** For a given set of entities $\mathcal{E}$, the existence of a representation oracle $\mathcal{O}_{\mathcal{E}}$ does not imply its uniqueness. For instance, a binary negation oracle (which transforms the zeros of a binary string into ones, and the ones into zeros), assigning to each string $x \in \mathcal{B}^*$ the entity $\mathcal{O}_{\mathcal{E}}(\neg x)$, would also qualify as a representation function. ■

Rather than deploying individual oracles, we could have employed a universal oracle machine. This is a machine $\mathcal{U}_{\mathcal{O}}$ which, given the encoding of an oracle $\mathcal{O}_{\mathcal{E}}$ and a string s as input, computes $\mathcal{U}_{\mathcal{O}}(\langle \mathcal{O}_{\mathcal{E}}, s \rangle) = \mathcal{O}_{\mathcal{E}}(s)$. Universal machines are particularly applicable to the universal set ξ, encompassing all entities. However, such an approach would complicate the process of scientific discovery in practical terms. Instead, we choose to work with entity sets $\mathcal{E}$ corresponding to different areas of knowledge, choosing a single oracle $\mathcal{O}_{\mathcal{E}}$ for each set $\mathcal{E}$ (the most suitable one according to our current knowledge and our practical needs).

■ **Example 2.4** Consider the case when the subjects of study are animals. Initially, one might use detailed physical descriptions of the animals as encodings. In this scenario, the oracle would be a hypothetical machine capable of reconstructing the original animal from its description. As our understanding of biology advances, we might instead adopt an alternative encoding based on the animals' DNA. Both of these encodings serve as valid representations of the entities. ■

As illustrated in Example 2.3 and Example 2.4, the entities in $\mathcal{E}$ can be encoded in multiple ways (see the problem of style in Section G.4). Different oracles accommodate different encoding schemes. Some strings provide more accurate representations of an entity than others (see the standard of accuracy in Section G.4). The optimal representation depends on the type of questions we aim to answer. Using a particular encoding style with an oracle designed for a different style may lead to unexpected outcomes. Our objective should be to employ representations that minimize the size of the oracle—that is, the amount of prior knowledge presumed to be embedded within it.

■ **Example 2.5** Consider $\mathbf{X}_t$ as a time series consisting of m measurements $x_1, \ldots, x_m$ collected at fixed intervals from a physical phenomenon exhibiting sinusoidal behavior. Suppose we have trained a multi-layer perceptron neural network nn that perfectly fits the data, meaning it returns x_t when given a time t as input. By analyzing the cycles in the time series, one would naturally identify a sine function as the most appropriate model for the underlying physical process. However, no existing machine learning methodology would arrive at this conclusion if provided solely with the neural network's architecture (i.e., the number of layers, their sizes, and the trained weights). Clearly, the oracle is sufficiently powerful to recognize this underlying structure. ■

Remember that the oracle operates as a partial function, meaning that not every string must represent an entity. The less information a representation contains, the more difficult it becomes to understand how the oracle works. It is essential to be cautious with representations that fail to capture the full structure of the original entities, as this can introduce bias into our analyses. Chapter 3 offers a detailed discussion of the types of errors arising from the miscoding of abstract entities, emphasizing that representations must not only correspond to entities, but also that entities must be relevant to their representations (see the requirement of directionality in Section G.4).

We employ an oracle function rather than an oracle relation $\mathcal{R}_{\mathcal{O}} \subset \mathcal{B}^* \times \mathcal{E}$, not to merely associate strings with their corresponding entities, but to reconstruct an entity from its representation. The oracle's ability to recover original entities underpins our capacity to make hypotheses about entities based on their representations (see surrogative reasoning in Section G.4). According to the theory of nescience, scientific inquiry involves not only learning how to encode entities properly but also understanding the mechanisms by which oracles decode them. For scientific inquiry to be practically effective, these oracles should ideally be minimal in size.

The purpose of encoding entities in the theory of nescience differs fundamentally from that in Shannon's information theory (see Chapter D), as illustrated in Example 2.6.

■ **Example 2.6** Take, for instance, a set $\mathcal{E}$ consisting of two books: "The Ingenious Nobleman Sir Quixote of La Mancha" and "The Tragedy of Romeo and Juliet". We might encode the first book with the string "0" and the second with the string "1". While these strings allow us to uniquely identify each book within the set, they do not qualify as valid encodings within the framework of the theory of nescience. In information theory, the goal is to uniquely identify an object based on a reference, assuming mutual agreement between the sender and the receiver about the mapping from references to objects. In contrast, the theory of nescience seeks representations that preserve the richness and detail of the original entities. For example, it would be impossible to hypothesize about Cervantes' influence on Shakespeare using only the strings "0" and "1". ■

One possible response to the limitation discussed in Example 2.6, where entities are encoded using overly simplistic strings that fail to capture their internal structure, would be to require the set $\mathcal{E}$ to be infinite, as is done in Kolmogorov complexity. This requirement avoids pathological cases in which too many entities are assigned trivial or arbitrary encodings. However, merely increasing the size of $\mathcal{E}$ does not solve the fundamental issue: even with an infinite set of entities, many encoding schemes still fall short of supporting surrogative reasoning. That is, they do not allow us to make meaningful inferences about the original entities based solely on their representations. To enable such reasoning, the encoding must preserve essential structural and semantic features of the entities, not just their identity.

We distinguish between *knowable* and *unknowable* entities. Knowable entities are those that can, in principle, be understood through scientific

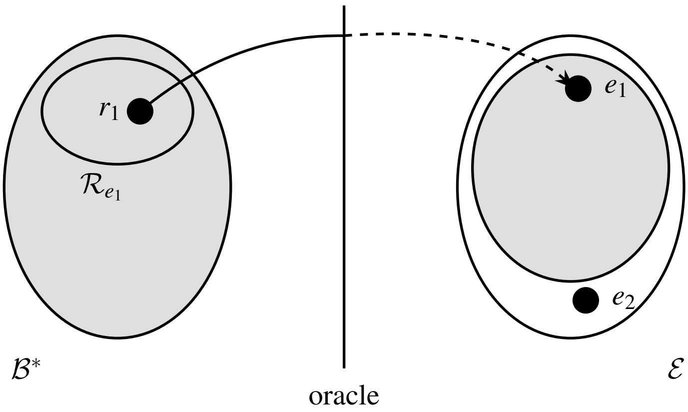


Figure 2.2: Encodings and Entities

inquiry (see Section G.2). Unknowable entities, on the other hand, lie beyond the reach of human comprehension—either because they are inherently inaccessible to observation and reasoning, or because they exceed the cognitive or methodological limits of science.

Definition 2.2.2 We say that an entity $e \in \mathcal{E}$ is *knowable* if there exists at least one $r \in \mathcal{B}^*$ such that $\mathcal{O}_{\mathcal{E}}(r) = e$. An entity $e \in \mathcal{E}$ is *unknowable* if it is not knowable.

A priori, it is not possible to determine whether an entity $e \in \mathcal{E}$ is knowable, unknowable, or only partially knowable. Identifying suitable knowable entities for study is a matter of trial and error. In this book, we say nothing further about unknowable entities, except to note that their unknowability can neither be proven nor discovered.

Definition 2.2.3 Let $e \in \mathcal{E}$ be a knowable entity. We define the *set of representations* for e, denoted by $\mathcal{R}_e$, as $\{r \in \mathcal{B}^* : \mathcal{O}_{\mathcal{E}}(r) = e\}$.

In Figure 2.2, we present a depiction of a hypothetical oracle mapping from the set of finite binary strings $\mathcal{B}^*$ to the set of entities $\mathcal{E}$. The figure also highlights a particular entity e_1, the subset of strings $\mathcal{R}_{e_1}$ that represent this entity, and a specific representation r_1. Since the set $\mathcal{E}$ is, in general, not well defined, the inverse function $\mathcal{O}_{\mathcal{E}}^{-1}(e_1)$ cannot be computed in practice.

A consequence of working with finite strings as representations is that some entities may not be encoded by any representation (see the gray areas in Figure 2.2; in particular, the entity e_2 is not encoded by any string). Intuitively, this reflects the fact that, in certain domains of knowledge, the number of possible problems far exceeds the number of available solutions.

■ **Example 2.7** If the collection of entities under study consists of real numbers, then there exist numbers that cannot be encoded using finite binary strings. This is because the set $\mathbb{R}$ has the cardinality of the continuum, whereas the set $\mathcal{B}^*$ is countable. ■

Since our knowledge of the entities and the internal workings of the oracle is incomplete, in practice we work with a different set of strings, denoted by $\hat{\mathcal{R}}_e$, which we believe are close approximations of the true representations $\mathcal{R}_e$ that encode the entity e. The elements of this set typically change over time, as our understanding of the entities in $\mathcal{E}$ and of how the oracle encodes them improves. The more abstract the set of entities is, the more difficult it becomes to approximate them as strings (see Chapter 3).

■ **Example 2.8** The entity "luminiferous ether" was a theoretical postulate describing a hypothetical medium through which light was believed to propagate. It was proposed to explain how wave-based light could travel through empty space. However, in 1887, the Michelson-Morley experiment provided strong evidence against the existence of ether. Later, Einstein's special theory of relativity offered a successful explanation for the propagation of light in a vacuum, leading to the complete abandonment of the ether concept. ■

If the chosen oracle is not minimal, determining whether a string is a valid representation of an entity requires understanding the internal workings of the oracle. A *non-minimal oracle* is one in which part of the information needed to reconstruct the original entity is embedded within the oracle itself, rather than being explicitly encoded in the representation string. Although using non-minimal oracles can simplify the research process by offloading complexity to the oracle, it obscures the boundary between what is encoded and what is assumed, making it harder to analyze or generalize the representation mechanism.

R One of the fundamental challenges in science—and in human intellectual activity more broadly—is the tendency to confuse symbols with the things they represent. The theory of nescience has been carefully designed to avoid this issue by clearly distinguishing between research entities and their representations. However, making this distinction explicit at every step would render the book unnecessarily difficult to read. We have aimed to strike a balance between clarity of exposition and rigor of definition. Occasionally, especially when introducing new ideas, we use the term *topic* to refer broadly to an entity, a representation, or both. Nevertheless, in all mathematical definitions and propositions, this distinction is made unambiguous. In case of any uncertainty, the formal definitions should be taken as the definitive reference.

2.3 Invalid Representations

It may happen that the representation we are using for an entity $e \in \mathcal{E}$ is incorrect. That is, instead of working with a string $r \in \mathcal{B}^*$ that perfectly encodes e, we are studying another string $r' \in \mathcal{B}^*$ which is, hopefully, close to r but not necessarily identical. We are interested in computing the distance between the string r' and the correct representation r as a quantitative measure of the error introduced by using an incorrect encoding (see Chapter 3). Unfortunately, we do not know r, since in most practical applications there does not exist a computable function from $\mathcal{E}$ to $\mathcal{B}^*$. The only tool at our disposal is an abstract oracle machine $\mathcal{O}_{\mathcal{E}}$ that knows which strings represent each entity. Recall from Section 2.2 that we propose to address the scientific representation problem by introducing an abstract oracle $\mathcal{O}_{\mathcal{E}} : \mathcal{B}^* \to \mathcal{E}$, which maps the set $\mathcal{B}^*$ of all finite binary strings to the set $\mathcal{E}$ of entities under study.

We begin by distinguishing between valid representations, strings that contain all the information required by the selected oracle to reconstruct an entity, and non-valid representations.

Definition 2.3.1 Let $\mathcal{E}$ be a collection of entities, and let $\mathcal{O}_{\mathcal{E}}$ be a decoding function. We define the set of *valid* representations for $\mathcal{E}$ with respect to the encoding function $\mathcal{O}_{\mathcal{E}}$, denoted by $\mathcal{R}^{\star}_{\mathcal{O}_{\mathcal{E}}}$, as the subset of representations that perfectly encode an entity in $\mathcal{E}$, according to $\mathcal{O}_{\mathcal{E}}$.

The set $\mathcal{R}^{\star}_{\mathcal{O}_{\mathcal{E}}}$ is generally unknown, as it is a subset of $\mathcal{B}^*$ whose definition depends on an abstract and not well-defined oracle. Intuitively, a representation is considered valid if it contains all the necessary information for the oracle to reconstruct the original entity without relying on any external sources. A valid representation must not include incorrect symbols, nor omit any relevant information, otherwise, the oracle would be unable to reconstruct the entity accurately.

Furthermore, we require that the oracle can not only reconstruct an entity from a representation, but also derive the set of valid representations for a given entity. From this perspective, a representation that includes non-relevant information cannot be considered valid, since that extraneous part cannot be generated by the oracle solely from the entity.

■ **Example 2.9** The astronomical data used during the time of Ptolemy to record the positions of celestial bodies throughout the year constituted a non-valid encoding of the entity "position of celestial bodies," due to its inaccuracy. A better encoding was later provided by the more precise observations of Tycho Brahe. Today, we possess even more accurate encodings. Adding the name of the person who collected the data to the dataset would be an example of a representation that includes non-relevant information. ■

Recall that, in our framework, we only allow representations of entities in the form of finite binary strings. Drawings, mathematical formulas, or datasets may serve as representations, provided they can be encoded as binary strings and are recognized as valid by the selected oracle. Each string represents one, and only one, entity. Naturally, different oracles may define different sets of valid representations. Throughout this work, we assume that a specific representation oracle $\mathcal{O}_{\mathcal{E}}$ has been chosen to encode the set $\mathcal{E}$ of entities under study.

Notation 2.2. *We will denote the set of valid representations of $\mathcal{E}$ by $\mathcal{R}^{\star}_{\mathcal{E}}$ when there is no ambiguity regarding the oracle $\mathcal{O}_{\mathcal{E}}$ in use.*

We can similarly define the set of valid representations for an individual entity e.

Definition 2.3.2 We define the set of valid representations for an entity $e \in \mathcal{E}$, denoted by $\mathcal{R}^{\star}_{e}$, as the subset of representations that perfectly encode the entity e; that is, $\mathcal{R}^{\star}_{e} = \mathcal{R}^{\star}_{\mathcal{E}} \cap \mathcal{R}_{e}$.

As we have seen in Example 2.4 there could be more than one valid representation for some entities, even it the oracle is restricted to a particular style. It might also happen that the set of valid representations is empty, that is, there is no valid representation for that entity. In that case the entity will be unknowable.

Notation 2.3. *We denoted by $r^{\star}_{e} \in \mathcal{R}^{\star}_{\mathcal{E}}$ the fact that r is a valid representation of the entity e.*

A consequence of working with approximations instead of true representations is that some of the candidate strings currently in use may encode a different entity than the one we intended to study.

■ **Example 2.10** In 1961, Soviet physicist Nikolai Fedyakin conducted a series of experiments that appeared to reveal a new form of water. This substance, named polywater, exhibited unusual properties: a higher boiling point, a lower freezing point, and much greater viscosity than ordinary water. However, later experiments demonstrated that polywater was simply ordinary water contaminated with small amounts of impurities. ■

We can safely assume (without logical contradiction) that the oracle machine not only knows which representations correspond to which entities, but also how far any string $r \in \mathcal{B}^*$ is from being a valid representation $r^{\star}_{e} \in \mathcal{R}^{\star}_{\mathcal{E}}$.

If a representation r is non-valid, the oracle will identify the closest valid representation and assume they both refer to the same entity.

The oracle defines an equivalence relation that partitions the set $\mathcal{B}^*$ into equivalence classes. Each class corresponds to an entity in $\mathcal{E}$, although it may happen that some entities in $\mathcal{E}$ do not have any associated class, these are what we call the unknowable unknowns. Every string is associated with some entity, but some representations are better than others (i.e., they yield lower nescience). No string can belong to more than one entity. Moreover, for any given collection $\mathcal{E}$, multiple valid oracles may exist.

Definition 2.3.3 Let $\mathcal{B}^*/\mathcal{O}$ be the quotient set defined by the oracle's equivalence relation over the set of binary strings. We call each class in this quotient set an *entity class*, denoted by $[e]$, that is, $[e] \in \mathcal{B}^*/\mathcal{O}$.

2.4 Joint Representations

We saw in the previous section that there is more than one way to encode an entity $e \in \mathcal{E}$, this collection of encodings is what we called the set $\mathcal{R}_e$ of representations of the entity. Some of these representations are of high quality, in the sense that they contain all the information required by the oracle to reconstruct (by whatever means the oracle employs) the original entity. However, the set $\mathcal{R}_e$ also includes low-quality representations, that is, representations that lack many of the details necessary to fully reconstruct the entity. Moreover, $\mathcal{R}_e$ may contain representations that include incorrect information: symbols that the oracle will automatically disregard during reconstruction but that may mislead us when trying to understand the entity.

If we want to increase our knowledge about an entity, we must identify the best possible representation for that entity, that is, one that is both complete and correct. One way to achieve this is to try different strings until we discover a high-quality representation. However, this method can be extremely time-consuming and impractical. A more efficient approach is to enhance a poor representation by adding missing symbols or by combining known representations that each contain partial information. Both approaches require introducing the concept of a joint representation.

Definition 2.4.1 Let $s,t \in \mathcal{R}_\mathcal{E}$ be two different representations. The *joint representation* of s and t is defined as the concatenated string st.

■ **Example 2.11** Suppose the research entity e of interest is the set of causes of lung cancer. To study this entity, we have measured a collection of risk factors in a random sample of the population (smoking, exercise, diet, age, etc.). However, due to a flaw in the sampling procedure, all the samples correspond to a specific subgroup of the population, for instance, males. This dataset constitutes a representation s of our entity e, but a poor one, as it is strongly biased. If we have a second representation t, corresponding to sample data from females, the joint representation st will be superior to either s or t considered in isolation. ■

It would be desirable for the set of representations $\mathcal{R}_{\mathcal{E}}$ to be closed under the operation of concatenation, meaning that if s and t are representations of an entity e, then their concatenation st would also be a representation of some entity (not necessarily the same one). Unfortunately, this is not the case, since the oracle function is partial; it does not assign an entity to every possible binary string. Moreover, we do not even require the set of representations $\mathcal{R}_e$ for a given entity e to be closed under concatenation. It is entirely possible that two strings $s \in \mathcal{R}_e$ and $t \in \mathcal{R}_e$ produce a concatenated string st that does not belong to $\mathcal{R}_e$.

The concept of joint representation is defined for any pair of strings $s,t \in \mathcal{R}_{\mathcal{E}}$, even if they do not belong to the same set of representations $\mathcal{R}_e$, that is, even when $\mathcal{O}_{\mathcal{E}}(s) \neq \mathcal{O}_{\mathcal{E}}(t)$. This ability to combine representations of different entities will prove particularly useful for the discovery of new research entities that are currently unknown (see Section **??**).

The operation of string concatenation is associative; that is, for all $r,s,t \in \mathcal{R}_{\mathcal{E}}$, we have $(rs)t = r(st)$. This property underlies the algebraic structure of the set of representations.

Proposition 2.4.1 The set $\mathcal{R}_{\mathcal{E}}$ of representations, together with the operation of concatenation, has the structure of a free monoid.

Proof. As shown in Section A.2, the operation of string concatenation on $\mathcal{R}_{\mathcal{E}}$ is associative, and the empty string λ serves as the identity element. ■

We do not require the operation of joining representations to be commutative with respect to the oracle function. Given representations $s,t \in \mathcal{R}_{\mathcal{E}}$, it may happen that the concatenated strings st and ts represent different entities—that is, $\mathcal{O}_{\mathcal{E}}(st) \neq \mathcal{O}_{\mathcal{E}}(ts)$.

The concept of joint representation can be extended to any arbitrary, but finite, collection of representations. This allows us to incorporate multiple partial representations into our research or to use them in the process of discovering new entities.

Definition 2.4.2 Let $r_1, r_2, \ldots, r_n \in \mathcal{R}_{\mathcal{E}}$ be a finite collection of representations. The *joint representation* of $r_1, r_2, \ldots, r_n$ is defined as the concatenated string $r_1 r_2 \ldots r_n$.

Unfortunately, the set $\mathcal{R}_{\mathcal{E}}$ is not closed under the operation of concatenation of multiple, finite, representations.

We have seen that the concatenation of two or more representations of an entity can result in a string that encodes a different entity from the original. Remarkably, this phenomenon can occur even when the individual representations being concatenated all correspond to the same entity. This non-trivial behavior opens the door to a novel strategy for scientific discovery: the generation of new, previously unknown entities through the systematic combination of representations of known entities.

■ **Example 2.12** Consider a research scenario in which the entities under study are chemical compounds, and the representations are strings encoding molecular descriptors. Suppose s encodes a compound known for its anti-inflammatory properties, and t encodes a structurally similar compound with anti-viral properties. While both s and t individually map to well-known compounds via the oracle, the concatenation st may correspond to a novel hybrid molecule whose biological activity has not yet been characterized. In this case, st represents a new research entity, possibly a candidate for drug discovery—that was not explicitly part of the original knowledge base. ■

2.5 Descriptions

So far, our goal in working with strings from $\mathcal{B}^*$ has been to construct encodings, or representations, that are as complete and detailed as possible for the entities in $\mathcal{E}$, regardless of their length. However, as stated in the preface of this book, human understanding requires the formulation of concise models of these entities, since human reasoning cannot operate effectively on lengthy representations.

■ **Example 2.13** In Example 2.11, we showed that a good representation of the entity "lung cancer" could be a dataset in which various risk factors are measured. However, smokers do not decide to quit smoking because they have studied and understood this extensive dataset. Rather, they do so because they understand the much simpler derived model: "smoking increases the risk of lung cancer." ■

A description or model[1] is a finite binary string that is mapped to a representation of an entity (see Figure 1.3 in Chapter 1). Importantly, descriptions do not directly model the entities themselves (i.e., the target systems); instead, they operate on representations of those entities (encodings in the form of strings) serving as approximations of the original entities through those representations.

In the theory of nescience, we require that descriptions be computable, so that the original representations can be fully and effectively reconstructed from them. This requirement of computability allows us to clearly define the limits of the concept of a "description." For example, paradoxes involving

[1] In the theory of nescience, the terms "description" and "model" are used interchangeably.

self-reference, such as the Berry paradox (i.e., "the smallest positive integer not definable in less than twelve words," see Chapter 1), can be addressed within the framework of computability.

Definition 2.5.1 — Model. Let $d \in \mathcal{B}^*$ be a binary string of the form $d = \langle TM, a \rangle$, where TM is the encoding of a prefix-free Turing machine and a is the input string to that machine. If $TM(a)$ is defined, then d is called a *description*.

Intuitively, a description consists of two parts: a Turing machine that captures and compresses the regularities present in the representation, and a string that contains what remains, that is, the incompressible or random part.

Definition 2.5.2 We define the *set of descriptions*, denoted by $\mathcal{D}$, as:

$$\mathcal{D} = \{d \in \mathcal{B}^* : d = \langle TM, a \rangle \wedge TM(a) \downarrow\}.$$

Let $r \in \mathcal{B}^*$ be a representation. We define the set of *descriptions for r*, denoted by $\mathcal{D}_r$, as:

$$\mathcal{D}_r = \{d \in \mathcal{D} : TM(a) = r\}.$$

Finally, given an entity $e \in \mathcal{E}$, we define the set of *descriptions for e*, denoted by $\mathcal{D}_e$, as:

$$\mathcal{D}_e = \{d \in \mathcal{D} : \exists r \in \mathcal{R}_e, TM(a) = r\}.$$

From an ontological point of view, descriptions are string-based representations that satisfy the additional requirement of being computable. In this sense, descriptions are a subset of representations, and thus, there can exist descriptions that describe other descriptions. However, in practice, it is not advisable to use descriptions as representations of entities, since what we seek in a good representation is the inclusion of as many details as possible about the original entities, not a concise encoding. Using descriptions in place of representations would make the task of scientific discovery considerably more difficult for humans.

Since each description corresponds to one, and only one, representation, we can define a function that maps descriptions to representations. Given that descriptions are encoded Turing machines, it is natural to define this mapping using a universal Turing machine. As a result, not only are individual descriptions of representations computable, but the function that maps descriptions to representations is also computable.

Definition 2.5.3 We call *description function*, denoted by δ, any universal Turing machine $\delta : \mathcal{D} \to \mathcal{B}^*$ that maps descriptions to their corresponding representations.

If $d = \langle TM, a \rangle$ is a description of the representation r, then we have that $\delta(d) = \delta(\langle TM, a \rangle) = TM(a) = r$.

Inspired by the Occam's razor principle[2], if two explanations are equivalent, we should prefer the shorter one. Accordingly, the limit of what can be known, or understood, about a representation, that is, its perfect model, is given by the shortest description that allows us to reconstruct that representation.

Definition 2.5.4 Let $\mathcal{D}_r$ be the set of descriptions of a representation $r \in \mathcal{R}_{\mathcal{E}}$, and let $d \in \mathcal{D}_r$ be a description of r. We say that d is a *perfect description* of the representation r if there is no other description $d' \in \mathcal{D}_r$ such that $l(d') < l(d)$.

Recall that what we know about an entity e depends on the quality of the representation r used. If the representation r is incorrect, we cannot achieve perfect knowledge of e, even if we have found the perfect description d for r.

Notation 2.4. *We denote by $d_r^\star$ that the description d is a perfect description of the representation r.*

The perfect description of a representation may not be unique; that is, there could be multiple optimal ways to compute r.

Definition 2.5.5 Let $\mathcal{D}_r$ be the set of descriptions of a representation $r \in \mathcal{R}_{\mathcal{E}}$. We define the *set of perfect descriptions* for r, denoted by $\mathcal{D}_r^\star$, as the subset of $\mathcal{D}_r$ consisting of all perfect descriptions of r.

Unfortunately, the set of perfect descriptions of a representation is generally unknown, and as Proposition 2.5.1 shows, there exists no algorithm to compute it. In practice, we must rely on approximations to estimate how far our current best description is from a perfect one, that is, to quantify how much we do not know about a particular representation of an entity (see Chapter 5).

Proposition 2.5.1 Let $r \in \mathcal{B}^*$ be a representation and let $d_r^\star$ be a perfect description of r. Then we have $l(d_r^\star) = K(r)$.

Proof. Apply Definition E.1.2 and note that the Turing machines TM used in descriptions of the form $\langle TM, a \rangle$ are required to be prefix-free. ■

[2] The Occam's razor principle refers to the number of assumptions in an explanation, not to the length of the explanation itself.

The actual length of a description $l(d)$ for a representation r depends on the specific encoding of Turing machines used. This encoding method is determined by the chosen description function δ. Fortunately, if we replace our description function with a different one, the length of perfect descriptions remains essentially unchanged, up to an additive constant that does not depend on the representation itself.

Corollary 2.5.2 Let $r \in \mathcal{R}_{\mathcal{E}}$ be a representation, and let δ and $\dot{\delta}$ be two different description functions. Let $d_r^\star$ be a perfect description of r under δ, and $\dot{d}_r^\star$ a perfect description under $\dot{\delta}$. Then $l\left(d_r^\star\right) \leq l\left(\dot{d}_r^\star\right) + c$, where c is a constant that does not depend on r.

Proof. Apply Proposition 2.5.1 and Theorem E.1.1. ■

In general, within the theory of nescience, we are not concerned with computing the exact value of nescience for an entity given a specific description and representation. Instead, our interest lies in the relative ordering of different possible pairs of descriptions and representations according to their nescience. In this sense, the specific details of the universal Turing machine used in practice are not relevant[3]. For the remainder of this book, we will assume that δ is fixed to a reference universal Turing machine Alternatively, the reader may consider that all theorems in this book involving the length of the shortest models are valid up to an additive constant that does not depend on the topics themselves.

A remarkable consequence of Proposition 2.5.1 is that perfect descriptions must be incompressible; that is, *perfect knowledge implies randomness* (see Section E.6).

Corollary 2.5.3 Let $d_r^\star$ be a perfect description of a representation r, then $K(r) = l\left(d_r^\star\right)$.

Proof. If $K(r) < l\left(d\_r^\star\right)$, then $d\_r^\star$ could be replaced by a shorter description, contradicting its minimality as a perfect description. ■

The converse does not generally hold: a description can be random without being the shortest possible one. That is, we may have a description d of a representation r such that $l(d) = K(d)$, yet $l(d\_r^\star) < l(d)$.

[3] Do not confuse the internal workings of the universal Turing machine that maps descriptions to representations, which are not of interest, with the internal workings of the universal oracle Turing machine that maps representations to entities, which are of interest, as understanding this mechanism is crucial to understanding how things work.

■ **Example 2.14** Consider a deep neural network with an input layer of one thousand nodes, ten hidden layers of fifty thousand nodes each, and an output layer of one thousand nodes. Suppose the network is trained to output a fixed string of one thousand 1's for any given input. The Kolmogorov complexity of this neural network is much greater than that of the output string itself, which consists of one thousand identical bits. ■

There is little value on descriptions that are longer than the representations they describe, that is, descriptions that do not compress the representations.

Definition 2.5.6 Let $r \in \mathcal{B}^*$ be a representation, and $d \in \mathcal{D}_r$ one of its descriptions. If $l(d) \geq l(r)$, we say that d is a *pleonastic description* of the representation r.

■ **Example 2.15** Consider the set of all possible finite graphs. Since graphs are abstract mathematical objects, we must represent them as strings, for instance, using a binary encoding of their adjacency matrices (see Section A.5 for an introduction to graphs). The description $d = \langle TM, r \rangle$, where r is the representation of a graph and TM is a Turing machine that simply halts, belongs to $\mathcal{D}_r$ because $TM(r) = r$. However, this description is of limited interest, as it is likely not the shortest possible description of r. ■

It may happen that there is no shorter possible description of a representation than the representation itself. This occurs when the representation is a random, or incompressible, string. As discussed in Section E.6, the overwhelming majority of strings are incompressible. Conducting research on random representations is unproductive, as it is not possible to find shorter models for such representations.

The concept of a perfect description can be generalized from individual representations to entire entities. This generalization allows us to study the nature and properties of the entities themselves.

Definition 2.5.7 Let $\mathcal{D}_e$ be the set of descriptions of an entity $e \in \mathcal{E}$. We define the *set of perfect descriptions* of the entity e, denoted by $\mathcal{D}_e^\star$ as the subset of $\mathcal{D}_e$ consisting of perfect descriptions. The elements of $\mathcal{D}_e^\star$ are denoted by $d_e^\star$.

If $d_e^\star \in \mathcal{D}_e^\star$ there must exists a representation $r \in \mathcal{R}_e^\star$ such that $d_e^\star \in \mathcal{D}_r^\star$.

An interesting case arises when all the descriptions in $\mathcal{D}_e$ are pleonastic, that is, there exists no model shorter than the representation for any of the possible representations of the entity. This situation would occur if all representations of the entity e are random strings. In such a case, scientific research would be fundamentally limited, as it would be impossible to find a suitable model for e. Our ability to understand and make predictions about e would then be constrained by the length of its incompressible representations.

2.6 Descriptions for Joint Representations

In Section 2.4, we introduced the concept of a joint representation ts, formed by combining two individual representations t and s. In this section, we aim to study how the length of the perfect description of a joint representation relates to the lengths of the perfect descriptions of the individual representations.

The length of the perfect description of a joint representation is greater than or equal to the length of the perfect description of either individual representation. In other words, the more information a representation contains, the longer it takes to describe.

Proposition 2.6.1 Let $t,s \in \mathcal{R}_{\mathcal{E}}$ be two representations, and let $m_t^\star$, $m_s^\star$, and $m_{ts}^\star$ denote the perfect descriptions of the representations t, s, and the joint representation ts, respectively. Then: $l\left(m_{ts}^\star\right) \geq l\left(m_t^\star\right)$ and $l\left(m_{ts}^\star\right) \geq l\left(m_s^\star\right)$.

Proof. The inequality $l\left(m_{ts}^\star\right) \geq l\left(m_t^\star\right)$ is equivalent to $K(ts) \geq K(t)$. The result then follows from Proposition E.3.3. ■

Intuitively, adding more information to a representation is beneficial if the additional information is relevant to describing the entity of interest. However, including irrelevant information leads to unnecessarily long models. Recall that joining representations can serve either to concatenate two partial representations of the same entity or to enrich a representation by adding missing symbols.

If the selected representations partially overlap, we can exploit this redundancy to produce a joint description that is shorter than the mere concatenation of the individual descriptions. In the worst-case scenario, the perfect description of a joint representation would be equal in length to the sum of the perfect descriptions of the individual representations.

Proposition 2.6.2 Let $t,s \in \mathcal{R}_{\mathcal{E}}$ be two representations, and let $m_t^\star$, $m_s^\star$, and $m_{ts}^\star$ denote the perfect descriptions of the representations t, s, and the joint representation ts, respectively. Then: $l\left(m_{ts}^\star\right) \leq l\left(m_t^\star\right) + l\left(m_s^\star\right)$.

Proof. The inequality $l\left(m_{ts}^\star\right) \leq l\left(m_t^\star\right) + l\left(m_s^\star\right)$ is equivalent to $K(ts) \leq K(t) + K(s)$. The result follows from Proposition E.3.2. ■

One interpretation of Proposition 2.6.2 is that including redundant information in the representation of an entity does not hinder our ability to find its shortest possible description. From the perspective of compression, redundancy can be eliminated during the modeling process. Therefore, in practice, we may prefer to work with representations that are longer but make the process of scientific discovery, i.e., finding the best model, easier, even if they contain superfluous information. In contrast, Proposition 2.6.1 highlights a different concern: adding irrelevant or non-informative symbols to a representation should be avoided, as they increase the complexity of the description without contributing useful information about the entity.

Finally, the following proposition shows that the order of the representations in the perfect description of a joint representation does not affect its length.

Proposition 2.6.3 Let $t,s \in \mathcal{R}_\mathcal{E}$ be two representations, and let $m^\star_{ts}$ and $m^\star_{st}$ be the perfect descriptions of the joint representations ts and st, respectively. Then: $l\left(m^\star_{ts}\right) = l\left(m^\star_{st}\right)$.

Proof. The equality $l\left(m^\star_{ts}\right) = l\left(m^\star_{st}\right)$ is equivalent to $K(ts) = K(st)$. The result follows from Proposition E.3.1. ■

It is important to note, however, that joining representations is not a commutative operation, there is no guarantee that the strings ts and st encode the same entity. Moreover, given only the concatenated string ts, it is generally not possible to recover the original representations t and s, since they are not self-delimiting.

Propositions 2.6.1, 2.6.2 and 2.6.3 can be generalized to any arbitrary, but finite, collection of representations $t_1, t_2, \ldots, t_n$.

Proposition 2.6.4 Let $t_1, t_2, \ldots, t_n \in \mathcal{R}_\mathcal{E}$ be a finite collection of representations. Then, we have that:

i $l(m^\star_{t_1 t_2 \ldots t_n}) \geq l(m^\star_{t_i}) \; \forall 1 \leq i \leq n$,
ii $l(m^\star_{t_1 t_2 \ldots t_n}) \leq l(m^\star_{t_1}) + l(m^\star_{t_2}) + \ldots + l(m^\star_{t_n})$,
iii $l(m^\star_{t_1 \ldots t_i \ldots t_j \ldots t_n}) = l(m^\star_{t_1 \ldots t_j \ldots t_i \ldots t_n}) + c \; \forall 1 \leq i \leq j \leq n$,
iv $l(m^\star_{t_1 \ldots t_{n-1}}) \leq l(m^\star_{t_1 \ldots t_{n-1} t_n})$.

Proof. Apply Propositions 2.6.1, 2.6.2 and 2.6.3 to individual pairs of representations i and j. ■

2.7 Conditional Descriptions

It is often cumbersome to include all the information required to reconstruct an entity within a single description, as this would typically result in very long strings for most entities. A more practical approach is to assume the existence of some background knowledge and to quantify our lack of knowledge about an entity relative to that background. In this section, we study the concept of *conditional descriptions*, that is, constructing a description given some prior description. Conditional descriptions also play a crucial role in the discovery of new knowledge: if conditioning a description on some prior knowledge significantly reduces the inaccuracy of a model, it indicates that this prior knowledge is relevant to understanding the entity.

Definition 2.7.1 Let $r, d, s \in \mathcal{B}^*$ be strings. We say that the string $\langle d, s\rangle$ is a *valid conditional description* of the representation r given the string s, denoted by $d_{r|s}$, if $d = \langle TM, a\rangle$ is a description, and $TM(\langle a, s\rangle) = r$.

The conditional description $d_{r|s}$ relies on two distinct strings: a and s, each fulfilling a different role. The string a is provided as input to the Turing machine TM and is intended to contain the portion of the representation r that cannot be derived from prior knowledge, that is, the incompressible or novel part. In contrast, the string s represents background knowledge: it is a description or representation of another entity that is assumed to be already known and that can facilitate the reconstruction or understanding of r. For example, as we will explain in Chapter 5, when evaluating the redundancy of a conditional description, the contribution of the string s is disregarded—only the length and content of a are taken into account.

Note that the conditional description $d_{r|s}$ does not belong to the set of valid descriptions $\mathcal{D}$ for the representation r, since computing r requires the additional string s, which is not part of the description itself. Therefore, a new definition is needed to formally capture this concept.

Definition 2.7.2 Let $r \in \mathcal{B}^*$ be a representation and $s \in \mathcal{B}^*$ an arbitrary string. We define the *set of conditional descriptions* of r given s, denoted by $\mathcal{D}_{r|s}$, as:

$$\mathcal{D}_{r|s} = \{d \in \mathcal{B}^*, d = \langle TM, a\rangle : TM(\langle a, s\rangle) = r\}.$$

For each representation $r \in \mathcal{B}^*$, there always exists a conditional description $d_{r|s}$ that describes r, as the following proposition shows.

Proposition 2.7.1 Let $r \in \mathcal{B}^*$ be a representation and $s \in \mathcal{B}^*$ an arbitrary string. If $d \in \mathcal{D}_r$ then $d \in \mathcal{D}_{r|s}$.

Proof. We can construct a conditional description $\langle\langle TM, a\rangle, s\rangle$ based on a Turing machine TM such that, when given the input $\langle a, s\rangle$, the machine safely ignores the string s. ■

The converse of Proposition 2.7.1 is not true. The fact that d is a conditional description (i.e., $d \in \mathcal{D}_{r|s}$) does not implies that d is also a valid description (i.e., $d \in \mathcal{D}_r$). Indeed, while we require that $TM(\langle a, s\rangle) = r$, we do not require that $TM(a) = r$, and in general, this may not hold.

We are interested in the concept of a perfect conditional description. The perfect conditional description of a representation, given some prior knowledge, is the shortest possible string that allows us to fully reconstruct the representation, assuming that the prior knowledge is already known.

Definition 2.7.3 Let $r \in \mathcal{B}^*$ be a representation, and let $d^\star_{r|s}$ be the shortest possible description of r given the string s. We call $d^\star_{r|s}$ the *perfect conditional description* of the representation r given the string s, or simply perfect conditional description of r given s for short.

Note that $d^\star_{r|s}$ is a perfect description of the representation r *conditional on* the string s. This does not imply that s is a perfect description itself; it may be an incomplete or partially irrelevant representation. In such a case, we would have achieved perfect knowledge with respect to the d component, but not with respect to the s component of the combined string $\langle d, s\rangle$.

The length of a perfect conditional description is always less than or equal to that of its unconditional counterpart. In other words, assuming the existence of some background knowledge can reduce the effort required to describe a representation.

Proposition 2.7.2 Let $r \in \mathcal{B}^*$ be a representation and $s \in \mathcal{B}^*$ an arbitrary string. Then $l\left(d^\star_{r|s}\right) \leq l\left(d^\star_r\right)$.

Proof. The inequality $l\left(d^\star_{r|s}\right) \leq l\left(d^\star_r\right)$ is equivalent to the well-known result $K(r \mid s) \leq K(r)$. The proposition follows directly by applying Proposition E.4.3. ■

The notions of unconditional, conditional, and joint descriptions are closely related. In particular, the availability of prior knowledge (as captured by a conditional description) can reduce the length of a description, while describing multiple entities jointly (via a joint description) typically requires more information than describing a single entity. The following proposition formalizes these relationships by comparing the lengths of the perfect conditional description, the perfect (unconditional) description, and the perfect joint description.

Proposition 2.7.3 Let $r, s \in \mathcal{B}^*$ two different representations. Then:

$$l\left(d^\star_{r|s}\right) \leq l\left(d^\star_r\right) \leq l\left(d^\star_{rs}\right)$$

Proof. The inequality $l\left(d^\star_{r|s}\right) \leq l\left(d^\star_r\right) \leq l\left(d^\star_{rs}\right)$ is equivalent to the Kolmogorov complexity relations $K(r \mid s) \leq K(r)$ and $K(r) \leq K(rs)$. The result follows directly by applying Proposition E.4.5. ■

As was the case with joint descriptions, the concept of conditional description can be naturally extended to finite collections of representations.

Definition 2.7.4 Let $r, d, s_1, s_2, \ldots, s_n \in \mathcal{B}^*$ be strings. We say that the string $\langle d, s_1, s_2, \ldots, s_n \rangle$ is a *valid conditional description* of the representation r given the strings $s_1, s_2, \ldots, s_n$, denoted by $d_{r|s_1,s_2,\ldots,s_n}$, if $d = \langle TM, a \rangle$ is a description, and $TM\left(\langle a, s_1, s_2, \ldots, s_n \rangle\right) = r$.

The following definition generalizes the notion of a perfect conditional description to the case of multiple conditioning strings.

Definition 2.7.5 Let $r \in \mathcal{B}^*$ be a representation, and let $d^\star_{r|s_1,s_2,\ldots,s_n}$ be the shortest possible description of r given the strings $s_1, s_2, \ldots, s_n$. We call $d^\star_{r|s_1,s_2,\ldots,s_n}$ the *perfect conditional description* of the representation r given the string $s_1, s_2, \ldots, s_n$, or perfect conditional description of r given $s_1, s_2, \ldots, s_n$ for short.

The next proposition generalizes Propositions 2.7.2 and 2.7.3 to any arbitrary (but finite) collection of strings $s_1, s_2, \ldots, s_n$. In particular, it shows that the more background knowledge we assume for a given representation, the shorter its perfect description becomes.

Proposition 2.7.4 Let $r, s_1, s_2, \ldots, s_n \in \mathcal{B}^*$ be a finite collection of strings. Then:

$$l\left(d^\star_{r|s_1,s_2,\ldots,s_n}\right) \leq l\left(d^\star_r\right) \leq l\left(d^\star_{r,s_1,s_2,\ldots,s_n}\right)$$

Proof. This follows from the Kolmogorov complexity inequalities $K(r \mid s_1, s_2, \ldots, s_n) \leq K(r) \leq K(r, s_1, s_2, \ldots, s_n)$, which generalize the results stated in Propositions 2.7.2 and 2.7.3. ■

The following proposition further generalizes the idea that assuming additional background knowledge cannot increase the length of a perfect conditional description.

Proposition 2.7.5 Let $r, s_1, s_2, \ldots, s_n, s_{n+1} \in \mathcal{B}^*$ be a finite collection of strings. Then:

$$l\left(d^\star_{r|s_1,s_2,\ldots,s_n,s_{n+1}}\right) \leq l\left(d^\star_{r|s_1,s_2,\ldots,s_n}\right)$$

Proof. This follows directly from the monotonicity property of conditional Kolmogorov complexity: adding more conditioning information cannot increase the complexity. Formally, $K(r \mid s_1, s_2, \dots, s_n, s_{n+1}) \leq K(r \mid s_1, s_2, \dots, s_n)$. ■

2.8 Research Areas

Entities can be grouped into research areas. The concept of an area is useful insofar as all the entities included in the area are related to a common subdomain of knowledge or share a common property. The specific criteria used for grouping depend on the practical application of the theory of nescience.

Definition 2.8.1 Given a set of entities $\mathcal{E}$, we define a *research area* $\mathcal{A}$ as a subset of entities, $\mathcal{A} \subset \mathcal{E}$.

If we want to quantify how much we do not know about a research area, we must first provide a representation for that area. In general, research areas are infinite, but the number of known representations is finite. Therefore, we can only describe an area with respect to our current state of knowledge.

Definition 2.8.2 Let $\mathcal{A} \subset \mathcal{E}$ be a research area. We define the *known subset of the area* $\mathcal{A}$, denoted by $\hat{\mathcal{A}}$, as the set of entities $e_1, e_2, \dots, e_n \in A$ for which at least one non-pleonastic description is known.

We must distinguish between the knowable subset of $\mathcal{A}$, composed of those entities for which a representation exists, and the known subset of $\mathcal{A}$, composed of those entities for which at least one non-pleonastic description is known, that is, entities about which some research has already been conducted. Clearly, the set of known entities is a subset of the set of knowable entities.

As our understanding of a research area evolves, the number of entities included in its known subset also changes. Throughout this book, the properties of research areas will always be considered relative to our current state of knowledge.

Definition 2.8.3 Let $\mathcal{A} \subset \mathcal{E}$ be a research area with known subset $\hat{\mathcal{A}} = \{e_1, e_2, \dots, e_n\}$, and let $R_{\hat{\mathcal{A}}} = \{r_1, r_2, \dots, r_n\}$ be a set of representations such that $r_i \in \mathcal{R}_{e_i}$. We call $R_{\hat{\mathcal{A}}}$ a *representation of the area* $\mathcal{A}$ given the known subset $\hat{\mathcal{A}}$, abbreviated as *representation of* $\mathcal{A}$.

In a similar manner to how we describe individual entities, we can also introduce the concept of a description for an entire research area. Since a research area is represented by a collection of known representations corresponding to its known subset, a description of the area must account for the generation of this entire set. Thus, we define a description of a research area as a program that, when executed, produces the sequence of representations associated with the known entities in that area.

Definition 2.8.4 Let $R_{\hat{\mathcal{A}}} = \{r_1, r_2, \ldots, r_n\}$ be the representation of an area $\mathcal{A}$. We call a *description of the area $\mathcal{A}$* given the known subset $\hat{\mathcal{A}}$, abbreviated as *description of $\mathcal{A}$*, and denoted by $d_{\hat{\mathcal{A}}}$, to any string in the form $\langle TM, a \rangle$ such that the Turing machine TM, when given input a, outputs the sequence $\langle r_1, r_2, \ldots, r_n \rangle$.

We can also consider all possible descriptions that generate the full set of known representations for a given research area. These descriptions differ in structure, length, or computational efficiency, but they all produce the same output: the sequence of representations associated with the known entities in the area.

Definition 2.8.5 Let $R_{\hat{\mathcal{A}}} = \{r_1, r_2, \ldots, r_n\}$ be the representation of an area $\mathcal{A}$. We define the set of *descriptions for $R_{\hat{\mathcal{A}}}$*, denoted by $\mathcal{D}_{R_{\hat{\mathcal{A}}}}$, as:

$$\mathcal{D}_{R_{\hat{\mathcal{A}}}} = \{d \in \mathcal{D} : TM(a) = \langle r_1, r_2, \ldots, r_n \rangle\}.$$

Finally, we are interested in identifying the perfect model for a research area, that is, the shortest possible string that fully describes its known subset. According to Definition 2.5.6, if we are aware of the existence of an entity $e \in A$, then e should be included in the known subset $\hat{A}$, even if no research has yet been conducted on that specific topic.

Definition 2.8.6 Let $A \subset \mathcal{E}$ be an area with known subset $\hat{A}$, and let $d^{\star}_{\hat{A}} \in \mathcal{D}_{R_{\hat{\mathcal{A}}}}$ be the shortest possible description of A. We call $d^{\star}_{\hat{A}}$ the *perfect description of the area A* given the known subset $\hat{A}$, abbreviated as *perfect description of A*.

The following proposition shows the relationship between the description of a research area and the descriptions of the individual entities that compose its known subset. In general, the models for an area are not simply the collection of the models for each individual topic; instead, a joint model may offer a more concise description.

Proposition 2.8.1 Let $A \subset \mathcal{E}$ be an area with known subset $\hat{A} = \{e_1, e_2, \ldots, e_n\}$, then we have that $l\left(d^{\star}_{\hat{A}}\right) \leq l(d^{\star}_{e_1}) + l(d^{\star}_{e_2}) + \ldots + l(d^{\star}_{e_n})$.

Proof. Apply Proposition 2.6.4-ii. ∎

Moreover, as shown in Proposition 2.6.4, the order in which the representations are listed in the description of an area does not affect the length of its perfect model.

Research areas can overlap; that is, given two areas A and B, it may be the case that $A \cap B \neq \varnothing$. Furthermore, one area can be a subset of another, forming a hierarchy of areas. In this context, we are particularly interested in how the length of perfect models for some areas compares to the length of perfect models for related areas.

Proposition 2.8.2 Let $A, B \subset \mathcal{E}$ be two areas such that $A \subset B$, and let $\hat{A}$ and $\hat{B}$ be their know subsets respectively, then we have that $l\left(d^\star_{\hat{A}}\right) \leq l\left(d^\star_{\hat{B}}\right)$.

Proof. Since $A \subset B$, it follows that $\hat{A} \subset \hat{B}$.Let

$$R_{\hat{A}} = \{r_1, r_2, \ldots, r_m\} \quad \text{and} \quad R_{\hat{B}} = \{r_1, r_2, \ldots, r_m, r_{m+1}, \ldots, r_n\}$$

be the sets of representations corresponding to $\hat{A}$ and $\hat{B}$ respectively, and let $d^\star_{\hat{B}}$ be the perfect description of $\hat{B}$. Then, we can construct a description d' of $\hat{A}$ by modifying $d^\star_{\hat{B}}$ to output only the subset $R_{\hat{A}}$. This can be achieved by appending a simple postprocessing step that discards the extra representations. The additional cost of this truncation is at most a constant number of bits, independent of the specific contents of $R_{\hat{B}}$.

Formally, we have:

$$l(d^\star_{\hat{A}}) \leq l(d') \leq l(d^\star_{\hat{B}}) + c$$

for some constant c. But since $d^\star_{\hat{A}}$ is the shortest possible description of $R_{\hat{A}}$, we conclude:

$$l(d^\star_{\hat{A}}) \leq l(d^\star_{\hat{B}}).$$

■

The following proposition shows how the length of the shortest possible description of two areas relates to the length of the description of their union and intersection.

Proposition 2.8.3 Let $A, B \subset \mathcal{E}$ be two areas with know subsets $\hat{A}$ and $\hat{B}$ respectively, then we have that $l\left(d^\star_{\hat{A}\cup\hat{B}}\right) = l\left(d^\star_{\hat{A}}\right) + l\left(d^\star_{\hat{B}}\right) - l\left(d^\star_{\hat{A}\cap\hat{B}}\right)$.

Proof. Let $R_{\hat{A}}$, $R_{\hat{B}}$, and $R_{\hat{A}\cap\hat{B}}$ be the sets of representations corresponding to the known subsets $\hat{A}$, $\hat{B}$, and $\hat{A} \cap \hat{B}$, respectively.

From the theory of Kolmogorov complexity, the minimal description length of the union of two finite sets of strings satisfies the following identity:

$$K(R_{\hat{A}\cup\hat{B}}) = K(R_{\hat{A}}) + K(R_{\hat{B}}) - K(R_{\hat{A}\cap\hat{B}}),$$

Since, by definition, the perfect description $d^\star_{\hat{A}}$ satisfies:

$$l(d^\star_{\hat{A}}) = K(R_{\hat{A}}), \quad l(d^\star_{\hat{B}}) = K(R_{\hat{B}}), \quad l(d^\star_{\hat{A}\cap\hat{B}}) = K(R_{\hat{A}\cap\hat{B}}),$$

it follows that:

$$l(d^\star_{\hat{A}\cup\hat{B}}) = K(R_{\hat{A}\cup\hat{B}}) = l(d^\star_{\hat{A}}) + l(d^\star_{\hat{B}}) - l(d^\star_{\hat{A}\cap\hat{B}}).$$

■

A consequence of Proposition 2.8.3 is that $l\left(d^\star_{\hat{A}\cup\hat{B}}\right) \leq l\left(d^\star_{\hat{A}}\right) + l\left(d^\star_{\hat{B}}\right)$, that is, when we combines two different research areas, how much we do not know about these areas decreases.

Just as we introduced a chain rule for entropy in Proposition D.4.5, we can also establish a chain rule for the shortest length of a description of a research area.

Proposition 2.8.4 Let $A,B \subset \mathcal{E}$ be two areas with know subsets $\hat{A}$ and $\hat{B}$, then we have that $l\left(d^\star_{\hat{A}\cup\hat{B}}\right) = l\left(d^\star_{\hat{A}}\right) + l\left(d^\star_{\hat{B}\backslash\hat{A}}\right)$.

Proof. Let $R_{\hat{A}}$ be the set of representations associated with $\hat{A}$, and let $R_{\hat{B}\backslash\hat{A}}$ be the set of representations corresponding to entities in $\hat{B}$ that are not in $\hat{A}$.

By definition, the known subset of the union $\hat{A}\cup\hat{B}$ corresponds to the set of representations:

$$R_{\hat{A}\cup\hat{B}} = R_{\hat{A}} \cup R_{\hat{B}\backslash\hat{A}}.$$

Let $d^\star_{\hat{A}}$ be the shortest (perfect) description that generates $R_{\hat{A}}$, and let $d^\star_{\hat{B}\backslash\hat{A}}$ be the shortest description that generates $R_{\hat{B}\backslash\hat{A}}$. Because the two subsets are disjoint, we can concatenate these two descriptions to produce a description of $R_{\hat{A}\cup\hat{B}}$.

Hence, the length of the shortest description of the union satisfies:

$$l\left(d^\star_{\hat{A}\cup\hat{B}}\right) \leq l\left(d^\star_{\hat{A}}\right) + l\left(d^\star_{\hat{B}\backslash\hat{A}}\right).$$

To prove equality, assume there exists a shorter description d' for $\hat{A}\cup\hat{B}$ such that:

$$l(d') < l\left(d^\star_{\hat{A}}\right) + l\left(d^\star_{\hat{B}\backslash\hat{A}}\right).$$

Then, one could extract from d' both $R_{\hat{A}}$ and $R_{\hat{B}\backslash\hat{A}}$, which would imply that at least one of $d^\star_{\hat{A}}$ or $d^\star_{\hat{B}\backslash\hat{A}}$ is not minimal—contradicting the assumption that they are perfect descriptions.

Therefore:

$$l\left(d^\star_{\hat{A}\cup\hat{B}}\right) = l\left(d^\star_{\hat{A}}\right) + l\left(d^\star_{\hat{B}\backslash\hat{A}}\right).$$

■

2.9 References

For more information about Russell's paradox, Cantor's theorem, and universal sets, refer, for example, to [Jec13]. This book also covers the Zermelo–Fraenkel system of axioms, including the Axiom of Choice. The idea of using a function to assign to each symbol and well-formed formula of a formal language a unique natural number (called a Gödel number) was introduced by Kurt Gödel in his proof of the incompleteness theorems [Göd31]. A detailed discussion of the Berry paradox from the perspective of computability can be found in [Cha95]. For a review of the problem of representation in Kolmogorov complexity, as well as a detailed account of the implications of Kolmogorov complexity being defined only up to an additive constant, see [LV13]. That oracle machines are not mechanical was originally stated by Turing when he introduced the concept of the oracle machine in [Tur39]. For a comprehensive review of oracle Turing machines, refer to [Rob15].

3. Miscoding

All great work is the fruit of patience and perseverance,
combined with tenacious concentration on a subject
over a period of months or years.
Santiago Ramón y Cajal

In many areas of science, the entities we aim to study (the set $\mathcal{E}$) often include abstract concepts or complex phenomena that are difficult to investigate directly. These may be ideas or processes that resist straightforward description or modeling. To gain insight into such entities, we must often rely on indirect methods. As discussed in the previous chapter, the theory of nescience suggests using representations, that is, sequences of symbols, rather than attempting to interact directly with the entities themselves.

However, this approach introduces its own challenges. Because our understanding of the elements in $\mathcal{E}$ is incomplete (otherwise, further research would be unnecessary), the representations we construct are typically imperfect, they lack the completeness and precision we would ideally desire. These imperfections can lead to significant problems: inaccuracies in representation can propagate into the models derived from them, potentially distorting our interpretation and understanding. It is therefore essential to recognize this source of error and to carefully consider its implications.

To address this issue, we introduce the concept of *miscoding*, a measure used to quantify the error that arises from misrepresenting or inaccurately encoding entities. Miscoding is defined in terms of the length of the shortest computer program capable of transforming an incorrect representation into a correct one. In essence, it measures the amount of effort, as reflected by the program's length, required to correct a faulty representation.

However, there is a significant complication: applying this idea in practice is not straightforward, since the perfect representations of entities are unknown. As a result, we cannot directly measure the gap between a given representation and an ideal one. Nevertheless, we propose a theoretical framework based on the oracle machine (an abstract construct) used to define the set $\mathcal{E}$. This oracle machine is assumed to be capable of recognizing valid representations for all entities in the set. It is important to note, however, the limitations of this approach; for instance, we cannot query the oracle about a specific entity unless we already possess a valid representation of it.

Getting a better grasp on scientific representation and the challenges in reducing miscoding could really push forward scientific research, helping us create better, more thorough models of the natural world. In this chapter, we are going to properly introduce the idea of miscoding and look into its various characteristics. We will examine how miscoding behaves when it comes to combined representations and discuss methods to reduce miscoding. We will delve into the idea that there are strings that do not represent any entity. And we will dig into why miscoding is important in different research areas and talk about its potential to open up new lines of inquiry.

Gaining a deeper understanding of scientific representation and the difficulties involved in reducing miscoding can significantly advance scientific research, enabling the development of more accurate and comprehensive models of the natural world. In this chapter, we formally introduce the concept of *miscoding* and explore its key properties. We will analyze how miscoding behaves in the context of combined representations and consider strategies for reducing it. We will also examine the notion that some strings fail to represent any entity and investigate the implications of this idea. Finally, we will highlight the relevance of miscoding across various research domains and discuss its potential to inspire new lines of inquiry.

3.1 Miscoding

In an ideal scenario, we would ask the oracle to determine how far a particular string r is from perfectly encoding an entity e. This, however, presents a complication: we can only refer to entity e through a valid representation in the set $\mathcal{R}_e^\star$. Unfortunately, we typically do not have access to these perfect representations and, therefore, cannot use them in our query.

To overcome this limitation, we propose an alternative approach. Rather than asking the oracle to assess the discrepancy between our current representation r and a valid representation of the specific entity e, we instead ask the oracle to identify the smallest distance between r and all valid representations of all entities in the set $\mathcal{E}$, that is, the elements of $\mathcal{R}^\star_{\mathcal{E}}$. As discussed in detail in Section 2.3, this type of query can, in principle, be handled by the oracle.

Definition 3.1.1 — Miscoding. Let $r \in \mathcal{B}^*$ be a representation. We define the *miscoding* of r, denoted by $\mu(r)$, as:

$$\mu(r) = \overset{o}{\min_{r_e^\star \in \mathcal{R}^\star_{\mathcal{E}}}} \frac{\max\{K(r \mid r_e^\star), K(r_e^\star \mid r)\}}{\max\{K(r), K(r_e^\star)\}}$$

where $\overset{o}{\min}$ indicates that the minimum is to be computed by an oracle.

Intuitively, our lack of knowledge about an entity is reflected in a higher miscoding value of its current representation. Conversely, a deeper understanding of the entity should lead to an encoding that is closer to a valid representation, and thus exhibits lower miscoding.

Miscoding is computed using a bidirectional approach: we require the oracle to determine both the length of the shortest computer program that can generate the valid representation $r_e^\star$ from our current representation r (i.e., $K(r_e^\star \mid r)$), and the length of the shortest program that can generate r from $r_e^\star$ (i.e., $K(r \mid r_e^\star)$). This bidirectionality captures the maximum difficulty of transforming one representation into the other. A high-quality representation should allow for an easy reconstruction of the correct representation and vice versa, implying that both of these conditional complexities are low. In other words, an ideal representation contains all the information needed to recover the correct encoding of the entity, without introducing any erroneous or irrelevant symbols.

While miscoding concerns whether the symbols in a representation are relevant, that is, whether they correctly refer to the intended entity, it is not concerned with how many symbols are used. In contrast, surfeit (as discussed in Chapter 5) focuses on whether the symbols are essential, aiming to minimize the number of unnecessary or redundant symbols. In this sense, miscoding relates to the correctness of the content, while surfeit relates to the efficiency of its expression. Although both concepts address flaws in representation, they capture fundamentally different types of representational inefficiency.

Our definition of miscoding is formulated as a relative measure rather than an absolute one. Instead of providing an isolated score for a single representation, it quantifies how far a representation is from the nearest valid representation, normalized by their respective lengths. This relative formulation allows us to meaningfully compare the miscoding of different representations of the same entity, and also to compare the miscoding values across representations of different entities, regardless of their size or complexity.

The miscoding value of a representation r always lies within the interval $[0,1]$.

Proposition 3.1.1 For all $r \in \mathcal{B}^*$, it holds that $0 \leq \mu(r) \leq 1$.

Proof. This follows directly from the inequality $0 \leq \frac{\max\{K(x|y),K(y|x)\}}{\max\{K(x),K(y)\}} \leq 1$ which holds for all $x, y \in \mathcal{B}^*$, as stated in Proposition E.5.5. ■

Miscoding is zero if, and only if, the representation r is a valid representation of some entity e.

Proposition 3.1.2 Given a representation $r \in \mathcal{B}^*$, we have $\mu(r) = 0$ if, and only if, $r \in \mathcal{R}^\star_{\mathcal{E}}$.

Proof. If $r \in \mathcal{R}^\star_{\mathcal{E}}$, then there exists an entity $e \in \mathcal{E}$ such that $r = r^\star_e$. In this case, $K(r \mid r^\star_e) = 0$, and thus $\mu(r) = 0$.

Conversely, if $\mu(r) = 0$, then there must exist some $r^\star_e \in \mathcal{R}^\star_{\mathcal{E}}$ such that $K(r \mid r^\star_e) = 0$ and $K(r^\star_e \mid r) = 0$, which implies that $r = r^\star_e$, and hence $r \in \mathcal{R}^\star_{\mathcal{E}}$. ■

According to Proposition 3.1.2, a miscoding value of zero implies that r perfectly encodes some entity e. However, identifying the exact entity that r represents remains a challenge. While scientific intuition may offer plausible hypotheses about the encoded entity, such guesses cannot be confirmed mathematically. Moreover, as scientific understanding evolves, our interpretation of what r encodes may also change over time (see Example 2.10).

It has been observed that an entity $e \in \mathcal{E}$ may possess multiple valid representations, as captured by the set $\mathcal{R}^\star_e$. Fortunately, the value of miscoding is invariant under the choice of valid representation (see the discussion on style in Section G.4).

Proposition 3.1.3 For any valid representation $r^*_e \in \mathcal{R}^\star_{\mathcal{E}}$, it holds that $\mu(r^\star_e) \leq \mu(r)$ for all $r \in \mathcal{B}^\star$.

Proof. This follows from the fact that $\mu(r^\star_e) = 0$ and $\mu(r) \geq 0$ for all $r \in \mathcal{B}^\star$. ■

For a given entity e, all valid representations in the set $\mathcal{R}_e^\star$ are equally adequate with respect to miscoding, as each yields a miscoding value of 0. From a practical standpoint, however, the most suitable representation is the one that best facilitates the discovery of new knowledge about the entity—specifically, the representation that most effectively supports the construction of explanatory models.

3.2 Joint Miscoding

Section 2.4 introduced the notion of a *joint representation*, which arises when two representations $s,t \in \mathcal{B}^*$ are concatenated to form a new string st. This section explores the properties of miscoding as they apply to such joint representations.

Since the concatenated string st is itself a valid representation, it is not necessary to introduce a separate definition of miscoding for joint representations. The miscoding of the joint representation is given by:

$$\mu(st) = \underset{r_e^\star \in \mathcal{R}_\mathcal{E}^\star}{\overset{o}{\min}} \frac{\max\{K(st \mid r_e^\star), K(r_e^\star \mid st)\}}{\max\{K(st), K(r_e^\star)\}}$$

Consistent with Proposition 3.1.1, the miscoding of a joint representation is a value between 0 and 1, i.e., $0 \leq \mu(st) \leq 1$.

It is important to note that supplementing an incomplete representation, that is, one with a positive miscoding value, with additional symbols does not necessarily lead to a reduction in miscoding. This is because the added symbols may introduce irrelevant or incorrect information. Conversely, miscoding does not necessarily increase either, since incorporating relevant and accurate symbols can reduce the miscoding of an incomplete representation.

From a formal perspective, given two arbitrary representations $s,t \in \mathcal{B}^*$, there is no guarantee that any of the following inequalities will always hold: $\mu(ts) \geq \mu(t)$, $\mu(ts) \leq \mu(t)$, $\mu(ts) \geq \mu(s)$, or $\mu(ts) \leq \mu(s)$.

■ **Example 3.1** Consider the text r of a biology research article that succinctly and accurately describes a newly discovered specimen, resulting in a low miscoding value $\mu(r)$. However, when additional text s, taken from a completely unrelated article about a second specimen from a different species, is appended, the resulting concatenated representation rs muddles the original focus. This inclusion of unrelated content increases the miscoding value to $\mu(rs)$, illustrating a case in which $\mu(rs) \geq \mu(r)$. Although the added text is scientifically valid on its own, it dilutes the clarity and precision of the original article, thereby increasing its miscoding.

Conversely, in a second scenario, consider another research article r' that exhibits a relatively high miscoding value $\mu(r')$, due to an incomplete description of the specimen. If this article is supplemented with additional text s', containing essential information previously omitted, the resulting concatenated representation $r's'$ becomes significantly more informative and coherent. As a result, the miscoding value decreases, demonstrating a case where $\mu(r's') \leq \mu(r')$. This highlights that enriching an incomplete representation with relevant and focused content can yield a more accurate and lower-miscoding representation. ■

Furthermore, it should not be assumed that the miscoding of a joint representation is less than or equal to the sum of the miscodings of the individual representations, i.e., $\mu(st) \leq \mu(s) + \mu(t)$. This inequality does not necessarily hold, even when both s and t encode the same entity. The reason is that the joint representation \$st\$ may end up encoding an entirely different entity from those represented by s and t individually.

■ **Example 3.2** In a medical research context, representation r describes a new drug compound A for treating a specific type of cancer, while representation s outlines a genetic mutation B associated with that cancer type. Both r and s have low miscoding values, denoting accurate, focused content. However, when concatenated, the combined representation rs unintentionally suggests a third entity C, implying a causal relationship between A and B. This unintended implication stems from the mixture of distinct information, leading to a higher miscoding value. In this instance, each of r, s, and rs essentially represents different research entities. r and s are clear in their individual contexts, but rs is ambiguous, exemplifying a case where concatenated information can inadvertently create a representation of an entirely different, unintended entity, thus increasing miscoding. ■

Given the non-commutative nature of joining two representations, it is not guaranteed that $\mu(ts) = \mu(st)$. This is because the composite strings ts and st may encode entirely different entities. This property holds true even when we restrict our attention to valid representations of a specific entity e. For example, if $r_e^\star, s_e^\star \in \mathcal{R}_e^\star$ are two valid representations of the entity e, there is no assurance that the concatenated string $r_e^\star s_e^\star$ will itself be a valid representation of e.

■ **Example 3.3** In environmental science, representation r thoroughly examines microplastics, their nature and harmful impacts on marine ecosystems, while representation s focuses on specific technologies and methodologies for detecting these pollutants in water. The concatenation rs presents a logical progression: first describing the pollutant and its effects, then outlining detection methods. This creates a coherent representation of a broader entity, one concerned with the pollutant, its impact, and how to detect it, an entity which may not yet be fully understood, hence yielding a higher miscoding value.

Conversely, the concatenation sr begins with technical methodologies for detection and then provides the contextual background on microplastics and their environmental effects. This ordering may be more familiar within a methodological framework and results in a more coherent and well-understood entity, yielding a lower miscoding value.

In this particular case, we observe that $\mu(rs) > \mu(sr)$. ■

The concept of miscoding can be naturally extended to joint representations formed from any finite collection of representations. Let $r_1, r_2, \ldots, r_n \in \mathcal{B}^*$ be a finite collection of representations. The miscoding of their concatenation, denoted by $r_1 r_2 \ldots r_n$, is defined as:

$$\mu(r_1 r_2 \ldots r_n) = \overset{o}{\min_{r_e^\star \in \mathcal{R}_\mathcal{E}^\star}} \frac{\max\{K(r_1 r_2 \ldots r_n \mid r_e^\star), K(r_e^\star \mid r_1 r_2 \ldots r_n)\}}{\max\{K(r_1 r_2 \ldots r_n), K(r_e^\star)\}}$$

As in the case of concatenating two representations, the miscoding of a joint representation composed of \$n\$ elements remains bounded within the unit interval $0 \leq \mu(r_1 r_2 \ldots r_n) \leq 1$. However, several caveats must be noted. There is no guarantee that $\mu(r_1 r_2 \ldots r_n) \leq \mu(r_i) \quad \text{or} \quad \mu(r_1 r_2 \ldots r_n) \geq \mu(r_i)$ for any $i = 1, \ldots, n$. Moreover, the miscoding of the joint representation is not necessarily less than or equal to the sum of the individual miscodings $\mu(r_1 r_2 \ldots r_n) \nleq \mu(r_1) + \mu(r_2) + \cdots + \mu(r_n)$. Finally, no general conclusions can be drawn regarding how the miscoding of a joint representation is affected by permutations of its components. That is, reordering the representations may increase, decrease, or leave unchanged the overall miscoding.

3.3 Decreasing Miscoding

A valid representation of an entity is a string that contains all the essential information required by the oracle to reproduce the entity, no more, no less. In contrast, an invalid representation, indicated by a miscoding value greater than zero, may result from missing critical information, the inclusion of incorrect symbols, or the presence of irrelevant symbols. To reduce the miscoding of a representation, one may attempt to supply the missing information or remove erroneous or non-pertinent symbols. However, it is generally not possible to determine in advance which of these actions will be effective. Nevertheless, as the following theorem shows, at least one of these approaches must be applicable.

Theorem 3.3.1 Let $r \in \mathcal{B}^*$ be a representation such that $\mu(r) > 0$, then one or both of the following conditions must hold:

(i) There exists a $s \in \mathcal{B}^*$ such that $\mu(rs) < \mu(r)$ or $\mu(sr) < \mu(r)$,

(ii) There exists an $s \in \mathcal{B}^*$ in the form $r = \alpha s \beta$ with $\alpha, \beta \in \mathcal{B}^*$ such that $\mu(s) < \mu(r)$.

Proof. Let $r \in \mathcal{B}^*$ be a representation with

$$\mu(r) = \min_{r_e^\star \in \mathcal{R}_\mathcal{E}^\star} \frac{\max\{K(r \mid r_e^\star),\, K(r_e^\star \mid r)\}}{\max\{K(r),\, K(r_e^\star)\}} > 0.$$

Fix one valid representation $r^\star \in \mathcal{R}_\mathcal{E}^\star$ at which the minimum is attained, and write

$$A := K(r \mid r^\star), \qquad B := K(r^\star \mid r), \qquad L := \max\{K(r), K(r^\star)\},$$

so that $\mu(r) = \frac{\max\{A,B\}}{L}$.

We distinguish two (exhaustive) cases. Case i). $B > 0$, that is, some information is missing in r. Because $B > 0$, a shortest self-delimiting program p of length B exists that, given r, outputs $r^\star$. Set $s := p$ and consider the concatenation $r' := rs$. Because s already is the program that converts r into $r^\star$,

$$K(r^\star \mid r') = O(1), \qquad K(r' \mid r^\star) \leq A + B + O(1).$$

Hence

$$\max\{K(r^\star \mid r'), K(r' \mid r^\star)\} \leq A + B + O(1) < A + L.$$

The description length of r' satisfies $K(r') \leq K(r) + B + O(\log B)$, so

$$\max\{K(r'), K(r^\star)\} \geq \max\{K(r), K(r^\star)\} = L.$$

Thus

$$\mu(r') = \frac{\max\{K(r^\star \mid r'),\, K(r' \mid r^\star)\}}{\max\{K(r'),\, K(r^\star)\}} < \frac{A + B + O(1)}{L} \leq \frac{\max\{A, B\}}{L} = \mu(r),$$

so either $\mu(rs) < \mu(r)$ (if we append) or, by symmetric reasoning, $\mu(sr) < \mu(r)$ (if we prepend). Hence condition (i) is satisfied.

Case ii). $B = 0$, that is, all information needed to produce $r^\star$ is contained in r; extra symbols remain. Now $A > 0$ because $\mu(r) > 0$. Since $K(r^\star \mid r) = 0$, a deterministic algorithm can scan r from left to right and halt as soon as it has seen a **shortest prefix** that already allows it to output $r^\star$. Let s

be that prefix and write $r = \alpha s \beta$ with $\beta \neq \lambda$ (otherwise $r = s$ and $A = 0$, contradicting $\mu(r) > 0$).

$$K(r^\star \mid s) = 0, \qquad K(s \mid r^\star) \leq K(r \mid r^\star) = A.$$

Because s is a proper prefix of r, $K(s) \leq K(r)$ (up to an $O(\log K(r))$ term). Therefore

$$\mu(s) = \frac{\max\{K(s \mid r^\star), K(r^\star \mid s)\}}{\max\{K(s), K(r^\star)\}} \leq \frac{A}{\max\{K(s), K(r^\star)\}} < \frac{\max\{A, B\}}{L} = \mu(r),$$

so condition (ii) holds with that substring s. ■

Refer to Example 2.11 for a case in which appending additional information to a representation improves its quality, that is, reduces its miscoding. Also, the following example illustrates the opposite situation: a case in which removing certain symbols from a representation can lead to a decrease in miscoding.

■ **Example 3.4** A historian compiles a representation r intended to narrate the events surrounding the signing of a pivotal treaty. However, the inclusion of speculative statements and personal interpretations about the intentions of the involved parties, statements not supported by primary sources, results in a high miscoding value. Although the document is rich in content, it is contaminated by erroneous or unverifiable information, rendering it an invalid representation of the historical event.

By removing these speculative and unsubstantiated segments, a revised version r' is produced. This refined representation presents a concise and factual account based solely on verifiable data and primary sources. The removal of misleading content reduces the miscoding value, making r' a more valid representation that more accurately reflects the historical event without the noise of uncorroborated interpretations. ■

3.4 Targetless Representations

In the most extreme scenario, the miscoding value can reach its upper bound of 1. This occurs when the current representation r does not contain a single symbol that contributes to the encoding of any entity in the set $\mathcal{E}$. In such a case, r is said to be a targetless representation, an abstract string with no concrete or meaningful interpretation.

Definition 3.4.1 Let $r \in \mathcal{B}^*$ be a representation. If $\mu(r) = 1$ we say that r is a *targetless* representation.

Although one could, in principle, assign a targetless representation to an arbitrary entity, doing so would violate the essential requirement of surrogative reasoning (see Section G.4). The following proposition formalizes this idea.

Proposition 3.4.1 Given a representation $r \in \mathcal{B}^*$, the miscoding $\mu(r)$ reaches its maximum value of 1 if and only if no symbol in r contributes to the encoding of any entity in $\mathcal{E}$.

Proof. Assume that r contains no symbol that contributes to the encoding of any entity $e \in \mathcal{E}$. Let $r_e^\star$ be a valid representation of some $e \in \mathcal{E}$. Then, the shortest program capable of generating $r_e^\star$ from r must encode the entirety of $r_e^\star$ without reuse of any symbols from r. Thus, $K(r_e^\star \mid r) = K(r_e^\star)$. Similarly, since no symbol in $r_e^\star$ contributes to the generation of r, we have $K(r \mid r_e^\star) = K(r)$. Substituting into the definition of miscoding:

$$\mu(r) = \frac{\max\{K(r \mid r_e^\star), K(r_e^\star \mid r)\}}{\max\{K(r), K(r_e^\star)\}} = \frac{\max\{K(r), K(r_e^\star)\}}{\max\{K(r), K(r_e^\star)\}} = 1$$

assuming $K(r) \neq 0$ and $K(r_e^\star) \neq 0$. Conversely, suppose that $\mu(r) = 1$. Then:

$$\max\{K(r \mid r_e^\star), K(r_e^\star \mid r)\} = \max\{K(r), K(r_e^\star)\}$$

which implies that neither r can help generate $r_e^\star$ nor $r_e^\star$ can help generate r. Therefore, there is no overlap in information, and r contains no symbol that contributes to the encoding of any entity in $\mathcal{E}$. ■

For every finite or countably infinite set of entities $\mathcal{E}$, there exists an infinite number of targetless representations. We will prove this result constructively by showing that at least one targetless representation exists and then defining a method to generate infinitely many more from it.

Proposition 3.4.2 For every finite or countably infinite set of entities $\mathcal{E}$, there exists an uncountably infinite set of targetless representations.

Proof. Let $\mathcal{R}$ denote the set of all valid representations of entities in $\mathcal{E}$, such that for each entity $e \in \mathcal{E}$, there exists a representation $r \in \mathcal{R}$ and vice versa. Since $\mathcal{E}$ is finite or countably infinite, $\mathcal{R}$ is also countable.

Now consider the set $\mathcal{B}^*$ of all finite binary strings. This set is countably infinite, as it includes all possible finite sequences over the alphabet $0, 1$. Because $\mathcal{R}$ is a subset of $\mathcal{B}^*$ and is countable, and $\mathcal{B}^* \setminus \mathcal{R}$ is non-empty and infinite, there must exist binary strings that are not valid representations of any entity in $\mathcal{E}$.

Let $r_0 \in \mathcal{B}^* \setminus \mathcal{R}$ be any such string. By definition, r_0 is a targetless representation.

Given any targetless representation r_i, we can construct a new targetless representation r_{i+1} by appending a symbol (either '0' or '1') to r_i. Since r_i does not encode any entity in $\mathcal{E}$, and $\mathcal{R}$ is prefix-free with respect to targetless extensions (i.e., extending a non-representation cannot turn it into a valid one), the new string r_{i+1} also does not correspond to any entity. Therefore, r_{i+1} is also targetless.

By iterating this process, we generate an infinite sequence of distinct targetless representations $r_0, r_1, r_2, \ldots \subset \mathcal{B}^* \setminus \mathcal{R}$. This proves that there exists a countably infinite set of targetless representations corresponding to any finite or countably infinite set of entities $\mathcal{E}$. ■

What constitutes a targetless representation for one oracle may not necessarily be targetless for another, as the following example illustrates.

■ **Example 3.5** Imagine two machines, A and B, each controlling a robotic arm capable of manufacturing nuts and bolts. Machine A operates using a low-level assembly language, whereas Machine B uses a more sophisticated high-level programming language. As a result, a particular set of instructions that fails to produce a valid output on Machine A—thus being considered a targetless representation—could be perfectly interpretable by Machine B, successfully yielding a finished bolt. ■

The normalized compression distance between a targetless representation and the closest valid (non-targetless) representation may be less than one. This indicates that the targetless representation shares some information with a valid one. However, this is not sufficient to ensure scientific progress, as the computational effort, reflected in the size or complexity of the Turing machine required to extract useful knowledge, may be larger.

3.5 Miscoding of Areas

The concept of miscoding can be extended to research areas to quantitatively measure the amount of effort required to correct an inaccurate representation of an area. Unfortunately, as discussed in Section 2.8, there is no reliable way to verify whether the strings included in an n-fold representation actually correspond to entities within that area. Moreover, it is not possible to prevent cases in which some of these strings represent the same entity.

Consider the strings $r_1, r_2, \ldots, r_n$, where each $r_i \in \mathcal{B}^*$ for $i = 1, 2, \ldots, n$. Recall that the expression $r_1 r_2 \ldots r_n$ refers to the concatenation of these strings into a single binary string. This operation may merge the individual components in a way that makes them inseparable. In contrast, the notation $\langle r_1, r_2, \ldots, r_n \rangle$ denotes a re-encoding of the individual strings into a single string that preserves the ability to recover each original component.

Furthermore, the joint representation $r_1 r_2 \dots r_n$ is assumed to encode a single entity, while the n-fold representation $\langle r_1, r_2, \dots, r_n \rangle$ may encode up to n distinct entities.

The following definition extends the concept of miscoding to n-fold representations.

Definition 3.5.1 Let $R = (r_1, r_2, \dots, r_n) \in \mathcal{B}^* \times \mathcal{B}^* \times \cdots \times \mathcal{B}^*$ be an n-fold representation. We define the *miscoding* of R, denoted by $\mu(R)$, as:

$$\mu(R) = \overset{o}{\min_{(r^\star_{e_1},\dots,r^\star_{e_n}) \in \mathcal{R}^\star_{\mathcal{E}} \times \cdots \times \mathcal{R}^\star_{\mathcal{E}}}} \frac{\max\left\{K\left(\langle r_1,\dots,r_n\rangle \mid \langle r^\star_{e_1},\dots,r^\star_{e_n}\rangle\right), K\left(\langle r^\star_{e_1},\dots,r^\star_{e_n}\rangle \mid \langle r_1,\dots,r_n\rangle\right)\right\}}{\max\left\{K\left(\langle r_1,\dots,r_n\rangle\right), K\left(\langle r^\star_{e_1},\dots,r^\star_{e_n}\rangle\right)\right\}}$$

where $\overset{o}{\min}$ indicates that the minimum is to be computed by an oracle.

The miscoding of the representation of an area falls within the range $[0, 1]$, as demonstrated by the following proposition.

Proposition 3.5.1 For all known subsets $R = (r_1, r_2, \dots, r_n) \in \mathcal{B}^* \times \mathcal{B}^* \times \cdots \times \mathcal{B}^*$, it holds that $0 \leq \mu(R) \leq 1$.

Proof. Since $\langle r_1, r_2, \dots, r_n \rangle$ is a string in $\mathcal{B}^*$, we can apply Proposition E.5.5, which guarantees that the normalized compression-based distance lies between 0 and 1. ∎

By extending the concept of miscoding to cover research areas, we gain a quantitative means of evaluating the quality of representations for specific subsets of entities. This mathematical framework provides a rigorous tool to assess and correct inaccuracies, both at the level of individual entities and across broader scientific domains.

References

Misrepresentation or inaccuracies in scientific representation have significant implications for scientific discovery, technological progress, policymaking, and other domains. However, no book or paper explicitly addresses the topic of "incorrect representations in science" from the perspective adopted in this work. Here, we decompose the problem of scientific representation into two complementary subproblems: the representation of entities and the description of those representations.

[Sup02] provides a formal foundation for scientific representation and emphasizes the role of structure-preserving mappings; his analysis is crucial for understanding when and how representations fail to capture relevant features of phenomena. [Van80] introduces the concept of "constructive empiricism" and highlights the model-dependent nature of scientific representation. [LSW13] offers an ethnographic study of how scientific representations are socially constructed—and, at times, distorted—in scientific practice.

Although the specific topic of incorrect representations has not been directly examined in this way, various researchers have addressed related concerns indirectly. Their discussions often focus on issues such as scientific fraud, the replication crisis, and the use of incorrect or misleading models. For example, [Ioa05] presents a widely cited empirical and philosophical analysis of how methodological biases, poor model design, and selective reporting contribute to unreliable or misleading scientific results.

4. Inaccuracy

A little inaccuracy sometimes saves
tons of explanations.
Saki

In Section 2.5, we introduced the notion of a description, or model, of an entity as a computer program. When executed, this program reproduces one of the representations encoding the entity in question. More precisely, a description d for a representation r of an entity e is a Turing machine that produces the string r when interpreted by a universal Turing machine δ. However, due to our typically incomplete understanding of the entity e, the actual output of the description, denoted as $r' = \delta(d)$, will generally resemble but not exactly match r.

In this chapter, we investigate the error introduced by flawed models, specifically, how closely the output r' approximates the intended representation r. We refer to this type of error as the *inaccuracy* of the description d.

Inaccuracy constitutes the second metric for assessing our understanding of a research entity. The underlying idea is that the more accurate our model, the closer r' is to r, and thus the better our understanding of the entity. Formally, the inaccuracy of a description d is defined as the normalized information distance between the original representation r and the output representation r' produced by the description. That is, inaccuracy measures the length of the shortest computer program needed to transform the erroneous output r' into the correct representation r.

Inaccuracy evaluates how well the output of a description aligns with the selected representation encoding the entity. However, as discussed in the preceding chapter, the representation itself may be flawed. Inaccuracy focuses exclusively on the description d, without accounting for potential miscoding in the representation r. Moreover, although its computation does not require an oracle, inaccuracy cannot always be calculated exactly in practice; instead, it must often be estimated—a topic we will address in Part II of this book.

In this chapter, we formally define inaccuracy and examine its key properties. We also analyze how inaccuracy behaves when conditional descriptions are used in place of unconditional ones. Finally, we extend the notion of inaccuracy from individual entities to entire research areas.

This investigation is not purely theoretical, it has significant practical relevance. Accurate models are essential across a wide range of domains, from climate prediction to the development of artificial intelligence systems. Understanding and quantifying inaccuracy can thus lead to better models, ultimately improving our ability to make reliable predictions and informed decisions.

4.1 Inaccuracy

In the process of studying an entity $e \in \mathcal{E}$ through a representation $r \in \mathcal{R}_e$, we may encounter situations in which our proposed description d fails to accurately produce r. That is, $d \notin \mathcal{D}_r$ (see Definition 2.5.2). In such cases, when the universal Turing machine δ receives d as input, it produces a string r' that differs from the original representation r.

Intuitively, one might say that d is an inaccurate description of the entity e. However, because descriptions refer to entities only indirectly, via representations, our formal notion of inaccuracy must be defined in terms of the representation, not the entity itself. Furthermore, we must account for the possibility that the representation r is itself flawed, as previously discussed through the concept of miscoding.

With these considerations in mind, we introduce the following definition of an inaccurate description.

Definition 4.1.1 Let $r \in \mathcal{B}^*$ be a representation, and let $d \in \mathcal{D}$ be a description, where $d = \langle TM, a \rangle$. If the output of $TM(a)$ is a string r' such that $r \neq r'$, we say that d is an *inaccurate* description for r.

Our proposed description d may fall outside the set of valid descriptions $\mathcal{D}_r$ for r (indicating positive inaccuracy), and the representation r may not belong to the set of valid representations $\mathcal{R}_e^\star$ for the entity e (indicating positive miscoding).

When a description is inaccurate, we aim to quantify the degree of inaccuracy. Within the computational framework, a natural approach is to measure how difficult it is to transform the incorrect representation r', obtained by executing d on the universal Turing machine, into the original representation r. This difficulty is captured by the normalized information distance between r' and r.

Definition 4.1.2 — Inaccuracy. Let $r \in \mathcal{B}^*$ be a representation, and let $d \in \mathcal{D}$ be a description, where $d = \langle TM, a \rangle$. We define the *inaccuracy* of the description d with respect to the representation r, denoted by $\iota(d,r)$, as:

$$\iota(d,r) = \frac{\max\{K(r \mid \delta(d)),\, K(\delta(d) \mid r)\}}{\max\{K(r),\, K(\delta(d))\}}$$

The use of a relative measure of inaccuracy, rather than an absolute one, enables meaningful comparisons between inaccuracies across different descriptions of the same representation, as well as between descriptions of different representations.

Similar to miscoding (see Definition 3.1.1), inaccuracy is computed using a bidirectional approach: we calculate the length of the shortest computer program that can generate the correct representation r from the erroneous one r', and vice versa, that is, the shortest program that can generate r' from r. In essence, a valid description should produce a representation that contains all the necessary information to reconstruct the intended entity, while excluding any erroneous or irrelevant content.

■ **Example 4.1** Inaccuracy primarily concerns the difficulty of correcting the *output* of a description, that is, the result produced by a computable model, rather than the difficulty of modifying the description itself.

For example, suppose we have a dataset generated by a system that is perfectly described by a quadratic function, but we choose a linear function as our model. In this case, inaccuracy evaluates how different the predicted dataset (produced by the linear model) is from the original quadratic dataset. It does not measure how difficult it is to transform the incorrect linear model into the correct quadratic one.

In this sense, if the original dataset consists of 10 points, a polynomial of degree ten that perfectly fits the data would also yield an inaccuracy of zero. Determining which model is preferable, the quadratic model with zero inaccuracy or the more complex degree-ten polynomial, also with zero inaccuracy, is a matter addressed by the surfeit metric (see Chapter 5). ▪

Given its basis in Kolmogorov complexity, inaccuracy is a quantity that, in general, cannot be computed exactly and must instead be approximated. The method used to approximate inaccuracy depends on the specific characteristics of the entities under study and the nature of their representations.

Conveniently, the inaccuracy of a description always falls within the range $[0,1]$, as established by the following proposition.

Proposition 4.1.1 For all representations $r \in \mathcal{B}^*$ and all descriptions $d \in \mathcal{D}$, it holds that $0 \leq \iota(d,r) \leq 1$.

Proof. This follows from the general inequality

$$0 \leq \frac{\max\{K(x \mid y),\ K(y \mid x)\}}{\max\{K(x),\ K(y)\}} \leq 1$$

for all $x, y \in \mathcal{B}^*$, as stated in Proposition E.5.5. ■

The proposition above applies to all pairs of descriptions d and representations r, even in cases where d is not intended to model r. In such instances, the inaccuracy $\iota(d,r)$ will typically be close to one.

Inaccuracy is exactly zero if and only if the description d is one of the valid descriptions of the representation r.

Proposition 4.1.2 Given a description $d \in \mathcal{D}$ and a representation $r \in \mathcal{B}^*$, we have that $\iota(d,r) = 0$ if and only if $d \in \mathcal{D}_r$, i.e., d is a valid description of r.

Proof. If $d \in \mathcal{D}_r$, then by definition, $\delta(d) = r$. Consequently, we have $K(r \mid \delta(d)) = K(\delta(d) \mid r) = 0$, and thus $\iota(d,r) = 0$.

Conversely, suppose $\iota(d,r) = 0$. Then,

$$\max\{K(r \mid \delta(d)),\ K(\delta(d) \mid r)\} = 0,$$

which implies that both conditional complexities are zero. Therefore, $r = \delta(d)$, and it follows that $d \in \mathcal{D}_r$. ■

Finally, given two representations r and s, we may also be interested in evaluating the inaccuracy of a description d when it is used to describe their joint representation rs. Since we require that rs is itself a valid representation, the extension of the inaccuracy concept to joint representations is straightforward and does not require a new definition:

$$\iota(d,rs) = \frac{\max\{K(rs \mid \delta(d)),\ K(\delta(d) \mid rs)\}}{\max\{K(rs),\ K(\delta(d))\}}$$

As a direct consequence of Proposition 4.5.1, for any representations $r, s \in \mathcal{B}^*$ and any description $d \in \mathcal{D}$, we have:

$$0 \leq \iota(d, rs) \leq 1.$$

4.2 Conditional Inaccuracy

In this section, we delve deeper into the concept of inaccuracy by considering its application to conditional descriptions. Specifically, we explore the inaccuracy of a description when evaluated in conjunction with pre-existing background knowledge, a notion we term *conditional inaccuracy*. As we will see, the inaccuracy of a conditional description can never exceed that of its unconditional counterpart; at worst, it remains unchanged. This property makes conditional inaccuracy a useful tool for evaluating new concepts or models and for assessing their explanatory power with respect to the entity of interest.

In Definition 2.7.1, we introduced the concept of a conditional description d for a representation r, given an arbitrary background string s. This is denoted by $d \mid s$ and defined as the self-delimiting concatenated string $\langle d, s \rangle$, where $d = \langle TM, a \rangle$ and $TM(\langle a, s \rangle) = r$. If $TM(\langle a, s \rangle) = r'$ with $r \neq r'$, then $d \mid s$ is referred to as an *inaccurate* conditional description of r.

It is important to note that $d \mid s$ must be defined for all possible background strings s. Additionally, we refer to the case in which s is the empty string, denoted $d \mid \lambda$, as the *unconditional* version of the description.

Building on the concept of inaccuracy introduced in Definition 4.1.2, we now define the notion of *conditional inaccuracy* to capture the error introduced when using an inaccurate conditional description.

Definition 4.2.1 Let $r \in \mathcal{B}^*$ be a representation, $s \in \mathcal{B}^*$ a background string, and $d \mid s$ an inaccurate conditional description. We define the *conditional inaccuracy* of the description d for the representation r given the string s, denoted by $\iota(d \mid s, r)$, as:

$$\iota(d \mid s, r) = \frac{\max\{K(r \mid \delta(d \mid s)),\ K(\delta(d \mid s) \mid r)\}}{\max\{K(r),\ K(\delta(d \mid s))\}}$$

Conditional inaccuracy is thus defined as the normalized information distance between the original representation r and the string produced by the conditional description $d \mid s$.

As a normalized measure, the conditional inaccuracy of a description lies within the interval $[0, 1]$.

Proposition 4.2.1 Let $r \in \mathcal{B}^*$ be a representation, $s \in \mathcal{B}^*$ a string, and $d \mid s$ a conditional description of r given s. Then $0 \leq \iota(d \mid s, r) \leq 1$.

Proof. This follows directly from the general inequality:

$$0 \leq \frac{\max\{K(x \mid y),\ K(y \mid x)\}}{\max\{K(x),\ K(y)\}} \leq 1$$

for all $x, y \in \mathcal{B}^*$, as established in Proposition E.5.5. ■

The conditional inaccuracy assumes a value of zero if and only if the conditional description $d \mid s$ is a valid model that correctly produces the representation r.

Proposition 4.2.2 Let $r \in \mathcal{B}^*$ be a representation, $s \in \mathcal{B}^*$ a string, and $d \mid s$ a conditional description of r given s, where $d = \langle TM, a \rangle$. Then $\iota(d \mid s, r) = 0$ if and only if $TM(\langle a, s \rangle) = r$.

Proof. If $TM(\langle a, s \rangle) = r$, then $\delta(d \mid s) = r$, which implies that

$$K(r \mid \delta(d \mid s)) = K(\delta(d \mid s) \mid r) = 0.$$

Hence, $\iota(d \mid s, r) = 0$. Conversely, if $\iota(d \mid s, r) = 0$, then

$$\max\{K(r \mid \delta(d \mid s)),\ K(\delta(d \mid s) \mid r)\} = 0,$$

which implies both conditional complexities are zero. Therefore, $\delta(d \mid s) = r$, which means $TM(\langle a, s \rangle) = r$. ■

Incorporating established prior knowledge into research does not increase the inaccuracy of a description. If this background knowledge is relevant to the representation being described, the oracle will use it accordingly. Conversely, if the prior knowledge is irrelevant, the oracle will simply disregard it. The following theorem formalizes this idea.

Theorem 4.2.3 Let $r \in \mathcal{B}^*$ be a representation, and $d \in \mathcal{D}$ a conditional description of r. Then

$$\iota(d \mid s, r) \leq \iota(d, r)$$

for all strings $s \in \mathcal{B}^*$.

Proof. Since $\iota(d, r)$ is equivalent to $\iota(d \mid \lambda, r)$, we need to prove that

$$\frac{\max\{K(r \mid \delta(d \mid s)), K(\delta(d \mid s) \mid r)\}}{\max\{K(r), K(\delta(d \mid s))\}} \leq \frac{\max\{K(r \mid \delta(d \mid \lambda)), K(\delta(d \mid \lambda) \mid r)\}}{\max\{K(r), K(\delta(d \mid \lambda))\}}.$$

This inequality follows from the fact that

$$K(r \mid \langle \delta(d), s \rangle) \leq K(r \mid \delta(d)),$$

as shown in Proposition E.4.3. ■

Theorem 4.2.3 represents a foundational result in the theory of nescience. It establishes the basis for developing a robust methodology aimed at deepening our understanding (i.e., reducing inaccuracy) of a research entity. In practical applications, our primary focus will typically be on prior knowledge directly related to the subject of study. However, the core insight of Theorem 4.2.3 is that incorporating concepts from seemingly unrelated domains will not compromise the accuracy of our investigation. This theorem becomes particularly powerful when such exploratory processes are automated (see Chapter 10).

■ **Example 4.2** The P vs. NP problem stands as one of the most significant unresolved questions in computer science. It asks whether every problem whose solution can be verified in polynomial time (class NP) can also be solved in polynomial time (class P). The relationship between these two complexity classes remains unsolved. Constructing a comprehensive, self-contained solution to this problem in a formal language is an immense challenge. However, leveraging relevant prior knowledge can significantly reduce the complexity of the required description. For instance, insights from Algorithm Theory, which deals with the classification and efficiency of algorithms, and from Formal Language Theory, which addresses the structure of computational problems (e.g., regular and context-free languages) and highlights the role of Turing machines, can be instrumental. Drawing upon such established knowledge may not only simplify our descriptions but also facilitate a deeper understanding and potentially contribute to resolving the P vs. NP problem. ■

Finally, given two representations r and t, the formalization of the concept of conditional inaccuracy, when applied to the joint representation rt, is straightforward and does not require a new definition:

$$\iota(d \mid s) = \frac{\max\{K(rt \mid \delta(d \mid s)), K(\delta(d \mid s) \mid rt)\}}{\max\{K(rt), K(\delta(d \mid s))\}}$$

As a normalized measure, $\iota(d \mid s)$ always takes a value in the interval $[0,1]$.

4.3 Decreasing Inaccuracy

Our objective is to reduce the inaccuracy of the current description d_1, thereby improving our understanding of the original entity. This improvement may involve either modifying d_1 to correct or eliminate its inaccuracies, or developing a completely new description based on a different approach to modeling the entity. In either case, the result is a new description d_2. In this section, we aim to analyze how the introduction of a new description d_2 affects the inaccuracy compared to the original description d_1.

Definition 4.3.1 Let $r \in \mathcal{B}^*$ be a representation, and let $d_1, d_2 \in \mathcal{D}$ be two descriptions. We define the *variation of inaccuracy* between the descriptions d_1 and d_2, with respect to r, denoted by $\Delta_\iota^a(d_1, d_2, r)$, as:

$$\Delta_\iota^a(d_1, d_2, r) = \iota(d_1, r) - \iota(d_2, r)$$

Since inaccuracy is bounded between 0 and 1, the maximum possible variation in inaccuracy is ± 1. A positive value of Δ_ι indicates that description d_2 is preferable to d_1 in terms of accuracy. Conversely, a negative value suggests that d_1 is more accurate than d_2. It is important to note that the new description may also introduce a substantial increase in surfeit, potentially outweighing the improvement in inaccuracy. For a detailed discussion of surfeit, refer to Chapter 5, and for an explanation of how inaccuracy and surfeit combine into the unified metric of nescience, see Chapter 6.

We can also introduce a relative measure of the variation in inaccuracy, when moving from description d_1 to d_2

Definition 4.3.2 Let $r \in \mathcal{B}^*$ be a representation, and $d_1, d_2 \in \mathcal{D}$ be two descriptions. We define the *relative variation of inaccuracy* between descriptions d_1 and d_2, denoted by $\Delta_\iota^r(d_1, d_2, r)$, as:

$$\Delta_\iota^r(d_1, d_2, r) = \frac{\iota(d_1, r) - \iota(d_2, r)}{\iota(d_1, r)}$$

provided that $\iota(d_1, r) \neq 0$.

A value of 0 indicates no change, while a value of 1 corresponds to a complete elimination of inaccuracy. Negative values, on the other hand, signify an increase in inaccuracy, indicating that the new description d_2 is less accurate than the original d_1. Note that the relative variation can be arbitrarily negative, diverging to $-\infty$ as $\iota(d_2, r)$ increases and $\iota(d_1, r)$ approaches zero.

As inaccuracy approaches zero, relative variations become increasingly unstable. A small absolute change can produce a large relative variation if the initial inaccuracy is very low. For instance, if $\iota(d_1, r) = 0.1$ and the inaccuracy decreases by 0.05, this corresponds to a relative improvement of 50%. In contrast, if $\iota(d_1, r) = 0.9$ and the same absolute improvement occurs, the relative reduction is only about 5.6%. Both absolute and relative variations are essential for evaluating the significance and magnitude of improvements.

An alternative strategy for reducing uncertainty about an entity involves modifying its representation rather than altering its description. While such a change might increase the miscoding of the entity, the potential reduction in inaccuracy could outweigh this drawback.

Definition 4.3.3 Let $r_1, r_2 \in \mathcal{B}^*$ be two representations, and let $d \in \mathcal{D}$ be a description. We define the *variation of inaccuracy* between representations r_1 and r_2, denoted by $\Delta_\iota^a(d, r_1, r_2)$, as:

$$\Delta_\iota^a(d, r_1, r_2) = \iota(d, r_1) - \iota(d, r_2)$$

As before, since inaccuracy is bounded between 0 and 1, the maximum possible variation is 1. A positive value of Δ_ι^a indicates a preference for representation r_2 over r_1 with respect to the fixed description d. Conversely, a negative value suggests that r_1 is more accurate than r_2. This comparison is based solely on inaccuracy, as miscoding is not considered here. Additionally, since the description remains unchanged, there is no risk of variation in surfeit.

Finally, we can also introduce a relative variation of inaccuracy with respect to a change in representation

Definition 4.3.4 Let $r_1, r_2 \in \mathcal{B}^*$ be two representations, and $d \in \mathcal{D}$ be a description. We define the *relative variation of inaccuracy* of the representations r_1, r_2, denoted by $\Delta_\iota^r(d, r_1, r_2)$, as:

$$\Delta_\iota^r(d, r_1, r_2) = \frac{\iota(d, r_1) - \iota(d, r_2)}{\iota(d, r_1)}$$

provided that $\iota(d, r_1) \neq 0$.

This quantity measures the proportional reduction in inaccuracy resulting from replacing representation r_1 with r_2, while keeping the description fixed. A value of 0 indicates no change in inaccuracy, and a value of 1 corresponds to a complete elimination of inaccuracy. However, Δ_ι^r can also take negative values, potentially diverging to $-\infty$, when the new representation r_2 performs worse than r_1. As the inaccuracy of the initial representation r_1 approaches zero, even minor absolute changes in inaccuracy can lead to large swings in the relative variation, making it increasingly volatile.

4.4 Inaccuracy-Miscoding Rate of Change

In the preceding section, we examined how the inaccuracy of a representation can be reduced by selecting a different description. We also explored an alternative strategy in which inaccuracy is minimized not by modifying the description, but by changing the representation itself. In this section, we turn our attention to a more general approach for reducing the inaccuracy associated with an entity. Rather than altering the description or the representation in isolation, it may be more effective to modify both simultaneously.

The balance between the amount of miscoding we are willing to accept in order to achieve a reduction in inaccuracy is referred to as the *miscoding-inaccuracy trade-off*. For a broader discussion of trade-offs in multi-objective optimization, refer to Section F.5.2.

Definition 4.4.1 Let $e \in \mathcal{E}$ be an entity, and $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{R}_e \times \mathcal{D}$ be two hypotheses, with $\mathbf{x}_1 = (r_1, d_1)$ and $\mathbf{x}_2 = (r_2, d_2)$. We define the *rate of change between the inaccuracy and the miscoding* of the hypothesis $\mathbf{x}_1, \mathbf{x}_2$, denoted by $\Delta_{\mu\iota}(\mathbf{x}_1, \mathbf{x}_2)$ as:

$$\Delta_{\iota\mu}(\mathbf{x}_1, \mathbf{x}_2) = \frac{\iota(d_2, r_2) - \iota(d_1, r_1)}{\mu(r_2) - \mu(r_1)}$$

provided that $\mu(r_2) - \mu(r_1) \neq 0$.

The ratio $\Delta_{\iota\mu}$ represents the rate of change between inaccuracy and miscoding when transitioning from the first hypothesis to the second. A positive value of $\Delta_{\iota\mu}$ implies that both quantities, miscoding and inaccuracy, either decrease (which is desirable) or increase (which is undesirable). The interpretation becomes more nuanced when $\Delta_{\iota\mu}$ is negative, indicating that one of the quantities decreases while the other increases. In such cases, two scenarios must be considered:

(i) Inaccuracy decreases and miscoding increases, we aim for $\Delta_{\iota\mu}(\mathbf{x}_1, \mathbf{x}_2) < M$, where $M < -1$, thereby ensuring that the reduction in inaccuracy compensates for the increase in miscoding.

(ii) Inaccuracy increases and miscoding decreases, we aim for $\Delta_{\iota\mu}(\mathbf{x}_1, \mathbf{x}_2) > M$, where $-1 < M < 0$, thereby ensuring that the reduction in miscoding justifies the increase in inaccuracy.

In both cases, caution is warranted when the change in miscoding is small, as it can disproportionately affect the ratio and potentially lead to misleading conclusions.

■ **Example 4.3** Let $\mathbf{x}_1$ and $\mathbf{x}_2$ be two hypotheses. For $\mathbf{x}_1$, the inaccuracy $\iota(d_1, r_1)$ is 0.40, and the miscoding $\mu(r_1)$ is 0.15. For $\mathbf{x}_2$, the inaccuracy $\iota(d_2, r_2)$ is 0.20 (a decrease from 0.40), and the miscoding $\mu(r_2)$ is 0.25 (an increase from 0.15). Using the definition of the rate of change, we compute:

$$\Delta_{\iota\mu}(\mathbf{x}_1, \mathbf{x}_2) = \frac{0.40 - 0.20}{0.15 - 0.25} = \frac{0.20}{-0.10} = -2$$

In this case, transitioning from hypothesis $\mathbf{x}_1$ to $\mathbf{x}_2$ results in a decrease of inaccuracy by 0.20 units and an increase in miscoding by 0.10 units. The rate of change is -2. ■

Having a very small change in miscoding can significantly amplify the value of the rate of change, potentially giving the misleading impression that inaccuracy and miscoding are varying at an extreme rate, even when the actual changes are minor. This phenomenon is illustrated in the following example.

■ **Example 4.4** Let $\mathbf{x}_1$ be a hypothesis with an inaccuracy $\iota(d_1, r_1)$ of 0.35 and a miscoding $\mu(r_1)$ of 0.20. Let $\mathbf{x}_2$ be a second hypothesis with an inaccuracy $\iota(d_2, r_2)$ of 0.30 (a slight decrease from 0.35) and a miscoding $\mu(r_2)$ of 0.2001 (a very small increase from 0.20). Applying the definition of the rate of change:

$$\Delta_{\iota\mu}(\mathbf{x}_1, \mathbf{x}_2) = \frac{0.35 - 0.30}{0.20 - 0.2001} = \frac{0.05}{-0.0001} = -500$$

The rate of change is -500, which may misleadingly suggest a dramatic shift. In reality, the inaccuracy only decreased by 0.05 units, and the miscoding increased by a negligible 0.0001 units. The extremely small denominator inflates the result, making the change appear far more significant than it actually is. ■

As we attempt to optimize both inaccuracy and miscoding, we inevitably encounter configurations (hypotheses) where improving one objective necessitates compromising the other. The set of such "best trade-off" configurations constitutes the Pareto frontier (see Section F.5). Points on the Pareto frontier are said to be Pareto optimal because any attempt to improve one objective leads to a deterioration in the other.

Definition 4.4.2 Let $e \in \mathcal{E}$ be an entity, and let $\mathbf{x} = (r, d) \in \mathcal{R}_e \times \mathcal{D}$ be a hypothesis. The hypothesis $\mathbf{x}$ is said to be a Pareto point with respect to inaccuracy ι and miscoding μ if there does not exist another hypothesis $\mathbf{x}' = (r', d')$ such that:

1 $\iota(d', r') \leq \iota(d, r)$ and $\mu(r') \leq \mu(r)$, and
2 $\iota(d', r') < \iota(d, r)$ or $\mu(r') < \mu(r)$.

In simpler terms, a hypothesis $\mathbf{x}$ is Pareto optimal if: (i) no other hypothesis is better in both inaccuracy and miscoding, and (ii) any improvement in one metric necessarily results in a worsening of the other.

The rate of change $\Delta_{\iota\mu}$ between any two Pareto optimal points provides insight into how the trade-off between inaccuracy and miscoding evolves along the Pareto frontier. If decision-makers are more sensitive to changes in inaccuracy than to miscoding, they may prefer configurations with a less negative $\Delta_{\iota\mu}$. Conversely, if miscoding is of greater concern, they may accept solutions where $\Delta_{\iota\mu}$ indicates a larger increase in inaccuracy in exchange for a smaller gain in miscoding.

4.5 Inaccuracy of Areas

An area $\mathcal{A}$ (see Section 2.8) is a subset $\mathcal{A} \subset \mathcal{E}$ of entities that are related or share a common property. The concept of inaccuracy can be extended to research areas in order to quantitatively measure the effort required to correct an inaccurate description of an area.

Given the strings $r_1, r_2, \ldots, r_n$, where each $r_i \in \mathcal{B}^*$ for $i = 1, 2, \ldots, n$, recall that we use $\langle r_1, r_2, \ldots, r_n \rangle$ to denote a self-delimited encoding of the individual strings r_i into a unified string, such that the original components can be fully recovered.

The following definition extends the concept of inaccuracy to research areas.

Definition 4.5.1 Let $\mathcal{A} \subset \mathcal{E}$ be an area with a known subset $\hat{\mathcal{A}} = r_1, r_2, \ldots, r_n$, and let $d \in \mathcal{D}$ be a description. We define the *inaccuracy of the area* given the description d, denoted by $\iota(d, \hat{\mathcal{A}})$, as:

$$\iota(d, \hat{\mathcal{A}}) = \frac{\max\{K(\langle r_1, r_2, \ldots, r_n \rangle \mid \delta(d)), K(\delta(d) \mid \langle r_1, r_2, \ldots, r_n \rangle)\}}{\max\{K(\langle r_1, r_2, \ldots, r_n \rangle), K(\delta(d))\}}$$

The inaccuracy of a description for an area falls within the interval from 0 to 1, as established by the following proposition.

Proposition 4.5.1 For all known subsets $\hat{\mathcal{A}} = r_1, r_2, \ldots, r_n$ and all descriptions $d \in \mathcal{D}$, we have that $0 \leq \iota(d, \hat{\mathcal{A}}) \leq 1$.

Proof. The result follows directly from the fact that $\langle r_1, r_2, \ldots, r_n \rangle$ is a string in $\mathcal{B}^*$, and from Proposition E.5.5. ■

By extending the concept of inaccuracy to cover areas, we can quantitatively evaluate the quality of a description for a specific subset of entities. This mathematical framework provides a rigorous tool for assessing and correcting inaccuracies not only at the level of individual entities but also across broader research domains.

References

A good introduction to the study of uncertainties (i.e., error analysis in models) in science (particularly in physics, chemistry, and engineering) is the best-selling textbook by Taylor [TAY22], which also features the same image of a crashed train used in the introduction to this chapter. Another excellent entry-level reference on error analysis, aimed at undergraduate students in science and technology, is the book by Hughes and Hase [HH10].

From a more philosophical perspective, Popper's work [Pop14] is highly influential. In it, he introduces the concept of falsifiability, asserting that for a theory to be regarded as scientific, it must be testable and subject to refutation.

5. Surfeit

Everything should be made as simple as possible,
but not simpler.
Albert Einstein

Surfeit is the final metric we introduce to quantitatively assess our understanding of a research entity. It measures the presence of superfluous symbols in the description used to model that entity. Intuitively, our lack of knowledge is often reflected in the length (i.e., number of symbols) of our current description. Lengthy descriptions tend to include erroneous or redundant elements. As our understanding of the subject improves, we should be able to identify and remove these unnecessary symbols, resulting in a more concise and accurate description.

We define the surfeit of a description for an entity as the difference in length between the given description and the optimal (i.e., shortest) one for that entity. Within the framework of the theory of nescience, we assume that the pinnacle of knowledge about an entity, its perfect description, is represented by the shortest description capable of fully reconstructing the entity's representation. This notion of perfection relies on both the validity of the representation and the accuracy of the description.

The length of the most concise description of an entity is determined by the Kolmogorov complexity of a representation of that entity. In practical scenarios, given that our knowledge of entities is typically incomplete, the most concise possible description remains unknown. Moreover, as previously discussed, Kolmogorov complexity is not computable in general. Consequently, surfeit is a metric that must be approximated in practice.

If we could construct a perfect description of an entity, it would necessarily be a random string; otherwise, it would contain redundant elements that could be eliminated. Within the framework of the theory of nescience, attaining perfect knowledge corresponds to reaching a state of randomness. This inherent randomness defines a boundary on the depth of understanding achievable for a given research topic. However, rather than constituting a limitation, recognizing and understanding this boundary opens new opportunities in both science and technology. For example, by assessing how far our current description deviates from a random string, we can estimate our proximity to realizing a perfect description.

In this chapter, we formally introduce the concept of surfeit and examine its properties, including conditional surfeit. We will also present the notion of redundancy as a practical approximation of surfeit. Strategies for reducing both surfeit and redundancy will be discussed, as well as the relationship between reductions in surfeit and changes in inaccuracy or miscoding. Finally, we extend the concept of surfeit to support the analysis of entire research areas.

5.1 Surfeit

Given the length of a description of a representation for an entity and the length of its shortest possible description, we can introduce a relative measure to quantify the unnecessary effort involved in explaining the entity using that particular description. We call this quantity *surfeit*. Surfeit is a key component of our definition of nescience, as it reflects the degree to which our current understanding of the research entity includes superfluous or redundant information.

> **Definition 5.1.1 — Surfeit.** Given a representation $r \in \mathcal{B}^*$, and a description $d \in \mathcal{D}$ for r, we define the *surfeit of the description d for the representation r*, denoted by $\sigma(d,r)$, as
>
> $$\sigma(d,r) = \frac{|l(d) - K(r)|}{l(d)}$$

For most descriptions, the length of the description $l(d)$ for r will exceed the length of its shortest possible description $K(r)$. Intuitively, the less we know about an entity, the longer our description tends to be. As our understanding of the entity improves, we should be able to remove all redundant elements from the description. There may also be cases where the description is shorter than the optimal one. In such instances, the description oversimplifies the problem, which can be equally problematic. This justifies the use of the absolute value $|l(d) - K(r)|$ rather than simply $l(d) - K(r)$. Naturally, the current description might also be inaccurate, or the representation may be invalid. These concerns are addressed separately by the metrics of inaccuracy and miscoding.

In our definition of surfeit, we chose a relative measure rather than an absolute one (i.e., $|l(d) - K(r)|$) because we aim to compare the surfeit not only among different models of the same entity but also across models of different entities. We prefer to use $K(r)$ instead of the equivalent $l(r^\star)$ to maintain consistency with the definition of inaccuracy provided in Section 4.1.

■ **Example 5.1** In a practical machine learning scenario, consider the task of classifying images of cats and dogs, where the representation consists of a set of training images. An initial complex model, burdened with excessive parameters and irrelevant features, can be seen as a lengthy "description" of the problem. The optimal model, by contrast, achieves a balance between accuracy and simplicity. Surfeit quantifies the excess complexity of the initial model relative to this optimal one. It measures the "extra" components that are not essential for accurate classification. A high surfeit indicates that the model is overly complicated, highlighting the need for simplification to improve both efficiency and generalization, a fundamental principle in machine learning for building models that perform well on unseen data. ■

The surfeit of a description is a number between 0 and 1.

Proposition 5.1.1 Let $r \in \mathcal{B}^*$ be a representation, and $d \in \mathcal{D}_r^\star$ one of its valid descriptions, then we have that $0 \leq \sigma(d,r) \leq 1$.

Proof. The numerator $|l(d) - K(r)|$ is non-negative for all d and r, and the denominator $l(d) > 0$ (as descriptions must be non-empty). Hence, the entire expression is non-negative $\sigma(d,r) \geq 0$.

To show that $\sigma(d,r) \leq 1$, observe that:

$$|l(d) - K(r)| = l(d) - K(r) \leq l(d).$$

since d is a valid description of r, and so $l(d) \geq K(r)$. Thus:

$$\sigma(d,r) = \frac{|l(d) - K(r)|}{l(d)} \leq \frac{l(d)}{l(d)} = 1.$$

■

The surfeit is zero when the length of the description $l(d)$ equals the Kolmogorov complexity $K(r)$ of the representation r of the entity, indicating that the description has achieved theoretical conciseness.

Proposition 5.1.2 Let $r \in \mathcal{B}^*$ be a representation, and $d \in \mathcal{D}_r^\star$ a valid description for r, then we have that $\sigma(d,r) = 0$ if and only if $l(d) = l(d^\star)$.

Proof. Assume $l(d) = l(d^\star) = K(r)$. Then:

$$\sigma(d,r) = \frac{|l(d) - K(r)|}{l(d)} = \frac{|K(r) - K(r)|}{K(r)} = \frac{0}{K(r)} = 0.$$

Assume $\sigma(d,r) = 0$. Then:

$$\frac{|l(d) - K(r)|}{l(d)} = 0.$$

This implies that the numerator must be zero, i.e.:

$$|l(d) - K(r)| = 0 \Rightarrow l(d) = K(r) = l(d^\star).$$

■

It is important to distinguish between conciseness and correctness. A surfeit of zero indicates that the description is as brief as theoretically possible, but not necessarily accurate. The accuracy of a description is evaluated using the inaccuracy metric. Thus, while a zero surfeit reflects the optimal compactness of a description, its correctness and reliability must be assessed separately through inaccuracy. Together, surfeit and inaccuracy provide a more complete assessment of the description's efficiency and validity.

The following example underscores the need to balance minimal surfeit with low inaccuracy in order to develop models that are both efficient and reliable.

■ **Example 5.2** In a machine learning scenario, consider a model designed to classify emails as spam or not. Suppose this model achieves a surfeit of zero, indicating optimal conciseness with no superfluous elements in its description. However, despite this streamlined complexity, the model exhibits high inaccuracy, frequently misclassifying emails. This illustrates the distinction between surfeit and inaccuracy: while the model is theoretically as concise as possible, reflected in its zero surfeit, its practical utility is compromised by incorrect classifications, as captured by the inaccuracy metric. ■

It is important to note that, in theory, more than one description may yield a surfeit of zero for the same representation. This occurs when two distinct, yet incompressible, descriptions have exactly the same length. In such cases, both descriptions are equally concise and minimal, meaning that neither contains redundant information that could be further compressed. Since surfeit measures the relative difference between the actual length of a description and the shortest possible one, any description whose length equals the Kolmogorov complexity $K(r)$ of the representation will result in $\sigma(d,r) = 0$. Therefore, while the perfect description is often referred to as unique, from a theoretical standpoint, multiple descriptions of equal minimal length and incompressibility may coexist.

5.2 Redundancy

Our definition of surfeit compares the length of a description with the Kolmogorov complexity of the representation, not with the Kolmogorov complexity of the description itself (i.e., $K(d)$). In other words, surfeit is not a measure of the redundancy within a description. It is possible to construct an incompressible description (i.e., one without any internal redundancy) that is not the shortest possible description of the representation it refers to (see Example 2.14). Such a description would not be redundant in the traditional sense, yet it would still exhibit surfeit according to the theory of nescience.

Moreover, it might happen that the description d under consideration does not describe the representation r; in other words, $d \notin \mathcal{D}_r$. For practical applications, it is useful to introduce an alternative, and arguably weaker, notion of redundancy that applies solely to the description itself, independently of any particular representation.

Definition 5.2.1 — Redundancy. Given a description $d \in \mathcal{D}$, we define the *redundancy* of the description d, denoted by $\rho(d)$, as

$$\rho(d) = 1 - \frac{K(d)}{l(d)}$$

The redundancy of a description d is a quantity related to the description itself, and it does not depend on the representation r being described. The following example shows that a description can have low redundancy (being incompressible) and still have high surfeit if it is longer than necessary to describe the underlying task.

■ **Example 5.3** Consider the task of computing the first n digits of π. Description d_1 is a program that implements an algorithm to generate and print these n digits. Description d_2 is a self-extracting compressed program that simply stores the first n digits of π as a hard-coded string, followed by a basic routine to print them.

Description d_2 does not exploit the mathematical structure of π, it merely reproduces the result. Therefore, relative to the representation of the task (computing π), the surfeit $\sigma(d_2, r)$ is high because $l(d_2) \gg K(r)$.

In contrast, description d_1 is significantly shorter since it captures the generative process behind π. While d_1 may still contain some redundancy $\rho(d_1) > 0$, for instance due to suboptimal coding practices, its surfeit remains low since it is near the minimal length required to describe the task effectively.
■

The redundancy of a description always falls within the range $[0, 1]$.

Proposition 5.2.1 We have that $0 \leq \rho(d) \leq 1$ for all $d \in \mathcal{D}$.

Proof. Since Kolmogorov complexity is always less than or equal to the length of the string, we have $0 \leq K(d) \leq l(d)$, which implies that $0 \leq \frac{K(d)}{l(d)} \leq 1$. Subtracting from 1 reverses the inequalities. ■

Finally, next proposition formalizes our intuition that the surfeit of a description is greater or equal than its redundancy.

Proposition 5.2.2 Let $r \in \mathcal{B}^*$ be a representation , and $d \in \mathcal{D}_r^\star$ one of its valid descriptions, then we have that $\rho(d) \leq \sigma(d, r)$.

Proof. Proving that $\rho(d) \leq \sigma(d, r)$ is equivalent to prove that $K(d) \geq K(r)$ for all d. Lets assume that there exist a d such that $K(d) < K(r)$, that would mean there exists a Turing machine $\langle TM, a \rangle$ such that $TM(a) = r$ but $l(< TM, a >) < K(r)$. That is a contradiction with the fact that $K(r)$ is the length of the shortest possible Turing machine that prints r. ■

It would be very nice if Proposition 5.2.2 applies to all possible description. Unfortunately, the proposition is true only when we deal with valid descriptions (from $\mathcal{D}_r^\star$).

5.3 Conditional Surfeit

We are interested in studying how the surfeit of a description for a representation is affected when some background knowledge is assumed. In particular, we examine the case where a description is constructed under the assumption that some prior information is already known. The surfeit of such a description is referred to as the *conditional surfeit*.

Definition 5.3.1 Let $r \in \mathcal{B}^*$ be a representation, $s \in \mathcal{B}^*$ a string, and $d \in \mathcal{D}$ a description of r given s. We define the *conditional surfeit* of the conditional description $d_{r|s}$, denoted by $\sigma(d_{r|s})$, as:

$$\sigma(d_{r|s}) = 1 - \frac{K(r \mid s)}{l\left(d_{r|s}\right)}$$

This definition is primarily motivated by practical considerations. When we assume perfect knowledge of s, we can isolate and study the informational content of r that is not already covered by s, that is, the new knowledge introduced by r relative to s. Conditional surfeit thus allows us to quantify the conciseness of a description in light of what is already known.

Conditional surfeit, being a relative measure, is a number between 0 and 1.

Proposition 5.3.1 Let $r \in \mathcal{B}^*$ be a representation, $s \in \mathcal{B}^*$ be a string, and $d \in \mathcal{D}$ be a description of r given s. We have that $0 \leq \sigma(d_{r|s}) \leq 1$.

Proof. Given that $l\left(d_{r|s}\right) > 0$ and that $K(r \mid s) > 0$, since they are the lengths of non-empty strings, and that $ll\left(d_{r|s}\right) \geq K(r \mid s)$. ■

Intuition tell us that the surfeit of a description could only decrease if we assume the background knowledge given by the description of another topic. This is because we require that this background knowledge must be a perfect description (it presents no surfeit). However, as it was the case of joint surfeit, we have to wait until Chapter 6 to formalize this intuition.

In the same way we introduced the concept of redundancy of a description as a weaker version of the concept of surfeit, we can also introduce the concept of conditional redundancy as a weaker version of the concept of conditional surfeit.

Definition 5.3.2 Let $s \in \mathcal{B}^*$ be a string, and $d \in \mathcal{D}$ be a conditional description given s. We define the *conditional surfeit* of the conditional description $d_{t|s^\star}$, denoted by $\sigma(d_{t|s^\star})$, as:

$$\rho(d_{r|s}) = 1 - \frac{K\left(d_{t|s^\star}\right)}{l\left(d_{t|s^\star}\right)}$$

Conditional surfeit is a relative measure, and so, a number between 0 and 1.

Proposition 5.3.2 We have that $0 \leq \rho(d_{t|s^\star}) \leq 1$ for all t, s and all $d_{t,s}$.

Proof. Given that $K(d_{t|s^\star}) \leq l(d_{t|s^\star})$ we have that $\frac{K(d_{t|s^\star})}{l\left(d_{t|s^\star}\right)} \leq 1$ and so, $1 -$

$\frac{K(d_{t|s^\star})}{l(d_{t|s^\star})} \geq 0$. Also, since $\frac{K(d_{t|s^\star})}{l(d_{t|s^\star})} > 0$ (both quantities are positive integers), we have that $1 - \frac{K(d_{t|s^\star})}{l(d_{t|s^\star})} \leq 1$. ■

Finally, we can extend our concepts of conditional surfeit and conditional redundancy to multiple, but fine, number of topics.

Definition 5.3.3 Let $t, s_1, s_2, \ldots, s_n \in \mathcal{T}$ be a finite collection of topics, and let $d_{t|s_1^\star, s_2^\star, \ldots, s_n^\star}$ any conditional description of t given $s_1, s_2, \ldots, s_n$. We define the *conditional surfeit* of the description $d_{t|s_1^\star, s_2^\star, \ldots, s_n^\star}$, denoted by $\sigma(d_{t|s_1^\star, s_2^\star, \ldots, s_n^\star})$, as:

$$\sigma(d_{t|s_1^\star, s_2^\star, \ldots, s_n^\star}) = 1 - \frac{K\left(t \mid s_1^\star, s_2^\star, \ldots, s_n^\star\right)}{l\left(d_{t|s_1^\star, s_2^\star, \ldots, s_n^\star}\right)}$$

And the *conditional redundancy* of the description $d_{t_1, t_2, \ldots, t_n}$, denoted by $\rho(d_{t_1, t_2, \ldots, t_n})$, as:

$$\rho(d_{t_1, t_2, \ldots, t_n}) = 1 - \frac{K(d_{t_1, t_2, \ldots, t_n})}{l\left(d_{t_1, t_2, \ldots, t_n}\right)}$$

It is easy to show that the properties of conditional surfeit and conditional redundancy apply to the case of multiple topics as well.

5.4 Decreasing Surfeit

Our objective is to reduce the surfeit of our current best description d_1, thereby enhancing our understanding of the original entity. This improvement may involve either refining d_1 to eliminate redundant symbols or developing an entirely new description based on a different modeling approach. In either case, the result is a new description d_2. In this section, we analyze how the introduction of a new description d_2 affects the surfeit relative to that of the original description d_1.

Definition 5.4.1 Let $r \in \mathcal{B}^*$ be a representation, and let $d_1, d_2 \in \mathcal{D}$ be two descriptions. We define the *variation of surfeit* between the descriptions d_1 and d_2, with respect to r, denoted by $\Delta_\sigma^a(d_1, d_2, r)$, as:

$$\Delta_\sigma^a(d_1, d_2, r) = \sigma(d_1, r) - \sigma(d_2, r)$$

Since surfeit is bounded between 0 and 1, the maximum possible variation is ± 1. A positive value of Δ_σ indicates that d_2 is preferable to d_1 in terms of surfeit. Conversely, a negative value suggests that d_1 is more concise than d_2.

It is important to emphasize that a new description may also introduce a substantial increase in inaccuracy, potentially offsetting the improvement in surfeit. For a detailed discussion of inaccuracy, refer to Chapter 4, and for an explanation of how inaccuracy and surfeit combine into the unified metric of nescience, see Chapter 6.

We can also introduce a relative measure of the variation in surfeit when transitioning from description d_1 to d_2.

Definition 5.4.2 Let $r \in \mathcal{B}^*$ be a representation, and $d_1, d_2 \in \mathcal{D}$ be two descriptions. We define the *relative variation of surfeit* between descriptions d_1 and d_2, denoted by $\Delta_\sigma^r(d_1, d_2, r)$, as:

$$\Delta_\sigma^r(d_1, d_2, r) = \frac{\sigma(d_1, r) - \sigma(d_2, r)}{\sigma(d_1, r)}$$

provided that $\sigma(d_1, r) \neq 0$.

A value of 0 indicates that there is no change in surfeit between the two descriptions. A value of 1 corresponds to a complete elimination of surfeit, meaning that the new description d_2 has zero surfeit, while the original description d_1 had a nonzero surfeit. Negative values indicate that surfeit has increased, suggesting that the new description d_2 either includes more irrelevant or redundant symbols than d_1, or is too short to adequately represent the entity, thus omitting important information. It is important to note that the relative variation can become arbitrarily negative. This occurs when the surfeit of the original description $\sigma(d_1, r)$ is close to zero, while the surfeit of the new description $\sigma(d_2, r)$ is significantly larger. In such cases, the denominator becomes very small, causing the relative variation to diverge toward $-\infty$.

As surfeit approaches zero, relative variations become increasingly unstable. A small absolute change can result in a large relative variation when the initial surfeit is very low. For example, if $\sigma(d_1, r) = 0.1$ and surfeit decreases by 0.05, the relative improvement is 50%. However, if $\sigma(d_1, r) = 0.9$ and the same absolute reduction occurs, the relative improvement is only about 5.6%. Therefore, both absolute and relative variations are important for assessing the significance and scale of changes in surfeit.

5.5 Surfeit-inaccuracy rate of Change

In the preceding section, we examined how the surfeit of a description can be reduced by modifying that description, either by adding missing symbols, or by removing redundant, or irrelevant symbols. In this section, we turn our attention to a more general approach for reducing the surfeit associated with an entity, by allowing a increase in the inaccuracy of the description. Rather than reducing the surfeit in isolation, it may be more effective to modify both, surfeit and inaccuracy, simultaneously.

The balance between the amount of inaccuracy we are willing to accept in order to achieve a reduction in surfeit is referred to as the *surfeit-inaccuracy trade-off*. For a broader discussion of trade-offs in multi-objective optimization, refer to Section F.5.2.

Definition 5.5.1 Let $d_1, d_2 \in \mathcal{D}$ be two descriptions, and $r \in \mathcal{B}^\star$ a representation. We define the *rate of change between the surfeit and inaccuracy* of the descriptions d_1, d_2 given the representation r, denoted by $\Delta_{\sigma\iota}(d_1, d_2, r)$ as:

$$\Delta_{\sigma\iota}(\mathbf{x}_1, \mathbf{x}_2) = \frac{\sigma(d_2, r) - \iota(d_1, r)}{\iota(d_2, r) - \iota(d_1, r)}$$

provided that $\iota(d_2, r) - \iota(d_1, r) \neq 0$.

The ratio $\Delta_{\sigma\iota}$ represents the rate of change between surfeit and inaccuracy when transitioning from the first description to the second. A positive value of $\Delta_{\sigma\iota}$ implies that both quantities, surfeit and inaccuracy, either decrease (which is desirable) or increase (which is undesirable). The interpretation becomes more nuanced when $\Delta_{\sigma\iota}$ is negative, indicating that one of the quantities decreases while the other increases. In such cases, two scenarios must be considered:

(i) Surfeit decreases and inaccuracy increases, we aim for $\Delta_{\sigma\iota}(d_1, d_2, r) < M$, where $M < -1$, thereby ensuring that the reduction in surfeit compensates for the increase in inaccuracy.

(ii) Surfeit increases and inaccuracy decreases, we aim for $\Delta_{\sigma\iota}(d_1, d_2, r) > M$, where $-1 < M < 0$, thereby ensuring that the reduction in inaccuracy justifies the increase in surfeit.

In both cases, caution is warranted when the change in inaccuracy is small, as it can disproportionately affect the ratio and potentially lead to misleading conclusions.

■ **Example 5.4** Let $d_1, d_2 \in \mathcal{D}$ be two descriptions, and $r \in \mathcal{B}^\star$ a representation. For d_1, the surfeit $\sigma(d_1, r_1)$ is 0.40, and the inaccuracy $\iota(d_1, r)$ is 0.15. For d_2, the surfeit $\sigma(d_2, r)$ is 0.20 (a decrease from 0.40), and the inaccuracy $\iota(d_2, r)$ is 0.25 (an increase from 0.15). Using the definition of the rate of change, we compute:

$$\Delta_{\sigma\iota}(d_1, d_2, r) = \frac{0.40 - 0.20}{0.15 - 0.25} = \frac{0.20}{-0.10} = -2$$

In this case, transitioning from description d_1 to d_2 results in a decrease of surfeit by 0.20 units and an increase in inaccuracy by 0.10 units. The rate of change is -2. ■

Having a very small change in inaccuracy can significantly amplify the value of the rate of change, potentially giving the misleading impression that surfeit and inaccuracy are varying at an extreme rate, even when the actual changes are minor. This phenomenon is illustrated in the following example.

■ **Example 5.5** Let $d_1 \in \mathcal{D}$ be a description and $r \in \mathcal{B}^\star$ a representation with an surfeit $\sigma(d_1, r)$ of 0.35 and a inaccuracy $\iota(d_1, r)$ of 0.20. Let $d_1 \in \mathcal{D}$ be a second description with an surfeit $\sigma(d_2, r)$ of 0.30 (a slight decrease from 0.35) and a inaccuracy $\iota(d_2, r)$ of 0.2001 (a very small increase from 0.20). Applying the definition of the rate of change:

$$\Delta_{\sigma\iota}(d_1, d_2, r) = \frac{0.35 - 0.30}{0.20 - 0.2001} = \frac{0.05}{-0.0001} = -500$$

The rate of change is -500, which may misleadingly suggest a dramatic shift. In reality, the surfeit only decreased by 0.05 units, and the inaccuracy increased by a negligible 0.0001 units. The extremely small denominator inflates the result, making the change appear far more significant than it actually is. ■

As we attempt to optimize both surfeit and inaccuracy, we inevitably encounter descriptions where improving one objective necessitates compromising the other. The set of such "best trade-off" configurations constitutes the Pareto frontier (see Section F.5). Points on the Pareto frontier are said to be Pareto optimal because any attempt to improve one objective leads to a deterioration in the other.

Definition 5.5.2 Let $d_1 \in \mathcal{D}$ be a description and $r \in \mathcal{B}^\star$ a representation. The description d_1 is said to be a Pareto point with respect to surfeit σ and inaccuracy ι if there does not exist another description d_2 such that:

1 $\sigma(d_2, r) \leq \sigma(d_1, r)$ and $\iota(d_2, r) \leq \iota(d_1, r)$, and
2 $\sigma(d_2, r) < \sigma(d_1, r)$ or $\iota(d_2, r) < \iota(d_2, r)$.

In simpler terms, a description is Pareto optimal if: (i) no other description is better in both surfeit and inaccuracy, and (ii) any improvement in one metric necessarily results in a worsening of the other.

The rate of change $\Delta_{\sigma\iota}$ between any two Pareto optimal points provides insight into how the trade-off between surfeit and inaccurac evolves along the Pareto frontier. If decision-makers are more sensitive to changes in surfeit than to inaccuracy, they may prefer configurations with a less negative $\Delta_{\sigma\iota}$. Conversely, if inaccuracy is of greater concern, they may accept solutions where $\Delta_{\sigma\iota}$ indicates a larger increase in surfeit in exchange for a smaller gain in inaccuracy.

5.6 Surfeit of Areas

The concept of surfeit can be extended to research areas, to quantitative measure the amount of extra effort we are using to describe the topics of the area.

Definition 5.6.1 Let $A \subset \mathcal{T}$ be an area with known subset $\hat{A} = \{t_1, t_2, \ldots, t_n\}$, and let $d_{\hat{A}}$ be a description. We define the *surfeit of the description* $d_{\hat{A}}$ as:

$$\sigma\left(d_{\hat{A}}\right) = 1 - \frac{K(\langle t_1, t_2, \ldots, t_n \rangle)}{l\left(d_{\hat{A}}\right)}$$

As it was the case of the concept of redundancy, in general we do not know the complexity of the area $K(\hat{A})$, and so, in practice, it must be approximated by the complexity of the descriptions themselves $K(\hat{d}_{\hat{A}})$. However, in the particular case of areas, we could have also problems with the quantity $\hat{d}_{\hat{A}}$, since it requires to study the conditional descriptions of the topics included in the area.

Definition 5.6.2 Let $A \subset \mathcal{T}$ be an area with known subset $\hat{A} = \{t_1, t_2, \ldots, t_n\}$, and let $d_{\hat{A}}$ be a description. We define the *weak redundancy of the description* $d_{\hat{A}}$ as:

$$\rho(d_{\hat{A}}) = 1 - \frac{K\left(d_{\hat{A}}\right)}{l\left(d_{\hat{A}}\right)}$$

References

The concept of redundancy has been also investigated in the context of information theory, since we are interested on using codes with low redundancy (see for example [Abr63]).

6. Nescience

There are known knowns. These are things we know that we know. There are known unknowns. That is to say, there are things that we know we don't know. But there are also unknown unknowns. There are things we don't know we don't know.

Donald Rumsfeld

Following the foundational Chapter 2, which introduced the core concepts of entity, representation, and description, and the subsequent Chapters 3, 4, and 5, which developed the new metrics of miscoding, inaccuracy, and surfeit, we are now prepared to delve into the central concept of nescience in this chapter, focusing on its fundamental properties.

Unlike Shannon entropy or Kolmogorov complexity, which measure information, nescience quantifies the absence of information, that is, what remains unknown. The theory of nescience characterizes our ignorance about a research entity through the three previously introduced metrics: miscoding, inaccuracy, and surfeit. Miscoding assesses how accurately an entity is represented as a string of symbols; inaccuracy measures how well our best available model describes this representation; and surfeit evaluates the descriptive efficiency of the model, as reflected in its length or symbol count.

These three metrics are inherently interdependent and often in conflict: reducing one can lead to an increase in another. The central challenge, therefore, is to develop a method for simultaneously minimizing all three. This requirement reflects, in our view, the fundamental nature of scientific inquiry as a multi-objective optimization problem.

One of the most significant outcomes of our definition of nescience, grounded in the metrics of miscoding, inaccuracy, and surfeit, is its capacity to partition the domain of research topics into two distinct areas. The first is the known unknown, which includes topics we are aware we do not fully understand, yet can recognize and acknowledge our incomplete knowledge. The second is the unknown unknown, comprising topics that have not yet been discovered or conceptualized. A key application of the theory of nescience is its use as a methodological framework for identifying and exploring what lies within the unknown unknown.

Another noteworthy implication of the nescience framework is the counterintuitive idea that, for certain topics, continued research may be counterproductive. In these cases, additional investigation may actually increase our ignorance rather than reduce it. This occurs when we reach a critical threshold beyond which our descriptions become more inaccurate, overly complex, or based on flawed representations, preventing any real progress toward understanding.

6.1 Nescience

Intuitively, our understanding of an entity should be based in the quality of the model we use to describe it, specifically, its ability to explain why things happen. Within the theory of nescience, we propose a quantitative measure of our ignorance concerning a research entity, based on three components: the miscoding of a string-based representation of the entity, and the inaccuracy and surfeit of the model describing that representation. Miscoding captures how accurately the representation encodes the entity, inaccuracy reflects how well the model describes the representation, and surfeit quantifies the extent of unnecessary effort embedded in the model. We argue that the goal of science should be to minimize all three quantities: miscoding, inaccuracy, and surfeit. Unfortunately, these metrics are inherently conflicting, reducing one may lead to an increase in one or both of the others.

According to the theory of nescience, science can be viewed as a multi-objective optimization problem[1] (see Section F.5):

[1]Technically speaking, science is a deterministic, discrete, nonlinear, nonconvex, nondifferentiable multiobjective optimization problem with a single decision maker.

The Science Problem

$$\begin{aligned} &\text{minimize} && \{\mu(r), \iota(d,r), \sigma(d,r)\} \\ &\text{subject to} && (r,d) \in \mathcal{B}^* \times \mathcal{D} \end{aligned}$$

A *scientific method*, further discussed in Chapter G, refers to any algorithm or computable procedure capable of solving, or closely approximating a solution to, the above minimization problem. This includes a broad class of techniques and methodologies aimed at systematically reducing the values of miscoding, inaccuracy, and surfeit. In doing so, scientific methods contribute to improving the accuracy and conciseness of our representations and models, thereby advancing our understanding of the world.

The feasible region is the Cartesian product $\mathcal{B}^* \times \mathcal{D}$, where $\mathcal{B}^*$ denotes the set of finite binary strings and $\mathcal{D}$ the set of descriptions. The decision vectors are pairs (r,d), referred to as *hypotheses*, consisting of a representation and a description. The objective functions to be minimized are miscoding, surfeit, and inaccuracy. The objective space is the subset $\mathbf{Z} \subset \mathbb{R}^3$, whose elements are the objective vectors.

In our formulation of science and the scientific method, we deliberately exclude the set $\mathcal{E}$ of entities. Requiring direct knowledge of an entity $e \in \mathcal{E}$ would render the scientific problem ill-posed for most research areas. Science, at its core, is a matter of manipulating strings of symbols. From a practical standpoint, it is about discovering strings that have meaningful interpretations in the real world and can be used to solve concrete problems. From a more theoretical perspective, the aim of science can be seen as the attempt to understand the workings of an unknown abstract oracle.

If the set $\mathcal{R}_e$ of representations for a particular entity e is known, or approximately known, we can restrict the science problem to:

$$\begin{aligned} &\text{minimize} && \{\mu(r), \iota(d,r), \sigma(d,r)\} \\ &\text{subject to} && (r,d) \in \mathcal{R}_e \times \mathcal{D} \end{aligned}$$

Within the theory of nescience, our primary focus lies in the decision space $\mathcal{B}^* \times \mathcal{D}$, the space of representations and descriptions, rather than in the objective space $\mathbf{Z} \subset \mathbb{R}^3$ of metric values. In the following definitions, we revisit key concepts from multiobjective optimization (see Section F.5) as they apply specifically to the science problem.

Pareto Optimality

If the representation and description currently used to characterize an entity are not perfect, our goal is to find an alternative representation or description that reduces at least one of the metrics miscoding, inaccuracy, or surfeit without increasing the value of any of the others.

Definition 6.1.1 We say that a hypothesis $(r,d) \in \mathcal{B}^* \times \mathcal{D}$ *dominates* another hypothesis $(r',d') \in \mathcal{B}^* \times \mathcal{D}$ if it improves at least one of the metrics miscoding, inaccuracy, or surfeit without worsening either of the other two.

For example, we might identify a new representation that encodes the entity more accurately without degrading the quality of its description. Alternatively, we could find a new description that improves accuracy without increasing surfeit, or a more concise description that preserves accuracy.

■ **Example 6.1** Consider an experiment in which we collect a set of observations r and apply a mathematical model f_1 from a model family $\mathcal{M}_1$, resulting in an inaccuracy of i_1. Later, we fit a second model f_2 from a different model family $\mathcal{M}_2$, which is smaller in size (i.e., has lower surfeit) but yields the same inaccuracy i_1. In this case, the hypothesis $B = (r, f_2)$ dominates the hypothesis $A = (r, f_1)$, even though it is not better in terms of inaccuracy alone. ■

For most entities, there does not exist a single solution that simultaneously minimizes all three metrics. Instead, we encounter a set of Pareto optimal solutions that define an optimal frontier.

Definition 6.1.2 We say that a hypothesis $(r,d) \in \mathcal{B}^* \times \mathcal{D}$ is *Pareto optimal* if there does not exist another hypothesis $(r',d') \in \mathcal{B}^* \times \mathcal{D}$ such that (r',d') dominates (r,d). The set of Pareto optimal solutions, denoted by $\mathbf{P}_{\mathcal{B}^* \times \mathcal{D}}$, is called the *Pareto frontier*.

In the realm of scientific research, the concept of the Pareto frontier, as defined by the set of Pareto optimal solutions $\mathbf{P}_{\mathcal{B}^* \times \mathcal{D}}$, plays a crucial role. It delineates the boundary of optimal trade-offs among the conflicting metrics of miscoding, inaccuracy, and surfeit, such that none can be improved without worsening at least one of the others. This frontier represents the spectrum of best-achievable balances, guiding researchers to identify models and representations that offer the most scientifically rigorous understanding of their subject matter (see Section 6.3).

However, in certain situations or specific applications, it may be reasonable to adopt a solution that is not Pareto optimal. For instance, one might choose to prioritize a particular metric due to its relevance or importance to the research objectives, accepting less favorable values for the remaining metrics as a necessary trade-off (see Section 6.2).

Building on the concept of Pareto optimality, where a solution is considered optimal if no other solution improves one objective without worsening another, we introduce the notion of weak Pareto optimality. A hypothesis is said to be weakly Pareto optimal if there is no other hypothesis that improves all objectives simultaneously. This concept is broader than Pareto optimality, as it includes solutions that may not be the best in any single objective but are not strictly outperformed in every dimension.

Definition 6.1.3 We say that a hypothesis $(r,d) \in \mathcal{B}^* \times \mathcal{D}$ *weakly dominates* another hypothesis $(r',d') \in \mathcal{B}^* \times \mathcal{D}$ if it improves all three metrics miscoding, inaccuracy, and surfeit simultaneously. That is, if $\mu(r') < \mu(r)$, $\iota(d',r') < \iota(d,r)$, and $\sigma(d',r') < \sigma(d,r)$.

A hypothesis is *weakly Pareto optimal* if there does not exist another hypothesis that improves all three metrics: miscoding, inaccuracy, and surfeit.

Definition 6.1.4 We say that a hypothesis $(r,d) \in \mathcal{B}^* \times \mathcal{D}$ is *weakly Pareto optimal* if there does not exist another hypothesis $(r',d') \in \mathcal{B}^* \times \mathcal{D}$ such that (r',d') weakly dominates (r,d). The set of weakly Pareto optimal solutions, denoted by $\mathbf{P}\_\mathcal{B}^* \times \mathcal{D}$, is called the *weakly Pareto frontier*.

If a hypothesis is weakly Pareto optimal, it means there is no other hypothesis that improves all three metrics simultaneously. However, it is still possible to find a hypothesis that improves one of the metrics without worsening the others, that is, a hypothesis that is Pareto optimal. Thus, the Pareto frontier is a subset of the weakly Pareto frontier. In the theory of nescience, we focus primarily on the set of Pareto optimal solutions rather than the set of weakly Pareto optimal ones.

■ **Example 6.2** Based on the assumptions of Example 6.1, hypothesis A could still be weakly Pareto optimal, but it cannot be Pareto optimal, since it is dominated by hypothesis B. However, it is not weakly dominated by hypothesis B. ■

The concepts of Pareto and weakly Pareto optimality can also be particuralized to the case in which the set $\mathcal{R}_e$ of representations of a particular entity e is known.

Range of Solutions

As discussed in Section F.5.1, an objective vector that achieves the minimum possible value for all objective functions is termed the ideal objective vector. For the science problem, this ideal vector is represented by the origin $(0,0,0)$, symbolizing the complete elimination of miscoding, inaccuracy, and surfeit.

Proposition 6.1.1 The ideal objective vector for the science problem is the origin $(0, 0, 0)$.

Proof. Proposition 3.1.1 established that miscoding is greater than or equal to zero, and Proposition 3.1.2 showed that it can be equal to zero. Likewise, Proposition 4.5.1 demonstrated that inaccuracy is non-negative, while Proposition 4.1.2 confirmed that a value of zero is attainable. Finally, Proposition 5.2.1 stated that surfeit is at least zero, and Proposition 5.1.2 verified that zero surfeit is achievable. ■

A hypothesis $(r,d) \in \mathcal{B}^* \times \mathcal{D}$ is said to be ideal if it exhibits zero miscoding, zero inaccuracy, and zero surfeit. This implies that the representation r is valid, the model d produces r as output, and there exists no shorter model d' that also achieves zero inaccuracy. Intuitively, a hypothesis (r,d) is ideal if there exists an entity $e \in \mathcal{E}$ such that r perfectly encodes e, and d is both an accurate and minimal model of r.

Ideal hypotheses embody the notion of perfect knowledge within the theory of nescience. Unfortunately, in most practical applications, reaching the ideal objective vector is not feasible due to the inherently conflicting nature of the metrics: miscoding, inaccuracy, and surfeit.

■ **Example 6.3** A research topic for which it is impossible to reach the ideal objective vector is weather prediction. In this case, the entity under study is the atmosphere over a geographical region. The representation of this entity (typically a set of meteorological measurements such as temperature, pressure, and humidity) is inherently flawed due to the limited spatial and temporal resolution of sensors, noise in the data, and incomplete coverage, particularly over oceans and remote areas. As a result, miscoding is strictly greater than zero. Furthermore, even the most sophisticated atmospheric models, which numerically approximate the physical laws governing weather dynamics, cannot produce perfectly accurate forecasts due to the chaotic nature of the system, the need for simplifying assumptions, and errors in initial conditions, ensuring that inaccuracy also remains greater than zero. Finally, these models are large, complex, and often include redundant components or overly general submodules, making them far from minimal in size; thus, surfeit is also non-zero. ■

The upper bound of the Pareto optimal set is given by the nadir objective vector. In the theory of nescience, the nadir vector is the point $(1,1,1)$, corresponding to maximum miscoding, maximum inaccuracy, and maximum surfeit.

Proposition 6.1.2 The nadir objective vector of the science problem is the vector $(1,1,1)$.

Proof. Proposition 3.1.1 demonstrated that miscoding is greater than or equal to zero, and Proposition 3.1.2 showed that it can be equal to zero. Similarly, Proposition 4.5.1 established that inaccuracy is greater than or equal to zero, and Proposition 4.1.2 indicated that a zero value is attainable. Finally, Proposition 5.2.1 showed that surfeit is greater than or equal to zero, and Proposition 5.1.2 confirmed that it can also reach zero. Therefore, since all three metrics are bounded between 0 and 1, the upper bound of the objective region is $(1,1,1)$. ■

The nadir vector represents a state of complete ignorance: a hypothesis (r,d) in which the representation r contains no meaningful information about the entity e under study, the description d generates a string entirely unrelated to r, and the description is of maximal length. This extreme point illustrates the worst-case scenario in terms of scientific knowledge: maximum miscoding, total inaccuracy, and maximum unnecessary complexity.

■ **Example 6.4** Consider the case of studying the physical law governing the motion of a pendulum. Suppose we define a hypothesis (r,d), where the representation r is a random binary string encoding information entirely unrelated to the pendulum, such as the binary representation of a shuffled deck of cards. The description d is a program that outputs an unrelated string, for example, one billion digits of π. In this scenario, miscoding is maximal because the representation bears no connection to the entity being studied, inaccuracy is maximal because the description produces a string entirely different from the representation, and surfeit is also maximal since the description is very long compared to the lenght of r. This hypothesis (r,d) reaches the nadir objective vector $(1,1,1)$, reflecting a state of complete ignorance about the entity. ■

Trade-offs

In Section 4.4, we analyzed the trade-off between inaccuracy and miscoding:

$$\Delta_{\iota\mu}(\mathbf{x}_1,\mathbf{x}_2) = \frac{\iota(d_2,r_2) - \iota(d_1,r_1)}{\mu(r_2) - \mu(r_1)}$$

where $\mathbf{x}_1 = (r_1,d_1)$ and $\mathbf{x}_2 = (r_2,d_2)$ are two hypotheses.

This ratio quantifies the rate at which inaccuracy changes relative to miscoding when transitioning between two hypotheses. A positive value of $\Delta_{\iota\mu}$ indicates that both metrics vary in the same direction, either improving or deteriorating together, whereas a negative value reflects a trade-off between them.

In Section 5.5, we similarly studied the trade-off between surfeit and inaccuracy:

$$\Delta_{\sigma\iota}(\mathbf{x}_1,\mathbf{x}_2) = \frac{\sigma(d_2,r) - \sigma(d_1,r)}{\iota(d_2,r) - \iota(d_1,r)}$$

This ratio captures how surfeit changes with respect to inaccuracy when the representation remains fixed and only the description changes. Again, a positive value of $\Delta_{\sigma\iota}$ indicates that both metrics are moving in the same direction, either improving or deteriorating together, whereas a negative value reflects a trade-off between them.

These trade-off ratios provide a local, quantitative tool for evaluating whether a change in hypothesis moves us toward Pareto optimality or away from it, and how it relates to the extreme points represented by the ideal and nadir objective vectors.

In this section we introduce a unified framework that provides a global trade-offs.

Definition 6.1.5 Let $\mathbf{x}_1 = (r_1, d_1)$ and $\mathbf{x}_2 = (r_2, d_2)$ be two hypotheses. We define the *nescience trade-off vector* between $\mathbf{x}_1$ and $\mathbf{x}_2$ as:

$$\Delta_{\text{nescience}}(\mathbf{x}_1, \mathbf{x}_2) = \left(\frac{\iota(d_2, r_2) - \iota(d_1, r_1)}{\mu(r_2) - \mu(r_1)}, \frac{\sigma(d_2, r_2) - \sigma(d_1, r_1)}{\iota(d_2, r_2) - \iota(d_1, r_1)} \right)$$

provided that $\mu(r_2) \neq \mu(r_1)$ and $\iota(d_2, r_2) \neq \iota(d_1, r_1)$.

This vector $\Delta_{\text{nescience}}(\mathbf{x}_1, \mathbf{x}_2)$ describes yhe rate of change of inaccuracy relative to miscoding, and the rate of change of surfeit relative to inaccuracy.

Definition 6.1.6 Given two hypotheses $\mathbf{x}_1 = (r_1, d_1)$ and $\mathbf{x}_2 = (r_2, d_2)$, we define the *unified trade-off magnitude*, denoted $\Theta(\mathbf{x}_1, \mathbf{x}_2)$, as:

$$\Theta(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{\left(\frac{\iota(d_2, r_2) - \iota(d_1, r_1)}{\mu(r_2) - \mu(r_1)} \right)^2 + \left(\frac{\sigma(d_2, r_2) - \sigma(d_1, r_1)}{\iota(d_2, r_2) - \iota(d_1, r_1)} \right)^2}$$

whenever both denominators are non-zero.

A small Θ value suggests an efficient trade-off: significant improvement in one metric with minor cost in others. A large Θ indicates a steep or unbalanced trade-off path in the nescience objective space. This formulation complements the concepts of Pareto dominance and optimality by quantifying how sharply a transition between hypotheses navigates the trade-offs among conflicting objectives.

6.2 Minimizing Nescience

From a mathematical perspective, any solution within the Pareto optimal set is considered a valid answer to the Science Problem. In fact, the problem is formally solved once all Pareto optimal solutions have been identified. However, in scientific practice, this is often not sufficient. Researchers usually seek a single, most appropriate solution that best aligns with the priorities or goals of the investigation.

In multi-objective optimization, a decision maker (see Section F.5) is an entity (either a human agent, a set of predefined criteria, or an algorithm) responsible for selecting one solution from the set of Pareto optimal hypotheses. The decision maker incorporates external preferences, priorities, or domain-specific constraints to guide the selection process. Its role is to introduce a preference relation that induces an ordering over the Pareto set, thereby allowing for the identification of the most suitable hypothesis according to the specific goals or values of the scientific inquiry.

To formalize this within the theory of nescience, we introduce the notion of a nescience decision maker, defined as a scalar-valued function that evaluates and ranks hypotheses based on their levels of miscoding, inaccuracy, and surfeit. This function reflects the relative preference for each hypothesis.

Definition 6.2.1 Let $(r,d) \in \mathcal{B}^* \times \mathcal{D}$ be a hypothesis. A decision maker for the science problem is a multivariate funcion $V : \mathbb{R}^3 \to \mathbb{R}$, that assings to each triplet $(\mu(r), \iota(d,r), \sigma(d,r))$ the real value $V(\mu(r), \iota(d,r), \sigma(d,r))$.

The function V is often referred to as a *value function* or *utility function*, and it encodes the preferences or priorities of the scientist or research community. Depending on the application, V may treat the three metrics equally, emphasize one over the others, or apply a more sophisticated transformation to reflect factors such as risk tolerance, interpretability, or domain-specific considerations.

This formalism enables the selection of a single hypothesis from the Pareto frontier, effectively transforming the multi-objective problem into a single-objective one guided by scientific judgment.

6.2.1 Global Criterion

The global criterion method (see Section F.5.3) is an approach to solving multi-objective optimization problems by minimizing the distance between a reference point and the feasible region in the objective space. The reference point is typically chosen to be the ideal vector, which in our case corresponds to the origin $(0,0,0)$.

Different distance metrics can be used in this framework. For example, the global criterion based on the origin and the Euclidean distance leads to the following minimization problem:

$$\begin{array}{ll} \text{minimize} & \sqrt{\mu(r)^2 + \iota(d,r)^2 + \sigma(d,r)^2} \\ \text{subject to} & (r,d) \in \mathcal{B}^* \times \mathcal{D} \end{array}$$

As shown in Proposition F.5.1, the solutions obtained through the global criterion method are guaranteed to be Pareto optimal. However, it is important to note that this method does not consider all Pareto optimal solutions. In particular, optimal points that lie far from the reference point are excluded.

■ **Example 6.5** Consider the following three Pareto optimal solutions:
- $A = (0.1, 0.8, 0.9)$
- $B = (0.8, 0.1, 0.9)$
- $C = (0.5, 0.5, 0.5)$

Although all three solutions are Pareto optimal, a global criterion based on Euclidean distance may select only C, as it is closest to the origin. However, A and B represent equally valid trade-offs. In particular, solution B achieves very low inaccuracy, which, in certain contexts, might make it the preferred option. ■

When working with a global criterion for optimization problems, it is customary to normalize the range of the objective values to prevent objectives with larger scales from disproportionately influencing the result. However, in the case of the theory of nescience, normalization is unnecessary. This is because the metrics we use (miscoding, inaccuracy, and surfeit) are already defined within the normalized range $[0,1]$. Consequently, all objectives contribute equally to the evaluation of candidate solutions under the global criterion.

Moreover, another important advantage of the theory of nescience is that all three metrics are inherently commensurable, meaning they are measured using the same units: lengths of computer programs. This shared unit of measurement allows for a coherent and meaningful comparison across the metrics, reinforcing the theoretical consistency and interpretability of the optimization framework.

The following are orther metrics that could be used as global criterion to minimize nescience:
- Arithmetic mean: $\frac{\mu(r)+\iota(d,r)+\sigma(d,r)}{3}$
- Geometric mean: $(\mu(r) \times \iota(d,r) \times \sigma(d,r))^{1/3}$
- Product: $\mu(r) \times \iota(d,r) \times \sigma(d,r)$
- Addition: $\mu(r) + \iota(d,r) + \sigma(d,r)$
- Harmonic mean: $\frac{3}{\mu(r)^{-1}+\iota(d,r)^{-1}+\sigma(d,r)^{-1}}$

Not all of these metrics qualify as distances, as the geometric mean, product, and harmonic mean do not satisfy the triangle inequality. Moreover, some are not even defined when one of the components is zero, for example, the harmonic mean becomes undefined in such cases. The following paragraphs describe the advantages and disadvantages of each of these metrics.

The Euclidean distance to the ideal vector $(0,0,0)$ offers a geometrically intuitive measure of closeness to perfect knowledge. It treats the three components symmetrically and accounts for their joint magnitude. However, it can bias the solution toward more centrally located points in the objective space and may exclude valid Pareto optimal solutions that lie further from the origin but with highly desirable properties in one metric.

The arithmetic mean provides a simple and interpretable way to aggregate the three metrics, treating each equally. It is widely used due to its mathematical convenience and stability. Nevertheless, it allows compensations (poor performance in one metric can be offset by better performance in others) making it unsuitable when balance among all metrics is crucial.

The geometric mean emphasizes balance by being more sensitive to high values than the arithmetic mean. It discourages solutions that perform poorly in any one metric, making it effective for encouraging uniformly low nescience. However, it is less intuitive and returns zero if any component is zero, which might unfairly suggest perfect knowledge even when other metrics are poor.

The product magnifies the penalty for imbalance: a single large value dominates the result, and a single zero collapses the result to zero. It strongly favors evenly low values across all metrics. While this strictness can be advantageous, it is overly sensitive to small changes, especially near zero, and may mask informative differences in otherwise competitive hypotheses.

The addition is mathematically equivalent to the arithmetic mean (up to scaling) and offers the same interpretability and ease of computation. It is particularly useful when metrics are already normalized, as in the theory of nescience. However, like the mean, it permits trade-offs that might be scientifically undesirable when balance across all three aspects is necessary.

The harmonic mean severely penalizes large values, making it ideal for enforcing balance and avoiding outliers. It is particularly well-suited when the worst-performing metric should drive the overall score. However, it is undefined when any component is zero, and it is more difficult to interpret than other averages.

6.2.2 Weighting Method

In the weighting method for solving multi-objective optimization problems, the idea is to associate a weighting coefficient to each objective function and minimize the weighted sum of the objectives. The weighting coefficients w_i are real numbers such that $w_i \geq 0$ for all $i = 1,\dots,k$. We also require that the weights are normalized, meaning $\sum_{i=1}^{k} w_i = 1$.

According to the weighting mehtod, the science problem is modified into the following problem:

$$\begin{aligned} &\text{minimize} \quad w_\mu \mu(r) + w_\iota \iota(d,r) + w_\sigma \sigma(d,r) \\ &\text{subject to} \quad \mathbf{x} \in \mathbf{S} \end{aligned}$$

where $w_\mu + w_\iota + w_\sigma = 1$.

A weighting coefficient of zero is not meaningful, as it would imply that one of the objective functions has no significance whatsoever, an assumption that contradicts the principles of the theory of nescience.

As shown in Proposition F.5.2, the solutions obtained through the weighted method are guaranteed to be Pareto optimal, although this approach does not capture all Pareto optimal solutions. In standard multi-objective optimization, it is customary to normalize the objective functions to prevent those with larger numerical ranges from disproportionately influencing the outcome. In the case of the theory of nescience, as previously discussed in the context of the global criterion, such normalization is unnecessary because the metrics we employ (miscoding, inaccuracy, and surfeit) are intrinsically defined within the normalized interval $[0,1]$.

If the weighting method is applied as an a priori approach, a natural question arises: what do the weighting coefficients actually represent within the context of the theory of nescience? These coefficients are often said to reflect the relative importance of the three objectives (miscoding, inaccuracy, and surfeit). However, the meaning of importance in this context is not well-defined and may lead to ambiguity. Rather than interpreting the weights as measures of absolute importance, it is more accurate to view them as expressing the rate at which the decision maker is willing to trade off one metric against another. That is, the weighting coefficients indicate how much increase in one metric the decision maker is willing to tolerate in exchange for a decrease in another, thereby quantifying their tolerance for imbalances among the three dimensions of nescience.

■ **Example 6.6** Suppose a scientist is studying the structure of a newly discovered biological molecule. The current best hypothesis (r,d) has a miscoding of $\mu(r) = 0.2$, an inaccuracy of $\iota(d,r) = 0.3$, and a surfeit of $\sigma(d,r) = 0.6$. The scientist is considering the use of the weighting method to guide the selection of the next hypothesis.

If the scientist assigns weights $w_\mu = 0.1$, $w_\iota = 0.7$, and $w_\sigma = 0.2$, this does not necessarily mean that inaccuracy is more important in some absolute sense. Rather, it reflects the scientist's current willingness to tolerate some miscoding or extra descriptive complexity (surfeit) in exchange for a more accurate model. For instance, the scientist might be aiming for predictive precision in experimental outcomes, even if the underlying representation is suboptimal or the model is longer than ideal.

This weighted preference would steer the optimization process toward hypotheses that reduce inaccuracy, even if they slightly increase miscoding or surfeit. In this way, the weighting coefficients quantify the scientist's subjective trade-offs in light of their practical research goals. ■

Employing the weighting method as an a priori method presumes that the decision maker's unerlying value function is or can be approximated by a linear function. It must be noted that altering the weighting vectors linearly does not have to mean that the values of the objective functions also change linearly. It is difficult to control the direction of the solutions by the weighting coefficients. Because $\mu, \iota, \sigma \in [0,1]$ but interact non-linearly, the drawbacks of the naive weighting scheme are amplified.

6.3 Perfect Knowledge

According to the theory of nescience, the fundamental aim of scientific research is to systematically reduce our ignorance concerning the topics under investigation. This ignorance is quantitatively expressed through the notion of nescience, which captures the combined deficiencies in our current understanding. Scientific progress, within this framework, is evaluated by the degree to which a hypothesis, defined as a pair consisting of a representation and a description, reduces the three interdependent components of miscoding, inaccuracy and surfeit. Perfect knowledge, in this context, is said to be achieved when further reductions in nescience are no longer possible. At this point, the nescience associated with the topic reaches its minimum value, signifying that our understanding is both complete and optimally efficient, and no further scientific improvement can be made.

We must distinguish between two notions of perfect knowledge. The first, ideal perfect knowledge, is a theoretical construct that represents a state in which all three components of nescience are exactly zero. This would require a representation that perfectly encodes the entity, a description that exactly reproduces the representation, and no shorter or simpler description being possible. However, this ideal is generally unattainable in practice due to limitations in representation, modeling, and the nature of the entities under investigation. In contrast, Pareto perfect knowledge, reflects the practical achievable implementation of the concept. It corresponds to hypotheses that lie on the Pareto frontier, where no further reduction in one component of nescience can be made without increasing at least one of the others. Thus, Pareto perfect knowledge represents the best feasible approximation to the ideal, balancing trade-offs among miscoding, inaccuracy, and surfeit.

Next, we formally define the concept of (theoretical) ideal perfect knowledge, which occurs when a hypothesis achieves zero miscoding, zero inaccuracy, and zero surfeit.

Definition 6.3.1 Let $(r,d) \in \mathcal{B}^* \times \mathcal{D}$ be a hypothesis. We say that we have attained *ideal perfect knowledge* for the hypothesis (r,d) if $\mu(r) = 0$, $\iota(d,r) = 0$, and $\sigma(d,r) = 0$.

While perfect knowledge can be achieved with respect to a given representation and its description, there is no mathematical or logical procedure to determine with certainty which entity this perfect knowledge pertains to. The mapping between representations and entities is mediated by an oracle, and since oracles are unknown, the identification of the underlying entity remains epistemologically inaccessible. Consequently, although we can verify that a hypothesis satisfies all the formal conditions for perfect knowledge, we cannot be certain of the true nature of the entity being perfectly known.

A consequence of our definition is that perfect knowledge implies randomness, in the sense of incompressible descriptions.

Proposition 6.3.1 Let $(r,d) \in \mathcal{B}^* \times \mathcal{D}$ be a hypothesis that yields ideal perfect knowledge. Then $K(d) = l(d)$.

Proof. Apply Proposition 5.1.2. ■

The common intuition is that a random string conveys no meaningful information, as randomness is often associated with noise or disorder. However, within the framework of the theory of nescience, a random description refers to a description that encodes the maximum amount of information in the smallest possible space—that is, one that contains no redundant elements. Such descriptions are incompressible and thus optimal in terms of descriptive efficiency.

The converse, however, does not generally hold, as the following counterexample demonstrates.

■ **Example 6.7** Aristotelian physics provides an inaccurate description of the physical world, as it makes predictions that are inconsistent with empirical observations, for instance, the claim that planets orbit the Earth. Suppose we take a description of Aristotelian physics and compress it using a standard compression algorithm. The resulting file would be a random description in the sense of having zero redundancy (i.e., it is incompressible). However, despite this lack of redundancy, our nescience would not be zero. That is, our knowledge would not be perfect, since the inaccuracy of the description is not zero. ■

Ideal perfect knowledge is unique in value, but not in representation or description, meaning that although there may be many different hypotheses (i.e., pairs of representations and descriptions) that all yield zero nescience, they are all equivalent in their informational content, they correspond to the same minimal level of uncertainty or ignorance (i.e., zero). However, these hypotheses can differ in their syntactic form: the representation of the entity or the syntax of the description may vary.

When continued research into a particular topic no longer yields improvements in any of these dimensions—i.e., when no further reduction in miscoding, inaccuracy, or surfeit can be achieved without worsening one of the others—we propose to say that a pareto perfect knowledge has been attained. This does not imply absolute or universal truth, but rather that we have reached the limit of what can be improved given our current symbolic framework. In such a state, the hypothesis lies on the Pareto frontier and corresponds to a point of local optimality, where no further refinement is scientifically justified within the constraints of the theory. The concept of perfect knowledge thus provides a formal stopping criterion for inquiry, signaling that the topic has been fully explored with respect to the goals of scientific understanding as defined by the theory of nescience.

Definition 6.3.2 Let $(r,d) \in \mathcal{B}^* \times \mathcal{D}$ be a hypothesis. We say that we have attained *Pareto perfect knowledge* if (r,d) is Pareto optimal.

When continued research into a particular topic no longer leads to improvement in any of the three components of nescience without worsening at least one of the others, we propose to say that Pareto perfect knowledge has been attained. This state does not imply an absolute or universal truth, but rather marks the boundary of what can be improved within the current symbolic and methodological framework. At this point, the hypothesis lies on the Pareto frontier, corresponding to a condition of local optimality where no further refinement is scientifically justified according to the principles of the theory of nescience. The concept of Pareto perfect knowledge therefore serves as a formal stopping criterion for scientific inquiry, indicating that the topic has been thoroughly explored with respect to the epistemic objectives defined by the theory.

Definition 6.3.3 Let $(r,d) \in \mathcal{B}^* \times \mathcal{D}$ be a hypothesis. We say that we have attained *Pareto perfect knowledge* if (r,d) is Pareto optimal.

It is important to emphasize that reaching Pareto perfect knowledge does not necessarily mean that our total ignorance, as measured by nescience, is zero. However, any attempt to reduce one of the components of nescience would unavoidably increase at least one of the others. In such cases, further scientific inquiry, understood as the pursuit of reduced overall nescience, ceases to be meaningful. Nevertheless, in certain practical contexts, we might still choose to prioritize one dimension over the others. For example, in highstakes engineering applications, it may be preferable to reduce inaccuracy even at the expense of greater miscoding or increased surfeit. Such trade-offs are driven by external goals or constraints, rather than the internal logic of the theory of nescience.

6.4 Current Best Hypothesis

Scientific discovery is inherently iterative. As we explore a topic, we accumulate a set of hypotheses, each composed of a representation and a description, aimed at approximating the underlying entity with increasing accuracy and efficiency. Within this evolving set of candidate hypotheses, it is both natural and practically useful to identify a preferred hypothesis. We refer to this distinguished hypothesis as the current best hypothesis. It represents the best approximation to perfect knowledge that we have found so far and serves as a concrete benchmark against which scientific progress can be measured.

Definition 6.4.1 Let $e \in \mathcal{E}$ be an entity, and let $\hat{\mathcal{H}}_e$ denote the collection of known hypotheses about e. We designate a distinguished element of $\hat{\mathcal{H}}_e$ as our *current best hypothesis*.

Our current best hypothesis should be minimal with respect to at least one of the three components (miscoding, inaccuracy, or surfeit) within the set $\hat{\mathcal{H}}_e$. The selection of a particular metric as the basis for minimization may lead to different hypotheses being identified as the current best. Ideally, the current best hypothesis would be minimal with respect to two, or even all three components simultaneously; however, this is not always attainable given the current set of known hypotheses for every entity.

■ **Example 6.8** Suppose we are studying a physical phenomenon such as planetary motion. We consider three competing hypotheses: (1) a geocentric representation with a descriptive model based on epicycles, (2) a heliocentric representation with elliptical orbits, and (3) a relativistic representation with spacetime curvature. Our current best hypothesis would the third one, as it achieves the lowest nescience given the representations and descriptions we have investigated so far. ■

In some scientific research scenarios, it is common to fix a particular representation, such as the result of an experiment or a dataset composed of measured data, and search only for the description that best models that representation. This motivates the definition of a related but more restricted notion: the best description for a given representation.

Definition 6.4.2 Let $r \in \mathcal{R}$ be a representation, and let $\hat{\mathcal{D}}_r$ denote the collection of known descriptions of r. We designate a distinguished element of $\hat{\mathcal{D}}_r$ as our *current best description*.

As in the case of the current best hypothesis, the current best description should be minimal with respect to at least one of the two components, inaccuracy and surfeit, within the set $\hat{\mathcal{D}}_r$. For most representations r, it is generally not possible to minimize both components simultaneously.

While this approach simplifies the search space and is often motivated by convenience or domain conventions, the theory of nescience discourages fixing the representation in advance. This restriction introduces a significant epistemological risk: one may fall into a local minimum of the nescience landscape, where improvements to the description cannot reduce ignorance further, even though a different representation might unlock a much lower nescience value when paired with an appropriate description. A more robust scientific methodology should simultaneously explore alternative representations and descriptions to maximize the chance of converging to a global minimum of nescience.

Excellent. Here's a revised version of your paragraph that includes a practical example more aligned with your preference—where selecting a different subset of attributes, possibly enhanced with external data, leads to a better model:

■ **Example 6.9** Consider a machine learning task to predict customer churn in a telecommunications company. A standard approach might involve using all available customer attributes, such as service usage metrics, demographic information, and past complaint history, as a fixed representation. A model is then trained to minimize prediction error on this data. Suppose that after exhaustive hyperparameter tuning and model selection, the best model still shows significant error. This may indicate that the current representation is suboptimal. A more insightful representation might focus on a carefully chosen subset of attributes, perhaps augmented with external data such as regional economic indicators or customer sentiment extracted from support call transcripts. ■

6.5 Unknonwn Unknown

In Chapter 1, we introduced the concept of the unknown unknown region, an area encompassing problems for which we not only lack solutions but are entirely unaware of their existence. Within the framework of the theory of nescience, one of the central objectives is to develop a systematic procedure for identifying and exploring potential research entities hidden within this region (refer to Chapter 7 for a detailed procedure on how to approach this task). In this section, we provide a formal characterization of the unknown unknown region and examine its properties.

To uncover what lies hidden within the unknown unknown region, we must first establish the boundary of what is already known. We define this boundary not merely by the existence of hypotheses about a topic, but by the quality of our current knowledge.

Definition 6.5.1 Let $e \in \mathcal{E}$ be an entity, and let $\hat{\mathcal{H}}_e$ denote the collection of known hypotheses about e. If there exists a hypothesis $h \in \hat{\mathcal{H}}_e$ that is Pareto optimal we say that e belongs to the set *known knowns* (denoted by $\mathcal{E}_{KK}$).

This definition identifies as known knowns those entities for which our current best hypotheses are not only available but have achieved a local optimum in the tradeoff between miscoding, inaccuracy, and surfeit. In practice, however, determining the exact set of known known entities is far from straightforward. Assessing whether a given hypothesis lies on the true Pareto frontier is, in general, undecidable. Consequently, our classification of entities as known knowns must be regarded as provisional and subject to revision as our knowledge evolves.

In addition to identifying what we already understand perfectly, we must also recognize the known unknowns, those entities or topics we acknowledge as scientifically relevant but for which our current understanding remains incomplete. These are areas where our ignorance is recognized, and active efforts are being made to reduce it through research.

Definition 6.5.2 Let $e \in \mathcal{E}$ be an entity, and let $\hat{\mathcal{H}}_e$ be the collection of known hypotheses about e. If $\hat{\mathcal{H}}_e \neq \varnothing$ and no hypothesis $h \in \hat{\mathcal{H}}_e$ is Pareto optimal, we say that e belongs to the set *known unknown* (denoted by $\mathcal{E}_{KU}$).

Known unknowns are entities for which we possess hypotheses, but none of them lie on the Pareto frontier. That is, each known hypothesis can be improved in at least one component of nescience without increasing the others. This implies that our current models are suboptimal and that further scientific progress is achievable. As before, identifying the set of known unknowns in practice is challenging. It requires not only recognizing which entities have been explicitly studied, but also verifying that hypotheses have been formally documented, typically through publications, datasets, or other structured records.

The unknown unknowns correspond to entities for which no hypothesis has ever been proposed. These are aspects of reality that lie entirely beyond the scope of our current scientific awareness. We are not only ignorant of their true nature, but also unaware of their very existence.

Definition 6.5.3 Let $e \in \mathcal{E}$ be an entity, and let $\hat{\mathcal{H}}_e$ be the collection of known hypotheses about e. If $\hat{\mathcal{H}}_e = \varnothing$, we say that e belongs to the set *unknown unknown* (denoted by $\mathcal{E}_{UU}$).

In the theory of nescience, all entities for which no hypotheses are currently known are considered part of the realm of the unknown unknown. This includes both entities that may become knowable in the future (given improved representations or descriptions), and those that might remain permanently inaccessible (see Section G.2). The theory of nescience does not distinguish between knowable and unknowable unknowns, as such a distinction is not operationally meaningful within a framework grounded in symbolic representations.

Every knowable entity belongs to exactly one of three epistemic categories: known knowns, known unknowns, or unknown unknowns. The following proposition formalizes this trichotomy.

Proposition 6.5.1 Let $\mathcal{E}$ be the set of all entities. Then:

$$\mathcal{E} = \mathcal{E}_{KK} \cup \mathcal{E}_{KU} \cup \mathcal{E}_{UU} \quad \text{and} \quad \mathcal{E}_{KK} \cap \mathcal{E}_{KU} = \mathcal{E}_{KK} \cap \mathcal{E}_{UU} = \mathcal{E}_{KU} \cap \mathcal{E}_{UU} = \varnothing$$

Proof. Let $e \in \mathcal{E}$ be arbitrary. By definition, the hypothesis set $\hat{\mathcal{H}}_e$ associated with e is either empty or non-empty. If $\hat{\mathcal{H}}_e = \varnothing$, then, by definition, $e \in \mathcal{E}_{UU}$. If $\hat{\mathcal{H}}_e \neq \varnothing$, then two cases are possible: i) if there exists $h \in \hat{\mathcal{H}}_e$ such that h is Pareto optimal, then $e \in \mathcal{E}_{KK}$; ii) if all $h \in \hat{\mathcal{H}}_e$ are not Pareto optimal, then $e \in \mathcal{E}_{KU}$. Therefore, every $e \in \mathcal{E}$ belongs to at least one of the three subsets.

To show that these subsets are pairwise disjoint, assume by contradiction that an entity e belongs to both $\mathcal{E}_{KK}$ and $\mathcal{E}_{KU}$. Then $\hat{\mathcal{H}}_e \neq \varnothing$, and both, $\exists h \in \hat{\mathcal{H}}_e$ that is Pareto optimal (by membership in $\mathcal{E}_{KK}$), and $\forall h \in \hat{\mathcal{H}}_e$, h is not Pareto optimal (by membership in $\mathcal{E}_{KU}$), which is a contradiction.

Similar contradictions arise if e belongs to both $\mathcal{E}_{KU}$ and $\mathcal{E}_{UU}$ or both $\mathcal{E}_{KK}$ and $\mathcal{E}_{UU}$, since $\mathcal{E}_{UU}$ requires $\hat{\mathcal{H}}_e = \varnothing$. ■

We are concerned not only with what we know or do not know, but also with the structural boundaries that separate these domains. The boundary that separates the set of entities for which at least one hypothesis is currently known (i.e., the known) from those for which no hypotheses exist (i.e., the unknown unknown) is referred to as the knowledge frontier.

Before doing so, we must introduce the concept of an anti-Pareto optimal hypothesis, which is one where no component of nescience can be made worse without improving at least one of the others. This notion mirrors the definition of Pareto optimality, but in reverse.

Definition 6.5.4 Let $\mathcal{H}_e$ be the collection of hypotheses about an entity $e \in \mathcal{E}$. We say that $(r,d) \in \mathcal{H}_e$ is *anti-Pareto optimal* for e if, for all $(r',d') \in \mathcal{H}_e \setminus (r,d)$, the following holds: if

$$\mu(r') > \mu(r), \quad \iota(d',r') \geq \iota(d,r), \quad \text{and} \quad \sigma(d',r') \geq \sigma(d,r),$$

then at least one of the following is strictly true:

$$\iota(d',r') < \iota(d,r), \quad \text{or} \quad \sigma(d',r') < \sigma(d,r).$$

The condition must also hold symmetrically for permutations involving ι and σ.

This definition captures the idea that the hypothesis lies at a point of locally maximal nescience, any attempt to increase ignorance along one dimension (e.g., adding more miscoding) will necessarily force a reduction in ignorance along at least one of the remaining dimensions (e.g., increased accuracy or reduced redundancy).

Definition 6.5.5 Let $\mathcal{E}_K$ be the set of known entities. The *knowledge frontier* is defined as the set:

$$\mathcal{F} = \{e \in \mathcal{E}_K \mid \text{the current best hypothesis is anti-Pareto optimal}\}.$$

This definition situates the knowledge frontier at the outermost edge of our current understanding. These are the entities for which: (i) at least one hypothesis is known; (ii) the best-known hypothesis is anti-Pareto optimal, meaning that any further degradation in one dimension of nescience necessarily leads to an improvement in at least one of the others; and (iii) no meaningful scientific degradation is possible without paradoxically improving the hypothesis. This configuration marks the conceptual boundary between the barely known and the unexplored.

A new research entity is any entity that lies beyond the current knowledge frontier. That is, it is an entity for which no hypothesis has yet been formulated, recorded, or studied. These entities exist within the realm of the unknown unknown, not only do we lack understanding of them, but we are not even aware of their existence. Identifying such entities represents the initial and most foundational step in expanding scientific knowledge, since they mark the points at which our current understanding fails to even formulate a question.

Definition 6.5.6 Let $\mathcal{E}$ denote the set of all knowable entities, and let $\hat{\mathcal{H}}_e$ be the collection of known hypotheses about an entity $e \in \mathcal{E}$. We say that e is a *new research entity* if $\hat{\mathcal{H}}_e = \varnothing$.

New research entities are, by definition, members of the unknown unknown region of the knowledge space. They have not been explicitly represented or described, and no attempt has yet been made to understand them through a scientific hypothesis. The identification and formalization of such entities is central to the methodology proposed by the theory of nescience: only by expanding the set of known entities can we ensure the continuous reduction of global ignorance.

A new research entitie refer to those entities for which no hypothesis has yet been proposed. By definition, such entities fall into the class of unknown unknowns. The following proposition formalizes this relationship.

Proposition 6.5.2 Let $\mathcal{E}_{NRE} \subseteq \mathcal{E}$ be the set of all *new research entities*, defined as entities $e \in \mathcal{E}$ such that $\hat{\mathcal{H}}_e = \varnothing$ and e has not yet been discovered or studied. Let $\mathcal{E}_{UU} \subseteq \mathcal{E}$ be the set of all *unknown unknowns*, defined by $\mathcal{E}_{UU} = \{e \in \mathcal{E} \mid \hat{\mathcal{H}}_e = \varnothing\}$. Then, $\mathcal{E}_{NRE} \subseteq \mathcal{E}_{UU}$.

Proof. Let $e \in \mathcal{E}_{NRE}$ be an arbitrary new research entity. By the definition of new research entity, we have $\hat{\mathcal{H}}_e = \varnothing$. But this condition is precisely the definition of membership in $\mathcal{E}_{UU}$. Therefore, $e \in \mathcal{E}_{UU}$. Since every element of $\mathcal{E}_{NRE}$ is also in $\mathcal{E}_{UU}$, it follows that: $\mathcal{E}_{NRE} \subseteq \mathcal{E}_{UU}$. ■

This result captures the foundational idea that research innovation arises from exploring the unknown unknown region. By definition, any new scientific entity must originate from an epistemically uncharted area, one where no hypotheses currently exist.

6.6 Science vs. Pseudoscience

In the theory of nescience, scientific progress is measured by the systematic reduction of ignorance. As we propose and validate hypotheses about previously unstudied entities, those entities transition from the unknown unknown region to either the known known or known unknown regions. From this perspective, the set of unknown entities should decrease over time.

Proposition 6.6.1 Let $\mathcal{E}_{UU}^{(t)}$ denote the set of unknown unknown entities at time t and $\mathcal{E}_{UU}^{(t+1)}$ at a posterior time. Then, $\mathcal{E}_{UU}^{(t+1)} \subseteq \mathcal{E}_{UU}^{(t)} \quad$ for all $t \in \mathbb{N}$.

Proof. At each time step t, let the process of scientific discovery introduce new hypotheses about entities in $\mathcal{E}$, thereby moving those entities from the unknown unknow region into the known known region (either known unknowns or known known). ■

In addition to the reduction in the cardinality of the unknown unknown region, we can also observe a progressive reduction in the nescience of individual entities as more refined hypotheses are introduced. Recall that the nescience of an entity is defined based on its current best hypothesis.

Proposition 6.6.2 Let $e \in \mathcal{E}$ be an entity such that $\hat{\mathcal{H}}_e^{(t)}$ and $\hat{\mathcal{H}}_e^{(t+1)}$ are the collections of known hypotheses about e at times t and $t+1$, respectively. Then, if a new hypothesis $h' \in \hat{\mathcal{H}}_e^{(t+1)} \setminus \hat{\mathcal{H}}_e^{(t)}$ is such that $\nu(h') < \nu(h)$ for all $h \in \hat{\mathcal{H}}_e^{(t)}$, the nescience of e satisfies:

$$\nu^{(t+1)}(e) < \nu^{(t)}(e),$$

where $\nu^{(t)}(e)$ denotes the nescience of the current best hypothesis at time t.

Proof. By definition, we have that $\nu^{(t)}(e) = \min_{h \in \hat{\mathcal{H}}_e^{(t)}} \nu(h)$ and $\nu^{(t+1)}(e) = \min_{h \in \hat{\mathcal{H}}_e^{(t+1)}} \nu(h)$. If a new hypothesis $h' \in \hat{\mathcal{H}}_e^{(t+1)}$ is added such that $\nu(h') < \nu^{(t)}(e)$, then $\nu^{(t+1)}(e) = \nu(h') < \nu^{(t)}(e)$. ■

This result reflects the iterative nature of scientific inquiry: as we formulate new hypotheses or improve existing ones, the combined errors associated with our representations and descriptions tend to diminish. Over time, and under continued research, the nescience of most entities should asymptotically approach its minimum, potentially reaching the Pareto frontier, or in rare cases, even ideal perfect knowledge.

This characteristic trend of decreasing nescience offers a powerful criterion for distinguishing scientific disciplines from pseudoscientific ones. In genuine scientific fields, the average nescience of topics demonstrably declines over time as knowledge improves. In contrast, pseudoscientific domains typically exhibit stagnation in nescience: either the number of proposed hypotheses remains static or their quality fails to improve, leading to no measurable reduction in ignorance. Thus, the presence or absence of a decreasing trend in nescience provides a formal, quantitative indicator for demarcating science from pseudoscience.

6.7 Nescience of Areas

As discussed in Section 2.8, entities can be grouped into research areas, defined as subsets $\mathcal{A} \subset \mathcal{E}$ of the overall entity space. The concept of a research area is meaningful when the entities in $\mathcal{A}$ share a common epistemic domain or possess a unifying property, such as belonging to the same scientific field or addressing a related phenomenon. To quantify how much we do not know about a research area $\mathcal{A}$, we must work with the subset of entities within $\mathcal{A}$ for which at least one hypothesis is currently known $\hat{\mathcal{A}} \subseteq \mathcal{A}$. A representation of the area $\mathcal{A}$ is then a symbolic encoding $R_{\hat{\mathcal{A}}}$ of the known entities in $\hat{\mathcal{A}}$, suitable for further descriptive analysis. Given this representation, we define a description of the area $\mathcal{A}$ as a string $d_{\hat{\mathcal{A}}}$ that models or summarizes the structure or content of $R_{\hat{\mathcal{A}}}$.

The concept of nescience can be extended from individual entities to entire research areas, allowing us to quantitatively assess how well a given area is understood. This extension relies on generalizing the core components of nescience to sets of entities. We use the notions of combined miscoding of the known subset (see Section 3.5), combined inaccuracy (see Section 4.5), and combined surfeit (see Section 5.6) to define a composite measure of nescience at the area level.

In practice, due to the difficulty of precisely identifying the entire known subset $\hat{\mathcal{A}} \subseteq \mathcal{A}$, it is often convenient to use approximations. One practical and interpretable approximation is the notion of average nescience, which provides a summary of the epistemic quality of the known entities within the area.

Definition 6.7.1 Let $\mathcal{A} \subset \mathcal{E}$ be an area, and $\hat{\mathcal{A}}$ be the subset of known entities. The *average nescience of the area* is defined as:

$$\bar{\nu}(\mathcal{A}) = \frac{1}{|\hat{\mathcal{A}}|} \sum_{e \in \hat{\mathcal{A}}} \nu(e),$$

where $\nu(e)$ denotes the nescience of the current best hypothesis about entity e given a particular decision maker.

For instance, when dealing with research topics, a research area may correspond to a broad disciplinary domain, such as biology, mathematics, or physics, each comprising a collection of entities that fall under that domain. In this context, the area of biology would include all research topics formally classified within the biological sciences. This classification allows us to compute and compare the nescience of distinct knowledge domains by aggregating the nescience of the individual topics they encompass (see Section 9.3). Such comparisons provide insight into which areas of human knowledge remain most poorly understood and where future research efforts might be most impactful.

References

Here are some selected references that are particularly relevant to the concept nescience, along with brief explanations of their relevance.

[LV13] is a foundational text in algorithmic information theory, central to defining concepts such as description length, randomness, and information content. These are directly used in our theory of nescience to formalize inaccuracy and surfeit. [Cha69] provides key ideas on the relationship between program length and algorithmic simplicity. This work contributes to the formal underpinnings of inaccuracy and model complexity in the theory of nescience. [CT12] A comprehensive treatment of classical information theory, including entropy, mutual information, and coding theorems. These concepts are foundational for measuring redundancy and assessing the informativeness of representations in our framework. [Grü07] is irectly relevant to the concept of surfeit in nescience. The MDL principle formalizes model selection based on description length, which parallels the idea of seeking non-redundant descriptions. [Sol64] Solomonoff's work on algorithmic probability underlies the notion of model uncertainty and prediction, both of which are implicitly addressed in our theory's pursuit of minimal ignorance. [Kol65] lays the groundwork for the use of Kolmogorov complexity as a measure of information, randomness, and compressibility, all essential in quantifying nescience. [Tur36] provides the foundational model of computation used throughout the theory of nescience. The theory's reliance on representations and oracle machines assumes the basic framework established by Turing. [Cal02] explores algorithmic complexity and randomness in depth, offering a broader perspective that connects well with our treatment of knowledge, representation, and incompleteness in the theory of nescience. [Cha95] illustrates limits of formal descriptions and links to incompleteness phenomena. This is relevant for understanding the boundaries of compressibility and the epistemological challenges in defining knowledge. [Mie12] is crucial for our use of Pareto and anti-Pareto frontiers in describing tradeoffs among miscoding, inaccuracy, and surfeit. Provides the theoretical tools for reasoning about optimality in multi-dimensional knowledge spaces. [Pop14] while not technical, this work provides a philosophical background on how scientific knowledge evolves through falsification, a process aligned with your model's notion of reducing nescience via hypothesis revision. [Sup02] addresses the problem of how scientific structures relate to the entities they describe, an issue directly relevant to your notion of representations, miscoding, and scientific models.

7. Interesting Questions

It is not the answer that enlightens,
but the question.
Eugène Ionesco

In this chapter, we introduce a set of metrics for classifying research topics according to their potential to generate interesting problems, along with a methodology for the assisted discovery of new research questions. The objective is to propose new directions, novel research ideas, that contribute to reducing nescience, that is, to diminishing the extent of the scientific unknown. The proposed methodology supports both the identification of new applications for existing tools to address open problems (the known unknown) and the discovery of entirely new and previously unexplored research directions (the unknown unknown). While the methodology is applicable to both intradisciplinary and interdisciplinary topics, the most impactful results typically arise in the latter case. In Chapter 10, we demonstrate the methodology in practice and propose several new questions and research topics.

We have already examined three dimensions for classifying research topics: miscoding (Chapter 3), inaccuracy (Chapter 4), and surfeit (Chapter 5). These metrics allow us to quantitatively assess our level of understanding of a topic, a concept we refer to as nescience. In this section, we introduce two additional metrics for characterizing topics: relevance (Section 7.1) and applicability (Section 7.2). Relevance measures the impact a topic has on people's lives and complements the existing metrics of nescience. Applicability quantifies how frequently a topic has been applied in other domains and helps identify new uses for existing technologies.

What is proposed in this chapter is an algebraic approach to the assisted discovery of potentially interesting research questions, grounded in the theory of nescience. The objective of this methodology is twofold. On the one hand, it aims to support researchers in their day-to-day work. The methodology can be used to uncover novel tools that may be applied to a given problem, or to identify new problems where existing tools could be effectively used. In its more advanced form, the methodology facilitates the exploration of the unknown unknown, that is, research areas that have not yet been conceptualized, described, or even imagined.

On the other hand, because the methodology is based on well-defined mathematical principles, it lends itself to automation. This opens the door for artificial intelligence systems to move beyond their current limitations, namely, their inability to autonomously generate truly novel research directions. By formalizing the process of question discovery, the methodology enables AI to propose interesting and previously unexplored research questions, and even to discover entirely new topics of scientific inquiry.

7.1 Relevance

In this chapter, we propose additional metrics to complement nescience in the task of evaluating the interest of research topics. These metrics will be useful not only for classifying individual topics, but also for developing a methodology for discovering potential solutions to open problems (Section **??**), as well as for identifying entirely new research topics (Section **??**).

One of these new metrics is *relevance*. Relevance quantifies the impact that a research topic has on people's lives. Intuitively, the greater the relevance of a topic, the higher its potential as a source of interesting problems, since it concerns issues that affect many individuals directly.

Before we can measure the relevance of a topic, that is, its impact on people's lives, we must introduce the concept of a *relevance graph*. The relevance graph (see Figure 7.1) captures the relationship between people and the research topics that affect them.

Definition 7.1.1 We define the *relevance graph*, denoted by **RG**, as the bipartite graph $\mathbf{RG} = (\mathcal{T}, \mathcal{P}, E)$, where $\mathcal{T}$ is the set of topics, $\mathcal{P}$ is the

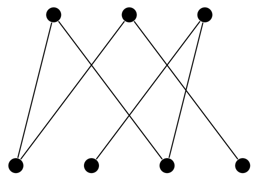


Figure 7.1: Relevance Graph

set of people, and $E \subseteq \{(i,j) : i \in \mathcal{T}, j \in \mathcal{P}\}$ is the set of edges between topics and people. An edge (i,j) belong to E if, and only if, person j is affected by topic i.

When we refer to the set of people $\mathcal{P}$, we mean all individuals in the world. A connection between a topic and a person indicates that the person is affected by the topic, not that they are necessarily interested in it. For example, someone researching a cure for diabetes would not be connected to the research topic "diabetes," but someone who actually suffers from the disease would be.

The higher the relevance of a topic, the greater its potential as a source of interesting problems to solve. In this sense, the research topic "how to cure diabetes" is more relevant than "how far dog fleas can jump," because more people are affected by the former than by the latter.

The precise meaning of "*being affected by*" is inherently abstract and must be approximated in practice. For instance, one could argue that the spouse of a person with diabetes is also affected by the disease in some way. In Section 10.1.2, we will explore how this concept can be operationalized in the context of scientific research topics.

Optionally, we can assign a weight $w_{ij} \in [0,1]$ to the edges of the graph to indicate the degree to which a person j is affected by a topic i. A weight of 1 could represent a life-or-death dependence, while a weight of 0 would mean that the person is not affected at all. Figure 7.1 shows an example of a relevance graph.

The relevance of a topic measures the extent to which it affects people. This can be assessed either by counting the number of affected individuals or by taking into account the magnitude of the effect.

Definition 7.1.2 Let $t \in \mathcal{T}$ be a topic, $\mathcal{P}_t \subseteq \mathcal{P}$ the set of people connected to t in the relevance graph, and $w_{tp} \in [0,1]$ the weight of the edge between

t and $p \in \mathcal{P}_t$. We define the *relevance* of t as

$$R(t) = \sum_{p:(t,p)\in E} w_{tp},$$

The unweighted relevance $R(t)$ (with $w_{tp} = 1$) counts the number of people affected by the topic, while the weighted relevance $R(t)$ reflects both the number of people and the severity of the effect. A higher relevance value indicates greater potential for generating important and impactful questions.

In practice it is useful to normalize the relevance of a topic so that the least relevant topic has a value of 0, the most relevant has a value of 1, and all others lie proportionally in between.

Definition 7.1.3 Let $t \in \mathcal{T}$ be a topic. We define the *min-max normalized relevance* of t as

$$\bar{R}(t) = \frac{R(t) - \min_{t'\in\mathcal{T}} R(t')}{\max_{t'\in\mathcal{T}} R(t') - \min_{t'\in\mathcal{T}} R(t')}$$

This transformation ensures that $\bar{R}(t) \in [0,1]$, with 0 assigned to the least relevant topic and 1 to the most relevant. In the degenerate case where all topics have the same relevance, all normalized values are set to 0.

We could also compute the weighted degree of a person p, denoted $R(p)$, defined as the sum of the weights of the edges that link p to topics in the relevance graph. This quantity measures the overall impact of all topics on a particular person. However, this measure is not used in the theory of nescience.

The relation between the weighted relevance of topics and the weighted degrees of people is given by the weighted degree sum formula:

$$\sum_{t\in\mathcal{T}} R(t) \;=\; \sum_{p\in\mathcal{P}} R(p) \;=\; \sum_{(t,p)\in E} w_{tp}.$$

In the unweighted case ($w_{tp} = 1$ for all edges), this formula reduces to the standard degree sum formula

$$\sum_{t\in\mathcal{T}} \deg(t) \;=\; \sum_{p\in\mathcal{P}} \deg(p) \;=\; d(E).$$

The next proposition shows that, in the weighted case, adding more topics to a research project can only increase its overall relevance. Of course, a research project dealing with "life, the universe, and everything" would be highly relevant, but also highly impractical. How to properly combine research topics will be described in Section **??**.

Proposition 7.1.1 Let $S \subseteq \mathcal{T}$ be a finite set of topics and let $t' \in \mathcal{T} \setminus S$ be an additional topic. Then

$$R(S \cup \{t'\}) \;\geq\; R(S),$$

where the total weighted relevance of a set of topics S is defined as

$$R(S) = \sum_{\substack{t \in S \\ p \in \mathcal{P} \\ (t,p) \in E}} w_{tp}.$$

Proof. We can write

$$R(S \cup \{t'\}) = \sum_{\substack{t \in S \cup \{t'\} \\ p \in \mathcal{P} \\ (t,p) \in E}} w_{tp} = R(S) + \sum_{\substack{p \in \mathcal{P} \\ (t',p) \in E}} w_{t'p}.$$

Since all weights w_{tp} are non-negative,

$$\sum_{\substack{p \in \mathcal{P} \\ (t',p) \in E}} w_{t'p} \geq 0,$$

which implies $R(S \cup \{t'\}) \geq R(S)$. ■

This property shows that weighted relevance is monotone with respect to topic inclusion: if you enlarge the set of topics under consideration, the total weighted relevance can never decrease. In other words, adding topics can only maintain or increase the number (or severity) of connections to people in the relevance graph.

7.2 Applicability

In this section, we introduce a new metric, applicability, which measures the potential of a research topic to serve as a tool for understanding or solving problems in other topics. The intuition is that some topics act as powerful enablers: mastering them allows progress to be made in many other areas.

From a formal standpoint, we say that a topic t_j can be applied to a topic t_i if the conditional nescience of t_i given t_j is smaller than the unconditional nescience of t_i (see Section **??**).

Before defining applicability formally, we introduce the applicability graph, which encodes which topics have been successfully applied to others. This is a directed graph whose nodes are research topics, and where an arc from t_j to t_i indicates that t_j has been successfully applied to explain or solve t_i.

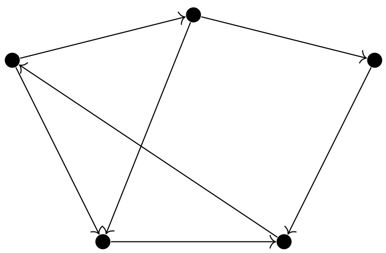


Figure 7.2: Example of an applicability graph.

Definition 7.2.1 We define the *applicability graph*, denoted by AG, as the directed graph $AG = (\mathcal{T}, E)$, where $\mathcal{T}$ is the set of research topics, and $E \subseteq \{(i, j) : i, j \in \mathcal{T}\}$ is the set of arcs. An arc (i, j) belongs to E if $N(t_i \mid t_j) < N(t_i)$, that is, knowing t_j reduces the nescience of t_i. The weight of the arc (i, j) is defined as $w_{ij} = N(t_i) - N(t_i \mid t_j)$, representing the reduction in nescience obtained by applying t_j to t_i.

The applicability of a topic measures the total reduction in nescience it has produced when applied to other topics.

Definition 7.2.2 Given the applicability graph $AG = (\mathcal{T}, E)$, the *applicability* of a topic $t_i \in \mathcal{T}$, denoted $A(t_i)$, is defined as

$$A(t_i) = \sum_{(i,j) \in E} w_{ij},$$

where the sum is over all arcs leaving t_i.

A topic with high applicability is a versatile tool, capable of contributing to the understanding of many other topics. Intuitively, if a tool has been successfully applied multiple times in the past, it is more likely to be useful for solving new problems in the future.

As with relevance, applicability is monotone with respect to topic inclusion: combining topics can only increase their total applicability.

Proposition 7.2.1 Let $S \subseteq \mathcal{T}$ be a finite set of topics and $t' \in \mathcal{T} \setminus S$ an additional topic. Then

$$A(S \cup \{t'\}) \geq A(S),$$

where

$$A(S) = \sum_{\substack{t \in S \\ (t,j) \in E}} w_{tj}.$$

Proof. We can write

$$A(S \cup \{t'\}) = A(S) + \sum_{(t',j) \in E} w_{t'j}.$$

Since all weights w_{ij} are non-negative,

$$\sum_{(t',j) \in E} w_{t'j} \geq 0,$$

which implies $A(S \cup \{t'\}) \geq A(S)$. ■

This property ensures that adding more tools to a research effort can only maintain or increase its applicability.

To compare applicability values across topics on a standard scale, we define a normalized measure using min-max normalization.

Definition 7.2.3 Given the applicability graph $AG = (\mathcal{T}, E)$, we define the *min–max normalized applicability* of a topic $t_i \in \mathcal{T}$, denoted $\tilde{A}(t_i)$, as

$$\tilde{A}(t_i) = \frac{A(t_i) - \min_{t_k \in \mathcal{T}} A(t_k)}{\max_{t_k \in \mathcal{T}} A(t_k) - \min_{t_k \in \mathcal{T}} A(t_k)}$$

where $A(t_i)$ is the applicability of t_i as in Definition 7.2.2.

This normalization ensures that $\tilde{A}(t_i) \in [0,1]$, with 0 assigned to the least applicable topic and 1 to the most applicable. In the degenerate case where all topics have the same applicability, all normalized values are set to 0. Note that min-max normalization can be sensitive to extreme values: if a single topic has exceptionally high applicability, the normalized scores of all other topics will be compressed toward zero.

In practice, computing the exact applicability graph is difficult because, for most topics, $N(t_i \mid t_j)$ is not known. We can approximate it by using a *simplified applicability graph*, where arcs are unweighted and represent known instances of one topic being applied to another.

Definition 7.2.4 We define the *simplified applicability graph*, denoted *SAG*, as the directed graph $SAG = (\mathcal{T}, E)$, where $\mathcal{T}$ is the set of research topics, and $E \subseteq \{(i,j) : i,j \in \mathcal{T}\}$ contains an arc (i,j) if topic j has been used to understand topic i.

Using the simplified applicability graph, we can define an unweighted applicability measure.

Definition 7.2.5 Given $SAG = (\mathcal{T}, E)$, the *simplified applicability* of a topic $t \in \mathcal{T}$, denoted $SA(t)$, is the outdegree of t in SAG, $SA(t) = \text{outdeg}(t)$.

Finally, we normalize simplified applicability to the range $[0,1]$:

Definition 7.2.6 Given the simplified applicability graph $SAG = (\mathcal{T}, E)$, we define the *min–max normalized simplified applicability* of a topic $t_i \in \mathcal{T}$, denoted $SA_n(t_i)$, as

$$SA_n(t_i) = \frac{SA(t_i) - \min_{t_k \in \mathcal{T}} SA(t_k)}{\max_{t_k \in \mathcal{T}} SA(t_k) - \min_{t_k \in \mathcal{T}} SA(t_k)}$$

where $SA(t_i)$ is the simplified applicability of t_i as in Definition 7.2.5.

This normalization ensures that $SA_n(t_i) \in [0,1]$, with 0 assigned to the least applicable topic and 1 to the most applicable. In the degenerate case where all topics have the same applicability, all normalized values are set to 0. As with the weighted case, min-max normalization may be sensitive to extreme values.

7.3 Maturity

When selecting topics to use as tools, we are primarily interested in those that are well understood. Relying on background knowledge that is poorly understood is generally unwise, even if it appears to significantly reduce the conditional nescience of our main problem.

We therefore introduce the concept of the maturity of a topic, which measures the degree to which a topic is understood. Maturity is defined as the inverse of the nescience of the topic: the lower the nescience, the higher the maturity.

Definition 7.3.1 Let $t \in \mathcal{T}$ be a topic, and let $N(t)$ denote its nescience. The *maturity* of t, denoted $M(t)$, is defined as $M(t) = \frac{1}{N(t)}$.

A higher maturity value indicates that the topic is better understood, and thus more suitable to be used as a tool in solving other problems. Conversely, highly immature topics (low $M(t)$) should be avoided as tools, since applying them would risk transferring our lack of understanding from one domain to another.

■ **Example 7.1** Linear regression is a highly mature topic, since its nescience is very small, and so, its maturity is large. ■

To compare maturity values across topics on a standard scale, we define a min-max normalized version. This transformation assigns 0 to the least mature topic, 1 to the most mature, and scales all others proportionally.

Definition 7.3.2 Given the set of topics $\mathcal{T}$, the *min-max normalized maturity* of a topic $t \in \mathcal{T}$, denoted $\tilde{M}(t)$, is

$$\tilde{M}(t) = \frac{M(t) - \min_{t' \in \mathcal{T}} M(t')}{\max_{t' \in \mathcal{T}} M(t') - \min_{t' \in \mathcal{T}} M(t')}$$

where $M(t)$ is the maturity of t as in Definition 7.3.1.

Min-max normalization ensures $\tilde{M}(t) \in [0,1]$, facilitating direct comparison between topics. However, as with other metrics, extreme outliers in maturity can compress the normalized values of the remaining topics toward zero.

7.4 Interestingness

We measure the interest of a topic in two complementary ways: as a tool, based on its usefulness in solving other problems; and as a problem, by studying its intrinsic research value.

The interestingness of a topic as a tool reflects how likely it is that the topic can be successfully applied to solve new problems. This likelihood depends on two key factors: maturity, or how well the topic is understood; and applicability, how widely it has been applied to other problems. We combine normalized measures of these two quantities into a single score:

Definition 7.4.1 We define the *interestingness as a tool* of t as

$$IT(t) = \frac{\sqrt{\tilde{M}(t)^2 + \tilde{A}(t)^2}}{\sqrt{2}}$$

A topic will have a high $IT_n(t)$ value when it is both well understood ($\tilde{M}(t)$ close to 1) and widely applicable ($\tilde{A}(t)$ close to 1). In other words, the most interesting tools are those that combine deep understanding with broad utility in solving other problems.

■ **Example 7.2** The Pythagorean theorem (in a right-angled triangle, the square of the length of the hypotenuse is equal to the sum of the squares of the other two sides) is undoubtedly one of the most widely used and applied theorems in various fields and practical situations, including but not limited to: engineering (calculating distances, angles, and forces in structures and mechanical systems), architecture (determining lengths and angles in building design and construction projects), land surveying (measuring distances and calculating areas of land parcels), physics (analyzing problems in mechanics, optics, and electromagnetism), computer graphics and game development (calculating distances and angles in 2D and 3D spaces) or trigonometry(serving as a foundation for the study of trigonometric functions and their applications). ∎

Some topics may have little utility as tools but are nonetheless highly valuable as research problems in their own right. To capture this idea, we define the interestingness of a topic as a problem, which reflects how compelling it is to investigate the topic itself. This depends on two main factors: relevance, or the degree to which the topic impacts people's lives; and nescience, as a measure of the extent to which the topic is not yet well understood.

Definition 7.4.2 The *interestingness as a problem* of t is

$$IP(t) = \frac{\sqrt{\tilde{N}(t)^2 + \bar{R}(t)^2}}{\sqrt{2}}$$

Intuitively, a topic is interesting as a problem worth investigating if it has a large relevance (it has high impact in people's life) and a large nescience (it is not very well understood). In this sense, we are borrowing ideas from Popper's falsificationism: the more risky is a conjecture, the higher the advance achieved in science given its confirmation.

∎ **Example 7.3** World War I is a very relevant topic, because it had a huge impact on many people's life, and also it is not very well understood topic, since it takes hundreds of pages to explain its causes, and there is no general agreement among the specialists. So, according to our definition, it is a very interesting research problem. ∎

7.5 Interesting Questions

In the theory of nescience we distinguish two kinds of unknowns, the known unknown and the unknown unknown. By known unknown we mean all those already known problems for which we do not know their solutions, for example, nobody knows how to cure diabetes, but we know what diabetes is and we are aware that nobody knows how to cure it. By unknown unknown we mean the collection of unknown problems, that is, all those problems that have not been found yet. In this section we focus on tools to takcle known unknown.

In our methodology, an interesting question emerges from the combination of two pre-existing topics. An interesting question is an ordered pair of topics t and p, where t has high interestingness as a tool, and p has high

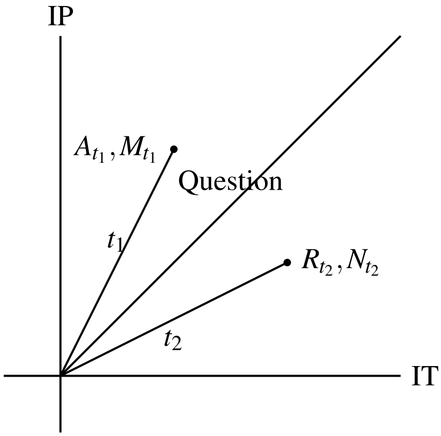


Figure 7.3: Example of an interesting quetion.

interestingness as a problem.

Definition 7.5.1 Given $t, p \in \mathcal{T}$, we call *question* the ordered pair $Q_{t \to p} = (t, p)$.

Given a pair of a topics in $t_1, t_2 \in \mathcal{T}$, the question can be framed as "can we apply the tool described by topic t_1 to solve the problem described by topic t_2?".

The most interesting questions arise when topic t_1 exhibits high interestingness as a tool, and topic t_2 exhibits high interestingness as a problem. We define the interestingness of a question using the Euclidean distance, considering the interestingness of topics t_1 and t_2 as points in a two-dimensional space. The coordinates of these points are (A_{t_1}, M_{t_1}) for the tool and (R_{t_2}, N_{t_2}) for the problem. The distance between these points reflects how promising the combination of t_1 as a tool and t_2 as a problem is.

Definition 7.5.2 We define the interestingness of $Q_{t \to p}$ as

$$IQ(t \to p) = \frac{\sqrt{IT(t)^2 + IP(p)^2}}{\sqrt{2}}$$

Using the Euclidean distance in this way provides a clear geometric interpretation of a question's interestingness in the two-dimensional interestingness space. The greater the magnitude of the resulting vector, the more interesting the question is likely to be.

In practice, we must calculate all possible combinations of topics with high interestingness as tools and those with high interestingness as problems. We then select the combinations with the highest interestingness as questions.

Naturally, most questions generated using this approach will be meaningless, much like those arising during brainstorming sessions when researchers attempt to identify new tools for tackling difficult problems.

This methodology can be applied in other scenarios as well. For instance, a researcher familiar with problem p might be interested in finding applicable tools to solve it. Similarly, a researcher specializing in tool t may be interested in discovering open problems where his expertise can be applied.

The above procedure can be easily generalized to encompass multiple tools and possibly multiple problems. This leads to the application of two tools to a given problem ($t_1 + t_2 \rightarrow p$), the application of a single tool to the combination of two problems ($t \rightarrow p_1 + p_2$), and so on. The exact meaning of these tool and problem combinations depends on the topics themselves.

An interesting question is intradisciplinary if it combines two topics that are studied in the framework of the same research area (e.g., computer science). An interesting question is interdisciplinary if it combines two topics of different research areas (e.g., computer science and philosophy). In principle, the most innovative questions would be interdisciplinary questions, because the probability that somebody has thought about them is lower, since it requires specialists in both research areas working together to come up with that particular question.

Definition 7.5.3 Let $\mathcal{A} \subseteq \mathcal{T}$ be a research area. The question $Q_{t \rightarrow p}$ is *intradisciplinary* if $t, p \in \mathcal{A}$; otherwise it is *interdisciplinary*.

■ **Example 7.4** We could combine the topics with high interestingness as tools found in the area of "computer science" with those topics with high interestingness as problems found in the area of "biochemistry" in order to find new interesting interdisciplinary questions. Some examples of the kind of questions we can find with this approach include: "can we use regular expressions to identify DNA genes?" or "can we use a recursive algorithm to characterize proteins tertiary structure?" ■

The most innovative questions tend to be interdisciplinary, as they have a lower likelihood of having been considered previously. This is because they require collaboration between specialists from different research areas.

7.6 New Topics

The area composed by the unknown unknown problems is a highly interesting one, since it contains those research topics that will be addressed in the future. One of the main goals of this book is to help scientists discover the topics that lay in this unknown unknown area, since that would bring to the present the research problems of the future. In this section we focus on how to indentify the topics hidden in the unknown unknown area.

Definition 7.6.1 Given $t_1, t_2 \in T'$, a (candidate) *new topic* from their combination is the unordered pair

$$S_{\{t_1,t_2\}} = \{t_1, t_2\}.$$

Associate $v(t) = (\tilde{N}(t), \bar{R}(t))$ and define the combination vector $v^{\oplus}(t_1, t_2) = v(t_1) + v(t_2)$.

The exact meaning of the new topic that results as the combination of topics t_1 and t_2 is left to the creative interpretation of the researcher.

Definition 7.6.2 We define the interestingness of $S_{\{t_1,t_2\}}$ as

$$IS(\{t_1, t_2\}) = \frac{\sqrt{IT(t_1)^2 + IT(t_2)^2}}{\sqrt{2}}$$

In practice, what we have to do is to compute all possible combination of those topics with very large interestingness as problems IP_t with themselves, and select the combinations with higher IS. Of course, some of the combinations generated would be totally meaningless. Advanced techniques from the area of natural language processing or machine learning could be used to try filter out those nonsense combinations.

Definition 7.6.3 Let $\mathcal{A} \subseteq \mathcal{T}$. The new topic $S_{\{t_1,t_2\}}$ is *intradisciplinary* if $t_1, t_2 \in \mathcal{A}$; otherwise it is *interdisciplinary*.

Again, the most innovative new topics would be by the combination of interdisciplinary topics, because the probability that somebody has already though about them is lower.

References

The following works provide theoretical and philosophical foundations for the concepts of interestingness, maturity, and the combination of topics as tools and problems.

[Cha13] An accessible introduction to the philosophy of science, addressing how scientific questions are formulated, evaluated, and justified.

[PM19] Introduces the principles of causal reasoning, crucial for determining whether applying one topic as a tool can effectively address another as a problem.

[Pop14] Discusses falsifiability, novelty, and the importance of bold conjectures—foundational ideas for the "new and original" criterion.

[Shm+10] Clarifies the distinction between explanatory and predictive goals, helping to differentiate between topics valuable as problems versus tools.

[Van80] Explores the aims of science, model construction, and empirical adequacy, offering a philosophical context for defining "interesting" research.

Part 2: Applications

8. Machine Learning

There are no difficult problems,
only lack of imagination.
Antonio García

We have seen that the most difficult problems to which we can apply the results of the theory of nescience arise when set of entities $\mathcal{E}$ under study is composed by abstract elements. The difficulty with abstract entities is that it does not exits a way to encode them as strings of symbols so we can effectively reconstruct them. In practice, a possible approach to deal with this problem is to run an experiment and collect the results, as we do in case of physics. An alternative approach would be to take a collection of measurements, like for example, by means of observing the behavior of users in an online social network.

This chapter is devoted to how to apply the concept of minimum nescience to the area of machine learning. We assume that the entities under study are encoded as a dataset $\mathbb{X}$ composed by n training vectors of p predictors and a response variable $\mathbf{y}$ (see Section F.2).

We will start by providing practical approximations for the concepts of miscoding, inaccuracy and surfeit when the entities are encoded as datasets, and then we will show how to combine them in the single quantity of nescience. These approximations will allow us to introduce the *minimum nescience principle*, a technique designed to automate the process of finding optimal models in machine learning (auto-machine learning).

Besides introducing these approximations, we will show how to apply them to solve practical problems. The examples will be based on the `nescience`[1] library, an open source python library that provides an implementation of the ideas included in this chapter.

8.1 Nescience Python Library

The `nescience` library is an open source Python library that provides an implementation of the ideas included in this book applied to the area of machine learning. The library follows the API and conventions of the highly popular `scikit-learn` machine learning tool suite, and so, it can be combined with the methods provided by this package.

The `nescience` library can be installed with the `pip` utility:

```
pip install nescience
```

In the web page that accompanies this book, the reader can find a collection of notebooks for the `jupyter-lab` environment describing how the library works. For each subsection of this chapter, there is a notebook that implements all the examples included, so that the reader can repeat and play with them. Additional information about the `nescience` library, and a reference of the API provided, can be also found in the web page of the book.

8.2 A Note About Compression

As it is customary, the Kolmogorov complexity $K(s)$ of a string s will be approximated by the length of the compressed version of that string using a standard compressor, that is, we will use the normalized compression distance:

$$E_Z(\mathbf{x}_j, \mathbf{y}) = \frac{\max\{\hat{K}_Z(\mathbf{x}_j \mid \mathbf{y}), \hat{K}_Z(\mathbf{y} \mid \mathbf{x}_j)\}}{\max\{\hat{K}_Z(\mathbf{x}_j), \hat{K}_Z(\mathbf{y})\}}$$

where $\hat{K}_Z(s)$ denotes the length of the compressed version of the string s using the compressor Z.

In the particular case of having a vector $\mathbf{x} = \{x_1, \dots, x_n\}$ of measurements, the string s to be compressed will be the concatenation of the encoded values

[1] `https://github.com/rleiva/nescience`

$s = \langle x_1, \ldots, x_n \rangle$. We prefer the following equivalent definition of normalized compression dinstance, since in practice it is easier to compute the joint distribution of two vectors than the conditional distribution:

$$E_Z(\mathbf{x}_j, \mathbf{y}) = \frac{\hat{K}_Z(\mathbf{x}_j, \mathbf{y}) - \min\{\hat{K}_Z(\mathbf{x}_j), \hat{K}_Z(\mathbf{y})\}}{\max\{\hat{K}_Z(\mathbf{x}_j), \hat{K}_Z(\mathbf{y})\}}$$

8.2.1 Compression of Strings

TODO: Pending

8.2.2 Compression of Datasets

Let $\mathbf{x} = x_1, \ldots, x_n$ be a vector to be compressed, representing either a feature or the target variable. As the compression technique, we employ a code C of minimal length, determined by the relative frequencies of the observed values (see Section D.3). We must distinguish between two cases: when the vector consists of discrete values and when it consists of continuous values.

If the variable is discrete, its values do not require further discretization. Suppose $\mathbf{x}$ is a qualitative vector taking values from a set of labels $\mathcal{G} = g_1, \ldots, g_\ell$, that is, $\mathbf{x} \in \mathcal{G}^n$. In this case, the empirical frequencies of the labels provide a natural basis for constructing the code. Specifically, let

$$f_i = \frac{1}{n} \sum_{j=1}^{n} I(x_j = g_i)$$

be the observed relative frequency of label g_i.

In the case where $\mathbf{x}$ is generated by a continuous random variable, we cannot directly assign probabilities to individual values x_j, since the underlying distribution of $\mathbf{x}$ is unknown and, moreover, $P(x_j) = 0$ for all j. To approximate the Kolmogorov complexity $K(\mathbf{x})$, we first discretize $\mathbf{x}$ into a finite set of intervals and then apply the same optimal coding scheme used in the discrete case.

A discretization algorithm maps a (potentially vast) set of numeric values into a reduced set of discrete categories, inevitably losing some information in the process. The choice of discretization method strongly affects the practical computation of nescience. Ideally, the procedure should balance bias and variance: it should use enough intervals to capture the structure of the data (low bias), but not so many that most bins remain empty (which would lead to high variance).

Common approaches include *equal-width discretization*, *equal-frequency discretization*, and *fixed-frequency discretization*. In the `mnplib` library we adopt an equal-width discretization strategy, enhanced with additional techniques that remove the need to manually optimize the hyperparameter controlling the number of bins, thereby enabling full automation of the discretization process.

Our approach begins by selecting the number of bins according to *Rice's rule*,

$$B \approx 2n^{1/3},$$

which is asymptotically motivated in the context of histogram density estimation and offers a good balance between resolution and robustness. This rule avoids the excessive granularity of the square-root heuristic (which can result in too few samples per bin when building joint encodings), while remaining less conservative than Sturges' logarithmic rule (see Section D.6).

Equal-width binning performs poorly in the presence of outliers, since extreme values can stretch the binning range, leaving large portions of the histogram empty. To address this issue, we adopt a *trimmed core range*: rather than spanning from $\min(x)$ to $\max(x)$, we restrict the binning interval to

$$[a,b] = \big[Q_\alpha(x),\, Q_{1-\alpha}(x)\big],$$

where $Q_\alpha(x)$ denotes the α-quantile (e.g., $\alpha = 0.005$). Two additional overflow bins, $(-\infty, a)$ and $(b, +\infty)$, capture the extreme tails, ensuring robustness against outliers.

To further prevent sparsity within the core, we impose a minimum occupancy threshold $m_{\min}$. If any bins fall below this threshold, the number of core bins is reduced until all bins contain at least $m_{\min}$ samples. This guarantees that each symbol represents a meaningful portion of probability mass (see Section D.6).

With this procedure, the estimated Kolmogorov complexity of a dataset is given by the length of its compressed representation under an optimal code. The discretization process combines Rice's rule for bin selection, robust trimming to handle outliers, and minimum occupancy enforcement to avoid empty bins. Together, these components ensure that the complexity estimates are (i) faithful to the observed distribution, (ii) robust to extreme values, and (iii) comparable across single and joint variables.

Given either a discretized continuous variable or a discrete variable with categorical labels, let c_i denote the number of samples in category or bin i, and let B be the total number of bins (or distinct labels). Instead of relying on the naive plug-in estimator $p_i = c_i/n$, we adopt the Krichevsky-Trofimov (or Jeffreys) smoothing:

$$p_i = \frac{c_i + \frac{1}{2}}{n + \frac{B}{2}}.$$

This Bayesian correction eliminates zero-probability events, stabilizes the estimation of code length, and achieves minimax-optimal redundancy in universal coding (see Section D.6). Intuitively, it can be interpreted as adding a "half-count" to every category or bin, ensuring that even rarely observed or unobserved outcomes contribute non-zero probability mass. The resulting compressed length is then

$$\hat{K}_C(\mathbf{x}) \;=\; -\sum_{i=1}^{B} c_i \log_2 p_i.$$

■ **Example 8.1** Consider the sample

$$\mathbf{x} = \{-1.2,\, -0.8,\, -0.5,\, -0.1,\, 0.0,\, 0.2,\, 0.4,\, 0.9,\, 1.1,\, 1.3,\, 1.5,\, 4.5\}$$

with $n = 12$, which contains an outlier at 4.5. We discretize using equal-width bins, with the bin count determined by Rice's rule:

$$B_{\text{core}} \;\approx\; \lceil 2n^{1/3} \rceil \;=\; \lceil 2 \cdot 12^{1/3} \rceil \;\approx\; \lceil 4.58 \rceil \;=\; 5.$$

Next, we apply a small trimming factor $\alpha = 0.05$. The core range is then defined as

$$[a,b] \;=\; \big[Q_{0.05}(x),\, Q_{0.95}(x)\big].$$

For this sample, the outlier 4.5 falls into the right tail, and the core can be taken as $[a,b] = [-1.2,,1.5]$. We divide this interval into $B_{\text{core}} = 5$ equal-width bins of size $h = (b-a)/5 = 0.54$:

$$[-1.2,-0.66),\; [-0.66,-0.12),\; [-0.12,0.42),\; [0.42,0.96),\; [0.96,1.5].$$

We also add two overflow bins, $(-\infty, a)$ and $(b, +\infty)$. With a minimum occupancy threshold $m_{\min} = 1$, all bins contain at least one observation, so no adjustment of B_{core} is required. Assigning each x_j to its bin (core bins are half-open except for the last) yields:

$$\text{Left tail} = 0, \quad \text{Core} = (2,\, 1,\, 4,\, 1,\, 3), \quad \text{Right tail} = 1.$$

Thus, the 7-bin count vector is

$$(c_1, \ldots, c_7) \;=\; (0,\, 2,\, 1,\, 4,\, 1,\, 3,\, 1), \qquad B = 7,\; n = 12.$$

Applying KT smoothing gives

$$p_i \;=\; \frac{c_i + \frac{1}{2}}{n + \frac{B}{2}} \;=\; \frac{c_i + \frac{1}{2}}{12 + 3.5} \;=\; \frac{c_i + \frac{1}{2}}{15.5},$$

so the smoothed probabilities are approximately

$$p \approx \big(0.0323, 0.1613, 0.0968, 0.2903, 0.0968, 0.2258, 0.0968\big).$$

Finally, the optimal data code length is

$$\widehat{K}_C(\mathbf{x}) = -\sum_{i=1}^{B} c_i \log_2 p_i \approx 28.9 \text{ bits}.$$

■

When compressing multiple variables jointly, for example $\mathbf{x}$ and $\mathbf{y}$, we first discretize each variable independently (if needed) using its own binning scheme, and then combine them into joint symbols. To preserve comparability, we use a *mixed-radix encoding*: if $\mathbf{x}$ has B_x bins and $\mathbf{y}$ has B_y, a pair (i, j) is mapped to the integer

$$z = i + B_x j.$$

This approach generalizes naturally to higher dimensions, providing a bijection between joint bins and integers while preserving the underlying probability distributions.

■ **Example 8.2** Let $\mathbf{x}$ and $\mathbf{y}$ be two samples of size n. Each axis is discretized independently, following the procedure described above, yielding B_x and B_y bins respectively (with the same trimming and occupancy rules applied). The joint space is then partitioned into $B_x \times B_y$ cells. To encode these joint cells, we use a mixed-radix mapping, where each pair (i, j) is mapped to a single index $z = i + B_x j$.

Let c_{ij} denote the joint counts and c_z the corresponding counts over the mapped indices. With KT smoothing, the joint code length is given by

$$\widehat{K}_C(\mathbf{x},\mathbf{y}) = -\sum_{z=1}^{B_x B_y} c_z \log_2\left(\frac{c_z + \frac{1}{2}}{n + \frac{B_x B_y}{2}}\right).$$

By using the same per-axis binning for $\mathbf{x}$, $\mathbf{y}$, and their joint grid, we ensure comparability under a consistent encoding scheme (the same "machine"). In practice, the relation

$$\widehat{K}_C(\mathbf{x},\mathbf{y}) \lesssim \widehat{K}_C(\mathbf{x}) + \widehat{K}_C(\mathbf{y})$$

holds up to small modeling constants, in accordance with the chain rule (see Section E.4.6). ■

8.3 Miscoding

In Section 3.1.1 we introduced the concept of miscoding as a quantitative measure of how well a string based encoding $r \in \mathcal{R}$ represents a research entity from $\mathcal{E}$. The miscoding of a representation r was defined as:

$$\mu(r) = \overset{o}{\min_{s \in \mathcal{R}_{\mathcal{E}}}} \frac{\max\{K(s \mid r), K(r \mid s)\}}{\max\{K(s), K(r)\}}$$

and we saw that this quantity cannot be computed in practice for the general case. First of all because it requires a computation from an abstract oracle machine, second because it is based on the uncomputable Kolmogorov complexity, and third because it does not take into account the entity e in which we are interested.

In this section we are going to see how this concept can be adapted in practice to compute the error made by using a dataset $\mathbf{X}$ as a representation of a response variable $\mathbf{y}$ (see Section F.2). Our goal is double, in one hand we are interested in measuring the quality of the dataset $\mathbf{X}$ as a predictor of the variable $\mathbf{y}$, and in the other we want to identify those features $\mathbf{x}_j$ of $\mathbf{X}$ that have the higher predictive power for $\mathbf{y}$. This is the problem addressed by discriminative models (see Section F.2.5) in which we want to estimate the conditional distribution $P(\mathbf{y} \mid \mathbf{X})$.

Given a training dataset $\mathbf{X}$, we can approximate the miscoding of a feature $\mathbf{x}_j$ for the target variable $\mathbf{y}$ by computing the normalized information distance between $\mathbf{x}_j$ and $\mathbf{y}$ (see Section E.5):

$$E(\mathbf{x}_j, \mathbf{y}) = \frac{\max\{K(\mathbf{x}_j \mid \mathbf{y}), K(\mathbf{y} \mid \mathbf{x}_j)\}}{\max\{K(\mathbf{x}_j), K(\mathbf{y})\}}$$

The Kolmogorov complexity $K(\mathbf{v})$ of a vector $\mathbf{v}$ will be approximated by the length of the compressed version of that vector $\hat{K}_C(\mathbf{v})$ using as compressor a minimal length code C (see Section 8.2).

Definition 8.3.1 Let $\mathbf{y}$ be a response variable, $\mathbf{X}$ a dataset composed by p features, and $\mathbf{x}_j$ the $j-th$ feature. We define the regular feature miscoding of $\mathbf{x}_j$ as a representation of $\mathbf{y}$, denoted by $\hat{\mu}(\mathbf{x}_j, \mathbf{y})$, as:

$$\hat{\mu}(\mathbf{x}_j, \mathbf{y}) = \frac{\hat{K}_C(\mathbf{x}_j, \mathbf{y}) - \min\{\hat{K}_C(\mathbf{x}_j), \hat{K}_C(\mathbf{y})\}}{\max\{\hat{K}_C(\mathbf{x}_j), \hat{K}_C(\mathbf{y})\}}$$

Intuitively, the quantity $\hat{\mu}(\mathbf{x}_j, \mathbf{y})$ is a measure of the effort, as the length of a computer program and in relative terms, required to fully encode $\mathbf{y}$ assuming a knowledge of $\mathbf{x}_j$, and the other way around. The lower this value, the better would be the quality of $\mathbf{x}_j$ as a predictor for $\mathbf{y}$.

■ **Example 8.3** Let's $\mathbf{y}$ be a target variable composed by 1.000 random samples that follows a normal distribution $N(3,1)$ with mean $\mu = 3$ and standard deviation $\sigma = 1$, $\mathbf{x}_1$ be a predictor feature that is equal to $\mathbf{y}$ with some random noise, that is $\mathbf{x}_1 = \mathbf{y} + N(3,1)/10$, and $\mathbf{x}_2$ be a second predictor based on random samples from a exponential distribution with a rate of $\lambda = 1$.

```
from scipy.stats import norm, expon

y  = norm.rvs(loc=3, scale=1, size=10000)
x1 = y + norm.rvs(loc=3, scale=1, size=10000) / 10
x2 = expon.rvs(size=10000)
```

We can use the Nescience library to compute the miscoding of the features $\mathbf{x}_1$ and $\mathbf{x}_2$ when they encode the target variable $\mathbf{y}$.

```
from fastautoml.miscoding import Miscoding
import numpy as np

X = np.column_stack((x1, x2))

miscoding = Miscoding()
miscoding.fit(X, y)
miscoding.miscoding_features(mode="regular")
```

The output of the library would be something similar to the following[2]:

```
array([0.27445364, 0.9934222])
```

As it was expected the miscoding of $\hat{\mu}(\mathbf{x}_1, \mathbf{y})$ is much smaller than the miscoding of $\hat{\mu}(\mathbf{x}_2, \mathbf{y})$. In this case, we should prefer $\mathbf{x}_1$ over $\mathbf{x}_2$ as a predictor of $\mathbf{y}$.

■

Sometimes we will use the normalized version of the complements of the individual miscodings, that is $\frac{1-\hat{\mu}(\mathbf{x}_i,\mathbf{y})}{\sum_{i=j}^{p} 1-\hat{\mu}(\mathbf{x}_j,\mathbf{y})}$, instead of the regular ones $\hat{\mu}(\mathbf{x}_i, \mathbf{y})$, because they are easier to compare with other feature selection techniques, and because they have a visually appealing interpretation. We call this version of miscoding the *adjusted* feature miscoding.

■ **Example 8.4** In this example we are going to generate a synthetic dataset where the target variable $\mathbf{y}$ is a collection of normally-distributed clusters of points, and the training set $\mathbb{X}$ is composed by both, relevant and irrelevant predictors. In particular we will generate 1.000 samples composed by 20 features that describe 10 clusters; only 4 of the features are relevant for prediction, and the other remaining 6 are just random values.

[2] Since we are generating a list of 1.000 random samples, the reader could get a slightly different result when running this example.

In Figure 8.1 we can see a two-dimensional projection of this dataset, along the hyperplane composed by features 8 and 10.

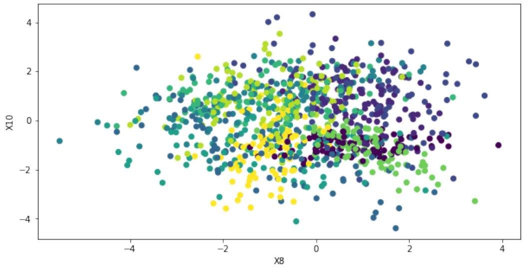


Figure 8.1: Gaussian Blob Cluster.

```
from fastautoml.miscoding import Miscoding
from sklearn.datasets.samples_generator import make_classification

X, y = make_classification(n_samples=1000, n_features=20, n_informative=4,
       n_redundant=0, n_classes=10, n_clusters_per_class=1, flip_y=0)

miscoding = Miscoding()
miscoding.fit(X, y)
msd = miscoding.miscoding_features(mode='adjusted')
```

We will use the adjusted version of the miscoding for an easier comparison with other feature selection techniques. If we plot the results (see Figure 8.2) we will see that the library has successfully identified the four relevant predictors ($\mathbf{x}_3$, $\mathbf{x}_8$, $\mathbf{x}_{10}$ and $\mathbf{x}_{16}$). Since we are using the adjusted version of miscodings, the higher the value the better, and mind that actual values have to be interpreted in relative terms.

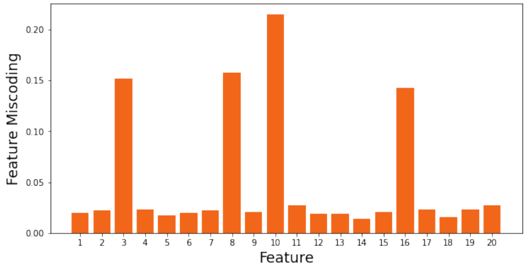


Figure 8.2: Miscoding of a Synthetic Dataset.

We can compare miscoding with correlation, a common technique used in machine learning to identify the most relevant features of a dataset. In Figure 8.3 is shown correlation between the individual features that compose

$\mathbf{X}$ and the target variable $\mathbf{y}$. As we can observe, correlation fails to properly identify one of the relevant features ($\mathbf{x}_3$).

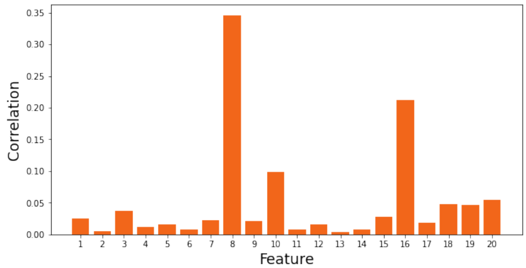


Figure 8.3: Correlation of a Synthetic Dataset.

■

Feature miscoding allow us to identify the most relevant features of a training dataset $\mathbf{X}$, but it cannot be used to compute the miscoding of the dataset itself. If we start with a miscoding of 1 (full unknown), and subtract the miscodings of the individual features, we will end up with a negative miscoding, something that it is not allowed by our theory. If we use the adjusted version, the dataset miscoding will be 0 for all datasets, which is against our intuition that not all possible datasets $\mathbf{X}$ represent equally well a target variable $\mathbf{y}$. According to the theory of nescience, we expect that non-relevant features add, instead of subtract, to the global miscoding of the dataset.

In order to address this problem, we have to introduce the concept of partial miscoding of a feature, as the difference between the adjusted and normalized miscodings.

Definition 8.3.2 Let $\mathbf{y}$ be a target variable, $\mathbf{X}$ a dataset composed by p features, and $\mathbf{x}_j$ the $j-th$ feature. We define the partial miscoding of $\mathbf{x}_j$ as a representation of $\mathbf{y}$, denoted by $\tilde{\mu}(\mathbf{x}_j, \mathbf{y})$, as:

$$\tilde{\mu}(\mathbf{x}_i, \mathbf{y}) = \frac{1 - \hat{\mu}(\mathbf{x}_i, \mathbf{y})}{\sum_{j=1}^{p} 1 - \hat{\mu}(\mathbf{x}_j, \mathbf{y})} - \frac{\hat{\mu}(\mathbf{x}_i, \mathbf{y})}{\sum_{j=1}^{p} \hat{\mu}(\mathbf{x}_j, \mathbf{y})}$$

A positive partial miscoding means that the feature contributes to describe the target variable, meanwhile a negative value means that the feature is not relevant.

■ **Example 8.5** We will use again the synthetic dataset of Example 8.4, but we will increase the number of relevant features from 4 to 14. Then, we will compute the list of partial miscodings.

```
from fastautoml.miscoding import Miscoding
from sklearn.datasets.samples_generator import make_classification

X, y = make_classification(n_samples=1000, n_features=20, n_informative=14,
       n_redundant=0, n_classes=10, n_clusters_per_class=1, flip_y=0)

miscoding = Miscoding()
miscoding.fit(X, y)
msd = miscoding.miscoding_features(mode="partial")
```

As we can see in Figure 8.4, not only the library has been able to correctly identify the relevant features, but also, non relevant features have now a negative contribution to the global miscoding.

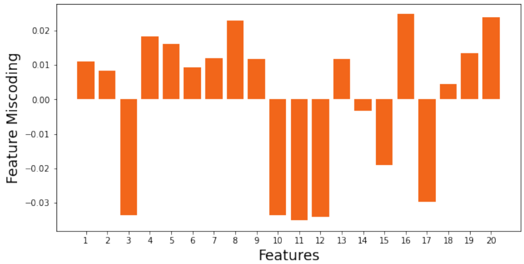


Figure 8.4: Partial Feature Miscoding.

■

Given the definition of partial feature miscoding we can provide a definition of the concept of miscoding of a target variable given a subset of predictors that it is closer to the original concept of miscoding defined by the theory of nescience.

Definition 8.3.3 Let $\mathbf{y}$ be a target variable, $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_p\}$ a dataset composed by p features, and $\mathbf{Z} = \{\mathbf{z}_1, \ldots, \mathbf{z}_k\}$ a subset of features, that is, $\{\mathbf{z}_1, \ldots, \mathbf{z}_k\} \subseteq \{\mathbf{x}_1, \ldots, \mathbf{x}_p\}$. We define the miscoding of $\mathbf{Z}$ as a representation of $\mathbf{y}$, denoted by $\hat{\mu}(\mathbf{Z}, \mathbf{y})$, as:

$$\hat{\mu}(\mathbf{Z}, \mathbf{y}) = \sum_{i=1}^{k} \tilde{\mu}(\mathbf{z}_i, \mathbf{y})$$

■ **Example 8.6** Based on the dataset and the partial features miscoding computed in Example 8.5, in Figure 8.5 we can see the evolution of the miscoding of the training subset $\mathbf{Z}$ as we add more features to the study.

■

In the following example we are going to compare the performance of a machine learning classifier when using a full dataset and a reduced version

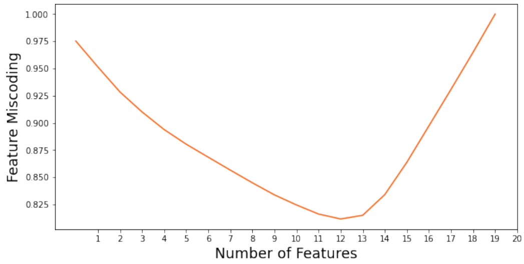


Figure 8.5: Accumulated Partial Feature Miscoding.

of the same dataset using only those features identified as relevant, i.e., with positive partial miscoding.

■ **Example 8.7** Let's train a neural network with the standard MNIST dataset in order to classify hand written digits. The evaluation criteria will be the score of the classifier, that is, the percentage of digits correctly classified, applied over a test dataset different from the dataset used for training. The neural network will be trained and evaluated using all the features that compose the dataset, and with a reduced version of the dataset composed by only those features with a positive partial miscoding.

```
import numpy  as np
from sklearn.model_selection import train_test_split
from sklearn.neural_network import MLPClassifier
from sklearn.datasets import load_digits
from fastautoml.fastautoml import Miscoding

data = load_digits()
X_raw = data.data
y_raw = data.target

miscoding = Miscoding()
miscoding.fit(X_raw, y_raw)
mscd = miscoding.miscoding_features(miscoding='partial')
X_red = X_raw[:,np.where(mscd > 0)[0]]
y_red = y_raw

X_raw_train, X_raw_test, y_raw_train, y_raw_test = train_test_split(X_raw,
             y_raw, test_size=.3)
X_red_train, X_red_test, y_red_train, y_red_test = train_test_split(X_red,
             y_red, test_size=.3)

clf = MLPClassifier(alpha=1, max_iter=1000)

clf.fit(X_raw_train, y_raw_train)
score_raw = clf.score(X_raw_test, y_raw_test)

clf.fit(X_red_train, y_red_train)
score_red = clf.score(X_red_test, y_red_test)
```

```
reduction = 1 - X_red_train.shape[1] / X_raw_train.shape[1]

print("Score raw:", score_raw, " Score Miscoding:", score_red,
      " Reduction:", reduction)

Score raw: 0.9833333333333333  Score Miscoding: 0.9814814814814815  Data Reduction: 0.4
```

If we run the above source code, we will see that the score of the neural network classifier is about the same for the two datasets, 98% of the digits are correctly classified using the test data. However, the reduced dataset used for training based on the optimal miscoding is 43% smaller than the original dataset. This size reduction could have a big impact in the training time of the neural network. Smaller datasets are also relevant when working with ensembles of models, like random forests, where hundreds or thousands of models have to be trained.

■

Intuitively, as Example 8.6 shows, we should prefer the subset $\mathbf{Z}$ of $\mathbf{X}$ composed by all those features whose partial miscoding are greater than zero. However, as we will see in the following sections of this chapter, this might not be the case. Feature selection is only one of the criteria used in the process of finding an optimal model for an entity represented by a dataset. It might happen that other elements, like inaccuracy or surfeit, suggest to use a different subset of predictors. The global optimization criteria we should use is the concept of nescience. A sensible approach to use partial miscoding would be to incrementally add to our model those features with higher miscoding, until all features with a positive value have been added, or an optimality criterion has been reached.

In case of having a generative model (see Section F.2.5), that is, a machine learning algorithm designed to find the joint probability $P(\mathbf{X},\mathbf{y})$, we could use miscoding to compute how the different features relate to each other, that is, the quantity $\hat{\mu}(\mathbf{x}_i,\mathbf{x}_j)$ for each pair of values $i,j \leq p$. The result would be a miscoding matrix (see Example 8.8).

■ **Example 8.8** The Boston dataset included in `scikit-learn` library contains a collection of variables that (potentially) could explain the price of houses in the area of Boston. In this example, instead of computing which are the factors that contribute the most to the price of houses, we are going to study the inter-dependence between these factors, using a miscoding matrix.

```
from fastautoml.fastautoml import Miscoding
from sklearn.datasets import load_boston

data = load_boston()
```

```
miscoding = Miscoding(X_type="numeric", y_type="numeric")
miscoding.fit(data.data, data.target)
mscd_matrix = miscoding.features_matrix(mode='regular')
```

In Figure 8.6 we can see a graphical representation using a heatmap of the miscoding matrix computed over the features. The darker values represent a lower miscoding (mind we are using the regular version of the concept of miscoding). In particular, the values of the main diagonal are equal to zero.

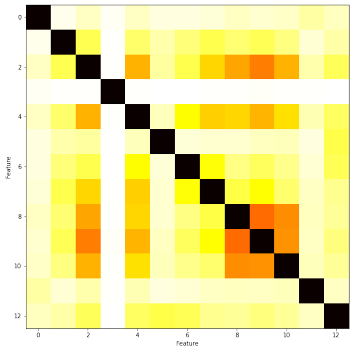


Figure 8.6: Regular Miscoding Matrix.

The minimum value of 0.52 is obtained with the pair $(8,9)$ that correspond to the features "index of accessibility to radial highways" and "full-value property-tax rate per \$10,000". These features are good candidates to evaluate in a predictive model, since they contain non-redundant information. The maximum value of 0.99 is achieved with the pair $(3,12)$ with the features "Charles River dummy variable" and "% lower status of the population". These features contains almost the same information, and so, including both in a model does not add nothing new, but increases the complexity of the model and the risk of over-fitting.

■

8.4 Inaccuracy

In Section 4.1 we defined the inaccuracy of a description $d \in \mathcal{D}$ for a representation $r \in \mathcal{R}$ as the normalized information distance between the representation r and the string $\Gamma(d)$ printed out by a universal Turing machine when given the description as input:

$$\iota(d,r) = \frac{\max\{K(r \mid \Gamma(d)), K(\Gamma(d) \mid r)\}}{\max\{K(r), K(\Gamma(d))\}}$$

Inaccuracy, being based in Kolmogorov complexity, is not computable for the general case, and so, it has to be approximated in practice. In this section we are going to see how this concept can be estimated in case of a model trained using a dataset. The approach will be similar to the one used in case of miscoding (see Section **??** for more information).

TODO: This definition correspond to the discriminative case. Introduce the generative case as well.

Definition 8.4.1 Let $\mathbb{X}$ be a dataset, $\mathbf{y}$ a response variable, m a model, and $\hat{\mathbf{y}} = m(\mathbb{X})$ the predicted values by m given $\mathbb{X}$. We define the *inaccuracy* of the model m for the target values $\mathbf{y}$, denoted by $\hat{\imath}(\hat{\mathbf{y}}, \mathbf{y})$, as:

$$\hat{\imath}(\hat{\mathbf{y}}, \mathbf{y}) = \frac{\hat{K}_C(\hat{\mathbf{y}}, \mathbf{y}) - \min\{\hat{K}_C(\hat{\mathbf{y}}), \hat{K}_C(\mathbf{y})\}}{\max\{\hat{K}_C(\hat{\mathbf{y}}), \hat{K}_C(\mathbf{y})\}}$$

Intuitively, the quantity $\hat{\imath}(\hat{\mathbf{y}}, \mathbf{y})$ is a measure of how far are the predicted values from real values. The lower this quantity, the better is the quality of m as a predictor for $\mathbf{y}$. With our new inaccuracy metric we are measuring not only how difficult is to reconstruct the original target vector $\mathbf{y}$ given the predicted values $\hat{\mathbf{y}}$, but also how much additional information $\hat{\mathbf{y}}$ contains that is not related to $\mathbf{y}$, being the latter a novelty with respect to other metrics used in machine learning to measure the accuracy of a model.

■ **Example 8.9** Inaccuracy, according to the minimum nescience principle, is given by the normalized compression distance between the actual targets $\mathbf{y}$ and the predicted targets $\hat{\mathbf{y}}$ by the model. In the following example we are going to compare the behavior of our new inaccuracy metric with a classical score metric. The experiment will be based on the MNIST dataset (hand written digits recognition) provided by scikit-learn.

```
from fastautoml.fastautoml import Inaccuracy
from sklearn.datasets import load_digits

X, y = load_digits(return_X_y=True)

inacc = Inaccuracy()
inacc.fit(X, y)
```

For this example we will train a decision tree classifier up to a pre-determined tree depth of i, where i goes from 1 to 20.

```
from sklearn.tree import DecisionTreeClassifier

scores       = list()
inaccuracies = list()

for i in range(20):

    tree = DecisionTreeClassifier(max_depth=i, random_state=42)
    tree.fit(X, y)
```

```
    scores.append(1 - tree.score(X, y))
    inaccuracies.append(inacc.inaccuracy_model(tree))
```

We are interested to compare the behavior of score (actually we are comparing against one minus score) and inaccuracy metrics. As we can see in Figure 8.7, both metrics present a similar behavior, having inaccuracy a larger value, due to a stronger emphasis in incorrectly predicted values.

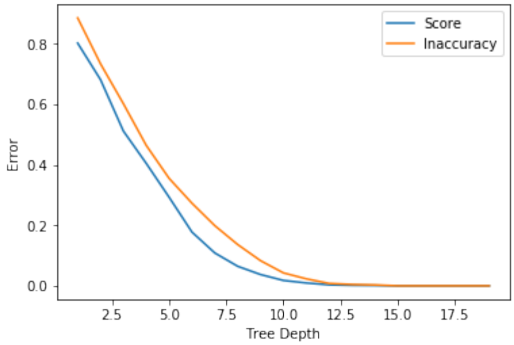


Figure 8.7: Inaccuracy vs. Score of Decison Trees

■

In Example 8.9 we have seen that the deeper the tree, the smaller is the training error. Of course, the higher the value of i, the higher the risk of overfitting the data. However, in case of inaccuracy we are not interested in avoiding overfitting, since overfitting is controlled by the metric of surfeit (see Section **??**).

We can see inaccuracy as the effort, measured as the length of a computer program, required to fix the predictions made by a model. In this sense, according to the minimum nescience principle, it is not the same a model that makes one hundred times the same error than a model that makes one hundred different errors, since it should be easier to fix the former than the later (see Example 8.10).

■ **Example 8.10** In this example we are going to use again a decision tree classifier, but this time it will be trained with the hyperparameter minimum number of samples per leaf node set to 5 (a common approach used in practice to avoid decision trees to overfit).

```
tree = DecisionTreeClassifier(min_samples_leaf=5)
tree.fit(X, y)
```

The inaccuracy of this new trained model is 0.17, and its score 0.08. Next we will artificially introduce one hundred errors in the dataset, simulating the case that the tree is not able to model correctly these data points. In this particular case all the errors are exactly the same.

```
X2 = X.copy()
y2 = y.copy()
for i in range(100):
    X2 = np.append(X2, [X[0]], axis=0)
    y2 = np.append(y2, (y[0]+1) % 10)
```

The inaccuracy of the decision tree, given this new dataset, has increased[3] from 0.17 to 0.21.

```
inacc.fit(X2, y2)
inacc.inaccuracy_predictions(pred)
```

Score has also increased, in this case from 0.08 to 0.13.

```
1 - tree.score(X2, y2)
```

Finally, we are going to repeat exactly the same experiment, but this time instead of adding one hundred times the same error, adding one hundred different errors.

```
X3 = X.copy()
y3 = y.copy()
for i in arange(100):
    index = np.random.randint(X.shape[0])
    X3    = np.append(X3, [X[index]], axis=0)
    y3    = np.append(y3, (y[index]+1) % 10)
```

In this last case the inaccuracy of the model has increased up to 0.25, meanwhile score remained the same. ■

In line with Example 8.10, an extreme case would be a model for a target binary variable (True and False) that always fails with its predictions, that is, if the value of the target is True, the model will predict False, and if it is False, it will predict True. The classical evaluation metrics would say that this model is the worst possible model, but our inaccuracy would claim that the model is perfect. We might be wondering what it is the value of a model that always fails to predict the correct target. But if we are the managers of an edge fund investing in the stock market, we will very happy to pay a huge amount of money for a model that predicts that the shares of IBM will go down whenever they go up, and the other way around.

[3] Note that we had to `fit()` again the class Inaccuracy in order to use the new dataset. Normally this is not the way we use this class; instead what we should do is to fit once a dataset, and then compute the inaccuracy of different models. We are doing here in this way to demonstrate an interesting property of the concept of inaccuracy.

In case of having a highly unbalanced dataset, that is, when some categories have a lot of more training data than others, the classical score metric can provide a misleading result, since a good score does not necessarily mean a good model, it might happen that the model is simply properly classifying the samples of the category with the higher number of training samples, and misclassifying the others. In practice, we solve this problem by using metrics specifically designed to deal with unbalanced datasets. In case of the new metric of inaccuracy, as Example 8.11 shows, a model that can not properly classify one of the categories is considered a bad model, even if this category has only a few points in the training dataset.

■ **Example 8.11** For this example, we will create a synthetic dataset using the `make_classification` utility of scikit-learn, with two classes in which one of then has 95% of the samples, and the other 5%.

```
from sklearn.datasets import make_classification

depth = list()
score = list()
inacc = list()

inaccuracy = Inaccuracy()

for i in np.arange(1, 100):

    X, y = make_classification(n_samples=1000, n_features=2,
                               n_informative=2, n_redundant=0,
                               class_sep=2, flip_y=0, weights=[0.95,0.05])

    inaccuracy.fit(X, y)

    tree = DecisionTreeClassifier(min_samples_leaf=i)
    tree.fit(X, y)

    depth.append(i)
    score.append(1 - tree.score(X, y))
    inacc.append(inaccuracy.inaccuracy_model(tree))
```

The experiment consists in training a decision tree classifier with a minimum number of samples per leaf of i, where i goes from 1 to 100. In Figure 8.8 we can see the behavior of inaccuracy and score. In case of large values of i, the score metric tell us that no more than a 5% of the samples is misclassified, however, the inaccuracy says that even if the total number of misclassified points is low, the inaccuracy of the model is very bad.

■

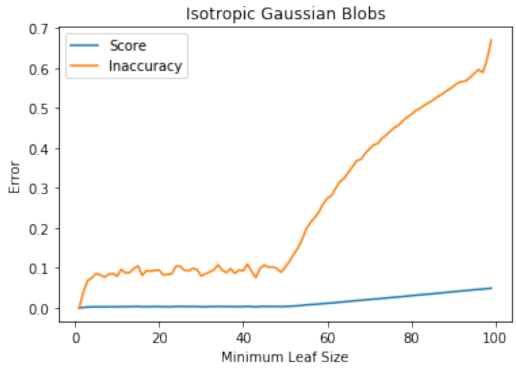


Figure 8.8: Inaccuracy of Decision Tree.

8.5 Surfeit

In Section 5.2 we defined the surfeit of the model $m \in \mathcal{M}$ for the representation $r \in \mathcal{R}$ as:

$$\sigma(m,r) = 1 - \frac{K(r)}{l(m)}$$

Since the length $K(r)$ of shortest possible model for the representation r is in general unknown, we have to approximate this concept in practice. In case of having a training dataset $\mathbb{X}$ and a target variable $\mathbf{y}$, we can approximate the surfeit of a model m for the representation $\mathbf{y}$ by means of computing:

$$\hat{\sigma}(m,y) = 1 - \frac{\hat{K}_C(\mathbf{y})}{l(m)}$$

Where $\hat{K}_C(\mathbf{y})$ is the length of the compressed version of the of the vector $\mathbf{y}$ using as compressor a minimal length code C, computed given the relative frequencies of the values observed in $\mathbf{y}$ (see Section **??**).

Definition 8.5.1 Let $\mathbf{y}$ be a response variable, $\mathbb{X}$ a dataset composed by p features and n samples. We define the surfeit of the model $m \in \mathcal{M}$ as a representation of $\mathbf{y}$, denoted by $\hat{\sigma}(m,\mathbf{y})$, as:

$$\hat{\sigma}(m,\mathbf{y}) = 1 - \frac{\hat{K}_C(\mathbf{y})}{l(m)}$$

The definition of surfeit requires a method of encoding the models as a string of symbols, so we can compute their length. Ideally, we should use as encodings Turing machines, and agree upon an universal Turing machine to interpret those models. However, that would make very difficult to add new models to the nescience library. Instead, we have used for the encoding of models a simplified version of the Python language, where not all the constructions are allowed, and we do not allow the use of libraries.

Surfeit is a metric that can help us to avoid overfitted models. The higher is the surfeit of a model, the higher is the probability that the model is an overfit of the training dataset, as Example 8.12 shows.

■ **Example 8.12** In this example we are going to generate a dataset composed by 900 samples of a sinusoidal curve, and we will fit the data using a n degree polynomial, where n goes form 1 to 15.

```
from sklearn.linear_model import LinearRegression
from sklearn.preprocessing import PolynomialFeatures

from Nescience.Nescience import Surfeit
from Nescience.Nescience import Inaccuracy

n_samples = 900
degrees = np.arange(1, 15)

X = np.sort(np.random.rand(n_samples) * 3)
y = np.cos(1.5 * np.pi * X)

linacc   = list()
lsurfeit = list()

for i in degrees:

    poly = PolynomialFeatures(degree=i, include_bias=False)
    newX = poly.fit_transform(X[:, np.newaxis])

    linear_regression = LinearRegression()
    linear_regression.fit(newX, y)

    inacc.fit(newX, y)
    inaccuracy = inacc.inaccuracy_model(linear_regression)

    sft.fit(newX, y)
    surfeit = sft.surfeit_model(linear_regression)

    linacc.append(inaccuracy)
    lsurfeit.append(surfeit)
```

In figure 8.9 we can see the results of this experiment. As it was expected, the higher the degree of the polynomial, the smaller is the error of the model. However, at the same time we see that the higher the polynomial, the higher the surfeit of the model. The ideal model is that one that has a low inaccuracy and a low surfeit.

■

Another advantage of the concept of surfeit is that it allows us to compare and decide between models that belong to different families. For example, in

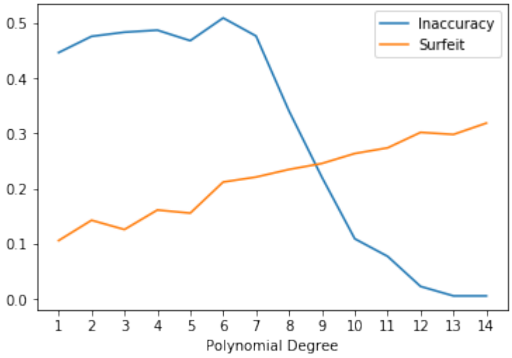
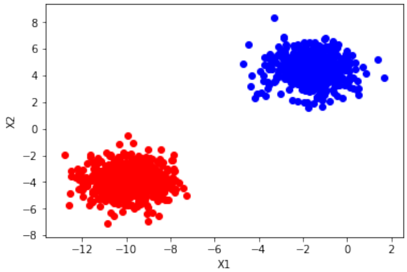


Figure 8.9: Surfeit vs Inaccuracy



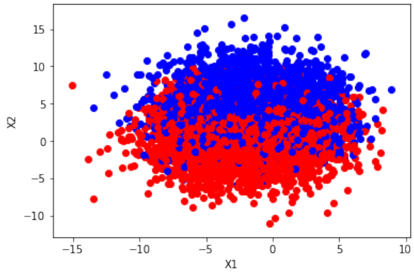


Table 8.1: Isotropic Gaussian blobs.

case of models having the same accuracy, shall we prefer a decision tree over a neural network, or a naive Bayes classifier over a support vector machine? Next example shows how we can decide about those questions.

■ **Example 8.13** In this example we are going to compare a decision tree with a neural network. We will use a synthetic dataset composed by two isotropic Gaussian blobs, and we will train our models to split them apart. In the first part of the example we will use a standard deviation of 1 and only two dimensions, so the two clusters are easy to classify (see figure on Table 8.1, left side).

```
from sklearn.tree import DecisionTreeClassifier
from sklearn.neural_network import MLPClassifier
from Nescience.Nescience import Surfeit
from Nescience.Nescience import Inaccuracy
from sklearn.datasets.samples_generator import make_blobs

X, y = make_blobs(n_samples=1000, centers=2, n_features=2, cluster_std=1)
```

```
tree = DecisionTreeClassifier()
tree.fit(X, y)
tree.score(X, y)

nn = MLPClassifier()
nn.fit(X, y)
nn.score(X, y)

sft = Surfeit()
sft.fit(X, y)

sft.surfeit_model(tree)
sft.surfeit_model(nn)
```

If we ran the above code we will see that both models have exactly the same accuracy of 1, that is, they are perfect classifiers. However the surfeit of the decision tree is 0.25, meanwhile the surfeit of the neural network is 0.73. In this particular case we should prefer the decision tree over the neural network.

If we perform the same experiment using a standard deviation of 3, so two clusters that are more difficult to split (see Table 8.1, right side), the situation will change.

```
X, y = make_blobs(n_samples=10000, centers=2, n_features=8, cluster_std=3)
```

In this second case, again, both models have the same accuracy (we have increased the number of samples, and the number of dimensions, so the models can still perform a perfect classification), but the surfeit of the decision tree has increased to 0.82, and the surfeit of the neural network is almost the same, 0.76. For this second dataset we should prefer the neural network over the decision tree.

■

In example 8.13 we have assumed that both models, decision tree and neural networks, have the same accuracy. When this is not the case, when the models do not have the same accuracy, we have to apply to the concept of nescience in order to decide between them.

R TODO: Mention the problem of the stability of the signal.

8.6 Nescience

In Chapter 6 we defined the concept of nescience as the solution to a non-linear multi-objective optimization problem, where we had to minimize the miscoding, inaccuracy and surfeit of representations and models. The solution to this problem is, in general, not unique, in the sense that we can find multiple pairs of representations and models that have the property that we can not improve one of these quantities without degrading the others (Pareto optimality). However, in practice, we expect that a machine learning library should provide a single solution when training a model over a dataset. In order to provide this unique solution, we have to resort to a utility function that selects one from the available solutions. The nescience library provide different alternatives of utility functions, being the default one the arithmetic mean the tree metrics.

R The nescience library implements the following utility functions to approximate the concept of nescience, that is, to compute $\hat{\nu}\left(\mathbb{Z}, m, \mathbf{y}\right)$:

- Euclid distance: $\left(\hat{\mu}(\mathbb{Z},\mathbf{y})^2 + \hat{\iota}(\hat{y},\mathbf{y})^2 + \hat{\sigma}(m,\mathbf{y})^2\right)^{1/2}$
- Arithmetic mean: $\frac{\hat{\mu}(\mathbb{Z},\mathbf{y}) + \hat{\iota}(\hat{y},\mathbf{y}) + \hat{\sigma}(m,\mathbf{y})}{3}$
- Geometric mean: $\left(\hat{\mu}(\mathbb{Z},\mathbf{y}) \times \hat{\iota}(\hat{y},\mathbf{y}) \times \hat{\sigma}(m,\mathbf{y})\right)^{1/3}$
- Product: $\hat{\mu}(\mathbb{Z},\mathbf{y}) \times \hat{\iota}(\hat{y},\mathbf{y}) \times \hat{\sigma}(m,\mathbf{y})$
- Addition: $\hat{\mu}(\mathbb{Z},\mathbf{y}) + \hat{\iota}(\hat{y},\mathbf{y}) + \hat{\sigma}(m,\mathbf{y})$
- Weighted mean: $w_\mu \hat{\mu}(\mathbb{Z},\mathbf{y}) + w_\iota \hat{\iota}(\hat{y},\mathbf{y}) + w_\sigma \hat{\sigma}(m,\mathbf{y})$
- Harmonic mean: $\frac{3}{\hat{\mu}(\mathbb{Z},\mathbf{y})^{-1} + \hat{\iota}(\hat{y},\mathbf{y})^{-1} + \hat{\sigma}(m,\mathbf{y})^{-1}}$

Euclid distance and addition have the drawback that they produce nescience values greater than one, something that it is against our theory. Geometric mean, product and harmonic mean have the problem that the nescience is zero, or not defined, if one of the three metrics (miscoding, inaccuracy or surfeit) is zero. And the weighted mean introduce three new hyperparameters that have to be optimized. It is still an open question which one is the best utility function to compute the nescience of a dataset and a model.

Example 8.14 shows how we can use the `nescience` library to compute the nescience of a dataset and a model.

■ **Example 8.14** This example shows how to compute in practice the nescience of a dataset and a model. In particular, we are going to compute the nescience of a decision tree classifier applied over the dataset digits (MNIST hand written digits classification problem) included in the `sklearn` library.

```
from sklearn.tree import DecisionTreeClassifier
from sklearn.datasets import load_digits
from Nescience.Nescience import Nescience

data = load_digits()

tree = DecisionTreeClassifier()
tree.fit(data.data, data.target)
tree.score(data.data, data.target)
[ ] 1
```

```
nescience = Nescience()
nescience.fit(data.data, data.target)

nescience.nescience(tree)
[ ] 0.5895603819965907
```

The score of the decision tree model is 1, meaning that all the samples have been properly classified. Of course, what happened is that the decision tree is overfitting the dataset. In order to avoid this kind of problems we usually split the data in separate training and testing subsets, or we perform a more advanced cross-validation. However, if we compute the nescience, we will get a value of 0.59, rising the flag that something is wrong with the model or the training dataset.

■

In Example 8.14 we have shown that one of the advantages of the concept of nescience is that we can evaluate the quality of a model without applying computationally expensive procedures like cross-validation, and without requiring to save part of the data as a test subset. Another advantage of the metric nescience is that it allows us to decide between competing models from different families of models, as it is shown in Example 8.15.

■ **Example 8.15** In this example we are going to compare two models from two different families of models: decision trees and neural networks. Both models will be trained with the breast cancer dataset provided by the `sklearn` library.

```
from sklearn.tree import DecisionTreeClassifier
from sklearn.neural_network import MLPClassifier
from sklearn.datasets import load_breast_cancer
from Nescience.Nescience import Nescience

data = load_breast_cancer()
X = data.data
y = data.target

tree = DecisionTreeClassifier(max_depth=3)
tree.fit(X, y)
tree.score(X, y)
[ ] 0.9789103690685413

nescience = Nescience()
nescience.fit(X, y)
nescience.nescience(tree)
[ ] 0.5945936419010083

nn = MLPClassifier()
nn.fit(X, y)
nn.score(X, y)
[ ] 0.9261862917398945
```

```
nescience.nescience(nn)
[ ] 0.7860523786210711
```

Both models have a similar score. In this case, not only the decision tree provide a better score, but also, the nescience is much lower than in case of the multi-layer perceptron, and so, we should prefer the former over the later.

■

Nescience is a metric that can be used to optimize the hyperparameters that define a (parametric) family of models. The advantage of nescience is that we can use a greeedy approach to select the best value for an hypeparameter, saving a lot of computational time and resources during the search. That is, if we have a model controlled by an hyperparameter such that the higher the value the better the score, we should select that value in which the nescience stops decreasing and starts to increase, since this is the point in which we are not longer learning anything new from that dataset (see Example 8.16).

■ **Example 8.16** For this example we will use again a decision tree classifier with the breast cancer dataset. We will train 10 different trees, setting the hyperparameter `max_depth` with values from 1 to 10. The `max_depth` hyperparameter controls how deep we allow the tree to grow in order to classify the samples of the dataset. The deeper the tree the higher the score of the model, but also, the higher the risk of overfitting the training data. For each tree we will compute the nescience of the model, and we will compare it with a cross validation score. The results are shown in Figure 8.10. As we can see in the figure, both, nescience and cross validation score, decrease are we increase the depth of the tree, until we reach a point in which it starts to increase. This inflection point is where the model begins to overfit the data. The nescience library suggests to use a tree with a maximum depth of 7, meanwhile with the cross validation we got an optimal level of 6.

■

It is interesting to note the behavior of the three metrics that define the concept of nescience in Figure 8.10. As it is expected the the deeper the tree the smaller is the inaccuracy of the model and the higher the surfeit. However, in case of miscoding, we have a sort of random evolution. This behavior is due to the fact that each candidate tree uses a different subset of features at the decision nodes. I would be very nice to have an decision tree building algorithm that takes into account miscoding in order to decide the best features for new branches. Such an algorithm is described in Section 8.11.

Finally, we are going to see how to use nescience in case of hyperparam-

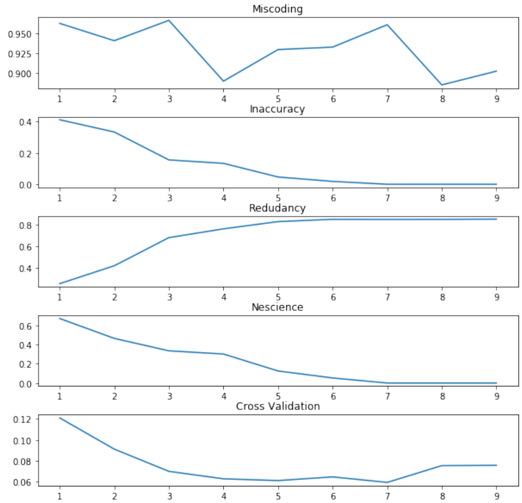


Figure 8.10: Evolution of Nescience with Tree Depth.

eter searches where we cannot apply a greedy approach, for example when the search is performed over a collection of (usually conflicting) hyperparameters. Hyperparameter search is a computationally expensive approach, since the number of possible combinations to test could be very large. Moreover, if for each candidate set we have to cross-validate the result, the search becomes prohibitive. As we have seen, nescience do not requires the use of crossvalidation to detect a situation of overfiting, and so, it can significantly speed up the process of searching for optimal hyperparameters. In Example 8.17 it is show how we can do that with the `nescience` library.

■ **Example 8.17** In this example we are going to see how we can use the `nescience` library to find the optimal hyperparameters for a model using a grid search. In particular, we are going to select the best hyperparameters for a multilayer perceptron classifer, including the number of hidden layers, and the size of those layers (what it is called Neural Architecture Search). The procedure will be demonstrated using the `digits` dataset.

```
from Nescience.Nescience import Nescience
from sklearn.neural_network import MLPClassifier
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import classification_report
from sklearn.model_selection import train_test_split
```

First of all we have to provide a custom loss function based on the concept of nescience to be integrated with the search procedure. The next code shows how to implement such a function.

```
def my_custom_loss_func(estimator, X, y):

    nsc = Nescience()
    nsc.fit(X, y)
    nescience = nsc.nescience(estimator)

    # scikit-learn expect that higher numbers are better
    score = -nescience

    return score
```

Second, we have to define the grid of hyperparameters over which we are going to do the search. The larger the grid, the better the result, but also, the more computer time is required to evaluate all possible combinations.

```
parameters = {'solver': ['lbfgs'],
              'max_iter': [1000, 1500, 2000 ],
              'alpha': 10.0 ** -np.arange(1, 10, 3),
              'hidden_layer_sizes':[(60,), (100,), (60, 60,), (100, 100,),
                                    (60, 60, 60,), (100, 100, 100,)]}
```

Next code show how to do a classical grid search using the score of the models. The search will be evaluated using a train/test split of the dataset.

```
clf_std = GridSearchCV(estimator=MLPClassifier(), param_grid=parameters,
                       cv=3, iid=True, n_jobs=-1)
clf_std.fit(X_train, y_train)
clf_std.best_params_

[] {'alpha': 0.1,
[]  'hidden_layer_sizes': (100,),
[]  'max_iter': 1000,
[]  'solver': 'lbfgs'}

y_true, y_pred = y_test, clf_std.predict(X_test)
print(classification_report(y_true, y_pred))

[] precision    recall  f1-score   support
[] avg / total       0.98      0.97      0.97       540
```

Next code show how to perform exactly the same search, but using the concept of nescience instead of the metric score.

```
clf_nsc = GridSearchCV(estimator=MLPClassifier(), param_grid=parameters,
                       cv=3, scoring=my_custom_loss_func, iid=True)
clf_nsc.fit(X_train, y_train)
clf_nsc.best_params_

{'alpha': 0.1,
 'hidden_layer_sizes': (60,),
 'max_iter': 1500,
 'solver': 'lbfgs'}

y_true, y_pred = y_test, clf_nsc.predict(X_test)
```

```
print(classification_report(y_true, y_pred))

                  precision    recall    f1-score    support
avg / total       0.98         0.98      0.98        540
```

As we can see, the results provided by the `nescience` library are slightly better in terms of train/test evaluations. However, what it is important is the library has opted for a smaller model (one layer of 60 neurons instead of one layer of 100 neurons) that provides a better result by increasing the maximum number of iterations (from 1000 to 1500). Nescience always select the smallest model that provides the best possible accuracy that does not overfit the training data.

■

8.7 Auto Machine Classification

The nescience library also includes a module for auto-machine learning (both for classification and regression problems). The auto-machine learning module returns the model, from a collection of families of models, that provides the smalles nescience. For each family of models, the class perform a greedy search over the hyperparameters required for each family. In Appendix XX is described the detail for each family of models.

Next example shows how to apply the automachine learning tools.

■ **Example 8.18** In this example we are going to see how to apply the nescience library to find the best model that describes the `digits` dataset.

```
from sklearn.datasets import load_digits
from sklearn.model_selection import train_test_split

from Nescience.Nescience import AutoClassifier

(X, y) = load_digits(return_X_y=True)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)

model = AutoClassifier()
model.fit(X_train, y_train)

model.score(X_test, y_test)
[] 0.9622222222222222
```

If we write `type(model.model)` we will see that the library has selected a linear support vector machine as the best model for this dataset.

■

TODO: Compare with other automl tools.

8.7.1 Surfeit of Algorithms

Decision Trees

For the representation of a tree as a string we use the following template:

```
def tree{[attrs]}:
    if [attr] <= [thresh]:
        return [label] || [subtree]
    else:
        return [label] || [subtree]
```

Where `[attrs]` is the list of attributes used, and only those used in the model,[4] `[attr]` is a single attribute represented by the letter `X` followed by a number (e.g. `X1`), `[thresh]` is the threshold used for the split, `[label]` is one of the valid labels from the set $\mathcal{G}$, and `|| [subtree]` means that the `return` statement can be replaced by another level of `[if - else]` conditions. We could have used a much shorter description of trees by replacing word tokens with symbols, e.g., by the ternary conditional operators `?` and `:` used in modern programming languages, or by dropping the `return` statement. This would produce shorter trees, but the complexity of the models would remain the same, up to an additive constant that does not depend on the model itself. Since the harmonic mean compares relative values instead of absolute ones, this additive constant can be safely ignored.

8.8 Auto Machine Regression

8.9 Time Series

TODO: Introduce this section

8.9.1 Automiscoding, Crossmiscoding and Partial Automiscoding

In this section we are going to study the application of the concept of miscoding to a time series and a delayed version of itself, or to a delayed version of a second time series.

Automiscoding is the application of miscoding to a time series and a delayed version of itself, as a function of this delay. Automiscoding is intended to estimate up to what extend previous observations of the time series can explain (or can be used to forecast) future observations. In this sense, automiscoding has a similar objective than autocorrelation in classical time series analysis (see Section F.2.8).

[4] If the dataset contains many attributes, listing all of them when dealing with very short models would make the length of the model's header greater than the length of the body.

Definition 8.9.1 Let $\{\mathbf{x}_t\}$ be a time series composed by n samples. We define lag k *regular automiscoding* of $\{\mathbf{x}_t\}$ as $\hat{\mu}(\mathbf{x}_{x_{k+1},x_{k+2},\ldots,x_n}, \mathbf{x}_{x_0,x_1,\ldots,x_{(n-k)}})$. We define in the same way the concepts of *adjusted automiscoding* and *partial automiscoding*.

On the contrary of what happened with the concept of autocorrelation, automiscoding is defined for all time series, including time series with a trend. Moreover, automiscoding is intepretable even in case of having a trending time series, for example, for the identification of seasonal components without requiring to apply a decomposition.

■ **Example 8.19** In this example we are going to study the presence of cycles in the number of passengers of a US airline. In Figure 8.11 is depicted a time series of monthly passengers from 1949 to 1960 (AirPassenger dataset, see References section bellow). As we can observe, there is a clear cycle that repeats every twelve months. We can apply the concept of auto-miscoding to validate analytically that this is the case.

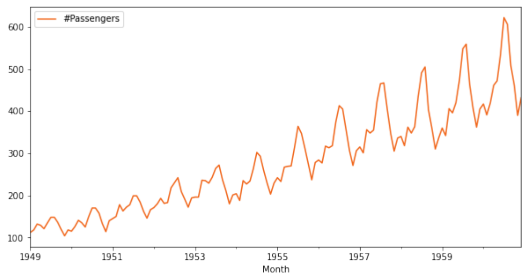


Figure 8.11: Air Passengers.

```
from nescience.timeseries import TimeSeries

data = pd.read_csv("data/AirPassengers.csv", index_col=["Month"], parse_dates=True)
X = np.array(data["#Passengers"]).reshape(-1, 1)

ts = TimeSeries(auto=False)
ts.fit(data)
mscd = ts.auto_miscoding(max_lag=36)
```

As we can see in Figure 8.12 there is a peak on the value of adjusted automiscoding every twelve months (the distance between both time series is minimal when we the lag is a multple of a year).

■

Crossmiscoding computes the inter-relation between a time series and a lagged version of a second time series. The objective is to detect if the first time series has a temporal predictive power over the second.

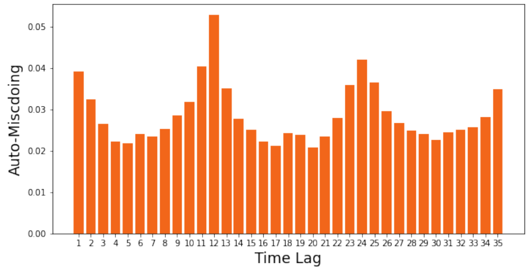


Figure 8.12: Auto-miscoding of Air Passengers.

Definition 8.9.2 Let $\{\mathbf{x}_t\}$ and $\{\mathbf{y}_t\}$ be two time series composed by n samples each. We define lag k *regular crossmiscoding* of $\{\mathbf{x}_t\}$ and $\{\mathbf{y}_t\}$ as $\hat{\mu}(\mathbf{x}_{x_{k+1},x_{k+2},\ldots,x_n}, \mathbf{y}_{x_0,x_1,\ldots,x_{(n-k)}})$. We define in the same way the concepts of *adjusted crossmiscoding* and *partial crossmiscoding*.

■ **Example 8.20** We are interested to determine if it possible to predict the energy consumption of the appliances of a house. The data set to study (appliances energy prediction dataset, see References below) is composed by the temperature and humidity conditions measured in the different rooms of the house every ten minutes, and the energy consumption of the appliances. The dataset also includes some information about the current weather, from a nearby weather station.

For every feature we will compute the optimal lag at which the features has the best prediction capabilities:

```
from fastautoml.fastautoml import Miscoding

X = pd.read_csv("../data/energydata_complete.csv", parse_dates=["date"], index_col="da
y = X["Appliances"]
X = X.drop(["Appliances", "lights"], axis=1)

miscoding = Miscoding()
miscoding.fit(X, y)

best_lag  = list()
for i in np.arange(X.shape[1]):
    mscd = miscoding.cross_miscoding(attribute1=i, min_lag=1, max_lag=30)
    best_lag.append(np.where(mscd == np.max(mscd))[0][0] + 1)
```

In Figure 8.13 we can see a plot of the results. As we can observe, in general, for the in-house measurements we should use small lag values. However, in case of the weather conditions, bigger lags provide better results. ■

R The approximation to the concept of miscoding introduced in this

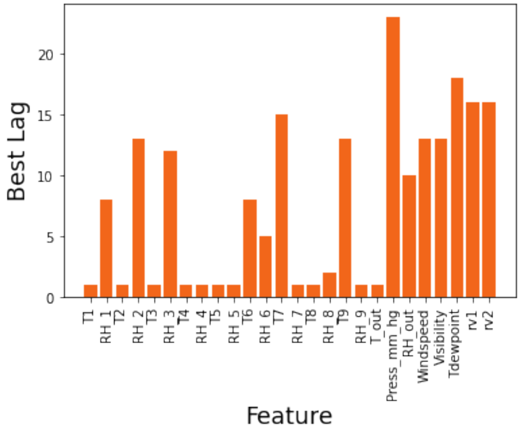


Figure 8.13: Cross Miscoding Lag

chapter estimates the quality of individual features as predictors of a target value, and the quality of the training dataset as a whole. However, the current approximation does not take into account the existing redundancy among the features themselves. For example, it might happen that two features $\mathbf{x}_i$ and $\mathbf{x}_j$ have very low miscoding with respect to the target variable $\mathbf{y}$, but at the same time they are redundant, in the sense that they contain almost the same information. It is still an open question how to extend the concept of miscoding to take into account feature redundancy, in such a way that it is close to the theoretical definition, it can be computed efficiently, and it does not require a huge number of samples.

8.9.2 Auto Time Series

TODO: Introduce the auto-time series models, and clearly state what it can be expect from such models (short story: nothing)

TODO: Introduce structural time series models, the state space representation, and the Kalman filter

structura approach [...] different unobserved components or building blocks responsible for the dynamics of the series such as trend, seasonal, cycle, and the effects of explanatory and intervention variables are identified separately before being put together in a state space model.

State space methods originated in the

eld of control engineering, starting with the groundbreaking paper of Kalman (1960). They were initially (and still are) deployed for the purpose of accurately tracking the position and velocity of moving objects such as ships, airplanes, missiles, and rockets [...] these ideas could well be applied to time series analysis generally as well.

In a state space analysis the time series observations are assumed to depend linearly on a state vector that is unobserved and is generated by a stochastically time-varying process (a dynamic system). The observations are further assumed to be subject to measurement error that is independent of the state vector. The state vector can be estimated or identified once a sufficient set of observations becomes available.

Definition 8.9.3 A linear Gaussian state space model for the multivariate time series $\mathbf{y} = \mathbf{y}_1, \ldots, \mathbf{y_n}$, where each observiation is a p dimensional vector $\mathbf{y}_i = \{y_{i1}, \ldots, y_{ip}\}$, is given by

$$\mathbf{y}_t = \mathbf{Z}_t \alpha_t + \mathbf{d}_t + \varepsilon_t \quad \varepsilon_t \sim N(0, \mathbf{H}_t) \tag{8.1}$$

called space? *orbservation or measurement equation*, and

$$\alpha_t = \mathbf{T}_t \alpha_{t-1} + \mathbf{c}_t + \mathbf{R}_t \eta_t \quad \eta_t \sim N(0, \mathbf{Q}_t) \tag{8.2}$$

called *state or transition equation*, where the individual summands correspond to:

- $\mathbf{y}_t$ observed or measured values,
- $\mathbf{Z}_t$ design matrix,
- α_t unobserved state,
- $\mathbf{d}_t$ observation intercept,
- ε_t observational disturbance,
- $\mathbf{H}_t$ observational disturbance covariance matrix,
- $\mathbf{T}_t$ transition matrix,
- $\mathbf{c}_t$ state intercept,
- $\mathbf{R}_t$ selection matrix,
- η_t state disturbance, and
- $\mathbf{Q}_t$ state disturbance covariance matrix

The $p \times m$ matrix Z_t links the observation vector y_t with the unobservable state vector α_t and may consist of regression variables. The $m \times m$ transition matrix T_t determines the dynamic evolution fo the state vector [...] the observation and state disturbances ε_t and eta_t are assumed to be serially independent and independent of each other at all time points [...] matrix R_t is an $m \times r$ selection matrix with $r < m$.

The initial state vector α_1 is assumed to be generated as $\alpha_1 \sim NID(a_1, P_1)$, independen of the observation and estate disturbances ε_t and η_t. Mean a_1 and variance P_1 can be treated as given konw.

Talk about initialization?

For example, if the time series $\mathbf{y}$ is unidimensional and the state space model is time invariant (only $\mathbf{y}_t$ and α_t depends on t, being the rest of the summands constant), a model with m unobserved stares will be given by

$$y_t = [z_1 \dots z_m] \begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix} + d_t + \varepsilon_t$$

Some of the most common time series models are particular cases of the state-space model (see Example XX).

■ **Example 8.21** ■

TODO: Explain the Kalman filter

The *Kalman filter* is a recursive formula that provides an optimal estimate for the unknown state in a state space model. At each time step t, the Kalman filter computes the predicted state conditional to the observations up to time $t-1$.

Kalman filter can be use for filtering, prediction and smoothing. Here we are only interested in prediction [...] forward pass [...] recursive formulas

Definition 8.9.4

$$\begin{aligned} \mathbf{a}_{t+1} &= \mathbf{T}_t \mathbf{a}_t + \mathbf{K}_t \mathbf{v}_t \\ \mathbf{K}_t &= \mathbf{T}_t \mathbf{P}_t \mathbf{Z}_t^T \mathbf{F}_t^1 \\ \mathbf{v}_t &= \mathbf{y}_t - \mathbf{Z}_t \mathbf{a}_t \end{aligned} \tag{8.3}$$

called *prediction equations*, and

$$\begin{aligned} \mathbf{F}_t &= \mathbf{Z}_t \mathbf{P}_t \mathbf{Z}_t^T + \mathbf{H}_t \\ \mathbf{L}_t &= \mathbf{T}_t - \mathbf{K}_t \mathbf{Z}_t \\ \mathbf{P}_{t+1} &= \mathbf{T}_t \mathbf{P}_t \mathbf{L}_t^T + \mathbf{R}_t \mathbf{Q}_t \mathbf{R}_t^T \end{aligned} \tag{8.4}$$

called *updating equations*.

■ **Example 8.22** TODO: Provide an example where we can see how the Kalman filter integrates the predicted probability distribution and observed probability distribution to make a prediction ■

TODO: Examplain the space search algorithm

■ **Example 8.23** TODO: Provide an example of auto-time series ■

8.10 Anomaly Detection

As we have seen in Section XXX, the main problem in the area of anomalies detection is that we do not have a precise mathematical definiton of what an anomaly is. Given a dataset, in this book we propose to equate the concept of abnormal samples with that of incompressible samples, and study its consequences. The essence of this chapter is that learning is about finding regularities in a dataset, and finding regularities is what data compression is about. We have also seen that the best model is the one that minimizes the sum of the length of the model plus the length of the data given the model. This optimal model divides our dataset into two disjoint subsets, the compressible part, and the incompressible part. It is the former in which we are interested in this section, since being incompressible means that they cannot be explained by the model, that is, they are model-based anomalies given the best possible model.

Fix the following definition.

Definition 8.10.1 Let X be a dataset composed by p features and n samples, $\mathbf{y}$ the target variable, and M a model such that the nescience $N(\mathbf{X}, M)$ is minimal. Let $\hat{y} = M(\mathbf{X})$ be the predicitons made by the model M over the vectors of $\mathbf{X}$. We define the *anomaly subset* of $\mathbf{X}$, denoted by $\mathcal{A}_M^{\mathbf{X}}$, to the set of X such that $y \neq \hat{y}$.

The `nescience.anomalies` class allow us to identify the anomaly subset, that is, the collection of samples that do not match the regularity patterns found in the rest of the dataset. In Example 8.24 we will see how to apply this class to indentify houses with abnormal low prices, and to explain why they are cheaper.

■ **Example 8.24** In this example we will use the Boston House Price dataset provided by the `scikit-learn` toolkit. The dataset contains 13 predictive features (both, numeric and categorical) measuring different characteristics of the houses, such as number of rooms, age, etc., and the target is the median value of owner-occupied homes. The dataset is composed by five hundred samples. We are interested in to identify those house that have an abnormally low price, that is, houses that given their characteristics (number of rooms, size, etc) should have a higher price.

```
from sklearn.datasets import load_boston

data = load_boston()
X    = data.data
y    = data.target
```

We have to train a "knowledge model", that is, find the best model that explains the target variable given the predictors, without overfitting. By default, the `anomalies` class uses the AutoML capabilities provided by the `nescience` library.

```
from nescience.anomalies import Anomalies

model = Anomalies(X_type="mixed", y_type="numeric")
model.fit(X, y)
```

Finally, we have to select those samples for which the actual price is smaller than the one predicted by the model.

```
anomalies = model.get_anomalies("smaller")
X.shape, anomalies.shape
((506, 13), (25,))
```

As we can see, there are 25 houses with abnormally low price. ■

The `anomalies` class also allow us to classify the identified anomalies according to the characteristics they share.

Let's see which are the best attributes that describe those abnormal houses.

```
model.get_classes(n_dims=1, an_type="smaller", filter_balancedness=True,
                  filter_redundancy=False, filter_repeated_attrs=False)

Attribute1 Attribute2 Inertia         N Class 0 N Class 1 Ratio
2         None         154.953975 9        16         0.36
4         None            0.090593 6        19         0.24
5         None         5.002437 17        8         0.68
7         None         20.352117 6        19         0.24
8         None         77.611111 18        7         0.72
9         None         41737.11111 7        18         0.28
10         None         26.577436 13        12         0.52
12         None         430.294828 18        7         0.72
```

According to the inertia, the best attribute that allow us to classify the anomalies is the number 4 (nitric oxides concentration). This attribute divides the abnormal houses into two clusters of size 6 and 19. Let's see how the house's price is affected by this dimension.

```
from sklearn.linear_model import LinearRegression
import matplotlib.pyplot as plt

lr = LinearRegression()
lr.fit(X[:,4].reshape(-1, 1), y)

plt.scatter(X[:,4].reshape(-1, 1), y)
plt.plot(X[:,4], lr.intercept_ + lr.coef_ * X[:,4], color="red")
plt.xlabel(data.feature_names[4])
plt.ylabel("Price")
```

The regression line suggest that the price of the houses is smaller in those

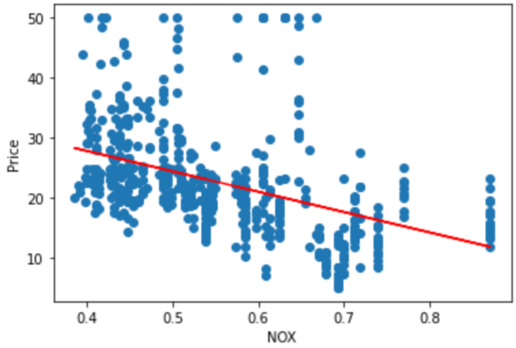


Figure 8.14: Price as a function of NOX.

areas with higher levels of nitric oxides concentration. Let's see how the anomalies are classified according to this dimension.

```
class0, class1 = model.get_class_points(attribute1=4, attribute2=None, an_type="smalle

plt.hist(class0)
plt.hist(class1)
plt.ylabel("Count")
plt.xlabel(data.feature_names[4])
plt.show()
```

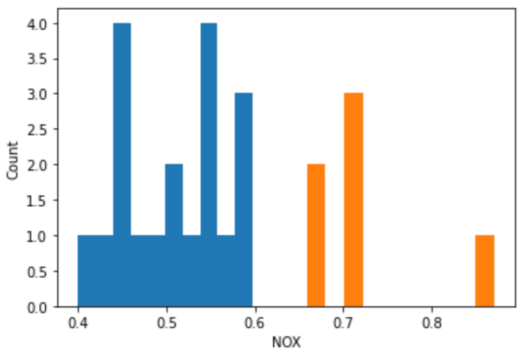


Figure 8.15: Histogram of anomalies NOX.

The analysis suggests that six of the houses have an abnormally low price because they are in an area with high levels of contamination. We can repeat the same analysis with the other attributes, although they have a higher inertia, so the class separation is not that evident. Please mind that there could be more than one reason why the price of a house is abnormally low.

8.11 Decision Trees

In the last sections we have seen how to use the concepts of miscoding, inaccuracy, surfeit and nescience to evaluate the quality of datasets and models, and to automatically select a family of models and search over its hyperparameters to find the best possible description of a topic. In particular, we have studied in detail the family of binary decision trees. The procedure used in the `fastautoml` library with trees was a mix between a classical approach (a CART algorithm combined with a cost-complexity pruning), and an evaluation of candidate trees using the minimum nescience principle. In this section we are going to see a new algorithm to derive optimal trees, both for classification and regression problems, that is entirely based on the theory of nescience. The new algorithm, by design, avoids the overfitting of the training dataset without losing accuracy, it does not require the optimization of hyperparameters, thus significantly reducing the training time, and it produces much smaller and more shallow trees than traditional algorithms, facilitating the interpretability of the results.

8.11.1 Algorithm Description

The following pseudocode shows the proposed algorithm to build a decision tree given a training dataset $(\mathbf{X}, \mathbf{y})$. The procedure is based on a breadth first traversal of trees combined with a greedy approach. It requires a function called BESTSPLIT() that returns the best split of a given subset of the data into two subsets; and a second function, called NESCIENCE() that provides an estimation of the nescience of the current tree. The algorithm is based on two nested loops: the external **while** loop keeps a list of the candidate nodes to grow, whereas the internal **for** loop finds the best node to grow the tree. The latter operation requires to check all possible growing options and select the one that minimizes the nescience. The exit point of the algorithm is when there are no more branches to grow. We keep track of the best nescience achieved during the building process and return the associated tree.

```
def BUILD_TREE(data)

    nodesList <- list()
    tree <- BESTSPLIT(data)
    bestNescience <- NESCIENCE(tree)
    nodesList.append(tree)

    while not nodesList.empty()

        nescience <- bestNescience
        bestNode <- None
        childNode <- None
```

```
        for i <- 1, nodesList.length()

            node <- nodesList[i]

            node.child <- BESTSPLIT(node.ldata)
            tmp <- NESCIENCE(tree)
            if tmp < nescience
                nescience <- tmp
                bestNode <- i

            node.left <- None

        if nescience < bestNescience
            node <- nodeList[bestNode]
            bestNescience <- nescience
            nodesList.append(node.left)

            if not node.left.empty() and not node.right.empty()
                nodesList.remove(bestNode)

    return tree
```

The main difference of our algorithm from other decision tree building algorithms is in the way the tree is evaluated. Instead of using only accuracy as most of the algorithms do, in addition, we take into account the complexity of the tree (surfeit) to avoid overfitting, and the quality of the subset of data used during the training process (miscoding).

Nescience

The calculation of the nescience implemented in the algorithm is based on a Euclidean distance utility function (see Section 8.6), because that one was the one that produced the best results in the tests we have performed. For the computation of miscoding and inaccuracy, we use the same techniques that the one used in the `fastautoml` library, described in Section 8.3 and Section 8.4 respectively. For the implementation of surfeit, we use the same template to describe trees that was used in the `DecisionTreeClassifier` of the `AutoClassifier` class, and that was described in Section 8.7.1. The only difference is that we also allow equalities in the nodes (`if [attr] = [thresh]`), something not supported by the `DecisionTreeClassifier` algorithm of the `scikit-learn` library.

The generic problem of the instability of inaccuracy due to very short models, also applies to this algorithm (see Section 8.5), and the particular problem of the algorithms to build decision trees, in which the best local split might not be that one that minimizes the error (see Section **??**) is also relevant in this case.

The concept of nescience is used in two different ways in our algorithm. For every iteration of the `for` loop we have to decide which one of the candidate branches of the tree we should develop. Recall that the order in which we develop the branches is important, since it might happens that one branch does not get develped because that would mean increase the sufeit without a sufficiently large decrease of the inaccuracy. The second place is a the end of the `while` loop, we we keep trac of the nescience of the different building steps, to decide at the end of the algorithm with wich tree we return.

We treat regression problems as classification problems in which we discretizes the continuous target variable $\mathbf{y}$ into n intervals given the number of samples, and using a uniform discretization (see Section). Once the target variable has been discretized, we train a regular classification tree.

Splitting Criteria

Given a subset $\mathbf{Q} \subseteq \mathbf{X}$ we have to find an split for $\mathbf{Q}$ such that the values of $\mathbf{y}$ are grouped together. Recall that a split is a pair $\theta = (j, w)$, were $1 \leq j \leq p$ is a feature index and w is the partition point (see Section F.2.7). A split divides the set $\mathbf{Q}$ into two disjoint subsets $\mathbf{Q}_l$ and $\mathbf{Q}_r = \mathbf{Q} \backslash \mathbf{Q}_l$. In case of a continuous variable we have that $\mathbf{Q}_l = \{\mathbf{x}_i \in \mathbf{Q} : x_{ij} \leq w\}$, and if the feature is categorical we define $\mathbf{Q}_l = \{\mathbf{x}_i \in \mathbf{Q} : x_{ij} = w\}$[5].

In Section F.2.7 we saw that a common splitting criteria used in practice is to minimize the weighted entropy $\tilde{H}$ of the subsets $\mathbf{Q}_l$ and $\mathbf{Q}_r$, that is, to find an split that it is minimal $\theta^\star = \arg\min_\theta \tilde{H}(\mathbf{Q}, \theta)$. More explicitly, if $\mathbf{y}$ is a target vector taking values from a set of k labels $\mathcal{G} = \{g_1, \ldots, g_k\}$ (either because is a categorical target or a continuous target that has been discretized into k intervals), and denoting the subsets of $\mathbf{y}$ as $\mathbf{y}^l = \{y_i : \mathbf{x}_i \in \mathbf{Q}_l\}$ and $\mathbf{y}^r = \{y_i : \mathbf{x}_i \in \mathbf{Q}_r\}$, and n_l and n_r are the number of elements of $\mathbf{y}^l$ and $\mathbf{y}^r$ respectively, we have that

$$\begin{aligned}\tilde{H}(\mathbf{Q}, \theta) = \frac{n_l}{n} & \left(- \sum_{i=1}^{k} \frac{\sum_{j=1}^{n_l} I(y_j^l = g_i)}{n_l} \log_2 \frac{\sum_{j=1}^{n_l} I(y_j^l = g_i)}{n_l} \right) \\ & + \frac{n_r}{n} \left(- \sum_{i=1}^{k} \frac{\sum_{j=1}^{n_r} I(y_j^r = g_i)}{n_r} \log_2 \frac{\sum_{j=1}^{n_r} I(y_j^r = g_i)}{n_r} \right) \qquad (8.5)\end{aligned}$$

In our nescience based decision tree algorithm, the splitting criteria is to minimize the total length of encoding the subsets $\mathbf{Q}_l$ and $\mathbf{Q}_r$ using optimal codes. We have to find the optimal split $\theta^\star = \arg\min_\theta \hat{K}_C(\mathbf{Q} \mid \theta) = \arg\min_\theta \{\hat{K}_{C_l}(\mathbf{Q}_l) + \hat{K}_{C_r}(\mathbf{Q}_r)\}$ where C_l and C_r are the optimal codes given the relative frequencies of the observed values of $\mathbf{y}^l$ and $\mathbf{y}^r$ respectively. The

[5] Ideally, for the categorical case, instead of a single feature w we should search over all the elements of the power set of the set of features $\mathcal{P}\{1, 2, \ldots, p\}$. Unfortunately, that would imply to check 2^p cases, something that is time-expensive from the computational point of view.

quantity $\hat{K}_C(\mathbf{Q} \mid \theta)$ is computed as:

$$\hat{K}_C(\mathbf{Q} \mid \theta) = \hat{K}_{C_l}(\mathbf{Q}_l) + \hat{K}_{C_r}(\mathbf{Q}_r) = -\sum_{i=1}^{k} \log_2 \frac{\sum_{j=1}^{n_l} I(y_j^l = g_i)}{n_l} - \sum_{i=1}^{k} \log_2 \frac{\sum_{j=1}^{n_r} I(y_j^r = g_i)}{n_r}$$

I this particular case (if we use as compression algorithm a code with optimal lengths, and continuous variables have been discretized) it turns out that both expressions are equivalent given the following relation:

$$\tilde{H}(\mathbf{Q}, \theta) = \frac{1}{n} \hat{K}_C(\mathbf{Q} \mid \theta)$$

We prefer to talk of encoding length instead of weighted entropy because it has an easier interpretation in the context of the theory of nescience.

R Strictly speaking, if we want to implement a decision trees search algorithm fully compliant with the minimum nescience principle, instead of using a total length encoding as splitting criteria, we should had computed the nescience at each split and select that one that makes it minimal. However, early experiments have shown that at local level it works better to group the values of y than to reduce the nescience. Further research is required to confirm and explain this point.

Practical Implementation

In the web page that accompanies this book[6] we provide an open-source implementation of our algorithm in Python. Our software can be used together with other machine learning tools from the `scikit-learn` library, since we adhere to the their API guidelines. For example, our algorithm can be used as part of an ensemble of classifiers, like the `BaggingClassifier` meta-estimator, or the results of the classification could be cross-validated with tools like `cross_val_score`. As an example, to provide a model for the breast cancer dataset, we could do something like the following:

```
from NescienceDecisionTree import NescienceDecisionTreeClassifier
from sklearn.datasets import load_breast_cancer

data = load_breast_cancer()

model = NescienceDecisionTreeClassifier()
model.fit(data.data, data.target)
print("Score: ", model.score(data.data, data.target))
```

[6] http://www.mathematicsunknown.com

8.11.2 Algorithm Evaluation

In this section we are going to evaluate our new algorithm, and compare its performance against the well-known algorithm CART. CART, *Classification and Regression Trees*, is the de-facto standard algorithm used in the machine learning industry for the derivation of decision trees. For this particular experiment we have used the CART implementation provided by `scikit-learn`.

Figure 8.16 shows a synthetic dataset consisting of 1000 random points lying on a two dimensional plane, where all the points with an $X1$ attribute less than 50 are colored blue, and the rest as red. We have artificially introduced a red point, simulating a measurement error, in the blue area. The black lines correspond to the decisions performed by CART. Since the CART algorithm will not stop until all the points have been properly classified, we have to specify an expected count condition to limit the number of splits. The figure correspond to the tree generated by CART setting the `min_samples_leaf` hyperparameter to 5.

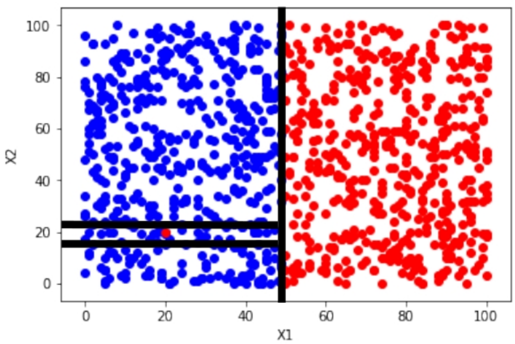


Figure 8.16: Synthetic dataset with CART algorithm splits.

The tree obtained by applying our algorithm to the dataset of Figigure 8.16 can be seen in Figure 8.17. The nescience based algorithm does not try to model the error point, since the gain due to an increment in the accuracy does not compensate the surfeit introduced in the model. Recall that the algorithm stops when the total nescience of the tree, based on the measures of miscoding, inaccuracy and surfeit, does not decrease when adding new nodes to the tree. Our algorithm presents a lower sensitivity to the errors found in datasets, at least if the number of errors is small compared with the number of valid points.

Our second experiment, again with synthetic dataset, is depicted in Figure 8.18. There, we create two isotropic Gaussian blobs that partially overlap.

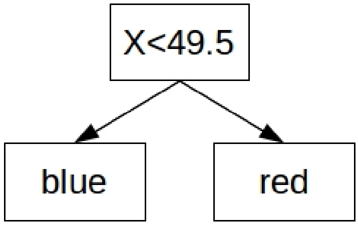


Figure 8.17: Decision tree obtained by the nescience algorithm.

We start with a standard deviation of 2.5 for each cluster, so they are easy to separate, and we increase the standard deviation in increments of 0.01, until we reach 4.5, which causes significant overlaps. For each value of the standard deviation, we run the experiment 100 times and we compute the average accuracy for the two algorithms using different datasets for training (70% of the data) and testing (30% of the data). The results of this experiment are shown in Figure 8.19.

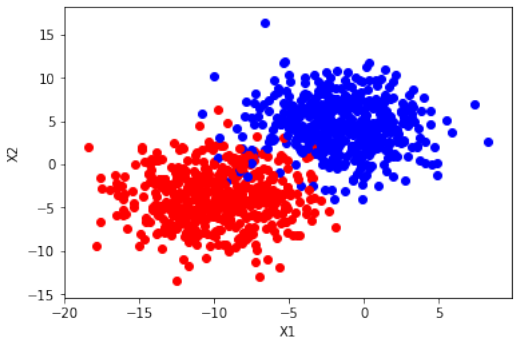


Figure 8.18: Isotropic Gaussian Blobs.

As we can see, the performance of both algorithms, in terms of accuracy, is similar. However we should note that the hyperparameter `minimum_leaf_size` of the CART algorithm has been optimized to achieve the best accuracy. For this particular experiment, the best value was achieved with a minimum leaf size of 26 points. By definition, given the fact that CART has one degree of freedom more than the nescicence algorithm, it should produce better accuracy; something that it is not observed (both algorithms have a mean accuracy of 0.87.

For each iteration of the experiment, we have also computed the average number of nodes, including internal and leaf nodes, required by the models to properly classify the clouds in the dataset. The results of this measurement

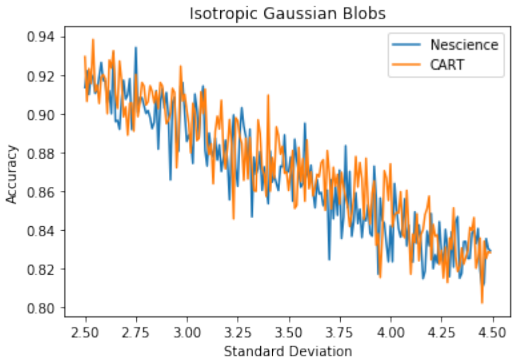


Figure 8.19: Accuracy of Isotropic Gaussian Blobs.

are show in Figure 8.20. Our algorithm requires an average of 4 nodes compared to 23 nodes for the CART algorithm. Moreover, our algorithm is more stable than CART, in the sense that it produces models of similar complexity when it gets similar input datasets (a standard deviation of 0.31 compared to 3.77 for CART).

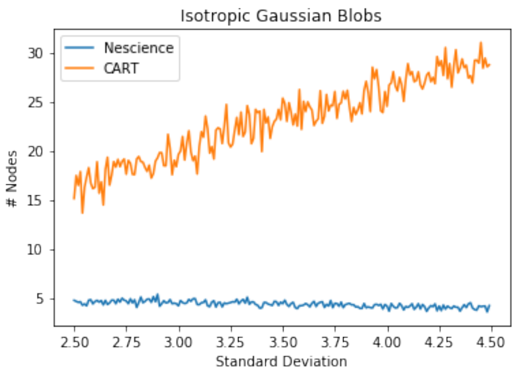


Figure 8.20: Number of Nodes.

In Figure 8.21 we show the maximum depth of the tree, defined as the longest path from the root of the tree to any of its leaves. The maximum depth of the tree is a good measure of the average time it will require for the model to provide a classification. The nescience algorithm has an average depth of 1.6 nodes, whereas the average depth yielded by the CART algorithm is 4.8 nodes.

The last part of the evaluation consists in comparing the performance of our algorithm and CART with a collection real datasets. More specifically,

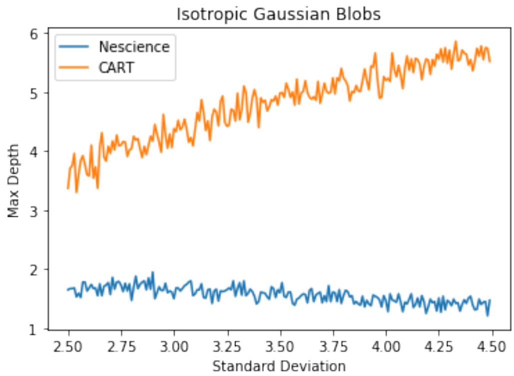


Figure 8.21: Maximum depth of the model.

we have selected 12 well known datasets from the UCI Machine Learning Repository. The selected datasets are: diagnosis of breast cancer (`cancer`), optical recognition of handwritten digits (`digits`), predicting protein localization sites in gram-negative bacteria (`yeast`), classification of NASA space shuttle data (`shuttle`), classification of blocks in web pages (`page`), segmentation of outdoor images (`image`), predicting the age of abalones from physical measurements (`abalone`), predicting the quality of red and white variants of Portuguese wine (`wine`), filter spam emails (`spam`), wall-following robot navigation (`wall`), classification of land use based on Landsat satellite images (`landsat`), and distinguishing signals from background noise in the MAGIC gamma telescope images (`magic`). For each dataset, we have repeated the experiment 100 times, by randomly selecting the training (70%) and testing (30%) subsets at each iteration.

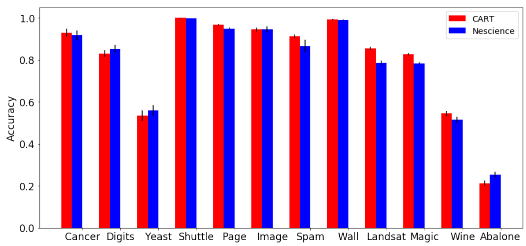


Figure 8.22: Maximum depth of the model.

In Figure 8.22 we compare the accuracy of the resulting models obtained by applying the CART algorithm and the nescience algorithm to the above datasets. In 4 of the 12 datasets, our algorithm provides better accuracy than CART. In the remaining 8 cases, the accuracy is, on average, less than 1%

smaller.

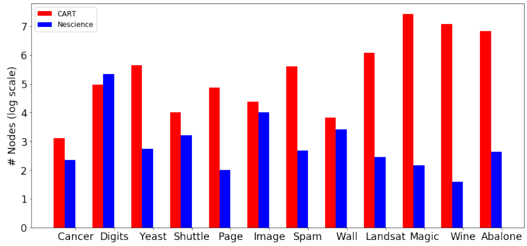


Figure 8.23: Maximum depth of the model.

In Figure 8.23 it is shown a comparison of the total number nodes (internal nodes plus leaf nodes) of the resulting models. Only for one of the datasets (`digits`), our model produces a slightly more complex tree that those generated by CART. In the rest of the cases, the number of nodes in the trees generated by the nescience algorithm have between two and three orders of magnitude fewer nodes (in this figure the y axis is in logarithmic scale).

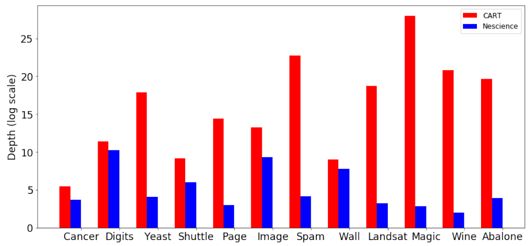


Figure 8.24: Maximum depth of the model.

Finally, in Figure 8.24 we provide a comparison of the depth of the tree of the resulting models. Our algorithm always yields a shallower tree than the CART algorithm.

We would like to mention that the nescience algorithm is hihgly robust with respect to the compressor selected or the nescience function implemented. In Table 8.11.2, we have apply the nescience algorithm to the datasets described above, and evaluate different alternatives for the definition of the nescience function $N(X,M)$: arithmetic mean $(\mu(M,D)+\iota(X,M)+\sigma(M,D))/3$, geometric mean $(\mu(M,D)+\iota(X,M)+\sigma(M,D))1/3$, harmonic mean $3/(\mu(M,D)+\iota(X,M)+\sigma(M,D))-1)$, Euclidean distance $(\mu(M,D)+\iota(X,M)+\sigma(M,D))1/3$, sum $\mu(M,D)+\iota(X,M)+\sigma(M,D)$, and product $\mu(M,D)+\iota(X,M)+\sigma(M,D)$. The table shows limited difference between the different functions.

	Euclid	**Arithmetic**	**Geometric**	**Product**	**Addition**	**Harmonic**
Accuracy	0.758	0.784	0.803	0.803	0.784	0.81
Stdev	0.051	0.041	0.033	0.033	0.041	0.038

Table 8.2: Comparison of nescience functions

Similarly, Table 8.11.2 shows the performance of our algorithm when using the LZMA, zlib, and bz2 compressors. We observe that all of them yield similar performance. The above results suggest that the performance our algorithm is independent of the specific choice made for either implementation aspect.

	bz2	**lzma**	**zlib**
Accuracy	0.813	0.804	0.81
Stdev	0.03	0.045	0.038

Table 8.3: Comparison of compressors

We emphasize that the CART algorithm requires to optimize a configuration hyperparameter in order to obtain good results, whereas the algorithm proposed in this book does not require from this optimization.

Shallower trees means faster forecasting times when the models used in production, since the number of `if-else` conditions to be evaluated is smaller. Moreover, smaller trees makes easier to interpret the results by human analysts. and much shorter training times, something very relevant in case of training ensembles of trees, like random forest or boosted trees (although the use of ensembles of models is highly discouraged by the theory of nescience, given their high surfeit).

8.12 Algebraic Model Selection

As it was the case for the definition of nescience based on the encyclopedic description of research topics, the nescience of structured datasets can be used to evaluate alternative descriptions of research topics (mathematical models), and to identify how far these descriptions are from an ideal perfect knowledge. This evaluation could be used to identify those topics which require further research. Moreover, the same methodology could be applied to collections of datasets to identify our current knowledge of research areas (collections of topics).

If we combine the concept of nescience of a model, with our concepts of relevance and applicability of research topics, we could apply our methodology for the assisted discovery of interesting questions to collections of datasets; a very useful methodology now that big datasets are becoming widely available.

In order to evaluate the methodology developed, we are going to apply it to a particular research topic: *Multipath Wave Propagation and Fading*. The problem at hand is to understand the effect of a propagation environment on a radio signal, such as the one used by wireless devices. The signals reaching the receiving antenna could follow multiple paths, due to atmospheric reflection and refraction, and reflection from water and objects such as buildings. The effects of these multiple wave paths include constructive and destructive interference (fading), and phase shifting of the original signal, resulting a highly complex received signal (see Figure 8.25).

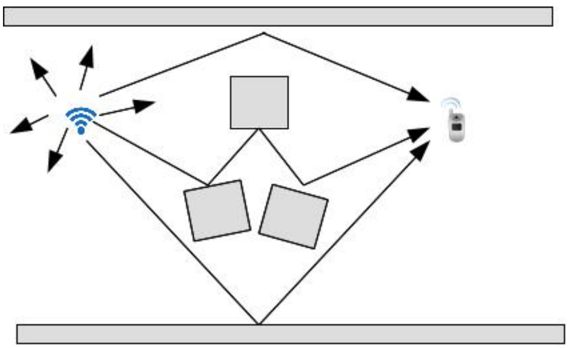


Figure 8.25: Multipath Signal Propagation

In many circumstances, it is too complicated to describe all reflection, diffraction and scattering processes that determine the different paths the signal will follow. Rather, it is preferable to describe the probability (stochastic model) that the received signal attains a certain value. We are interested in to analyze how well these stochastic models (our current knowledge) are able to describe what happen in reality.

The *Rayleigh fading model* assumes that the magnitude of a signal will vary randomly, or fade, according to a Rayleigh distribution (the radial component of the sum of two uncorrelated Gaussian random variables). The Rayleigh probability density function of the power signal is given by:

$$P_{\sigma}(x) = \frac{1}{\sigma} \exp\left[-\frac{x}{\sigma}\right]$$

where σ is the mean of the received signals. Rayleigh fading is viewed as a reasonable model for the effect of heavily built-up urban environments, when there is no dominant propagation along a line of sight between the transmitter and receiver.

The Rice or *Rician distribution* describes the power of the received signal when the target consists in many small scatterers of approximately equal strength, plus one dominant scatterer whose individual received signal equals all that of all the small scatterers combined (there is a dominant line of sight). The probability density function of the power of the received signal is given by:

$$P(x) = \frac{1}{\bar{\sigma}}\left(1+a^2\right)\exp\left[-a^2 - \frac{x}{\bar{\sigma}}\left(1+a^2\right)\right] I_0\left[2a\sqrt{\left(1+a^2\right)\frac{x}{\bar{\sigma}}}\right]$$

where $\bar{\sigma}$ is the mean of the received signals, and it is equal to $\bar{\sigma} = \left(1+a^2\right)\bar{\sigma}_R$, being $a^2\bar{\sigma}_R$ the power of the dominant scatterer, and I_0 is the modified zeroth order Bessel function of the first kind.

An experiment (see Figure 8.26) was set up to collect a real dataset to analyze. The experiment was run on a $135m^2$ office full of obstacles (interacting objects). The transmitter was an Odroid C1 Linux computer with a Ralink RT5370 USB Wifi adapter. The receiver was a (fixed in space) Motorla Moto G mobile phone. Data was collected using the Kismet [7] platform (an 802.11 layer2 wireless network detector, sniffer, and intrusion detection system), with some ad hoc, home made, software extensions, mostly for data aggregation. A total of 3,177 samples (power level measured in dBm) were collected during one hour experiment.

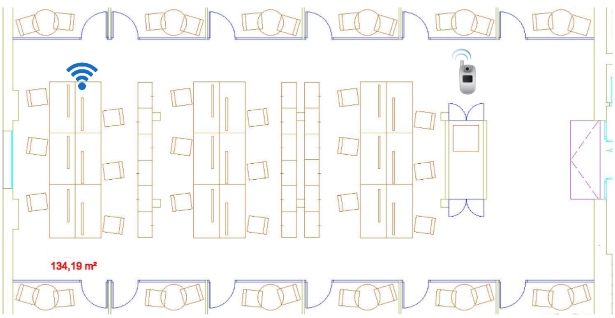


Figure 8.26: Experimental Set Up

Next table summarizes the results of applying the three considered models (uniform, Raylegh and Rice) and the optimal encoding using a Huffman code:

[7] https://www.kismetwireless.net/index.shtml

Model	LDM	Nescience
Uniform	17,351	1.30
Rayleigh	13,229	0.75
Rice	11,118	0.47
Huffman	7,541	-

Table 8.4: Nescience of Models

The uniform model, that is, assuming zero knowledge about the topic covered by the dataset, has a nescience of 1.30. This value is a kind of upper level for the nescience associated with that particular topic and dataset; any model with a higher nescience should be classified as zero knowledge model. If we introduce the knowledge that in a environment with multiple obstacles the signal propagation can be described as a Gaussian process (Rayleigh distribution), we are able to decrease our nescience to 0.75, that is, there were a 43% improvement in our understanding of the topic. If we add the knowledge that there is usually a strongly dominant signal seen at the receiver caused by a line of sight between the antenna and the mobile phone (Rician distribution), the nescience decreases to 0.47, and so, we have achieved an additional 23% gain in our understanding. Given that numbers we can conclude that the Rayleigh model increases our knowledge with respect to the uniform model, and that the Rice model does so with respect to Rayleigh. However, the nescience of this last model is 0.47. That means that there still patterns in the dataset that are not explained by the Rice model, or what it is equivalent according to our methodology, there is still some knowledge to discover and learn.

The methodology has been applied to a dataset gathered in a single experiment under a controlled environment, since the goal of this Chapter was to provide a methodology to quantify the nescience of structured datasets, not to evaluate models for signal propagation and fading. In order to to conclude that, in general, the Rice model is an improvement over Rayleigh, a more realistic experiment is required, with multiple datasets gathered in real environments.

8.13 The Analysis of the Incompressible

As we have said in Chapter chap:Introduction, one of the reasons to understand how things work is to understand the cause-effect relation in systems. We are interested in this cause/effect relation in two ways. That is, if we want to see an effect in a system, we want to understand wich causes trigger that effect. Also, and perhaps more interesting, if we have observed an (probably undesired effect) in a system we would like to discover what has caused that effect, so we can fix it, and revert the normal situation.

We could use the theory of nescience to model, and modify, those uncommon effect, by means of training a model and looking at the incompressible part of the data.

A model $\mathcal{M}$ for a dataset $\mathcal{D} = (X, y)$ is a compressed version of that dataset, since the length of the dataset given the model $l(\mathcal{D} \mid \mathcal{M})$ is smaller that then length of the original dataset $l(\mathcal{D})$. The model $\mathcal{M}$ is composed by the regularities found in the dataset (subject to the algorithm used and the families of models considered). What it is left, $\mathcal{D} \mid \mathcal{M}$ is the incompressible part of the dataset, that is, those samples that have no regularity at all, or present a regularity that requires a description longer than the length of the raw data.

In this section we are going to show the practical applications of analyzing what it is left, that is, the incrompressible samples of a dataset. An element that is incompressible represents a very unlikely, or uncommon, situation of the entity being studied. A incompressible element does not necessarily means a problem, since if a problem is sufficiently common, it can be compressed. An incompressible element is something than cannot be explained given the normal behaviour of the system. Of course, all of this is assuming that our dataset has no errors.

Once we have found a model that has the lowest possible nescience for a dataset, we could separate those elements that have not been compresed, denoted by XX, and fit a second model. We could argue that it does not make any sense to model the incompressible part, since, it is incompressible. However, the incompressible part is incompressible with respect to the original entity under study, that is, the global systen. And in this new case, we are studying a different entity, namely, the uncommon parts of an entity. It might happen that we can find regularities in this new entity.

References

A insightful description of the differences between explanation models and predictive models, how these models are used in different scientific disciplines, and what are the implications for the process of statistical modeling can be found in [Shm+10].

The application of the minimum description length principle to the identification of optimal decision trees have been proposed in [QR89], further refined and clarified in [WP93]; however the coding method proposed by those authors is different from the one used in this book.

In our web page can be found an implementation of the decision tree following the guidelines defined in [].

The Minimum Description Length [Grü07] and the Minimum Message Length [Wal05] techniques have been applied to the problem of inferring decision trees in [QR89], later on clarified and extended in [WP93], in [MRA+95] as a technique for pruning, and in [RS98], among others. Although the underlining concepts behind the cost function proposed in this chapter are the same (namely, that learning is equivalent to the capability to compress), our approach is very different from the ones described in these works.

TODO: Find the original reference of the AirPassengers dataset.

TODO: Find the original reference of the Appliance energy consumption dataset. https://archive.ics.uci.edu/ml/datasets/Appliances+energy+prediction

```
The normalized compression distance of two vectors $x$ and $y$ comput
\[
NCD_C\left(\mathbf{x},\mathbf{y}\right)=1-\frac{I\left(\mathbf{x};\ma
\]
The quantity $1 - \frac{I\left(\mathbf{x};\mathbf{y}\right)}{\max\lef
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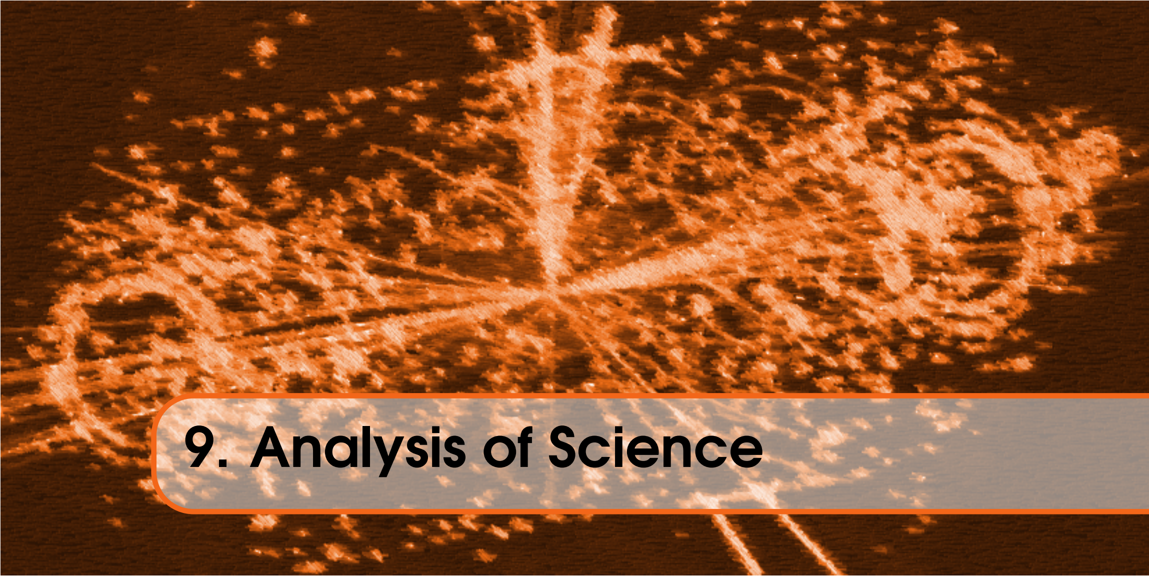


9. Analysis of Science

Science may be regarded as the art of data compression.
Li & Vitányi

TODO: Write this introduction

In this chapter we will use our theory of nescience to study our current scientific knowledge

We will see how he can approximate the concept of nescience in practice. The concept of surfeit will be based, as it was described in Chaper XX, on the concept of redundancy, and redundancy will be computed in practice based on starndar text compressors.

A historical analyis of the evolution of nescience is also covered in the chapter.

At the end of the chapter we will extend the analysis from individual research topic to research areas, in order to understand

9.1 Describing Current Knowledge

According to the theory of nescience, evaluating our current knowledge begins by selecting a specific set of entities we want to understand. Within this framework, universal sets that include every possible entity, whether known or unknown, are not permitted. This restriction arises from the logical paradoxes associated with such sets, including Cantor's theorem, which demonstrates that the set of all subsets has a strictly greater cardinality than the set itself, and Russell's paradox, which involves sets that are not members of themselves (see Section 2.1). Therefore, in this chapter, since our objective is to assess the current state of human knowledge, we focus on a finite set composed of entities that are already known and have been studied by science. These entities are suitable for analysis because humanity possesses at least some information about them.

The next step involves identifying the best available encoding of the selected entities as representations, typically composed of data or facts, followed by determining the most accurate descriptions we have, such as models, theories, and laws. In the theory of nescience, we maintain a clear distinction between representations and descriptions because this separation facilitates the discovery of new knowledge: either by improving the representation or by refining the description. However, since our aim here is to evaluate rather than expand our knowledge, we simplify the process by using only descriptions. These descriptions serve both as the representation and the description of an entity (see Section XX, which explains why descriptions can fulfill both roles). Moreover, we will drop the requirement that these descriptions be computable, since very few scientific descriptions in practice are actually computable. Requiring computability would severely limit the scope of our analysis and exclude a significant portion of scientific knowledge.

For our analysis, we use descriptions derived from the collection of scientific pages from Wikipedia. Wikipedia is a free, collaborative online encyclopedia launched in 2001 that allows anyone with internet access to create, edit, and update articles on a wide array of topics. It is maintained by a global community of volunteer contributors and aims to provide reliable, neutral, and verifiable information to the public. Several features make Wikipedia particularly suitable for analyzing scientific knowledge: it maintains a transparent version history that tracks content changes over time; supports collaborative validation that reduces individual bias; enforces strict citation requirements to ensure information is verifiable and based on authoritative sources; offers broad and consistent coverage across scientific disciplines; and is dynamically updated to reflect new findings and corrections.

Wikipedia is fundamentally a tertiary source. It compiles and synthesizes information from primary sources, such as firsthand accounts of events or discoveries, and secondary sources, which interpret and evaluate those primary materials. Tertiary sources play a key role in academia by summarizing information that has already been thoroughly discussed and vetted. High-quality Wikipedia articles strive to be comprehensive, covering all major aspects of a topic in appropriate detail while avoiding undue emphasis on minor or peripheral information.

Furthermore, Wikipedia is inherently citational. Every statement included in a Wikipedia article must be supported by a published, reliable, and verifiable source. Original research is not allowed, meaning that novel claims, hypotheses, or breakthroughs must already be published in credible sources such as academic journals or books before being included. Wikipedia also employs a form of peer review, where one or more editors review and suggest improvements to an article. While this process is not anonymous or uniformly applied like traditional academic peer review, it still acts as a quality control mechanism that enhances the coverage, clarity, and accuracy of articles through community oversight.

Wikipedia pages are written in the MediaWiki Markup Language, a simplified system for formatting text that allows users without technical knowledge of XHTML or CSS to easily edit articles. Before we can analyze the content of a scientific page, it is essential to remove all markup tags and formatting elements to isolate only the meaningful textual information. To achieve this, we used the Python library `wikitextparser`, which allows us to parse and process the raw wikitext of Wikipedia articles to extract the relevant content. In addition to stripping out the markup, the library was configured to eliminate other non-relevant elements, such as images, references, and lists, which do not contribute directly to our analysis of knowledge.

Wikipedia articles are written in the MediaWiki Markup Language, a simplified formatting system that allows users without technical expertise to contribute easily. Before we can analyze this content, it is necessary to remove all markup tags and formatting elements to isolate only the meaningful text. To do this, we used the Python library `wikitextparser`, which parses raw wikitext and extracts relevant content. In addition to removing markup, the library was configured to exclude other non-essential elements such as images, references, and lists, which do not directly support our knowledge analysis.

Wikipedia hosts a vast collection of articles covering disciplines such as history, literature, politics, entertainment, and science. Since our goal is to evaluate scientific knowledge specifically, we limited our analysis to articles categorized under the "Science" category. This subset includes topics related to the natural and formal sciences—such as physics, biology, chemistry, and mathematics—ensuring that our study remains aligned with the goal of assessing scientific understanding. We further refined this selection by excluding articles focused on individuals, organizations, awards, lists, portals, and similar metadata-oriented content. This filtering ensures that our analysis includes only those articles centered on scientific concepts, processes, or phenomena.

Both the list of articles and the full content of each article were retrieved directly from Wikipedia using the MediaWiki API. This API provides programmatic access to Wikipedia's content, allowing automated queries for page metadata, article text in wikitext format, category information, and revision history. It ensures we are working with the most current and accurate versions of each article while offering a reproducible and efficient method for gathering large-scale data[1]. A detailed explanation of the entire extraction and preparation process can be found in Appendix **??**, allowing any interested reader to reproduce the steps and ensure the consistency of the analysis.

9.2 Measuring Knowledge

As mentioned in the previous section, to evaluate our current knowledge in practice, we used the collection of scientific pages from Wikipedia, which we pre-processed to extract the relevant information for our analysis. We focused exclusively on the topic descriptions, treating descriptions and representations as equivalent. In this context, since descriptions and representations are considered the same, the inaccuracy of a topic is effectively zero, leaving miscoding and surfeit as our primary metrics of interest.

To demonstrate how our theory can be practically applied to assess the current state of knowledge, we selected a collection of topics listed under the Theoretical Computer Science category on Wikipedia. This includes all pages within the main category, as well as those in its subcategories and their respective subcategories, up to a depth of five levels. Figure 9.1 illustrates the Theoretical Computer Science category (Level 1) alongside all its Level 2 subcategories, such as Theory of Computation, Graph Theory, and Logic in Computer Science.

Only pages classified as "GA" have been considered. Articles in the GA class are considered complete, and they have been examined by one or more impartial reviewers. From these list, we have removed pages related to non-relevant topics, such as journals, symposiums, associations, or awards. Additionally, we have removed articles too generic pages (e.g. parallel computing) or pages describing multiple algorihtms (e.g. Tropical cyclone forecasting). For a detailed description of the Wikipedia page preprocessing, please refer to Appendix **??**.

[1] The articles analized in this chapter correspond to April 2025.

Figure 9.1: Categories in Theoretical Computer Science

Only pages classified as "GA" (Good Article) have been considered. GA articles are regarded as complete and have been reviewed by one or more impartial evaluators. From this list, we excluded pages related to non-relevant topics, such as journals, symposiums, associations, or awards. We also removed overly generic articles (e.g., Parallel Computing) and pages describing multiple algorithms (e.g., Tropical Cyclone Forecasting). For a detailed description of the Wikipedia page preprocessing, please refer to Appendix **??**.

The topics analyzed cover a wide range of areas within theoretical computer science and mathematics. In graph theory, we explored topics such as graph coloring (Greedy coloring), structural properties and special classes

(Snark, Perfect graph, Halin graph, Laves graph, Rook's graph, Rado graph, Well-covered graph, Pseudoforest, Component, Unit distance graph, Cop-win graph), graph transformations (Graph homomorphism, Logic of graphs), and graph-based theorems (Steinitz's theorem, De Bruijn–Erdős theorem, Turán's brick factory problem). In algorithms and data structures, we considered classical techniques like Binary search, Selection algorithm, Euclidean algorithm, Fast inverse square root, Farthest-first traversal, Linear probing, Trie, as well as more specialized algorithms such as the Gale–Shapley algorithm, Widest path problem, and data structures like the Cartesian tree. Topics in logic and computational foundations included 2-satisfiability, the Rule of inference, and the BIT predicate. In mathematical methods and theorems, we covered results such as Pick's theorem, Viète's formula, Sylvester–Gallai theorem, Sylvester's sequence, Shapley–Folkman lemma, and the Handshaking lemma. The list also touches on applied mathematics and modeling, through topics like the Dirac delta function, Earth–Moon problem, Tropical cyclone forecast model, Finite subdivision rule, and Network synthesis. Furthermore, in machine learning and computational complexity, we included Reinforcement learning from human feedback and the Small set expansion hypothesis. Finally, some topics address computer science system design and principles, such as the Allocator (C++), Book embedding, Three utilities problem, the Commutative property, and visualization techniques like the Arc diagram. Overall, the list covers a broad spectrum of topics within the area of theoretical computer science, highlighting its diversity and interdisciplinary connections.

9.2.1 Surfeit

In Section 5.2, we introduced the concept of surfeit as a relative measure to quantify the unnecessary effort involved in explaining an entity using a particular description. The surfeit of a description d for a representation r is defined as:

$$\sigma(d,r) = \frac{|l(d) - K(r)|}{l(d)}$$

where $r \in \mathcal{B}^*$ and $d \in \mathcal{D}$ is a description of r. Intuitively, the less we know about an entity, the longer our description tends to be. As our understanding of the entity improves, we should be able to remove all redundant elements from its description.

In practice, when descriptions and representations are considered equivalent, the concept of surfeit simplifies to:

$$\rho(d) = 1 - \frac{K(d)}{l(d)}$$

Algorithm	Analysis of Boolean functions	Automated r
Farthest-first traversal	Gale–Shapley algorithm	Widest path
Cartesian tree	Viète's formula	Dirac delta
Euclidean algorithm	Fast inverse square root	Rule 1
Binary search	Linear probing	Selection al
2-satisfiability	Graph homomorphism	Logic of g
Steinitz's theorem	De Bruijn–Erdős theorem	Earth–Moon
Turán's brick factory problem	Laves graph	Rook's g
Snark	Perfect graph	Clique pr
Feedback arc set	Euclidean minimum spanning tree	Compo
Unit distance graph	Halin graph	Cop-win
Pseudoforest	Well-covered graph	Rado gr
Network synthesis	Telephone number (mathematics)	Book emb
Three utilities problem	BIT predicate	Pick's the
Sylvester–Gallai theorem	RL from human feedback	Finite subdiv
Sylvester's sequence	Tropical cyclone forecast model	Shapley–Folkr
Theil–Sen estimator	Trie	Rule of inf
Commutative property	Allocator (C++)	Handshakin

Table 9.1: Topics in Theoretical Computer Science

This is referred to as the redundancy of a description.

The Kolmogorov complexity of the Wikipedia pages was estimated by compressing the raw text. For compression, we used `bzip2`, a free and open-source program based on the Burrows–Wheeler algorithm. bzip2 is commonly used in practice to estimate Kolmogorov complexity because it employs a very large compression buffer. It is well known that if the buffer size is too small, the estimation of a text's Kolmogorov complexity can be significantly distorted. For example, the `gzip` compressor uses a 32 KB buffer, which is too small for our purposes. In contrast, `bzip2` offers a buffer size of 900 KB at its highest compression setting (compression level of 9), which is more than sufficient for compressing Wikipedia pages.

Figure 9.2 (left) depicts an histogram of the redundancy for the 50 theoretical computer science articles studied. The histogram shows that, once markup and boiler-plate are stripped, redundancy of articles is tightly concentrated between ≈ 0.75 and 0.82, peaking near 0.80. In practical terms, even the clean prose of these pages can typically be shrunk to about three-quarters of its original size, indicating a common stock of recurring phrases, technical jargon, and definitional patterns across the corpus. The scatter plot in figure 9.2 (rigth) adds a systematic dimension: redundancy rises by roughly 2–3

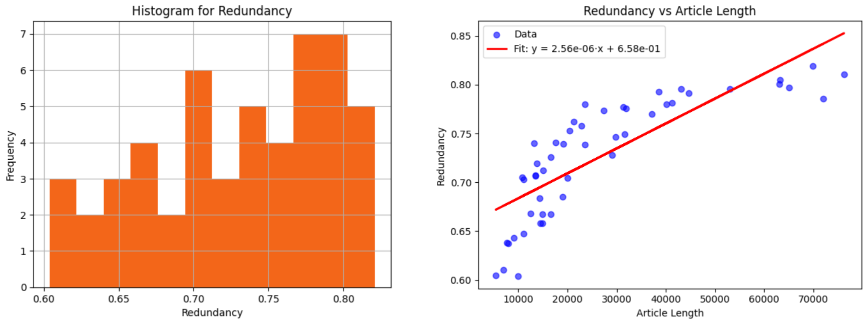


Table 9.2: Redundancy of Topics

percentage points for every additional 10000 characters. Because every file fits inside the single 900 kB block used at `bzip2`'s highest setting (-9), block-size effects are neutralised and the only compressor artefacts left—headers and model warm-up—explain at most a few tenths of that increase. The bulk of the slope therefore reflects the prose itself: longer articles increasingly reuse terminology, theorem–proof templates, and explanatory scaffolding, making them intrinsically more compressible. In short, both figures together show that theoretical-computer-science pages share a fairly uniform baseline of linguistic redundancy, and that this redundancy grows gradually with article length because the writing becomes more internally self-similar rather than because of any quirk of the compression tool.

Table 9.3 lists the ten topics from Wikipedia within the area of Theoretical Computer Science that exhibit higher redundancy. Each page revolves around a single, well-defined object—a classic algorithm (binary search, Euclidean algorithm, clique problem), a mathematical construct (Dirac delta, Rado graph), or a concise metatheorem (2-SAT, Shapley–Folkman lemma). Pages of this kind inevitably iterate the same symbol palette, definitions, and step-by-step explanations: every subsection restates the object, walks through an example, then re-expresses the same idea in a different formalism (pseudocode, recurrence, proof sketch, code snippet). That self-similar scaffolding gives compressors a wealth of repeated n-grams to exploit, driving redundancy up to 0.79 – 0.82 even after boiler-plate has been stripped. While the list includes some of the longer articles in the corpus (e.g. Dirac delta at 117 kB), it also contains mid-sized pages such as Rado graph (38 kB). In other words, high redundancy is not just a by-product of length; rather, it emerges when a compact conceptual core is expanded through multiple parallel presentations (history, intuition, formal statement, variations, applications, proof, pseudocode).

Table 9.4 lists the ten topics that exhibit lower redundancy. These articles

Topic	Redundancy	Page Length	Length Compressed
Dirac delta function	0.821	117121	20969
Binary search	0.819	69838	12634
Euclidean algorithm	0.811	113242	21455
2-satisfiability	0.811	76225	14442
Shapley–Folkman lemma	0.805	63172	12323
Clique problem	0.801	63125	12574
RL from human feedback	0.797	64981	13160
Book embedding	0.796	53046	10831
Rule of inference	0.795	43158	8826
Rado graph	0.793	38626	7989

Table 9.3: Topics with higher redundancy

sit in the low–redundancy tail (between 0.60 and 0.67) differ from the high-redundancy ones in both size and content mix. (i) Every entry is under 17 kB—well below the corpus median. Because bzip2's fixed header and model "warm-up" overhead account for a larger share of such small files, their redundancy starts a few percentage points lower even before content is considered. This matches the positive slope in the scatter-plot: shorter pages naturally cluster toward the left-hand foot of the trend line. (ii) Many of these topics centre on a single formula, sequence, or code idiom (e.g. Viète's formula, Sylvester's sequence, Allocator). They pack unique symbols, numeric constants and one-off identifiers that appear only once or twice, so compressors see far fewer repeated n-grams than in algorithm-walk-through articles. Others, such as "Tropical cyclone forecast model" and "Finite subdivision rule", read more like concise surveys, stringing together disparate subtopics rather than iterating one core definition from multiple angles; that heterogeneity also suppresses repetition.

Together, the list illustrates the floor of the redundancy spectrum: pages that are (i) short enough for compression overhead to matter and (ii) information-dense or eclectic enough to avoid recycling the same prose patterns never reach the 0.70–0.80 plateau seen elsewhere. Their position reinforces the earlier finding that rising redundancy with length is not merely a compressor artefact; it also depends on how much authors reuse terminology and explanatory scaffolding as an article grows.

9.2.2 Inaccuracy

Inaccuracy serves as the second metric in assessing our understanding of a research entity. The underlying idea is that the more accurate our model, the

Topic	Redundancy	Page Length	Length Compressed
Tropical cyclone forecast model	0.667	16675	5550
Allocator (C++)	0.658	14887	5085
Finite subdivision rule	0.658	14416	4933
Snark (graph theory)	0.648	11020	3882
Theil–Sen estimator	0.643	9171	3275
Earth–Moon problem	0.638	7640	2762
Halin graph	0.637	7953	2885
Viète's formula	0.61	7016	2733
Turán's brick factory problem	0.605	5427	2146
Sylvester's sequence	0.604	9994	3960

Table 9.4: Topics with Lower redundancy

better our understanding of the entity. Formally, we calculate the inaccuracy of a description d as the normalized information distance between the original representation r and the output representation r' generated by our description d. That is, inaccuracy is quantified as the length of the smallest computer program capable of correcting the erroneous output of our model.

Inaccuracy, serving as the second gauge to measure our comprehension of a research entity, is based on the principle that the more precise our model, the better our grasp of the entity. Formally, the inaccuracy of a description d is computed as the normalized information distance between the original representation r and the output representation r' generated by the description d. Thus, inaccuracy is assessed as the extent of the smallest computer program that can rectify the incorrect output of our model.

Inaccuracy evaluates how well the output of our description aligns with the selected representation encoding the entity. However, this representation could be flawed itself, as discussed in the preceding chapter. Inaccuracy focuses solely on the description d, neglecting the potential miscoding within the representation r. Furthermore, even though it doesn't require an oracle, inaccuracy cannot be calculated for every case, so it needs to be estimated in practical situations, as we will explore in Part III of this book.

Let us consider $r \in \mathcal{B}^*$ as a representation, and $d \in \mathcal{D}$ as a description, where $d = \langle TM, a \rangle$. We then define the *inaccuracy* of the description d with respect to the representation r, denoted as $\iota(d,r)$, according to the following formula:

$$\iota(d,r) = \frac{\max\{K(r \mid \delta(d)), K(\delta(d) \mid r)\}}{\max\{K(r), K(\delta(d))\}}$$

Intuitively, accuracy measures the difficulty in converting an incorrect representation r' produced by a desription d into the original representation r. In essence, this involves the computation of the normalized information distance between r' and r.

In practice, and in the particular case of descriptions based on the scientific articles of Wikipedia, we cannot apply this definition, because an article of Wikipedia is not a Turing machine that produces a string based output.

Figure 9.8 left depicts a histogram showing the inaccuracy of the analyzed topics, and right side shows a scatterplot of the article lenghts vs. the length of the correspondign talk pages, toghether with a regression line fitted to the data. The two plots suggest that, within this sample of good-quality theoretical computer science pages, talk pages chatter is generally modest and becomes proportionally smaller as articles grow. Inaccuracy, approximated as talk / (article + talk), is highly right-skewed. Roughly half the pages fall below 0.05 and more than three-quarters below 0.15, meaning their talk pages contain at most one word of discussion for every six to twenty words of main-text content. Only a small tail of articles pushes beyond 0.40, indicating a handful of topics that still attract extensive debate or revision despite their "good" label. In the scatter plot we can observe that the best-fit line ($y \approx -2.44 \times 10^{-6} \dot{l}ength + 0.271$) slopes downward, so predicted inaccuracy drops from about 0.27 for a 0-length stub to ≈ 0.10 at 70 kB. Empirically, short articles (< 15 kB) show the widest spread—from virtually no talk to talk pages two-thirds the size of the article—whereas long articles (> 50 kB) cluster below 0.15 with only rare outliers. In other words, once an article expands to tens of thousands of characters, the relative volume of unresolved discussion shrinks, suggesting that length correlates with maturity and consensus. Taken together, the figures imply that most good theoretical-CS pages are comparatively settled, that the few contentious ones are disproportionately short, and that growing an article tends to absorb or resolve the issues reflected on its talk page rather than magnifying them.

Table 9.9 lists topics exhibiting the lowest levels of nescience. The topics with the lowest inaccuracy values (≤ 0.04) look like settled science. They cover classical, mathematically-rigorous results—matching algorithms (Gale–Shapley), structural graph properties (perfect graphs, Steinitz's theorem), and well-studied data-structures or routing primitives (Cartesian tree, widest-path problem). For such topics there is little room for interpretive dispute: statements are either formally correct or not, and once a clean exposition is in place subsequent editors rarely need lengthy back-and-forth. That is why some talk pages are only a few dozen words long (25 for Gale–Shapley) even when the article itself spans tens of kilobytes. Length alone does not guarantee a quiet talk page—the list includes both mid-sized texts (≈ 20 kB) and the 72 kB Network synthesis article—yet all of them keep the ratio of

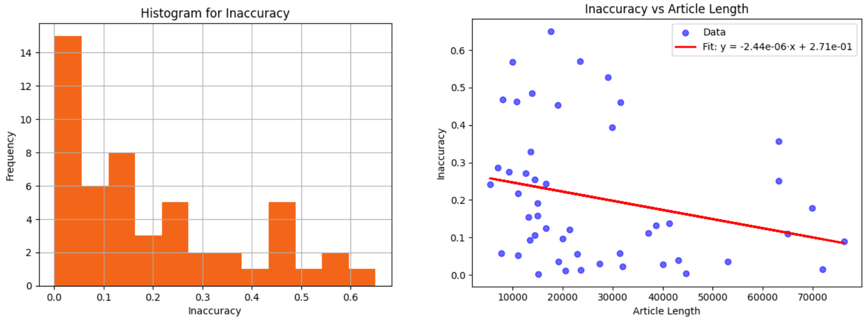


Table 9.5: Inaccuracy of Topics

Topic	Inaccuracy	Article length	Talk length
Gale–Shapley algorithm	0.001656	15072	25
Perfect graph	0.004412	44683	198
Unit distance graph	0.012203	20479	253
Rook's graph	0.013267	23576	317
Network synthesis	0.014493	71945	1058
Logic of graphs	0.022260	31933	727
Steinitz's theorem	0.027765	40094	1145
Cartesian tree	0.030849	27395	872
Widest path problem	0.035644	19128	707
Book embedding	0.036141	53046	1989

Table 9.6: Topics with lower inaccuracy

discussion to content below 4%. Where talk does appear (e.g. 1 989 words for Book embedding or 1 145 for Steinitz's theorem) it is still dwarfed by the main text, implying that open issues tend to be minor wording tweaks, sourcing details, or peripheral expansions rather than fundamental disagreements. In short, low-inaccuracy articles are those whose subject matter is uncontroversial, formally locked-down, and already presented in a stable, comprehensive fashion, leaving editors with little need for ongoing debate.

Finally, Table 9.7 lists the topics with the highest nescience values. The articles with the highest inaccuracy scores are not necessarily the most error-ridden; rather, they are the ones whose talk pages have become arenas for protracted discussion because their subjects invite disagreement or continual refinement—foundational concepts like the commutative property and tries that draw many first-time editors, folklore-tinged algorithms such as the fast inverse square root, or theorems and graph classes (e.g., Sylvester–Gallai, pseudoforests, Halin graphs) that have multiple equivalent statements, proofs,

Topic	Inaccuracy	Article length	Talk length
Sylvester–Gallai theorem	0.394610	29810	19431
Pseudoforest	0.454130	18999	15806
Selection algorithm	0.461374	31578	27049
BIT predicate	0.463016	10817	9327
Halin graph	0.467671	7953	6987
Three utilities problem	0.485948	13846	13089
Fast inverse square root	0.528723	29001	32536
Sylvester's sequence	0.567808	9994	13130
Trie	0.570980	23503	31280
Commutative property	0.650826	17583	32773

Table 9.7: Topics with higher inaccuracy

or naming conventions. In every case the talk page approaches or even exceeds the size of the main text, so anywhere from 40% to 65% of the combined bytes are debate rather than exposition; this ratio is amplified by the fact that most of these articles are relatively short ($\approx$ 10˘30 kB), meaning even modest amounts of conversation loom large. Together they illustrate that a high inaccuracy score chiefly signals ongoing editorial contention—about scope, presentation order, historical credit, or performance claims—rather than a simple lack of factual correctness, and that such contention is most pronounced where definitions are ambiguous, folklore collides with formalism, or broad audiences repeatedly revisit basic material.

9.2.3 Nescience

According to the theory of nescience, our understanding of an entity should be based on the quality of the description used to explain it. In Chapter 6, we introduced a quantitative measure of our ignorance regarding a research entity. This measure depends on the miscoding of a string-based representation of the entity, as well as the inaccuracy and surfeit of the model describing this representation. Ideally, we seek representations and descriptions that simultaneously minimize these three aspects.

In practical terms, particularly when entities correspond to topics covered by scientific Wikipedia pages, we consider only the surfeit and inaccuracy of a description. In this scenario, the representation of a topic coincides with its description, rendering the computation of miscoding irrelevant.

To address the multi-objective optimization problem posed by nescience, we apply a global criterion approach (see Section F.5.3). This method solves multi-objective optimization problems by minimizing the distance between a chosen reference point and the feasible region of the objective space. We select the origin vector $(0,0)$ as our reference point. The distance metric used will be the harmonic mean of surfeit and inaccuracy, defined as:

$$\frac{2}{\iota(d,r)^{-1}+\sigma(d,r)^{-1}}$$

As described in previous sections, surfeit is approximated by the redundancy of the topic's description (the Wikipedia page), while inaccuracy is estimated by the length of the corresponding Talk page.

As it was explained in Section XX, since we are using a decision maker to compute nescience based on redundancy and inaccuracy, and since these quantities do not have the same scale, it is highly convenient to apply the following additional transformation to them:

$$\mu_t^{'} = \frac{\mu_t - \min(\mu)}{\max(\mu) - \min(\mu)}$$

where μ_t refers to the considered metric (nescience, relevance, ...).

Figure 9.8 left depicts a histogram showing the nescience levels of the analyzed topics, and right side shows a scatterplot of the article lenghts vs. the nescience, toghether with a regression line fitted to the data. The two panels paint a mixed picture of how much "unknown-ness" remains in these 50 "good" theoretical-CS articles once both redundancy (compressibility of the prose) and inaccuracy (relative size of the talk page) are factored in. Histogram — a long, uneven tail. Roughly one-third of the articles cluster below nescience ≈ 0.10, meaning they are simultaneously concise (low redundancy) and largely uncontested (little talk). Frequency then stays fairly flat through the 0.15 – 0.35 band and drops again, before a second bump appears between 0.60 and 0.75. That small peak corresponds to pages that are both highly repetitive and heavily debated—the same ones that topped the earlier redundancy and inaccuracy lists. In short, while many good-class pages are well understood, a non-trivial minority still exhibits a pronounced knowledge gap. Scatter plot — almost length-neutral. The best-fit line rises only 0.007 points for every additional 10 000 characters (slope $\approx 7.5 \times 10^{-7}$), so article length alone is not a strong predictor of nescience. Short pages can swing from near-zero to 0.7, depending on how contentious they are, whereas long pages (> 50 kB) compress more (pushing nescience up) but also attract proportionally less talk (pushing it down), leaving them parked in a mid-range around 0.25–0.35. The gentle upward tilt therefore reflects the fact that redundancy grows with length a bit faster than inaccuracy falls, but the wide vertical spread shows that editorial stability—rather than size—is the decisive factor. Overall, "good" status keeps most theoretical-CS articles

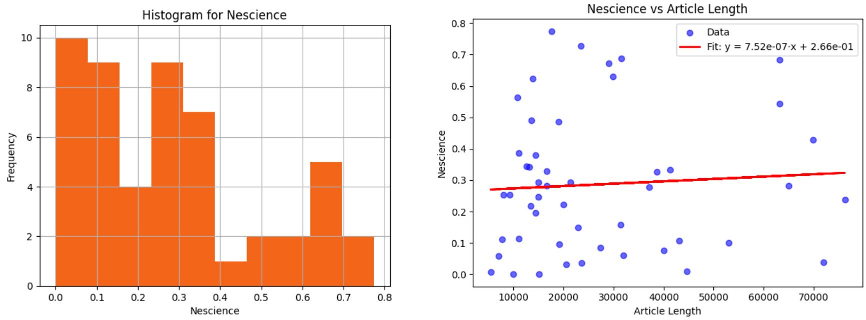


Table 9.8: Nescience of Topics

in a low-to-moderate nescience zone, yet about a quarter of them still suffer from enough repetition and unresolved discussion to signal that our coverage of those topics remains less mature than the label might suggest.

Table 9.9 lists topics exhibiting the lowest levels of nescience. The articles that score best on the nescience metric fall into two complementary archetypes, each driving the harmonic mean down by making one of the two ingredients—redundancy or inaccuracy—almost vanish. The first archetype is epitomised by "Sylvester 's sequence" and "Turán's brick-factory problem": they are short, information-dense pages whose prose compresses poorly (normalized redundancy ≈ 0), so even a rather lively talk page cannot lift their nescience above zero. The second archetype—illustrated by "Gale–Shapley algorithm", "Perfect graph", "Network synthesis", and several other graph-theoretic topics—shows the opposite pattern: their text is highly repetitive (normalized redundancy $\approx$ 0.8˘0.86), but the talk pages are almost silent, so inaccuracy is near zero and the harmonic mean again collapses. Taken together, the list reveals that low lack-of-knowledge can arise either from concise, debate-heavy but non-redundant expositions or from long, internally repetitive but well-settled treatments; what matters for nescience is that at least one dimension of uncertainty is squeezed to the floor.

Finally, Table Finally, Table 9.10 lists the topics with the highest nescience values. The upper tail of the nescience scale is populated by pages that score high on both axes at once —they are repetitive and heavily debated—so the harmonic mean refuses to average the trouble away. Half of the list ("BIT predicate", "Three-utilities problem", "Fast inverse square root", "Selection algorithm", "Trie", "Commutative property") shows normalized-inaccuracy ≥ 0.70, signalling talk pages that rival the article in size; the same set attracts a steady stream of newcomers or folklore-laden claims, which keeps discussion alive. The other half ("Shapley–Folkman lemma", "Clique problem", "Sylvester–Gallai theorem", "Farthest-first traversal") earns its

Topic	Nescience	Norm. Inaccuracy	Norm. Redundancy
Sylvester's sequence	0.000000	0.872117	0.000000
Gale–Shapley algorithm	0.000000	0.000000	0.499166
Turán's brick factory problem	0.007362	0.370945	0.003718
Perfect graph	0.008448	0.004245	0.864084
Unit distance graph	0.031744	0.016248	0.686717
Rook's graph	0.035003	0.017887	0.812327
Network synthesis	0.038635	0.019774	0.836612
Viète's formula	0.057626	0.437415	0.030845
Logic of graphs	0.061030	0.031738	0.791546
Steinitz's theorem	0.076638	0.040219	0.811139

Table 9.9: Topics with lower nescience

Topic	Nescience	Norm. Inaccuracy	Norm. Redundancy
Farthest-first traversal	0.490109	0.505215	0.475880
Shapley–Folkman lemma	0.543853	0.384947	0.926181
BIT predicate	0.562673	0.710692	0.465683
Three utilities problem	0.622535	0.746017	0.534125
Sylvester–Gallai theorem	0.629670	0.605318	0.656063
Fast inverse square root	0.671295	0.811908	0.572197
Clique problem	0.683333	0.548081	0.907206
Selection algorithm	0.688247	0.708163	0.669420
Trie	0.727080	0.877003	0.620932
Commutative property	0.774591	1.000000	0.632109

Table 9.10: Topics with higher nescience

place chiefly through very high redundancy (≈ 0.90 in the case of the clique problem), reflecting articles that restate definitions, proofs and examples in multiple near-duplicate forms. In every case the other dimension is still uncomfortably large (≥ 0.38), so neither trimming repetition nor settling open talk-page issues alone would be enough to pull these topics out of the danger zone. In short, high-nescience entries are those where unresolved editorial contention co-exists with a self-similar writing style—pages that simultaneously need consensus-building and structural tightening before they can be considered well understood.

9.2.4 Conclusion

Across the 50 "good-class" Wikipedia pages in theoretical computer science, our indicators tell a nuanced story about what the encyclopaedia can reveal—and obscure—about collective understanding. Talk-page activity, captured by our inaccuracy ratio, does a credible job of flagging articles whose content is still contested: pages with minimal discussion almost always cover settled, formally unambiguous material, whereas those whose talk pages rival the main text correspond to concepts riddled with naming ambiguity, folklore or pedagogical disagreement. Redundancy, distilled from compression ratios after stripping boiler-plate, complements this view by signalling how tightly authors have distilled the topic: low values align with concise, information-dense expositions, while high values mark articles that re-iterate definitions, proofs and code snippets in multiple guises. Each metric thus illuminates a different facet—editorial consensus on one side, stylistic efficiency on the other—yet neither by itself captures "knowledge quality" outright.

Their harmonic mean, which we dubbed nescience, succeeds as a triage tool because it punishes a topic the moment either dimension becomes extreme. Articles that are both verbose and hotly debated—such as those on the fast inverse square root or the clique problem—cluster at the high end, clearly pointing to areas where Wikipedia's coverage remains unsettled. Conversely, pages with either crisp, irredundant prose or near-empty talk pages sink to the bottom, reflecting mature, well-understood subjects like the Gale–Shapley algorithm or perfect graphs. In that sense, nescience offers a practical snapshot of our residual ignorance as reflected in the encyclopaedia: it reliably highlights where clarification, consolidation or further research are still needed, even if it cannot, on its own, disentangle whether the root cause is factual dispute, pedagogical complexity, or simple editorial neglect.

9.3 Measuring Research Areas

In this section, we evaluate the nescience of entire research areas rather than individual topics, measuring how much knowledge each discipline encompasses. We examined all English-language "good-class" articles in six broad disciplines (biology, chemistry, mathematics, philosophy, physics, and psychology) comprising roughly 600 pages (see Table 9.11). For each discipline, we assessed three metrics: inaccuracy, redundancy, and nescience.

Wikipedia organizes articles into categories by topic to simplify navigation and discovery. Rather than a strict hierarchy, categories form an interconnected network: each category can have multiple subcategories, and a subcategory may belong to multiple parent categories. Editors avoid

Area	Num. Topics
Biology	214
Philosophy	33
Psychology	44
Mathematics	127
Chemistry	138
Physics	52

Table 9.11: Number of topics analyzed per area

circular links, where a category would indirectly include itself through its descendants. Conceptually, this structure resembles a partially ordered set in mathematics and computer science, and it allows diverse classification schemes to coexist within a unified framework. When one category clearly falls under another, it is designated as a subcategory to preserve a logical "is-a" relationship. Articles are typically placed only in their most specific relevant category to avoid redundancy. For example, the article on Claude Shannon appears in "Category:American information theorists," not directly under the broader "Category:Mathematicians."

The top level of Wikipedia's category system is "Category:Contents," which has no parent. From there, the path we have used proceeds as: Contents → Articles → Main topic classification → Academic disciplines → Science → Branches of Science (Applied Sciences, Formal Sciences, Natural Sciences, Social Sciences). Our analysis focuses on five scientific areas: Mathematics, which falls under Formal Sciences; Biology, classified within Life Sciences under Natural Sciences; Physics and Chemistry, both part of Physical Sciences in the Natural Sciences; and Psychology, included in Social Sciences. We also analyze Philosophy, categorized under Humanities within Academic disciplines. These selections ensure comprehensive coverage of both theoretical and empirical fields.

First, we looked at redundancy (see Figure 9.2), which shows how much an article repeats itself. We took out templates, lists, and other markup, then compressed each page using bzip2 at its highest setting. Pages with more repeated text stay larger after compression. We found that most good articles in every field fall in a redundancy range of about 0.70 to 0.80, so they repeat text at similar rates. Biology had the widest range, from about 0.52 up to over 0.90, meaning some articles are very concise while others include many standard sections. Chemistry was the most consistent group, clustering around 0.72, possibly because of regular naming rules and reaction sections. Mathematics, philosophy, physics, and psychology were all in the middle, with medians near 0.75 but small differences in spread. For example,

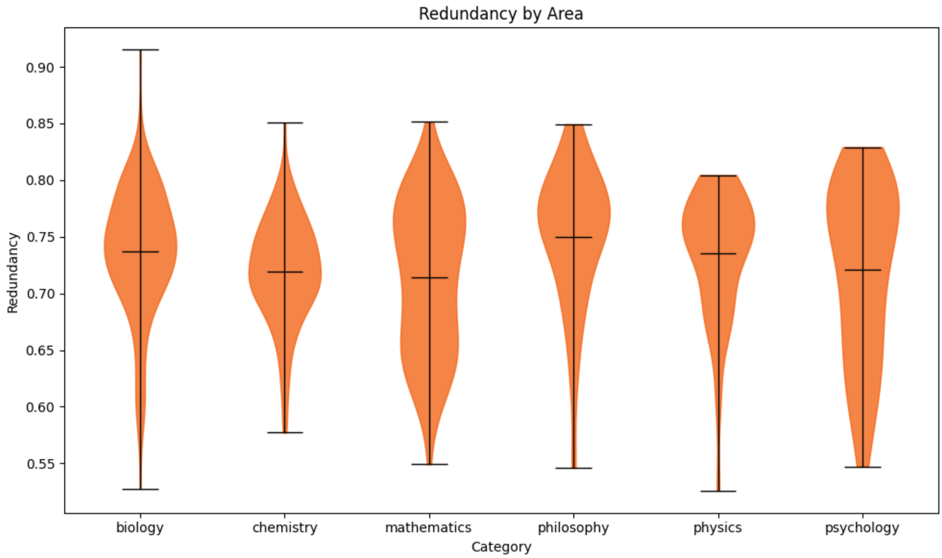


Figure 9.2: Redundancy by Area

math and philosophy pages sometimes repeat proofs or arguments, raising their upper range, while psychology has some short experiment-focused articles. Physics looks like psychology but with a slightly lower median. In short, redundancy is similar across fields: most good articles keep about three-quarters of their text after compression, showing that writing style and citation rules has a higher impact than the topic itself.

Next, we estimated inaccuracy by looking at editorial debate rather than factual error (see Figure 9.3). We looked at each article's talk page size and compared it to the total size of both the talk page and the article. A larger talk page means more discussion or disagreement. The violin plot shows that most articles in every field spend only a small part of their bytes on talk pages, but a few pages have much longer debates. In chemistry, most articles keep their talk pages below about 0.1 of the total bytes, and the median is just above that. Only a few articles reach up to 0.80. Biology, philosophy, and psychology also have most pages under roughly 0.15, but these fields have taller plots in the upper half. That means a few topics, like controversial medical issues in biology or big theoretical arguments in philosophy and psychology, spark long discussions. Mathematics and physics have the highest and widest range of debate. Their median sits around 0.25, and many pages go up to 0.5 or even 0.9, showing that some articles have as much discussion as main content. Overall, most scientific topics settle into low debate, but math and physics pages often have more back-and-forth about

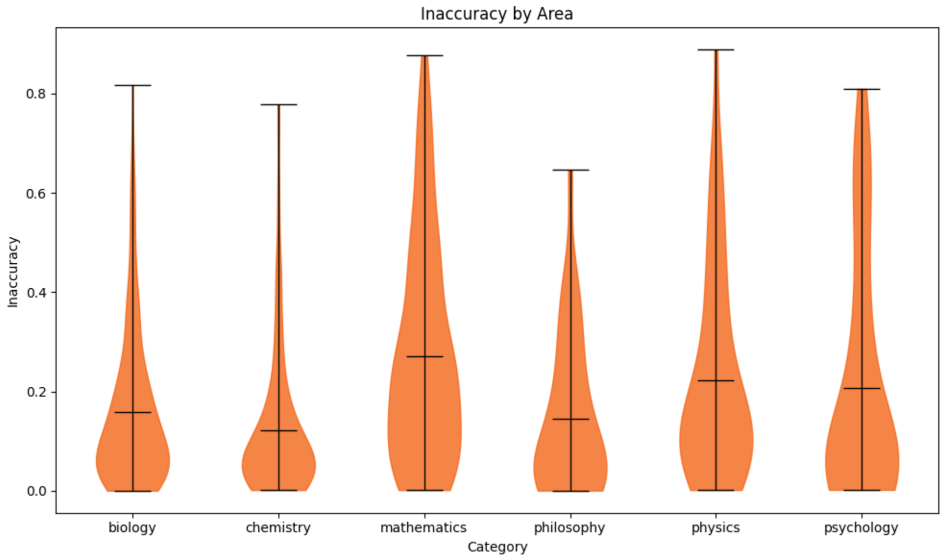


Figure 9.3: Inaccuracy by Area

definitions, notation, and sources, while chemistry articles are more stable.

Finally, we combined redundancy and inaccuracy into one score, nescience (see Figure 9.4). We first scaled each measure to range from 0 to 1, then took their harmonic mean. This score highlights pages that are either very repetitive, heavily debated, or both. In the violin plot, chemistry articles have low nescience (mostly under 0.20), showing they are concise and rarely debated. Biology is similar but has a few articles with higher scores, reflecting some ongoing talk-page discussions. Mathematics has the highest median nescience (around 0.40) and reaches up to 0.90, because many pages repeat concepts and have active debates over definitions. Philosophy and physics each show two peaks. one for well-settled articles near zero and one above 0.50 for more contested topics. Psychology mainly has low nescience, but some articles still face long debates. Overall, while every field has many well-covered pages, our nescience score shows that gaps in knowledge are biggest in mathematics and, to a lesser degree, in philosophy, physics, and psychology.

Table 9.12 shows the average scores for each discipline. The numbers show that redundancy is almost the same across all six fields, ranging from 0.71 to 0.75, but inaccuracy varies more than a factor of two, from 0.12 in chemistry to 0.27 in mathematics. Because redundancy stays nearly constant, the differences in the combined nescience score come mostly from inaccuracy. In other words, after removing repeated boilerplate, the

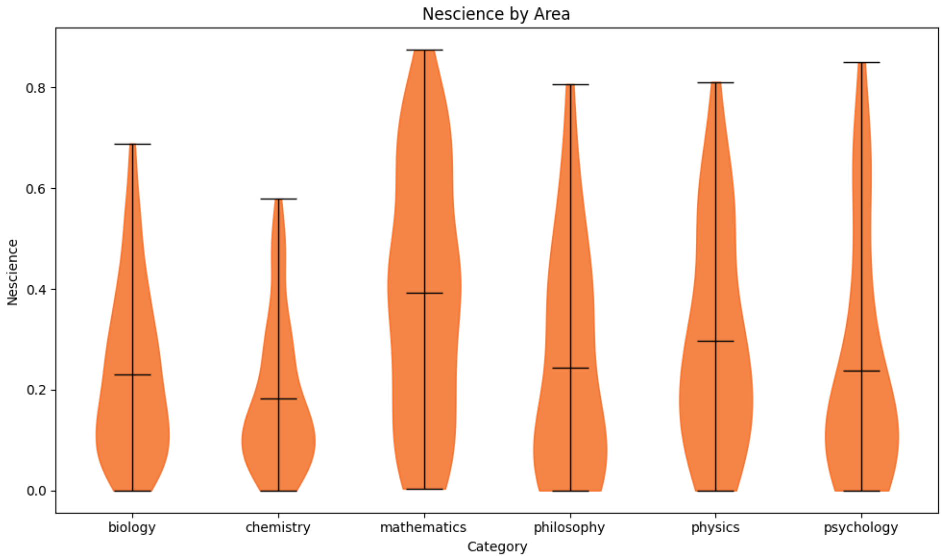


Figure 9.4: Nescience by Area

Category	Inaccuracy	Redundancy	Nescience
Biology	0.157773	0.736704	0.229765
Chemistry	0.122821	0.719500	0.183116
Mathematics	0.271307	0.714365	0.392008
Philosophy	0.144690	0.750007	0.244622
Physics	0.223447	0.735314	0.297802
Psychology	0.207355	0.721208	0.237835

Table 9.12: Average metrics by area

writing style is similar across subjects; what really changes is how much editors discuss or disagree on the talk pages. For example, chemistry's low inaccuracy (0.12) gives it the smallest nescience (0.18), even with average redundancy. In contrast, mathematics has the highest inaccuracy (0.27) and therefore the highest nescience (0.39), despite slightly lower redundancy. Physics and psychology have similar redundancy (around 0.72–0.74), but physics sees more talk-page debate (0.22 vs. 0.21), so its nescience is higher than psychology's. Philosophy shows the highest redundancy (0.75) but only a medium nescience (0.24) because its talk pages are quieter. Overall, this table tells us that for high-quality articles, the main difference between fields is how much editors argue, not how the text is written.

Putting together the redundancy and inaccuracy measures gives a single nescience score. This shows that all fields have similar writing patterns, most high-quality articles compress to about 70–80% of their original length, but they differ in how much they spark online discussions. Chemistry and biology have the quietest talk pages, so they score lowest on nescience. Mathematics and physics have more debates, so they score highest, even though their writing density is similar. Philosophy and psychology fall in between. These gaps happen because each field has many settled articles and a smaller group that need more discussion. In short, Wikipedia's top science articles are usually concise and well written, but the talk pages reveal where editors still disagree most. The biggest knowledge gaps remain in math topics heavy on definitions and in physics areas open to different interpretations.

9.4 The Evolution of Knowledge

Our understanding of a scientific topic typically improves through sustained research efforts over time, resulting in a reduction of the topic's nescience, our lack of knowledge. Specifically, this improvement occurs through reductions in redundancy (repeated, unnecessary information) and inaccuracy (incorrect or misleading information), without significant increases in either component offsetting these improvements. New explanatory frameworks may emerge from innovative theories, refinements of existing theories, or simplified models. Ideally, each successive explanation will become more concise and accurate, removing previously redundant details and errors. Occasionally, new descriptions may temporarily lengthen as additional factual information is incorporated, causing a temporary increase in nescience. Nevertheless, the overall trend in scientific research should consistently be a progressive decrease in nescience as our knowledge advances.

To demonstrate how our theory can be used to characterize the evolution of our understanding of a scientific topic, that is, how nescience decreases with time, we have selected three highly relevant research topics as illustrative examples: graphene, CRISPR, and deep learning. Graphene is a single layer of carbon atoms arranged in a two-dimensional honeycomb lattice, known for its exceptional strength, conductivity, and versatility. CRISPR (Clustered Regularly Interspaced Short Palindromic Repeats) is a revolutionary gene-editing technology that allows for precise, targeted modifications to DNA. Deep learning is a subset of machine learning based on artificial neural networks, enabling complex pattern recognition and predictive modeling. These topics were chosen for their scientific importance and the richness of their associated descriptions, allowing us to apply our methodology and illustrate its effectiveness.

Figure 9.13 illustrates the evolution over time of redundancy, inaccuracy,

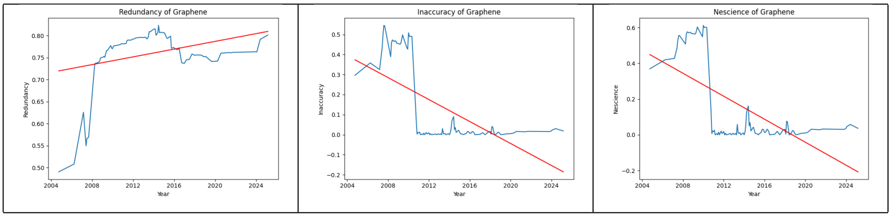


Table 9.13: Knowledge evolution of graphene

and nescience metrics for the topic of Graphene. Each point on the graph corresponds to the analysis of a cleaned-up version of the Wikipedia page at a specific point in time. The early history of the graphene article shows the classic growth-and-turmoil phase of a fast-moving research topic. Between 2005 and 2010 redundancy climbed from ≈ 0.5 to just over 0.7 as the page ballooned with additional sections, figures and repeated explanations, while inaccuracy, our proxy for debate, spiked above 0.5. That surge coincides with the period when graphene research exploded in the literature, patents, and the popular press, so editors were actively negotiating scope, terminology and sourcing. The high redundancy plus high inaccuracy pushed the nescience curve to its peak near 0.9 in 2009-2010, signalling that the encyclopaedia's coverage lagged behind the field's rapid advances.

A sharp inflection occurs in 2011. The talk-page ratio collapses almost to zero-likely because extensive discussion was archived or split into sub-pages after the article stabilised-driving inaccuracy, and therefore nescience, down to negligible levels. From that point on the page continues to lengthen: redundancy drifts upward into the 0.78-0.82 band as definitions, production methods and applications are reiterated for different audiences. Yet talk-page activity remains a small fraction of total bytes, so nescience stays close to zero with only minor blips when new findings (e.g., commercial production techniques around 2014 or 2019) briefly rekindle debate. The negative regression slope on both the inaccuracy and nescience plots confirms a long-term convergence toward consensus, while the positive slope on redundancy simply reflects a mature, template-rich article that keeps accumulating detail without reopening fundamental disputes.

CRISPR's Wikipedia trajectory (see Figure 9.14) mirrors the arc of a scientific whirlwind maturing into mainstream knowledge. When the page first took shape (2010 - 2013) redundancy sat in the low-to-mid 0.60, reflecting a compact article that still compressed poorly, while inaccuracy-driven by an energetic talk page-hovered around 0.40. Those years coincide with the burst of laboratory discoveries that turned CRISPR-Cas9 from an obscure bacterial defence into a headline-making gene-editing tool, so

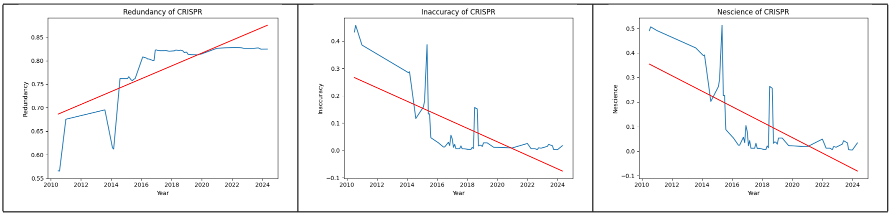


Table 9.14: Knowledge evolution of CRISPR

editors were constantly renegotiating scope and sourcing. Both factors pushed nescience above 0.70, signalling a large knowledge gap between fast-moving science and the encyclopaedia's ability to consolidate it.

A decisive shift occurs in 2015-2016. The talk-page share collapses, dropping inaccuracy to near zero almost overnight; the page was substantially rewritten and much of the debate was archived once standard terminology, mechanism diagrams and milestone experiments had stabilised. Redundancy, meanwhile, jumps above 0.75 and keeps inching up as new sections on ethics, patents and clinical trials are added-material that inevitably repeats the core biology and acronyms. With one input shrinking and the other growing only slowly, nescience plummets and stays near the floor, apart from brief spikes that map neatly onto external flashpoints (the 2018 gene-edited-babies scandal, for example).

The overall downward regression slopes for both inaccuracy and nescience confirm a steady convergence toward consensus, while the upward slope in redundancy simply records the article's swelling, template-rich structure. By 2020 the CRISPR page looks much like that of graphene in its mature phase: highly compressible, rarely contested, and updated incrementally rather than rewritten from scratch each time the field advances.

The deep-learning article (see 9.15) traces a pattern typical of a field that shifted from niche research to global headline status almost overnight. In its early years (2011-2014) the page was compact and still being drafted: redundancy climbed from ≈ 0.40 to the low 0.70 as basic definitions, algorithm lists and seminal breakthroughs were added and often restated, while inaccuracy oscillated but stayed below 0.30, reflecting moderate talk-page traffic. The real turbulence began in 2017: the talk-page share abruptly jumped above 0.40 and stayed there for nearly five years, mirroring the community's debates over benchmark claims, ethics, and the hype surrounding "AI booms." Because redundancy had already settled in the mid-0.70s, this burst of discussion drove nescience to a sustained plateau above 0.85, marking the article as one of Wikipedia's most actively contested science pages during the height of deep-learning publicity.

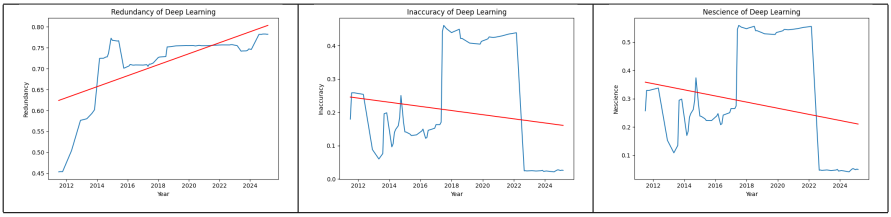


Table 9.15: Knowledge evolution of deep learning

A dramatic correction occurs in late 2022. Large chunks of deliberation were apparently archived or spun off, slashing inaccuracy to near zero almost overnight and dropping nescience with it. Since then the page has remained highly compressible (redundancy $\approx$ 0.75 - 0.78) but largely uncontested; only small upticks appear as new foundation-model milestones are folded in. The negative regression slopes for inaccuracy and nescience therefore chart a long-run movement toward consensus, even though the five-year plateau of high nescience serves as a reminder that Wikipedia's knowledge gap can stay wide for a protracted period when a discipline's methods, jargon and social implications are evolving faster than editors can lock down a stable narrative.

Across three emblematic case studies (graphene, CRISPR and deep learning) the time-series confirm that Wikipedia's nescience reliably chronicles the lifecycle of a scientific topic: initial growth brings a surge of redundancy as material is layered on, and a spike of inaccuracy as editors negotiate scope and sourcing; once consensus forms, talk-page activity collapses, redundancy stabilises in the high-0.70s, and nescience falls toward zero. Graphene reached this mature phase around 2011, CRISPR around 2016, while deep learning lingered in a high-gap state from 2017 to 2022 before a mass archiving of debate produced an abrupt convergence. The trajectory is thus quantifiable: rising redundancy without rising inaccuracy signals steady accretion of detail, whereas persistent high nescience marks periods when the science itself, or its social framing, is still in flux.

9.5 The Demarcation Problem

In this section, we propose a practical method, based on the theory of nescience, to address the demarcation problem, specifically, the challenge of distinguishing scientific from non-scientific knowledge in real-world contexts. Although demarcation is a longstanding philosophical issue, our aim is not to conclusively solve this complex problem but rather to provide insights into its nature and outline potential paths toward future solutions through practical and operational methods.

For our experiments and analysis, we have selected six scientific topics and six pseudoscientific topics to evaluate our approach to the demarcation problem. Our analysis is based on the descriptions of these topics provided by Wikipedia and their associated `Talk` pages. As in previous analyses conducted in this chapter, we have preprocessed the Wikipedia pages by using the `wikitextparser` Python library to remove Wikimedia tags and other irrelevant elements such as tables and images.

The six scientific topics selected are: Climate Change (the long-term alteration of temperature and weather patterns), Graphene (a single-layer carbon material with extraordinary physical properties), Dark Matter (a hypothesized form of matter making up approximately 85% of the universe), Deep Learning (a subset of machine learning using neural networks with multiple layers), Lithium-ion Battery (a type of rechargeable battery widely used for portable electronics and electric vehicles), and Brain-Computer Interface (a technology enabling direct communication between the brain and external devices). These scientific topics have been selected due to their intensive research activity over the past 20 years.

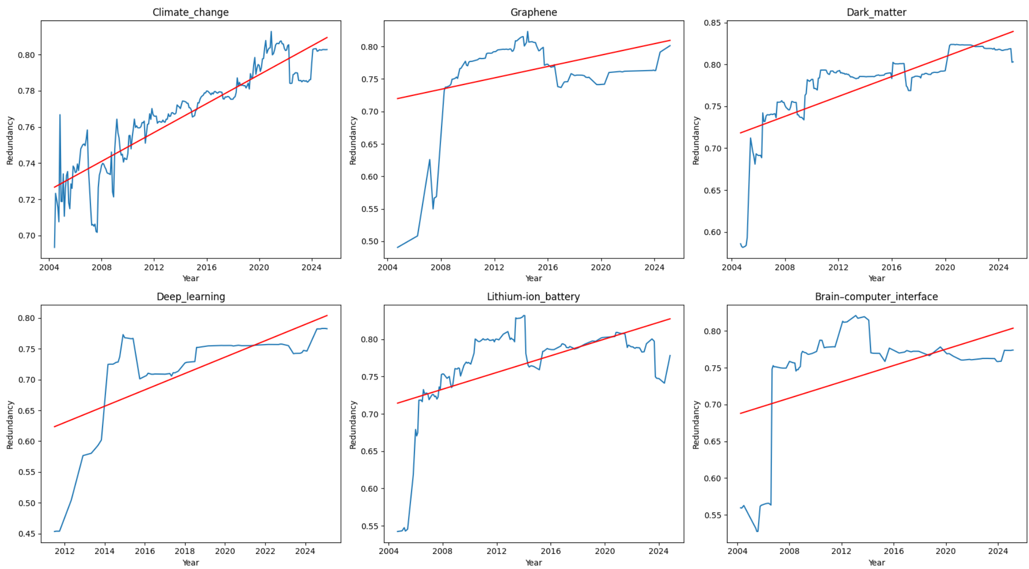


Figure 9.5: Evolution of Redundancy in Scientific Topics

Redundancy, as an approximation of the concept of surfeit, is computed, as in the previous case, by comparing the ratio of the length of a text to its compressed version. Figure 9.5 shows the evolution of redundancy for these selected scientific topics over the past 20 years. As observed, redundancy for these topics demonstrates an increasing trend, as confirmed by the computed regression line. Although one might generally expect redundancy to decrease as our understanding improves, new discoveries and emerging knowledge frequently necessitate additional details and explanations, thus increasing redundancy in descriptions.

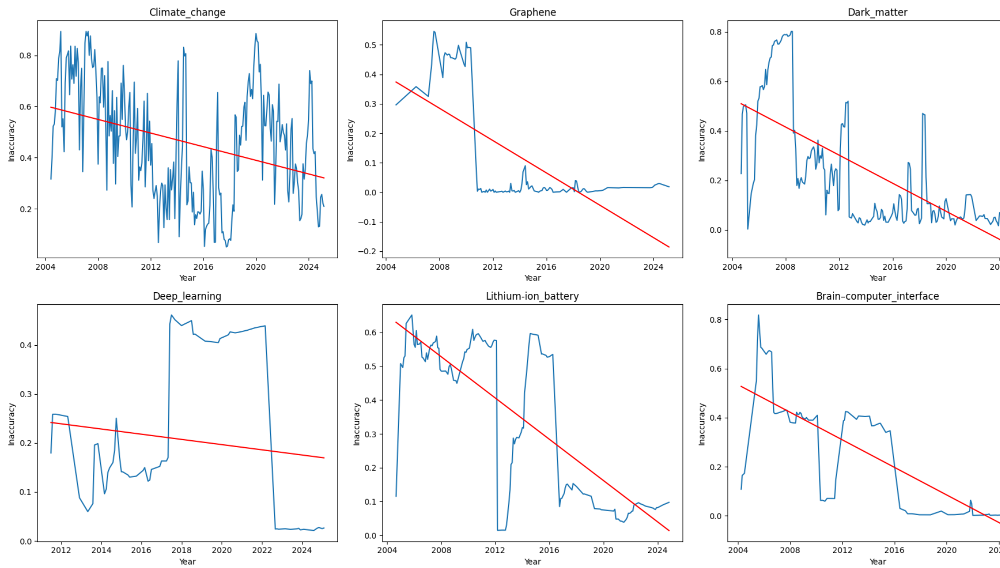


Figure 9.6: Evolution of Inaccuracy in Scientific Topics

Inaccuracy is computed based on the ratio length_talk / (length_talk + length_article), where length_talk represents the length of the Talk page for each topic, and length_article is the length of the corresponding Wikipedia article, as done in the previous sections. Utilizing Talk pages is an effective method for approximating article inaccuracy since these pages typically contain discussions, disputes, and clarifications regarding inaccuracies or controversies in the articles. Figure 9.6 illustrates the evolution of inaccuracies for the selected scientific topics, showing a clear decreasing trend across all topics.

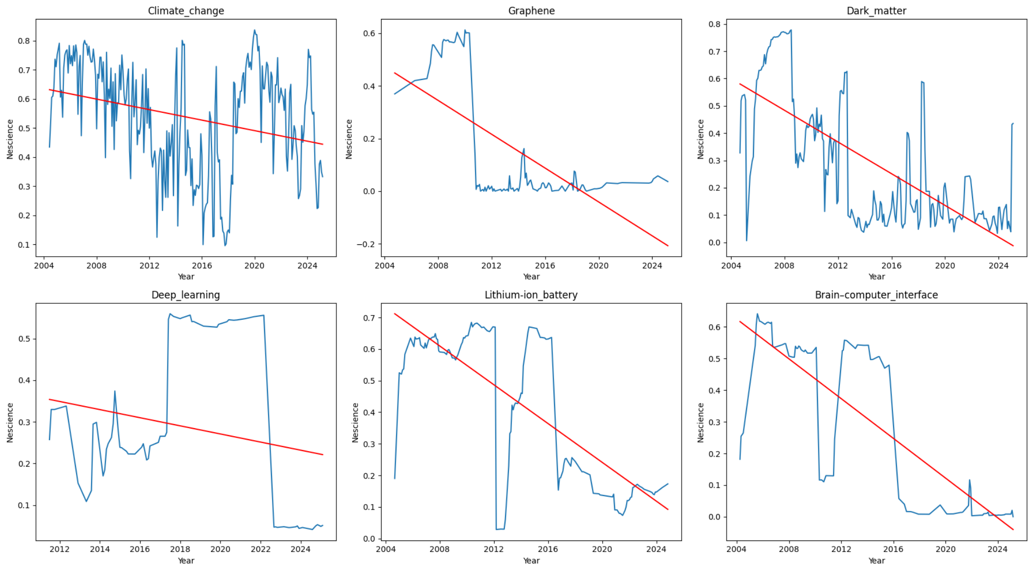


Figure 9.7: Evolution of Nescience in Scientific Topics

Finally, Figure 9.7 shows the evolution of nescience for all selected scientific topics, where nescience is estimated as the harmonic mean of the metrics of redundancy and inaccuracy. As depicted, despite the positive trend in redundancy, nescience exhibits a decreasing trend, suggesting our overall understanding of these topics improves over time.

Additionally, we have selected six pseudoscientific topics to further evaluate our demarcation method: Lunar Effect (the belief that lunar cycles influence human behavior), Water Memory (the claim that water retains a memory of substances previously dissolved in it), Astral Projection (the claimed ability of consciousness to leave the physical body and travel in the astral plane), Enneagram of Personality (a model describing personality types based on a geometric figure with nine interconnected points), Perpetual Motion (the hypothetical concept of a machine that operates indefinitely without energy input), and Dowsing (a technique claiming the ability to locate water, minerals, or other hidden substances through intuitive means). These topics represent different pseudoscientific categories—Lunar Effect (Astrology), Water Memory (Homeopathy), Astral Projection (Parapsychology), Enneagram of Personality (Numerology), Perpetual Motion (Physics-related pseudoscience), and Dowsing (Divination)—and were selected based on classifications from Wikipedia itself as pseudoscience.

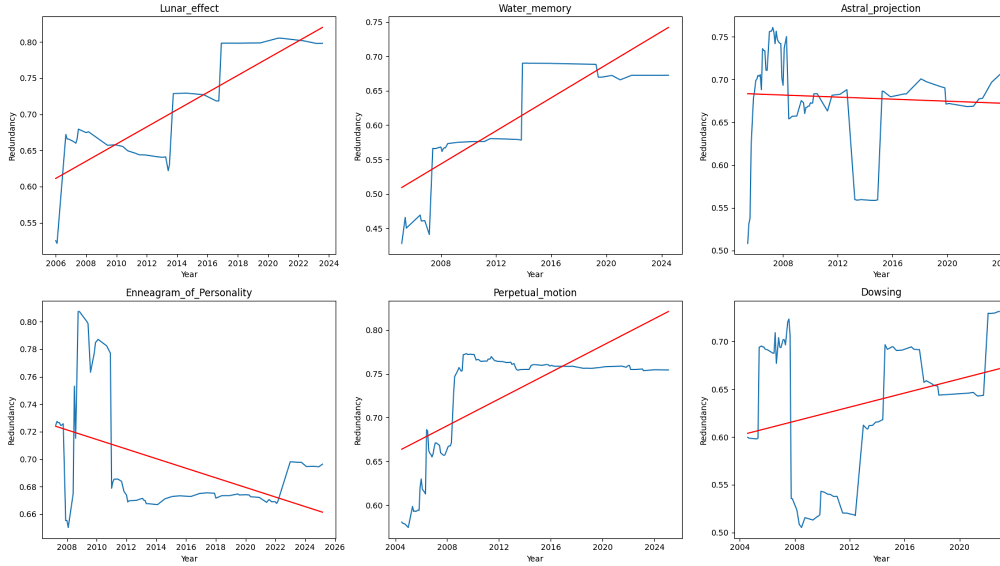


Figure 9.8: Evolution of Redundancy in Pseudoscientific Topics

Figure 9.8 shows the evolution of redundancy for these selected pseudoscientific topics over the past 20 years. As it was the case of scientific topics, redundancy for these topics demonstrates an increasing trend for "Lunar Effect", "Water Memory", "Perpetual Motion", and "Dowsing", and a rather surprising non-increasing trend for "Astral Projection" and "Enneagram of Personality". This decrease in redundancy for the latter two topics may indicate that their Wikipedia articles have undergone substantial editing aimed at streamlining or simplifying the content.

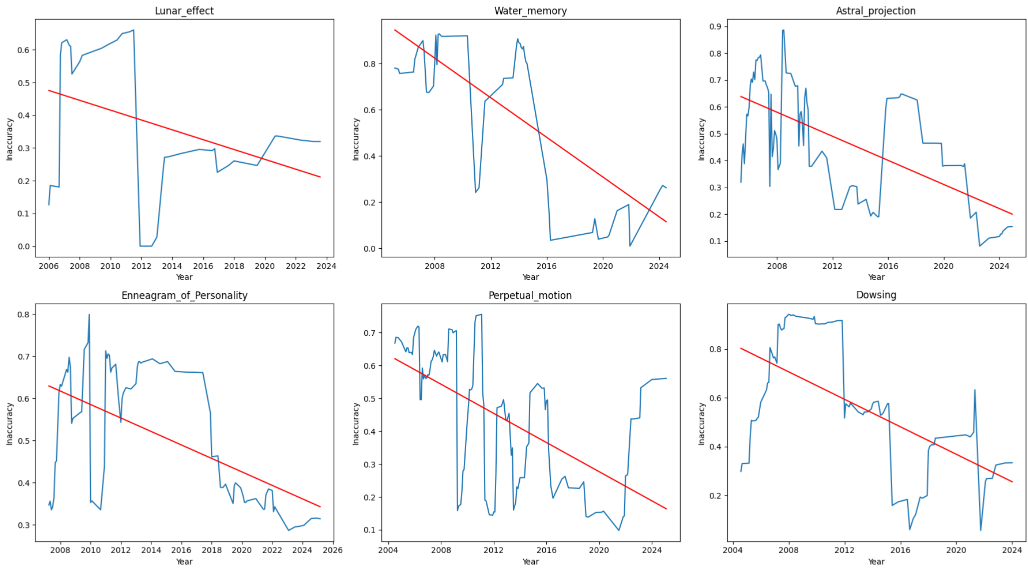


Figure 9.9: Evolution of Inaccuracy in Pseudoscientific Topics

Figure 9.9 illustrates the evolution of the estimated inaccuracies for the same pseudoscientific topics. A clear decreasing trend in inaccuracies is observable across most topics, suggesting, somewhat unexpectedly, that controversies regarding these topics have started to settle down.

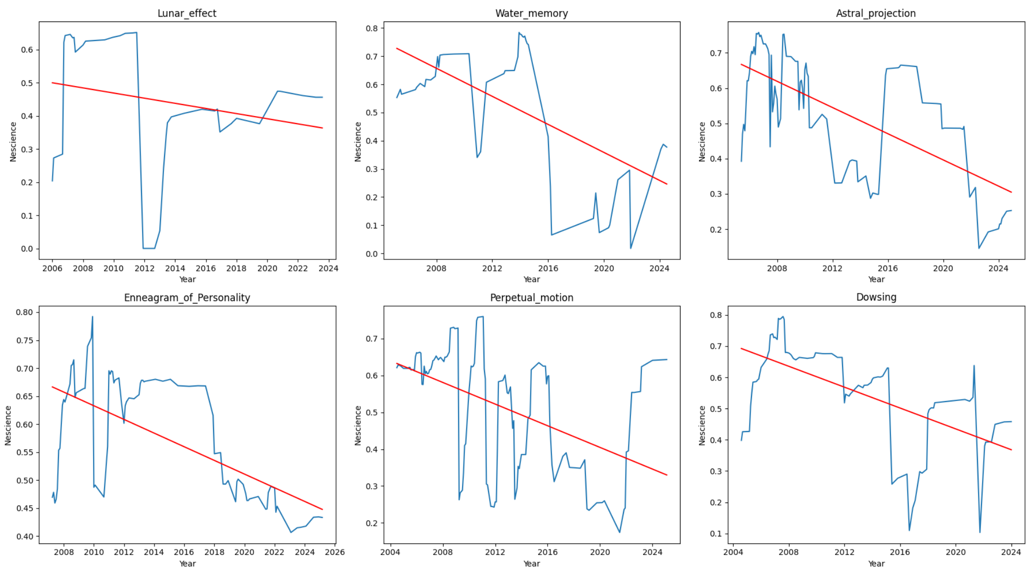


Figure 9.10: Evolution of Nescience in Pseudoscientific Topics

Finally, Figure 9.10 shows the evolution of the estimated nescience for all selected pseudoscientific topics. As expected, given the previous figures for redundancy and inaccuracy, a decreasing trend is observed for most topics, suggesting that our knowledge about this topics has, in fact, decreased with time.

Our preliminary analysis is too superficial to draw definitive conclusions. A more detailed analysis, employing randomized controlled experiments and rigorous hypothesis testing, needs to be conducted. Additionally, the approximations for redundancy and inaccuracy could be refined further (e.g., citation analysis, scientific community surveys, bibliometric analysis). Based on our initial findings, there appear to be no significant practical differences between science and pseudoscience—both communities seem capable of increasing our knowledge about their respective topics. The essential distinction between science and pseudoscience may lie in the validity and truthfulness of claims, rather than in their methodologies. Alternatively, demarcation could also be based on science's demonstrated capability to transform theoretical results into practical, real-world applications—a capability generally lacking in pseudoscience.

9.6 Perfect knowledge

Philosophers of science deal with the problem of how knowledge about our world is gathered trough our senses, and if we can trust our perceptions. Also, they address the difficult issue of how knowledge is derived from facts (for example, by means of applying the principle of induction), and if it is sound, from a logic point of view, to make those derivations. Finally, philosophers are interested in how scientific theories are generated based in this knowledge. Any of these problems is covered by the theory of nescience, since we assume that theories (or descriptions in our own terminology) are already known. We do not provide any method to create those theories. What the theory of nescience provides is a set of metrics to quantitatively evaluate, and compare, existing scientific theories.

It might appear that the descriptions in which the theory of nescience is based are truly objective, in the sense that they must be so clear and well stated that even a computer can reconstruct the original topic given its description. Although this point is true, the problem that prevents the theory to provide an absolute knowledge about our world is the way we choose the entities to study, and how we encode as strings those entities. As we have seen (see Chapter 2), the accuracy of our descriptions depend on how good is our encoding of the abstract entities we are studying. Unless the entities are strings themselves, we must assume that our encoding could not be perfect.

Moreover, we could be wrong about our assumption that the selected set of entities covers all possible entities of that kind. That is, the set of entities are subject to change as our scientific understanding about them develops. The same might happen in case of encodings.

Although the theory of nescience does not say anything about how we can reach an absolute knowledge about an entity, it can tell us if we have reached a perfect description (that we make equal to a perfect knowledge). That is, the theory of nescience can answer the question if we have reached a perfect knowledge about a topic, subject that the the entity under study has been properly identified, and the encoding of this entity has no errors.

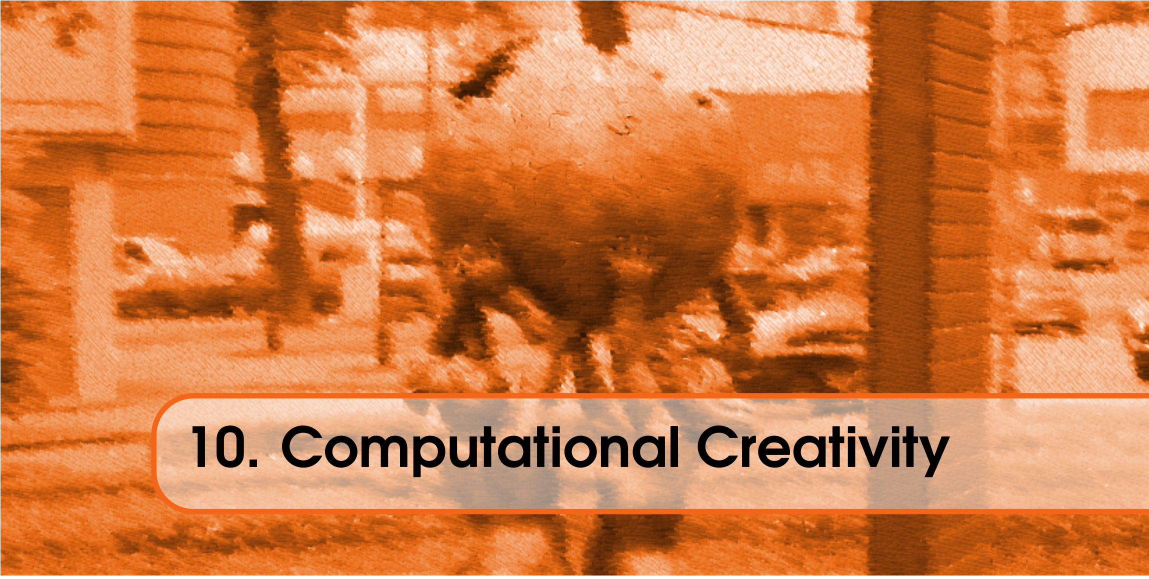
9.7 Uknown-unknown

References

Provide a reference to Wikpedia

The behavior of compressors depending of the size of objects and window (buffer) size is studied in detail in [CAO+05] with applications to the normalized compression distance (a measure of similarity between objects proposed in [Li+04]).

Add a reference to the Burrows–Wheeler algorithm and to bzip2, and gzip. Perhaps a comparison, or more bib in NCD in practice.



10. Computational Creativity

To be surprised, to wonder,
is to begin to understand.
José Ortega y Gasset

In this Chapter we are going to see how to apply in practice our methodology for the assisted discovery of interesting research questions. As it was the case of previous chapter, in which we studied the concept of nescience from a practical point of view, ...

In the first part of this chapter we will see how to approximate the new metrics introduced: relevance and applicability. The relevance of a topic will be based on the number of web pages on Internet that link to the topic's page on Wikipedia (external links), and applicability will be estimated by the number of links from the Wikipedia's scientific pages to themselves (internal links). We will provide some practical examples of both quantities for the set of topics that compose the research area of theoretical computer science. Then, we will describe how to apply in practice our methodology for the discovery of interesting questions, and we will come up with some examples of new research questions that, in principle, could be addressed by science. The new questions proposed will be both, intradisciplinary, coming from the area of theoretical computer science, and interdisciplinary, by means of combining the area of theoretical computer science with the area of philosophy and the area of biochemistry. Finally, we will derive some new interesting research topics, according to our subjective interpretation of the combinations found, that are enough interesting to deserve to be the subject of new research activities. We will also evaluate if the proposed topics fulfill the requirements that we proposed in Chapter 7 for a question to be classified as interesting.

In the last part of the chapter, we will apply the set of metrics defined for the classification of individual research topics to full research areas. In this way, we will compute the interestingness of the different research disciplines as source of new problems, and their interestingness as a source of useful tools to solve open problems. These metrics will allow us to compare the relative merits of different knowledge disciplines. Some examples of research areas in decay will be shown as well.

10.1 Maturity

The maturity of a topic is estimated based on the length of the Wikipedia article (only the text), and the length of the compressed version. Figure 10.1 shows a plot of the maturity of the selected set of topics after the normalization process.

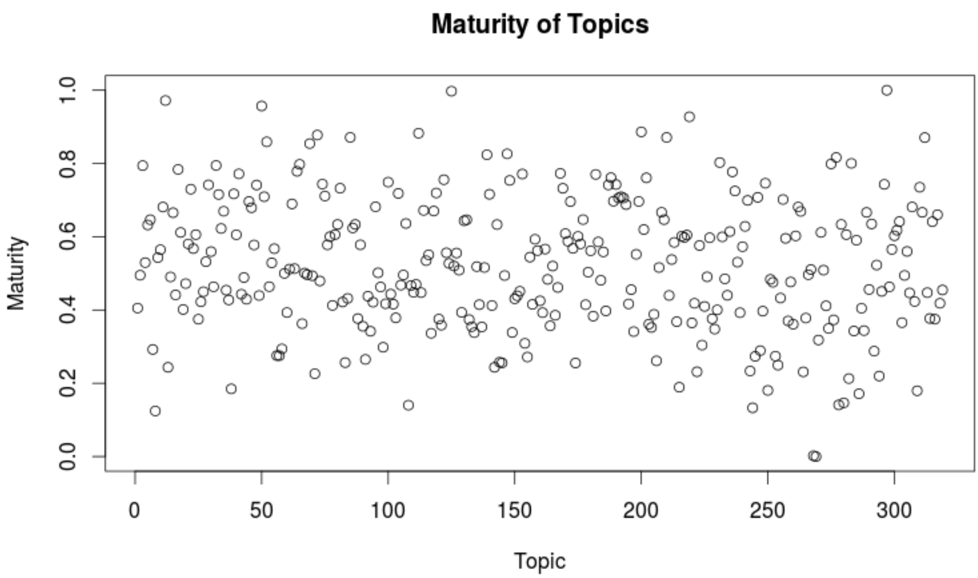


Figure 10.1: Maturity of topics

Topic	Maturity	Norm.
Carry operator	5.34	1.00
Binade	4.54	0.99
Comm. X-Machine	3.01	0.97
PowerDEVS	2.35	0.94
MPIR	2.00	0.92
Constraint automaton	1.84	0.90
RO right moving TM	1.73	0.89
P”	1.71	0.89
Crossing sequence (TM)	1.63	0.88
Microsoft Binary Format	1.53	0.86

Table 10.1: Maturity of topics

Table 10.1 contains the ten most relevant topics according to its maturity. For each topic it is shown the maturity and the normalized version of this number. Well classified topics, that is, topics that our intuition tell us that are well understood, could include *Read-only right moving Turing machines*, *Crossing sequence (Turing machines)*, and perhaps the *P” language*. Other topics that perhaps are misclassified include *communication X-Machine*, *Power DEVS*, *MIPR*, and *constraint automaton*.

10.1.1 Applicability

Applicability measures how likely is that a research topic can be applied to solve open problems. If a tool has been already applied to solve multiple problems, then there is a high probability that it can be used again to solve new problems. The number of problems in which a tool has been applied is computed with the aid of the applicability graph (see Definiton 7.2.1), and applicability is formally defined as the out-degree of the topic in this graph (see Definiton 7.2.2). We have approximated the applicability graph by means of using the graph of internal links between the scientific pages of Wikipedia. That is, we approximate the applicability of a topic by counting the number of pages from Wikipedia domain that links to the topic's page (we have used the *“What links here”* facility from Wikipedia, a tool to see the list of the pages that link to, but not redirect to, the current page).

TODO: Perhaps we could include a nice picture of the graph of Wikipedia internal links

The applicability of a topic Figure 10.2 shows an histogram of the applicability of the selected set of topics. The histogram's shape is dominated by an enormous spike in the very first bin and a sparsely populated, elongated right-hand tail. Roughly three-quarters of the theoretical-CS topics attract fewer than $\tilde{5}0$ incoming Wikipedia links, while only a sprinkling reach the triple-digit range and just one or two break past 300. That steep drop-off is the signature of a power-law (or at least heavy-tailed) distribution: applicability, as measured here, is concentrated in a tiny set of "super-connectors," with the median topic enjoying only modest reuse. In practical terms, the average link count is a misleadingly rosy figure—pulled upward by a few giants—whereas the typical topic remains niche.

Such inequality has several implications. First, it reinforces the idea that a small core of foundational ideas underpins a large share of problem-solving across the field; investing effort in those hubs yields the greatest leverage. Second, the emptiness of the mid-range hints that rising topics face a kind of applicability "valley of death": they must clear a substantial gap before joining the elite club of widely referenced concepts. Finally, the long tail highlights opportunity—numerous specialised notions wait at low link counts, potentially poised for breakout if new cross-disciplinary applications emerge.

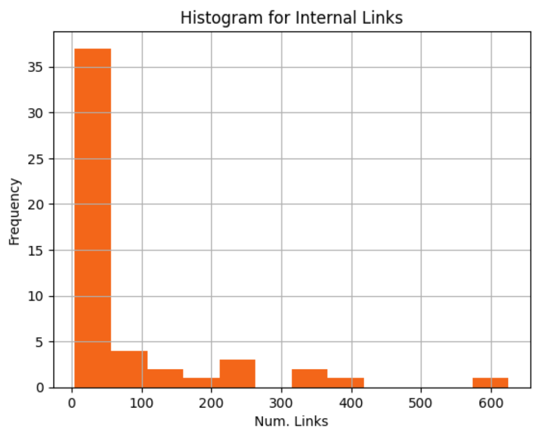


Figure 10.2: Applicability of topics

Table 10.2 contains the ten most relevant topics according to its applicability. The backlink data confirm the long-tailed picture hinted at by the histogram: applicability—at least as proxied by Wikipedia's "What links here" counts—is highly unequal. A single super-hub (the **Dirac delta function**, 625 links) dwarfs the rest, while only a handful of topics even cross the 200-link mark. This means that when researchers look for broadly reusable tools, the "return on attention" is greatest in a very small set of concepts that already function as connective tissue across many areas.

Topic	Internal Links
Dirac delta function	625
Rule of inference	409
Reinforcement learning from human feedback	351
Euclidean algorithm	343
Trie	244
Telephone number (mathematics)	228
Commutative property	214
Tropical cyclone forecast model	195
Cartesian tree	155
Binary search	116

Table 10.2: Applicability of topics

Equally striking is *who* those hubs are. Alongside classic algorithmic staples such as the **Euclidean algorithm**, **Trie**, and **Binary search**, we see foundational math/logic notions (e.g., **Rule of inference**, **Commutative property**), a fast-rising AI methodology (**Reinforcement learning from human feedback**), and even a domain-specific meteorology model. In other words, high applicability favors breadth rather than disciplinary purity: ideas that spill into multiple conversations—whether introductory, theoretical, or applied—accumulate the most links. For anyone mapping future research bets, this suggests monitoring backlink growth over time (to catch newcomers like RLHF early) and normalizing counts by sub-field size to filter out topics whose popularity is driven by narrow, self-referential clusters.

10.1.2 Relevance

In Definition 7.1.2 we introduced the concept of relevance of a research topic as a measure of the impact that this topic could have in people's life. The idea was that the higher the relevance, the higher its potential as a source of interesting questions, since we would be addressing a problem that affects many people. Relevance was defined as the degree of the research topic in the relevance graph, a bipartite graph connecting topics and people (see Definition 7.1.1). Of course, this relevance graph is a mathematical abstraction that it is very difficult to compute in practice, since we do not have information about how people is affected by each topic.

As an approximation of the relevance of a topic we have used the number of links (URLs) from external web pages on the whole Internet that point to the topic's web page on Wikipedia. The rationale is that the more relevant is a topic, the more people will be talking about it on Internet, and the more URLs there will be linking to Wikipedia, since Wikipedia is a well known source of information to which many people refer. In fact, we are not interested in knowing the absolute relevance of research topics, since what we need is a measure of relative relevance between different topics. An underestimate of the relevance is not harmful as long this underestimation is equally distributed among all the topics. It requires further research to fully understand how well the the theoretical concept of relevance is approximated by this URLs counting procedure.

Another problem is that we do not know the number of links to a web page on Internet, and so, we have to apply a second approximation. In this case, the number of links was estimated using Google's `link:` facility in searches. Google's `link:` lists the links that Googlebot discovered during its crawling and indexing process of Internet. For example, the number of external pages that link to the *Computer Science* article in Wikipedia is given by:

```
link:http://en.wikipedia.org/wiki/Computer_science
```

As Google recognizes in its web page, not all links to a site may be listed. The number of links could vary due to redirections, crawling errors, and other problems. How these errors affect to the accuracy of the links counting is not clear, since the details of the Google's crawling algorithm are not public.

Figure 10.3 shows a plot of the relevance of the set of topics after the application of the normalization process described in XXX. A practical problem is that there are too many topics with a very low number of links (as indexed by Google). That should not be a problem since we are not using at any moment those topics with very low relevance.

Table 10.3 contains the ten most relevant topics according to its relevance. For each topic it is shown it relevance (number or external links) and the normalized version of this number. The list includes basic concepts (*binary number, floating point*), advanced concepts (*Turing machine*, *finite-state machine, cellular automaton, lambda calculus*, *Turing completeness*), highly popular tools (*recursion*, *regular expression*) and classical problems (*halting problem*). All those topics could fit into our intuitive idea of highly relevant, although some authors could perfectly disagree that some of them are the most relevant ones in the area of theory of computation (for example, *floating point*).

10.2 Interesting Research Questions

Before to compute the new interesting questions, it is highly convenient to normalize the metrics of the topics involved in the study, otherwise, a very

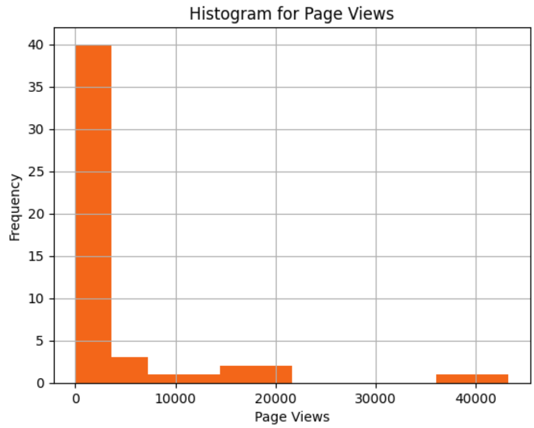


Figure 10.3: Relevance of topics

Topic	Relevance	Norm.
Regular expression	409	1.00
Turing machine	159	0.90
Binary number	141	0.89
Recursion	133	0.88
Finite-state machine	118	0.86
Halting problem	108	0.85
Cellular automaton	104	0.85
Floating point	99	0.84
Lambda calculus	95	0.84
Turing completeness	93	0.83

Table 10.3: Relevance of topics

reduced set of topics could dominate all the questions. For the normalization process we have used the BoxCox method, that it is based on the identification of the best transformation from a family of power transformations.

TODO: Explain the BoxCox method

The most difficult part of the identification of topics as tools, that is, topics with very high maturity (or very low nescience), is to distinguish when the description of a topic is short because it is well understood (for example, a mathematical theorem), or when it is short because it is a unfinished or poorly written article. Our work is based on the classification of Wikipedia articles as stubs, however, this classification is not very reliable, since many stubs articles are not classified as such (many of the misclassified topics suffer from this problem). How to automatically distinguish between a well-understood

Tool	Problem	Interestingness
Ternary numeral system	Regular expression	1.21
GNU MPAL	Arithmetical hierarchy	1.19
IEEE 854-1987	Arithmetical hierarchy	1.17
Quantum computer	Regular expression	1.17
Ternary numeral system	Arithmetical hierarchy	1.15
Division by zero	Regular expression	1.15
Turing machine	Regular expression	1.14
GNU MPAL	Regular expression	1.13
Ternary numeral system	Halting problem	1.13
Recursion	Halting_problem	1.13

Table 10.4: Interesting Intradisciplinary Questions

topic and a poorly written description is still an open question.

By combining the elements of Table 10.8 and Table 10.9 we could come up with new interesting ideas of how to apply existing tools to open problems. As it was said above, the goal of the approach described in this article is to identify highly potential interesting applications, but is up to the researcher to decide if certain combination of topics make sense or not, and if they deserve the effort to pursuit them. The results of the combination is in Table 10.4.

Most of the interesting questions identified have very low quality. As it was said before, the problem is that it is very difficult to distinguish (automatically and unsupervised) between a poorly written article from a very well understood topic. In this section we review some on the interesting intradisciplinary questions identified with the aim to clarify what we mean as interesting question and how interesting questions should be interpreted. Some combinations worth examining could be:

- Interesting Question 7: *Can we apply* Turing machines *to* regular expressions*?* The answer to this question is yes, since it is a very well know question. Regular expressions are recognized by finite automata, and finite automata can be simulated by Turing machines.
- Interesting Question 10: *Can we apply* recursion *to the* halting problem*?* Again the answer is yes, since the proof of the halting problem is based on a machine that call itself.

Note that both questions have well known answers, and so, we have failed to provide original questions.

The most interesting questions arise when we combine topics from two different disciplines. However, the probability that the identified questions are meaningful is lower than in the case of intradisciplinary analysis.

Tool	Problem	Interestingness
State space	Action potential	1.17
Turing machine	Action potential	1.16
Quantum computer	Action potential	1.16
Abstract machine	Action potential	1.14
Computational model	Action potential	1.13
State space	Membrane potential	1.12
State space	Meiosis	1.11
Arithmetic logic unit	Meiosis	1.11
GNU MPAL	Flashbulb memory	1.11
Ternary numeral system	Working memory	1.10

Table 10.5: Interesting Interdisciplinary Questions

For the interdisciplinary analysis we have used the collection of pages from the theory of computation already used in the intradisciplinary analysis, and a new collection of topics from the area of bioinformatics. The topics were selected using the Wikipedia category *natural sciences*, *biology*, *bio*logical *processes*. In total, there were more than 10^5 combinations analyzed. Table 10.5 contains the list of the most relevant intradisciplinary applications.

The set of interdisciplinary questions also suffer from the problem of the stub articles, and so, the quality of the results is low. Some interdisciplinary applications could be:

- Interesting question 1: *Can we apply state space to action potential?* Questions 1, 2, 3, 4 and 5, all of them, suggest the same idea, that is, if it is possible to formalize the concept of action potential, in such a way that can be reproduced by a computer.
- Interesting question 7: *Can we apply state space to meiosis?* Question 7 is similar to question 1, and it asks about the possibility of formalize the concept of meiosis using a computer.

10.2.1 Intradisciplinary Questions

The interest of a topic as a tool measures how likely is that this tool can be applied to other problems. Figure 10.4 shows a plot of the interestingness of the selected set of topics after the normalization process.

Table 10.6 shows the average applicability and average maturity of each of the selected areas, and the average interestingness of each area as a source of interesting tools. The table largely fits our intuitive idea of which areas are more important as a source of tools: computer science is the area of highest

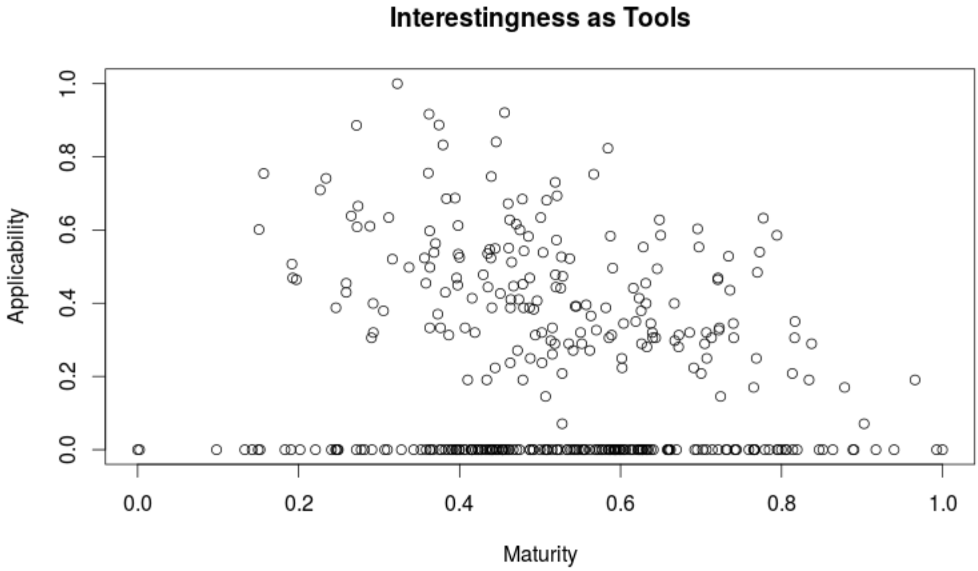


Figure 10.4: Interestingness of Tools

interest, and sociology is the area with less interest. The only extrange elements is that epistemology appears as a source of very interesting tools, even more interesting, on average, than topics from mathematics (probably because it contains a large ratio of poorly written articles).

Finally, Table 10.7 shows the relevance and nescience of the selected areas, and their interest as a source of interesting problems. Again, the results largely match our intuitive idea of which areas are less understood: sociology is the area with the highest number of interesting problems, and mathematics is the area with the lower number of problems.

Table 10.8 contains the ten most relevant topics according to its interestingness as a source of interesting tools. Out of the ten topics, only two (*ternary numeral system* and *recursion*) appear in the list of top ten mature topics or top ten applicable topics; the rest of topics are new. In the list we can find topics like the *GNU Multiple Precision Arithmetic Library* and the *standard for radix-independent floating-point arithmetic* (IEEE 854-1987) that are definitely tools, but not in the sense of tool that we are looking for our methodology. Some other topics are not clear that can be considered as tools, like *arithmetic logic unit*, *barrel shifter*, or *arithmetic overflow*. Topics that match or intuitive idea of tool include *recursion*, *state space*, *abstract machine*, and *ternary numeral system*. There are also some topics,

Research Area	Applicability	Maturity	Tools
Sociology	1.00×10^{-3}	2.93×10^{-3}	3.09×10^{-3}
Biology	9.20×10^{-4}	4.65×10^{-3}	4.74×10^{-3}
Chemistry	3.11×10^{-3}	5.01×10^{-3}	5.90×10^{-3}
Psychology	1.14×10^{-3}	6.91×10^{-3}	7.00×10^{-3}
Mathematics	9.32×10^{-3}	9.47×10^{-3}	1.32×10^{-2}
Epistemology	1.55×10^{-3}	1.75×10^{-2}	1.76×10^{-2}
Computer_science	9.93×10^{-3}	1.90×10^{-2}	2.15×10^{-2}

Table 10.6: Interestingness of Areas as Tools

	Relevance	Nescience	Problems
Mathematics	4.22×10^{-2}	3.51×10^{-1}	3.53×10^{-1}
Computer_science	2.35×10^{-2}	4.43×10^{-1}	4.44×10^{-1}
Chemistry	5.95×10^{-2}	4.66×10^{-1}	4.70×10^{-1}
Biology	3.85×10^{-2}	4.75×10^{-1}	4.77×10^{-1}
Psychology	5.06×10^{-2}	5.28×10^{-1}	5.31×10^{-1}
Epistemology	4.54×10^{-2}	5.30×10^{-1}	5.32×10^{-1}
Sociology	4.21×10^{-2}	5.43×10^{-1}	5.44×10^{-1}

Table 10.7: Interestingness of Areas as Problems

like *computational model*, too broad to be considered in a question.

Finally, Figure 10.5 contains a plot of the interestingness of the topics considered as potential interesting problems.

Table 10.9 shows the ten most interesting topics as interesting problems. Topics that fit our intuitive idea of problem, that is, not very well understood concepts with a high relevance, could include *arithmetical theory*, *halting problem*, *floating point*, *quantum computer*, and *computable function*. The topic *recursion* appears both as a tool and as a problem. However in case of tools it refers to the concept of recursion in general, and in case of problems it refers to the implementation of the concept of recursion in the particular case of computer science. The case of *regular expression*, a topic that intuitively should be classified as a tool and not as a problem, can be explained due to the length of the article in Wikipedia, that provides a detailed description of the language used for regular expressions. This problem rises the question of how to distinguish in Wikipedia between introductory articles and reference articles. Finally, there are topics like *computability theory*, *lambda calculus* and *computability* that are too broad to be analyzed as problems.

R Based on the given definition of "Interestingness of a topic as a tool",

Topic	Interestingness
GNU MPAL	0.49
Ternary numeral system	0.48
IEEE 854-1987	0.47
Arithmetic logic unit	0.43
Recursion	0.42
Barrel shifter	0.42
State space	0.42
Abstract machine	0.41
Computational model	0.39
Arithmetic overflow	0.39

Table 10.8: Interestingness of Tools

Topic	Interestingness
Arithmetical hierarchy	0.72
Regular expression	0.68
Computability theory	0.65
Halting problem	0.65
Recursion (CS)	0.64
Lambda calculus	0.63
Floating point	0.61
Quantum computer	0.57
Computability	0.55
Computable function	0.55

Table 10.9: Interestingness of Problems

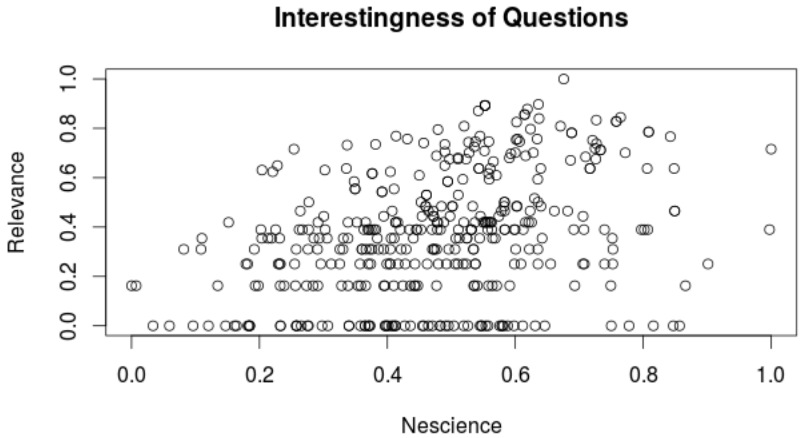


Figure 10.5: Interestingness of Questions

we can explore various mathematical properties and concepts derived from this idea. Some possibilities include:

- Normalization: To compare different topics fairly, we can normalize their interestingness values by scaling them to a specific range, e.g., [0, 1]. This normalization can help compare the relative interestingness of various topics.
- Weighted Interestingness: We can introduce weights to the maturity and applicability dimensions to emphasize one over the other depending on the specific context or application. This would allow us to fine-tune the interestingness measure for different scenarios.
- Correlation: Studying the correlation between maturity and applicability could provide insights into how these dimensions are related and possibly reveal trends across different research topics.
- Cluster Analysis: By examining topics in the two-dimensional vector space defined by maturity and applicability, we can perform cluster analysis to identify groups of topics with similar levels of interestingness. This can help identify areas of research that share characteristics and possibly suggest interdisciplinary research opportunities.
- Rate of Change: Investigating the rate of change of interestingness over time can provide insights into the evolving landscape of a research field. This analysis could reveal emerging topics or those that are becoming less relevant.
- Optimization: Using the interestingness metric, we can explore optimization techniques to find the most interesting topics given certain constraints or within specific domains. This could be useful for research prioritization and resource allocation.

> These derived mathematical properties and concepts can provide a deeper understanding of the interestingness of research topics and their potential application as tools for solving problems.

10.2.2 Interdisciplinary Questions

10.3 New Research Topics

If we combine the list of highly relevant and not very well understood problems with themselves, it might happen that we come up with a new topic that lies in the new unknown unknown area.

In Figure 10.6 it is shown a plot[1] of the interestingness of the (potential) new topics compared with the interestingness of the topics that generated them.

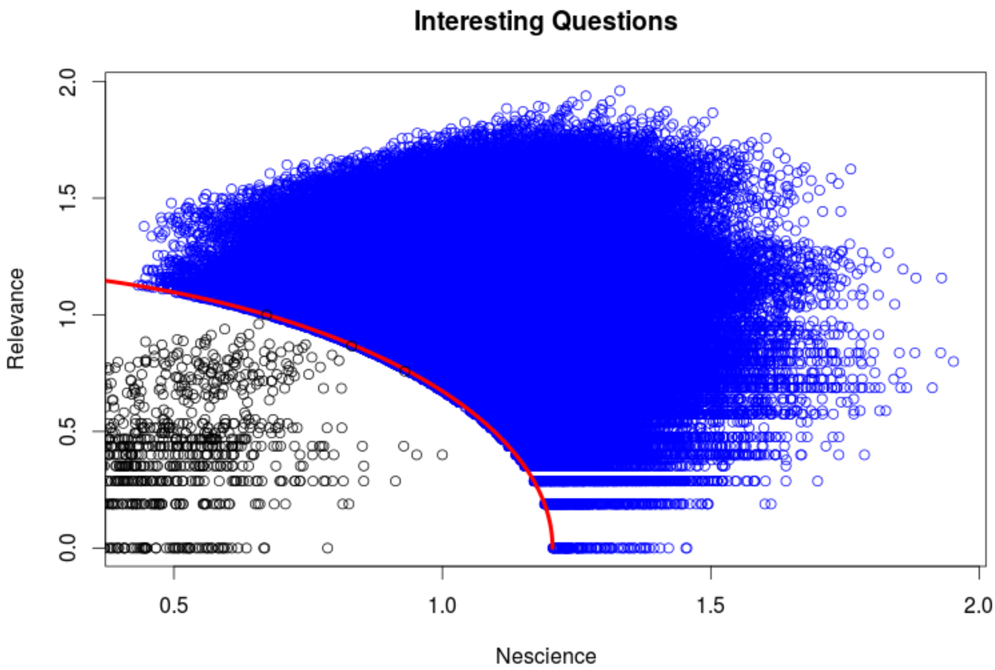


Figure 10.6: Interesting Intradisciplinary Questions

Table 10.10 contains a list of the top 25 candidates to become new topics topics according to their interestingness. In this analysis we have included all the topics from all the knowledge areas. Most of the questions deal with

[1]With the aim to make the figure clear, only a reduced set of the topics is depicted.

the concept of intellectual property (*copyright*, *open access*, *public domain*, and perhaps, *wiki*), suggesting that this is an area where there are still a lot of things to discover, much more that we are aware of. Perhaps, it could be also a problem of a certain bias of Wikipedia to these, and related, topics. Further investigation is required to clarify this point.

In order to understand how new topics are generated, we have selected the following two examples:

- New topic 17: *Public domain* + *Earth*. This question rises the issue if the Earth should be considered as a public resource; it touches the very concept of private property. The methodology suggest that this is not a very well understood topic.
- New topic 18: *Public domain* + *Internet*. Raises the same issue that Question 17, but in this case restricted to Internet and its governance.

Unfortunately, in both cases we fail to provide a well defined, innovative, and previously unseen, research topic.

We could also restrict our search of new topics to a reduced number of knowledge categories. For example, in Table 10.11 contains the ten most interesting new topics corresponding to the already studied areas of *theory of computation* and a new area of *phenomenology* (from Level 2 *philosophy of mind*, and Level 1 *cognitive science*). Given the list of topics contained in the table, we could come up with, for example, the following potential new topics:

- New topic 2: *Turing machine* + *synesthesia*: this new topic could be about a new kind of Turing machine that incorporates synesthesic properties. These new s*ynesthesic Turing machines* could be defined as the union of a group of Turing machines that are linked together in such a way that when one machines read a symbol from its tape, it produces an automatic change in the state of another machine. The property of synesthesia could be also extended to the case of non-deterministic Turing machines.
- New topic 4: *Kolmogorov Complexity* + *Self-awarenes*: This topic could be interpreted as investigating the minimum complexity required for a computer program to have the capacity of self-awareness.

10.4 References

Papers about the BoxCox method ...

10.5 Future Work

Problem	Problem	Interestingness
Public domain	Open access	1.71
Public domain	REST	1.70
Public domain	Wiki	1.70
Open access	REST	1.70
Copyright	Public domain	1.69
Open access	Wiki	1.69
Public domain	QR code	1.69
Copyright	Open access	1.68
Wiki	REST	1.68
Open access	QR code	1.68
Public domain	Transport Layer Security	1.68
Copyright	REST	1.68
QR code	REST	1.67
Open access	Transport Layer Security	1.67
Copyright	Wiki	1.67
Wiki	QR code	1.67
Public domain	Earth	1.67
Public domain	Internet	1.67
REST	Transport Layer Security	1.66
Copyright	QR code	1.66
Earth	Open access	1.66
Internet	Open access	1.66
Public domain	Open source	1.66
Public domain	Web 2.0	1.66
Wiki	Transport Layer Security	1.66

Table 10.10: New Topics

Question	Question	Interestingness
Kolmogorov complexity	Change blindness	1.24
Turing machine	Synesthesia	1.23
Kolmogorov complexity	Qualia	1.23
Kolmogorov complexity	Self-awareness	1.22
Turing machine	Qualia	1.22
Kolmogorov complexity	Synesthesia	1.21
Turing completeness	Synesthesia	1.20
Turing machine	Self-awareness	1.20
Turing completeness	Qualia	1.20
Turing completeness	Self-awareness	1.18

Table 10.11: Restricted New Topics

Apendix

A. Discrete Mathematics

Mathematics may be defined as the subject in which
we never know what we are talking about,
nor whether what we are saying is true.
Bertrand Russell

The majority of mathematical concepts used throughout this book belong to the domain of *discrete mathematics*. This field focuses on mathematical objects that take on distinct, separate values, as opposed to continuous ones. In this book, we make use of various discrete structures, including integers, strings, graphs, and computer programs. A key feature of discrete sets is their countability, meaning they can be put into one-to-one correspondence with the natural numbers. By contrast, continuous mathematics, such as calculus, will play only a minimal role in the theoretical development of the theory of nescience.

Our primary interest in discrete mathematics arises from its direct relevance to computation. The theory of nescience draws upon various aspects of computer science, including algorithms, coding, and string complexity. Computers operate in discrete steps and manipulate information stored in discrete memory units. Our interest in computers stems from the aspiration to apply our theoretical framework to a broad range of real-world entities.

We consider computers to be the most suitable tools for modeling the world around us. While pure mathematics often engages with abstract objects independent of their representations, the theory of nescience places significant emphasis on the representation (or encoding) of objects.

This chapter provides a brief overview of the fundamental concepts of discrete mathematics, introducing topics such as sets, strings and languages, counting methods, matrices, and graphs. While we do not present formal definitions or prove theorems in this overview, these subjects lay the groundwork for the theories and ideas explored in later sections. Discrete mathematics is a broad and diverse field; here, we focus only on those elements essential for understanding the theory of nescience. More advanced topics (such as computability, information theory, and complexity) require a deeper treatment and are addressed in dedicated chapters.

The References section provides a list of recommended books that explore the topics introduced in this chapter in greater depth. Readers interested in further developing their understanding can use this list to delve more deeply into each subject, thereby complementing the foundational overview presented here.

A.1 Sets, Relations and Functions

The sets of *natural*, *integer*, *rational*, and *real* numbers are denoted by $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{Q}$, and $\mathbb{R}$, respectively. Each of these sets includes the number 0. The *positive integers* are represented by $\mathbb{Z}^+$, and the *positive reals* by $\mathbb{R}^+$; both sets also include 0. Let A be a *set*. We indicate that x is an *element* of A using the notation $x \in A$, and that x is not an element of A with $x \notin A$. Elements of a set can be listed explicitly using braces, as in $A = \{0,1,2,3\}$, or defined by a condition using *set-builder* notation, for example, $A = \{x \in \mathbb{N} : x < 4\}$, provided that the *universe* of discourse is clearly specified.

Suppose A and B are two sets. We use the notation $A = B$ to indicate that the sets are *equal*. The expression $A \subseteq B$ signifies that A is a *subset or equal* to B, while $A \subset B$ denotes that A is a *proper subset* of B (meaning that A is contained in B but is not equal to B). The condition $A = B$ holds if and only if both $A \subseteq B$ and $B \subseteq A$ are true. The symbol $\varnothing$ denotes the *empty set*, which is the set containing no elements.

■ **Example A.1** For every set A, we have that $\varnothing \subseteq A$ and $A \subseteq A$. ■

The term *cardinality* refers to the number of elements in a finite set A, denoted by $d(A)$. Accordingly, the cardinality of the empty set $\varnothing$ is 0, since it contains no elements. For any two sets A and B, the notation $A \cup B$ denotes the *union* of A and B, while $A \cap B$ represents their *intersection*. For a collection

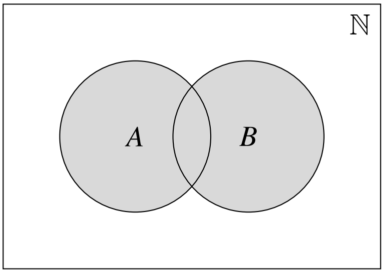


Figure A.1: Representation of $A \cup B$ as a Venn Diagram

of n sets $A_1, A_2, \ldots, A_n$, we write their union and intersection as $\cup_{i=1}^{n} A_i$ and $\cap_{i=1}^{n} A_i$, respectively. For an arbitrary collection of sets indexed by a set I, we use the notations $\cup_{i \in I} A_i$ and $\cap_{i \in I} A_i$. When dealing with an infinite collection of sets, we may use the shorthand $\cup_{i=1}^{\infty} A_i$ and $\cap_{i=1}^{\infty} A_i$. Occasionally, we will make use of *Venn diagrams* to visually represent set operations, as illustrated in Figure A.1.

Given any two sets A and B, the *set difference* is denoted by $A \backslash B$, and the *complement* of the set A is written as A^c. *De Morgan's laws* state that for any sets A and B, we have $(A \cup B)^c = A^c \cap B^c$ and $(A \cap B)^c = A^c \cup B^c$.

Two sets A and B are said to be *disjoint* if their intersection is empty, i.e., $A \cap B = \varnothing$. A collection of sets $A_1, A_2, \ldots, A_n$ is disjoint if $A_i \cap A_j = \varnothing$ for all $i \neq j$. A *partition* of a set A is a collection of nonempty, pairwise disjoint subsets $A_1, A_2, \ldots, A_n$ such that $A = \cup_{i=1}^{n} A_i$. The *power set* of A, denoted by $\mathcal{P}(A)$, is the set of all possible subsets of A. If the cardinality of A is n, i.e., $d(A) = n$, then the cardinality of its power set is 2^n, so $d(\mathcal{P}(A)) = 2^n$.

■ **Example A.2** Given the set $A = \{1, 2, 3\}$, its power set is:

$$\mathcal{P}(A) = \{\varnothing, \{1\}, \{2\}, \{3\}, \{1,2\}, \{1,3\}, \{2,3\}, A\}$$

■

Consider a non-empty set A and a collection $\mathcal{F}$ of subsets of A. The pair $(A, \mathcal{F})$ is called a *field* over A if it satisfies the following conditions: it contains the empty set, that is, $\varnothing \in \mathcal{F}$; it is closed under complementation, meaning that for every $F \in \mathcal{F}$, the complement F^c also belongs to $\mathcal{F}$; and it is closed under finite unions, meaning that for any subsets $F_1, \ldots, F_n \in \mathcal{F}$, the union $F_1 \cup \ldots \cup F_n$ is also in $\mathcal{F}$. Additionally, it can be shown that a field also satisfies two further properties: the universal set A itself belongs to $\mathcal{F}$, and it is closed under finite intersections, so that $F_1 \cap \ldots \cap F_n \in \mathcal{F}$ for all subsets $F_1, \ldots, F_n \in \mathcal{F}$.

Consider two elements, x and y. An *ordered pair*, denoted as (x, y), is a pairing in which the order of the elements matters. Generalizing this idea, an *n-tuple* is an ordered sequence of n elements, written as $(x_1,\dots,x_n)$. The *Cartesian product* of two sets A and B, denoted by $A\times B$, is the set of all ordered pairs (x,y) such that $x\in A$ and $y\in B$. This concept extends naturally to n sets $A_1,A_2,\dots,A_n$, where the Cartesian product is expressed as $A_1\times A_2\times\cdots\times A_n$. Additionally, the *n-fold Cartesian product* of a set A with itself is denoted as A^n.

Let R be a subset of the Cartesian product of a set A with itself, i.e., $R\subseteq A\times A$. Such a subset is called a *binary relation*. We write aRb to indicate that the ordered pair (a,b) belongs to R. A binary relation is said to be *reflexive* if, for every element $a\in A$, it holds that aRa. It is called *symmetric* if, for all $a,b\in A$, the condition aRb implies bRa. A relation is *antisymmetric* if, for all $a,b\in A$, the coexistence of aRb and bRa implies $a=b$. It is *transitive* if, for all $a,b,c\in A$, the conditions aRb and bRc together imply aRc. A relation is *total* if, for every pair $a,b\in A$, either aRb or bRa holds. Binary relations can also be defined between two different sets A and B, in which case R is a subset of $A\times B$. Furthermore, the concept can be generalized to *n-ary* relations, represented as $R\subseteq A_1\times A_2\times\cdots\times A_n$.

Let R be a binary relation that is a subset of the Cartesian product $A\times A$, i.e., $R\subseteq A\times A$. If this relation is reflexive, symmetric, and transitive, it is called an *equivalence relation*, typically denoted by the symbol $\sim$. Under an equivalence relation, two elements $a,b\in A$ are said to be *equivalent* if $a\sim b$. The *equivalence class* of an element a, denoted by $[a]$, is the set of all elements in A that are equivalent to a. That is, the equivalence class of a is defined as $[a]:=\{b\in A : a\sim b\}$. An equivalence relation partitions the set A into disjoint subsets known as *equivalence classes*, collectively forming what is called the *quotient set*. The quotient set is denoted by $A/\sim$ and is defined as the set of all equivalence classes: $A/\sim\,:=[a]:a\in A$.

A binary relation that is reflexive, transitive, and antisymmetric is known as a *partial order*, typically denoted by the symbol $\preceq$. A set equipped with a partial order is called a *partially ordered set*, or *poset* for short. In a poset, an element $a\in A$ is considered *minimal* if there is no element $b\in A$ such that $b\preceq a$ and $b\neq a$. Similarly, an element a is said to be *maximal* if there is no element $b\in A$ such that $a\preceq b$ and $b\neq a$. A relation that is reflexive, transitive, antisymmetric, and total is called a *total order*, often denoted by the symbol $\leq$. A set endowed with a total order is referred to as a *totally ordered set*. In such a set A, the *maximum element*, denoted by $\max(A)$, satisfies $\max(A)\geq x$ for all $x\in A$, and the *minimum element*, denoted by $\min(A)$, satisfies $\min(A)\leq x$ for all $x\in A$.

■ **Example A.3** Let R be a relation that is a subset of the Cartesian product of the set of natural numbers $\mathbb{N}$ with itself, i.e., $R\subset\mathbb{N}\times\mathbb{N}$. In this relation, an ordered pair (a,b) belongs to R if and only if a is a divisor of b. The set

$\mathbb{N}$, together with the relation R, forms a partially ordered set. In this context, 1 is the unique minimal element, and every prime (e.g. 11) is maximal. ■

A *function* is defined as a binary relation $f \subseteq A \times B$ such that for each element $x \in A$, there exists at most one $y \in B$ for which $(x,y) \in f$. In this context, elements $(x,y) \in f$ are written as $f(x) = y$, and the function is denoted by $f : A \to B$. The set A is called the *domain* of f, and B is the *codomain*. The set $y \in B : \exists x \in A$ such that $f(x) = y$ is known as the *range* of f. If the relation is not defined for every $x \in A$, the function is called a *partial function*, and we write $f(x) \uparrow$ to indicate that f is undefined at x.

A function is said to be *injective* if, for all elements x and y, the condition $f(x) = f(y)$ implies that $x = y$. A function is *surjective* if, for every y in the codomain, there exists at least one x in the domain such that $f(x) = y$. A function is described as *bijective* if it is both injective and surjective. The *identity* function $I_A : A \to A$, defined by $I_A(a) = a$ for all $a \in A$, is an example of a bijective function. These concepts (function, partial function, injective, surjective, and bijective) can be extended to n-ary functions, which are functions of the form $f : A_1 \times A_2 \times \cdots \times A_n \to B$.

The *inverse* of a bijective function f, denoted by f^{-1}, is defined as $f(f^{-1}(x)) = f^{-1}(f(x)) = x$, for all x in the domain of f^{-1} and the range of f, respectively. Given two functions f and g, where the domain of f includes the range of g, the *composition* of f with g, denoted by $f \circ g$, is defined as $(f \circ g)(x) = f(g(x))$.

■ **Example A.4** In Section C.4, we will explore an alternative interpretation of a function as a procedure or algorithm that assigns an element of B to each element of A. For example, the following C code defines a partial function from $\mathbb{R}$ to $\mathbb{R}$, which is partial because $inv(0) \uparrow$:

```
double inv(double x) {
    return 1 / x;
}
```

■

The *characteristic function* of a set A is denoted by $1_A : A \to \{1, 0\}$, where $1_A(x) = 1$ if $x \in A$ and $1_A(x) = 0$ otherwise.

An infinite set A is said to be *countable* if there exists a bijective function that maps the elements of A onto the set of natural numbers $\mathbb{N}$. In contrast, a set is considered *uncountable* if it is neither finite nor countable. A set is said to have *countably many* elements if it is either finite or countably infinite.

■ **Example A.5** The sets $\mathbb{N}$, $\mathbb{Z}$, and $\mathbb{Q}$ are countable, whereas $\mathbb{R}$ is uncountable. ■

Considering a real number $x \in \mathbb{R}$, its *absolute value*, denoted by $|x|$, is defined as x if $x \geq 0$ and $-x$ if $x < 0$. The *ceiling* function of x, written as $\lceil x \rceil$, is the smallest integer greater than or equal to x. The *floor* function of x, denoted by $\lfloor x \rfloor$, is the largest integer less than or equal to x. Given two positive integers a and b, the *modulo* operation, written as $a \bmod b$, yields the remainder when a is divided by b.

For two functions f and g defined as $f, g : \mathbb{N} \to \mathbb{R}^+$, we say that $f(n)$ is of the *order of* $g(n)$, denoted $f(n) = O(g(n))$, if there exist positive constants $c > 0$ and m such that $f(n) \leq cg(n)$ for all integers $n \geq m$. In this context, g is called an *upper bound* for f.

A.2 Strings and Languages

Consider a non-empty finite set $\mathcal{S} = \{s_1, s_2, \ldots, s_q\}$, referred to as the *alphabet*. The elements of this set are called *symbols*. A *sequence* over $\mathcal{S}$ is defined as an ordered arrangement of symbols $x_1 x_2 \ldots x_n$, where each x_i belongs to $\mathcal{S}$. In the special case where the alphabet is $\mathcal{B} = \{0, 1\}$, such sequences are known as *binary sequences*. We use the term *string* to denote a finite sequence. This book primarily focuses on binary strings.

The *length* of a string s, denoted by $l(s)$, refers to the total number of symbols contained in s. The symbol λ is used to denote the *empty string*, which is defined as the unique string over $\mathcal{S}$ with length 0. Given a symbol $x \in \mathcal{S}$, the string consisting of x repeated n times is denoted by x^n. If $s = x_1 x_2 \ldots x_n$ is a string, its *reverse*, denoted by s^R, is given by $x_n x_{n-1} \ldots x_1$.

The set of all strings $s\_1s\_2 \ldots s\_n$ of length n over the alphabet $\mathcal{S}$ is denoted by $\mathcal{S}^n$[1]. We denote by $\mathcal{S}^+$ the union of all $\mathcal{S}^n$ for $n \geq 1$, and by $\mathcal{S}^*$ the set $\mathcal{S}^+ \cup \lambda$. Note that all strings in $\mathcal{S}^*$ have finite length. The term *Kleene closure* refers to $\mathcal{S}^*$.

■ **Example A.6** The following relations hold: the cardinality of the set of binary strings of length n is $d(\{s \in \mathcal{B}^* : l(s) = n\}) = 2^n$, and the cardinality of the set of binary strings of length up to n is $d(\{s \in \mathcal{B}^* : l(s) \leq n\}) = 2^{n+1} - 1$. ■

Given two strings s and t from $\mathcal{S}^*$, the *concatenation* of s and t, denoted as st, is the sequence obtained by placing the sequence of symbols in t immediately after the sequence in s. Consequently, the length of the concatenated string, $l(st)$, is the sum of the lengths of s and t. This indicates that $\mathcal{S}^*$ is closed under the operation of concatenation. Moreover, the set $\mathcal{S}^*$, together

[1] It is important to avoid confusing the set of strings of length n over an alphabet, $\mathcal{S}^n$, with the n-fold Cartesian product of a set, S^n. The use of calligraphic fonts helps distinguish between alphabets and other sets.

with concatenation, forms a *free monoid*. This means that concatenation is associative ($s(tr) = (st)r$), and that there exists an identity element, specifically, the empty string λ, for which $\lambda a = a\lambda = a$ holds for any string a.

A string s is called a *substring* of a string t if there exist strings u and v (possibly empty) such that $t = usv$. If there exists a string u such that $t = su$, then s is said to be a *prefix* of t, denoted by $s <_p t$. A subset $S \subset \mathcal{S}^*$ is described as *prefix-free* if, for any $s,t \in S$, the condition $s <_p t$ implies $s = t$. Given two sets of strings $S,T \subset \mathcal{S}^*$, the (left) *quotient* $S^{-1}T$ is defined as the set of residual strings obtained from T by removing a prefix in S; formally, $S^{-1}T = \{t \mid st \in T \wedge s \in S\}$.

We denote the *self-delimited* form of a string $s \in \mathcal{S}^*$ by $\bar{s}$, and define it as $\bar{s} = 1^{l(s)}0s$. Consequently, the length of $\bar{s}$, denoted $l(\bar{s})$, is given by $l(\bar{s}) = 2l(s) + 1$, meaning it is twice the length of s plus one.

■ Example A.7 The set $\bar{\mathcal{S}}^*$, consisting of all self-delimited strings from $\mathcal{S}^*$, is prefix-free. ■

In cases where $\mathcal{S}$ is a totally ordered set, we can define a total order on $\mathcal{S}^*$. This ordering, known as *shortlex ordering*, arranges sequences primarily by length, with shorter sequences appearing first. Among sequences of the same length, lexicographical order is used to break ties.

■ Example A.8 Given $\mathcal{S} = a,b,c$ with $a < b < c$, the shortlex order on $\mathcal{S}^*$ produces the sequence $\lambda < a < b < c < aa < ab < \ldots < cc < aaa < aab < \ldots < ccc < \ldots$ ■

For any arbitrary object O, we use the notation $\langle O \rangle$ to denote its string based representation, assuming the existence of a standard encoding scheme. For objects $O_1, O_2, \ldots, O_k$, the expression $\langle O_1 O_2 \ldots O_k \rangle$ refers to the plain concatenation of their string representations: $\langle O_1 \rangle \langle O_2 \rangle \ldots \langle O_k \rangle$. By contrast, the notation $\langle O_1, O_2, \ldots, O_k \rangle$ indicates a structured concatenation that allows for the decoding and unique identification of each individual object. For example, this may be implemented as $\langle \bar{O}_1 \rangle \langle \bar{O}_2 \rangle \ldots \langle \bar{O}_k \rangle$.

■ Example A.9 Natural numbers can be represented by binary strings via the following encoding method: $\langle 0 \rangle = \lambda$, $\langle 1 \rangle \to 0$, $\langle 2 \rangle \to 1$, $\langle 3 \rangle \to 00$, $\langle 4 \rangle \to 01$, $\langle 5 \rangle \to 10$, $\langle 6 \rangle \to 11$, $7 \to 000$, and so on. Therefore, the pair of numbers $\langle 3,7 \rangle$ would be represented as 110001110000. Given this particular encoding, it follows that $l(\langle n \rangle) = \lfloor \log_2(n+1) \rfloor$. ■

A *language*, denoted by L, over an alphabet $\mathcal{S}$, is defined as a subset of strings, that is, $L \subseteq \mathcal{S}^*$. The individual elements of L are called *words*. The unique language that contains no words is referred to as the *empty language*, and is denoted by $L = \varnothing$.

Consider two languages L_1 and L_2 over a common alphabet $\mathcal{S}$. Several standard operations can be applied to these languages. The *union* of L_1 and L_2 is defined as $L_1 \cup L_2 = w \in \mathcal{S}^* \mid w \in L_1$ or $w \in L_2$. The *intersection* of L_1 and L_2 is given by $L_1 \cap L_2 = w \in \mathcal{S}^* \mid w \in L_1$ and $w \in L_2$. The *complement* of L_1 is defined as $\overline{L_1} = w \in \mathcal{S}^* \mid w \notin L_1$. Finally, the *Kleene closure* of L_1, denoted L_1^*, is defined as $L_1^* = \lambda \cup wz \mid w \in L_1$ and $z \in L_1^*$.

Languages can be systematically generated using a finite set of string rewriting rules, commonly referred to as grammars. A *grammar*, denoted by G, is defined as a 4-tuple (N, Σ, P, S), where: $N \subseteq \mathcal{S}$ is a finite set of *nonterminal symbols*; $\Sigma \subseteq \mathcal{S}$ is a finite set of *terminal symbols*; P is a finite set of *production rules* of the form $(\Sigma \cup N)^* N (\Sigma \cup N)^* \to (\Sigma \cup N)^*$; and $S \in N$ is a distinguished *start symbol*. Each production rule allows one string of symbols to be rewritten into another, beginning with the start symbol and proceeding through successive applications of the rules.

■ **Example A.10** Consider the alphabet $\mathcal{S} = \{S, a, b\}$, and define the grammar (N, Σ, P, S) where $N = \{S\}$, $\Sigma = \{a, b\}$, $P = \{S \to aSb, S \to ba\}$, and the start symbol is $S \in N$. This grammar generates the language $L = \{a^n bab^n \mid n \geq 0\} = \{ba, abab, aababb, aaababbb, \ldots\}$. ■

The *Chomsky hierarchy* is a classification scheme for grammars, organized according to their expressive power, that is, the types of languages they are capable of generating. The hierarchy, arranged from the most to the least restrictive class of grammars, is described as follows (where a denotes a terminal symbol; A, B are nonterminal symbols; and α, β, and γ are strings composed of terminals and/or nonterminals):

Type-3 Known as *regular grammars*. In these grammars, the left-hand side of each production rule consists of a single nonterminal symbol. The right-hand side must be either the empty string, a single terminal symbol, or a terminal symbol followed by a nonterminal symbol. Formally, the rules are of the form $A \to \lambda$, $A \to a$, or $A \to aB$.

Type-2 Referred to as *context-free grammars*. In this class, the left-hand side of each production rule is exactly one nonterminal symbol. The general form of the rules is $A \to \alpha$.

Type-1 These are *context-sensitive grammars*. Here, production rules allow a nonterminal to be replaced by a string in a specific context. The rules take the form $\alpha A \beta \to \alpha \gamma \beta$.

Type-0 This category includes *recursively enumerable grammars*, which place no restrictions on the structure of production rules. These can be written in the general form $\gamma \to \alpha$.

■ **Example A.11** The grammar presented in Example A.10 is a Type-2 grammar, that is, a context-free grammar. ■

The *Backus-Naur form* (BNF) is a notation system specifically designed to describe context-free grammars. It is widely used in computer science to formally specify the syntax of programming languages and communication protocols. A BNF grammar consists of a set of production rules structured as follows:

```
<symbol> ::= __expression__
```

Here, <symbol> denotes a non-terminal symbol, __expression__ represents a sequence of terminal and/or non-terminal symbols, and ::= signifies that the symbol on the left-hand side can be replaced by the expression on the right. Multiple alternatives for the expression can be provided in a single rule by separating them with a vertical bar |, indicating that any one of the alternatives may be chosen during substitution. Symbols that never appear on the left-hand side of any production rule are considered terminal symbols. In contrast, those that do appear on the left-hand side are non-terminal symbols and are conventionally enclosed in angle brackets <>. The non-terminal symbol on the left-hand side of the first production rule is designated as the start symbol.

■ **Example A.12** The grammar introduced in Example A.10 can be expressed in Backus-Naur form using the following production rule:

```
<string> ::= a <string> b | ba
```

■

A.3 Counting Methods

Combinatorics, a specialized branch of mathematics, is primarily concerned with the study of discrete objects and the relationships among them. Its central themes include the counting, arrangement, and selection of such objects, along with the methods used to carry out these tasks. Combinatorics provides a powerful set of tools for analyzing large collections of objects that satisfy specific properties. In this section, we revisit the most important results in combinatorics, focusing on their interpretation in terms of sets and ordered lists.

The *multiplication rule* is a fundamental principle that determines the number of possible outcomes in the Cartesian product of sets. According to this rule, if there are k sets $A_1, A_2, \ldots, A_k$, and each set A_i contains n_i elements (for $i = 1, \ldots, k$), then the Cartesian product $A_1 \times A_2 \times \ldots \times A_k$ contains exactly $n_1 n_2 \ldots n_k$ elements. In particular, if a set A has n elements, then the k-fold Cartesian product A^k contains n^k elements.

The *inclusion-exclusion principle* determines the cardinality of the union of multiple sets based on the sizes of the individual sets and all possible intersections among them. Given k sets $A_1, A_2, \ldots, A_k$, the formula is:

$$d\left(\bigcup_{i=1}^{k} A_i\right) = \sum_{i=1}^{k} d\left(A_i\right) - \sum_{i<j} d\left(A_i \cap A_j\right) + \sum_{i<j<l} d\left(A_i \cap A_j \cap A_l\right) - \\ - \sum_{i<j<l<m} d\left(A_i \cap A_j \cap A_l \cap A_m\right) + \ldots + (-1)^{k+1} d\left(A_1 \cap \ldots \cap A_k\right)$$

Permutations refer to the number of distinct ways in which the elements of a set can be arranged. Let A be a set with n elements. The number of ordered selections of k elements from n distinct elements without replacement, denoted by $P_{n,k}$, is given by $P_{n,k} = n(n-1)\ldots(n-k+1)$. In the case where $k = n$, the total number of permutations is $P_{n,n} = n(n-1)\cdots 1 = n!$ where $n!$ is read as "n factorial".

■ **Example A.13** Consider the set $\{a, b, c\}$. There are six distinct permutations of its elements: $\{a, b, c\}$, $\{a, c, b\}$, $\{b, a, c\}$, $\{b, c, a\}$, $\{c, a, b\}$, and $\{c, b, a\}$. Each permutation represents a unique ordering of the elements in the original set. ■

The *pigeonhole principle* is a simple yet powerful concept. It asserts that if there are more pigeons than pigeonholes, then at least one pigeonhole must contain more than one pigeon. More formally, if n items are distributed among m containers and $n > m$, then at least one container must hold more than one item.

The logarithmic form of *Stirling's* approximation is particularly effective for estimating large factorials:

$$\log(n!) \approx \frac{1}{2}\log(2\pi) + \left(n + \frac{1}{2}\right)\log(n) - n$$

Numerous counting problems involve determining the number of subsets of a specific size within a given set. For a set with n elements, the total number of possible subsets is 2^n, including both the empty set and the set itself. The number of subsets of size k, also known as the number of *combinations* of k elements from a set of n, is denoted by $C_{n,k}$ and computed using the formula $C_{n,k} = \frac{P_{n,k}}{k!} = \frac{n!}{k!(n-k)!}$. The symbol $\binom{n}{k}$ also represents the value $C_{n,k}$, which is known as the *binomial coefficient*. It is known that $\binom{n}{0} = \binom{n}{n} = 1$ for all n, and $\binom{n}{k} = \binom{n}{n-k}$ for all $k = 0, 1, \ldots, n$. Additionally, $\binom{n}{k} = 0$ whenever $k > n$.

■ **Example A.14** Consider the set $\{a, b, c, d\}$. There are 4 combinations of size 3: $[a, b, c]$, $[a, b, d]$, $[a, c, d]$, and $[b, c, d]$. Since combinations disregard order, $[a, c, d]$ and $[d, c, a]$ represent the same combination. ■

The *multinomial coefficient*, a generalization of the binomial coefficient to more than two categories, represents the number of ways to partition a set of objects into a fixed number of subsets, each containing a specified number of elements. Suppose we have a set with n elements that is to be divided into k subsets of sizes $n_1, n_2, \ldots, n_k$, respectively. The multinomial coefficient, denoted as $\binom{n}{n_1, n_2, \ldots, n_k}$, gives the number of such possible partitions and is calculated by the formula:

$$\binom{n}{n_1, n_2, \ldots, n_k} = \frac{n!}{n_1! n_2! \ldots n_k!}$$

where $n_1 + n_2 + \cdots + n_k = n$.

The different combinations of replacement and ordering lead to four distinct counting scenarios, as summarized below. These conditions depend on whether the order of selection matters and whether elements can be selected more than once.

	Without replacement	With replacement
Ordered	$\frac{n!}{(n-r)!}$	n^r
Unordered	$\binom{n}{r}$	$\binom{n+r-1}{r}$

In the first row, we consider ordered selections: without replacement, the number of ways corresponds to the number of permutations of r elements from a set of n; with replacement, each of the r positions can independently be filled with any of the n elements. In the second row, we consider unordered selections: without replacement, the count is given by the standard binomial coefficient; with replacement, the result corresponds to the number of multisets of size r formed from n distinct elements.

A.4 Matrices

A *matrix*, denoted by A, of order $m \times n$ is a rectangular array consisting of m *rows* and n *columns*, filled with a sequence of mn scalars. It is typically written as:

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{pmatrix}$$

The *entry* a_{ij} denotes the element located at the i-th row and j-th column of the matrix A. The *set of all matrices* of order $m \times n$ is denoted by $\mathcal{M}_{m \times n}$. A *row matrix* is any matrix in the set $\mathcal{M}_{1 \times n}$, while a *column matrix* belongs to $\mathcal{M}_{m\times 1}$. A *square matrix* is an element of $\mathcal{M}_{n\times n}$. The entries a_{ii} of a square matrix form its *main diagonal*. A *diagonal matrix* is a square matrix in which all entries outside the main diagonal are zero. The *identity matrix*, denoted by I, is a special diagonal matrix with all diagonal entries equal to 1.

The *transpose* of a matrix $A \in \mathcal{M}_{m\times n}$ is defined as the matrix $A^T \in \mathcal{M}_{n\times m}$, whose entry at position (i,j) is equal to the entry at position (j,i) in A. If $A = A^T$, then A is called a *symmetric matrix*. A *submatrix* of a matrix is obtained by deleting one or more rows and/or columns.

■ **Example A.15** Consider the square matrix $A = \left(\begin{smallmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{smallmatrix}\right)$. The entry in position $(2,3)$ is 6, and the main diagonal consists of the elements 1, 5, and 9. The transpose of A is $A^T = \left(\begin{smallmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{smallmatrix}\right)$. The matrix $B = \left(\begin{smallmatrix} 1 & 3 \\ 4 & 6 \end{smallmatrix}\right)$ is a submatrix of \$A\$. ■

The addition of two matrices A and B of the same size produces a new matrix $A+B$, where each entry at position (i,j) is defined as $(A+B)_{ij} = a_{ij} + b_{ij}$. Matrix addition is associative, i.e., $(A+B)+C = A+(B+C)$, and commutative, i.e., $A+B = B+A$. It has a neutral element, the zero matrix, such that $A + 0_{m\times n} = A$, and each matrix has an additive inverse, since $A + (-A) = 0_{m\times n}$.

The product of a scalar λ and a matrix A yields another matrix, denoted by λA, in which each entry at position (i,j) is given by $(\lambda A)_{ij} = \lambda a_{ij}$. Scalar multiplication is distributive over matrix addition, i.e., $\lambda(A+B) = \lambda A + \lambda B$, and over scalar addition, i.e., $(\alpha+\beta)A = \alpha A + \beta A$. It is also associative with respect to scalar multiplication, i.e., $(\alpha\beta)A = \alpha(\beta A)$, and has a multiplicative identity, since $1A = A$.

The product of two matrices $A_{m\times n}$ and $B_{n\times p}$ results in a matrix $AB_{m\times p}$, where each entry at position (i,j) is given by $(AB)_{ij} = \sum_{k=1}^{n} a_{ik}b_{kj}$. Matrix multiplication is associative, meaning that $(AB)D = A(BD)$. It has a left identity element: $AI_n = A$, and a right identity element: $I_m A = A$. It is also compatible with scalar multiplication, so that $\alpha(AB) = (\alpha A)B = A(\alpha B)$. Furthermore, matrix multiplication is distributive over addition: from the right, $A(B+C) = AB + AC$, and from the left, $(B+C)D = BD + CD$.

The transpose operation satisfies the following properties: $(A+B)^T = A^T + B^T$, $(\lambda A)^T = \lambda A^T$, and $(AB)^T = B^T A^T$.

■ **Example A.16** Given the matrices $A = \left(\begin{smallmatrix} 1 & 2 \\ 3 & 5 \end{smallmatrix}\right)$ and $B = \left(\begin{smallmatrix} 5 & 6 \\ 7 & 8 \end{smallmatrix}\right)$ we have that $A+B = \left(\begin{smallmatrix} 6 & 8 \\ 10 & 13 \end{smallmatrix}\right)$, $2A = \left(\begin{smallmatrix} 2 & 4 \\ 6 & 10 \end{smallmatrix}\right)$ and $AB = \left(\begin{smallmatrix} 19 & 22 \\ 50 & 58 \end{smallmatrix}\right)$. ■

A square matrix A is said to be *invertible* or *non-singular* if there exists a matrix B such that $AB = BA = I$. If A is non-singular, the matrix B is unique and is called the *inverse* of A, denoted by A^{-1}. A matrix A is called *orthogonal* if its transpose is equal to its inverse, that is, $A^T = A^{-1}$. The columns and rows of an orthogonal matrix are referred to as *orthonormal vectors*.

The *determinant* is a special scalar value that can be computed from the elements of a square matrix. For a matrix A, the determinant is denoted by $\det(A)$. It can be calculated using the Leibniz formula:

$$\det(A) = \sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) \cdot a_{1,\sigma(1)} \cdot a_{2,\sigma(2)} \cdots a_{n,\sigma(n)}$$

where S_n denotes the set of all permutations of the integers 1 to n, and $\operatorname{sgn}(\sigma)$ is the sign of the permutation σ, equal to $+1$ for even permutations and -1 for odd permutations. A matrix is invertible if and only if its determinant is nonzero.

■ **Example A.17** The determinant of a 3×3 matrix $A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix}$ is computed as:

$$\det(A) = aei + bfg + cdh - ceg - bdi - afh$$

■

For a given matrix A, the *rank*, denoted as $\operatorname{rank}(A)$, is the maximum number of linearly independent rows or columns in the matrix.

A number λ and a nonzero vector $\mathbf{v}$ such that $A\mathbf{v} = \lambda\mathbf{v}$ are called an *eigenvalue* and an *eigenvector* of A, respectively.

Matrix decomposition is the process of transforming a matrix into a more tractable form while preserving certain properties, such as the determinant or rank. The *singular value decomposition* (SVD) of a matrix A of order $m \times n$ is a factorization of the form $A = U\Sigma V^T$, where U is an $m \times m$ orthogonal matrix, Σ is an $m \times n$ diagonal matrix with nonnegative entries, and V^T is the transpose of an $n \times n$ orthogonal matrix.

A.5 Graphs

A *graph*[2] G is defined as an ordered pair (V, E), where V is a set of *vertices*, and E is a set of *edges*. Each element of E is an unordered pair $\{u, v\}$, where $u, v \in V$ are distinct (loops are not allowed). Two vertices u and v are said to be *adjacent* if $\{u, v\} \in E$; in that case, they are referred to as the *endpoints* of the edge. If the set V is infinite, the graph is called an *infinite graph*. In this book, however, we consider only finite graphs. Given a graph $G = (V, E)$, its

[2]The definition of a graph given here corresponds to that of a *simple graph*, as commonly found in discrete mathematics literature.

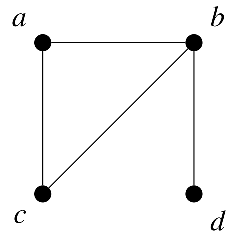


Figure A.2: An Example of Graph

adjacency matrix is a square matrix of size $d(V) \times d(V)$, denoted A, where $A_{uv} = 1$ if $\{u, v\} \in E$, and $A_{uv} = 0$ otherwise.

Graphs are typically depicted as a set of dots (vertices) connected by lines (edges).

■ **Example A.18** Let $V = a, b, c, d$ and $E = a, b, a, c, a, d, b, c$. The graph $G = (V, E)$ is illustrated in Figure A.2. ■

When a vertex v is an endpoint of an edge e, the edge e is said to be *incident* on v. The *degree* of a vertex v, denoted $\deg(v)$, is the number of edges incident on v. A vertex with degree zero is called an *isolated vertex*, while a vertex with degree one is termed a *pendant vertex*. The *neighborhood* of a vertex v, denoted $N(v)$, is the set of all vertices adjacent to v. For a subset $A \subset V$, the neighborhood of A is defined as $N(A) = \bigcup_{v \in A} N(v)$. A *path* in a graph is a sequence of distinct vertices $v_0, v_1, \ldots, v_k$ such that v_i and v_{i+1} are adjacent for each $0 \le i < k$. The path is called a *simple path* if no vertex is repeated. A graph is said to be *connected* if there exists a path between every pair of vertices. If $v_0 = v_k$, the path is called a *cycle*. A cycle is *simple* if it includes at least three vertices and only the first and last vertices are repeated.

■ **Example A.19** In a graph $G = (V, E)$, the *handshaking theorem* states that $\sum_{v \in V} \deg(v) = 2m$, where $m = d(E)$, since each edge contributes to the degree count of two vertices. ■

If the vertex pairs (u, v) are arranged as ordered pairs, the graph is called a *directed graph*. In this context, u is referred to as the *initial vertex* and v as the *terminal vertex*. For a directed graph G, the *in-degree* of a vertex v, denoted by $\text{indeg}(v)$, is the number of edges for which v is the terminal vertex. The *out-degree* of a vertex v, denoted by $\text{outdeg}(v)$, is the number of edges for which v is the initial vertex. A directed graph is said to be *strongly connected* if there exists a directed path from every vertex to every other vertex. Directed graphs are typically represented using arrows instead of lines to indicate the direction of edges.

A graph G is classified as emphbipartite if its vertex set V can be partitioned into two subsets V_1 and V_2 such that every edge of G connects a vertex from V_1 to a vertex from V_2. Bipartite graphs are commonly denoted as $G = (V_1, V_2, E)$. The degrees of the vertices in a bipartite graph satisfy the *degree sum formula*, $\sum_{u \in V_1} \deg(u) = \sum_{v \in V_2} \deg(v) = d(E)$.

A graph $G(V', E')$ is called a *subgraph* of a graph $G(V, E)$ if $V' \subseteq V$ and $E' \subseteq E$, where every edge in E' has both endpoints in V'. A graph G is said to be a *labeled graph* if its edges and/or vertices are assigned specific data. In particular, if each edge e in G is assigned a nonnegative number $w(e)$, then $w(e)$ is referred to as the *weight* of the edge e.

A specific type of graph that plays a fundamental role in this book is the *tree*. A tree is defined as a non-empty graph in which any pair of vertices is connected by a unique path. A tree typically includes a specially designated vertex known as the *root*, and every edge is conceptually oriented away from this root.

■ **Example A.20** An alternative definition of a tree, grounded in set theory, characterizes it as a partially ordered set $(T, <)$ such that for every $t \in T$, the set $S = s \in T : s < t$ has a least element, that is, an element smaller than all other elements in S. ■

Given a tree T, for any vertex v other than the root, the *parent* of v is the unique vertex u such that there is an edge directly connecting u to v. Conversely, if u is the parent of v, then v is called a *child* of u. Any other vertex in the tree that shares the same parent as v is referred to as a *sibling* of v. The *ancestors* of a vertex consist of all vertices along the unique path from the root to that vertex, excluding the vertex itself but including the root. The *descendants* of a vertex v are all vertices that have v as an ancestor. A vertex with no children is called a *leaf*, whereas vertices that have one or more children are known as *branches*. The *depth* of a vertex v is the length of the unique path from the root to v. The *height* of the tree is the maximum depth among all its vertices.

■ **Example A.21** For the tree illustrated in Figure A.3, the root vertex is a; c is the parent of d, so d is a child of c; d and g are siblings; the ancestors of d are a and c; the descendants of c are d, e, and f; the leaf vertices are b, e, f, and g; a and c are branches; the depth of d is 3; the height of the tree is 4. ■

Given a vertex v in a tree, the *subtree* rooted at v is the subgraph that consists of v, all its descendants, and all edges connecting these vertices. A tree is called a *k-ary tree* if each branch has at most k children. If every branch has exactly k children, the tree is referred to as a *full k-ary tree*. A k-ary tree with $k = 2$ is specifically known as a *binary tree*. A k-ary tree of

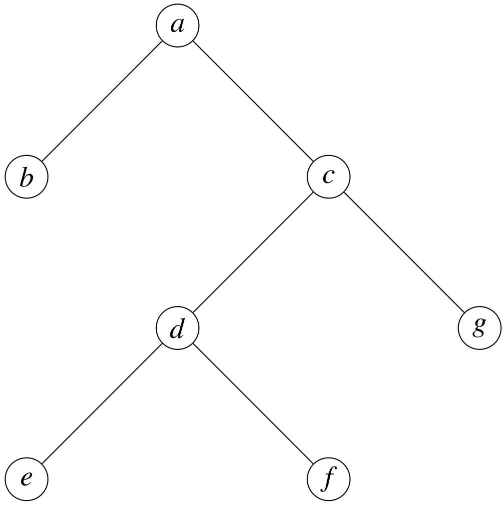


Figure A.3: An Example of a Tree

height h is said to be *balanced* if all its leaves are located at depth h or $h-1$.

■ **Example A.22** A tree with n vertices contains exactly $n-1$ edges. A full k-ary tree with i branches contains $m = ki+1$ vertices. ■

The procedure of visiting each node in a tree exactly once is known as *tree traversal*. Traversal methods are categorized based on the order in which nodes are visited, with the two main types being *depth-first* and *breadth-first*. In a *depth-first traversal*, the algorithm starts at the root node and explores as far as possible along each branch before backtracking to explore siblings. There are three common strategies for visiting nodes in a depth-first manner: *in-order*, *pre-order*, and *post-order*.

The following code snippet, written in a C-like syntax, demonstrates a recursive pre-order depth-first traversal algorithm used to print the nodes of a binary tree:

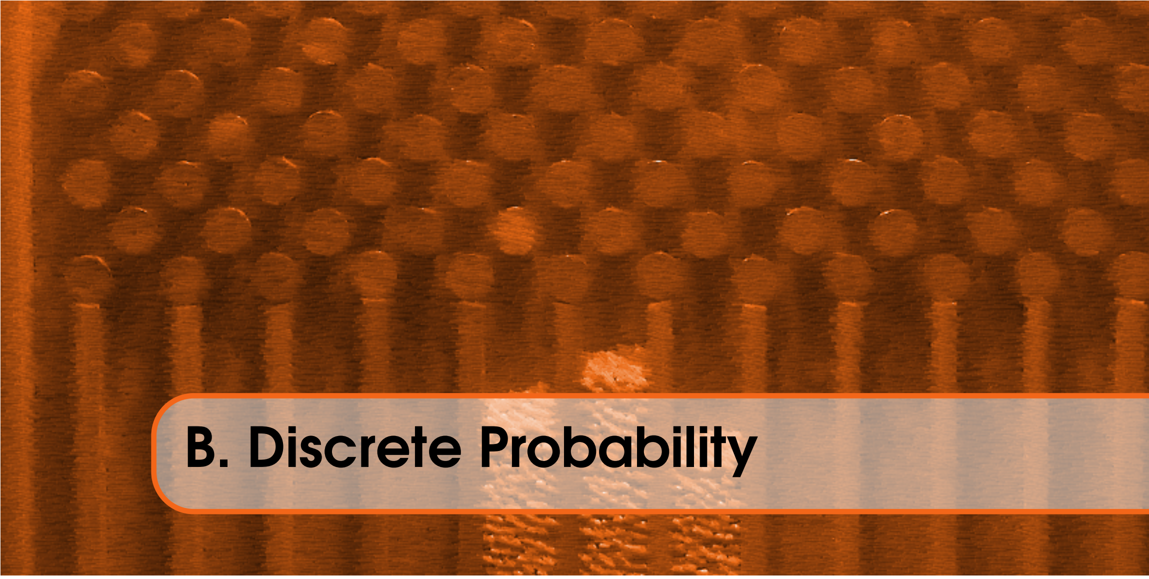
```
void print_tree(binary_tree *tree) {
    if (!is_empty(tree)) {
        printf("%c\n",tree->node);
        print_tree(tree->left_branch);
        print_tree(tree->right_branch);
    }
}
```

Conversely, in a *breadth-first traversal*, the algorithm begins at the root of the tree and explores all nodes at the current depth level before proceeding to nodes at the next depth level. Implementing breadth-first traversal typically requires the use of auxiliary data structures, such as queues. For examples and implementation details of such algorithms, please refer to the references section.

■ **Example A.23** For the tree described in Example **??**, a pre-order depth-first traversal produces the string "abcdefg". In contrast, a pre-order breadth-first traversal yields the string "abcdgef". ■

References

The book *Discrete Mathematics* by Johnsonbaugh [Joh09] is designed for undergraduate students enrolled in a one- or two-semester course in discrete mathematics, and it provides thorough coverage of fundamental topics in the field. *Introduction to the Theory of Computation* by Sipser [Sip12] offers a comprehensive and accessible introduction to key topics in computational theory. It is widely praised for its clear presentation and in-depth treatment of automata, formal languages, and complexity theory. *Introduction to Algorithms* by Cormen et al. [Cor+90], often referred to as "CLRS" after the initials of its authors, is a foundational text in the study of algorithms. It covers a broad range of subjects, including graph algorithms, and is known for its depth and rigor. Lastly, *Matrix Computations* by Golub and Van Loan [GV13] focuses on a wide array of topics in matrix theory, with particular emphasis on computational techniques—making it especially valuable for those involved in numerical and computational studies.



B. Discrete Probability

The purpose of models is not to fit the data
but to sharpen the questions.
Samuel Karlin

Probability theory is the branch of mathematics that studies random experiments and phenomena. It assigns a numerical value to each possible outcome of an experiment, reflecting how likely that outcome is to occur. Even when the outcome of a specific experiment cannot be predicted in advance, probability theory allows us to analyze its properties and derive meaningful insights. For example, while we cannot foresee the next number drawn in a lottery, probability theory helps explain why spending all our savings on lottery tickets is an unwise strategy for becoming wealthy.

The significance of probability theory goes far beyond games of chance. It forms the mathematical foundation of statistical inference, allowing us to draw conclusions from data, and it underpins many machine learning algorithms used for classification and prediction with large datasets. Moreover, probability theory plays a vital role in fields such as finance, risk management, and the natural sciences, where understanding uncertainty and variability is crucial.

In this chapter, we focus on the area of discrete probability. In this version of the theory, the possible outcomes of an event are either finite or, at most, countably infinite. Our interest in discrete probability arises for two main reasons: first, due to its practical applications in learning from data; and second, because it has deep connections to several theoretical concepts explored in this book, such as the length of optimal codes, the probability that a random machine will halt, and the derivation of universal distributions based on Kolmogorov complexity. All of these connections are directly relevant to our theory of nescience.

We will cover only the most important concepts and results of probability theory. The material has been selected based on its relevance to the theory of nescience. For instance, moment-generating functions are not included. For a more comprehensive introduction to probability theory, refer to the references at the end of this chapter.

Our approach to probability theory will be formal and axiomatic. We will begin by stating a basic set of fundamental axioms, from which we will derive the main results and properties. Axioms are essential in mathematical theory, as they provide the foundation for constructing a consistent, universal, and rigorous framework. In the context of probability theory, they allow us to define and manipulate the elusive concept of probability in a way that is both precise and widely applicable.

B.1 Interpretations of Probability

The concept of *probability* presents a profound intellectual challenge. Consider the case of rolling a die and computing the probability of obtaining an even number. The die has six distinct outcomes, and since half of them are even, we conclude that the probability is $3/6$, or equivalently $1/2$. This reflects the *classical interpretation* of probability, which states that in an experiment where all finite outcomes are equally likely, the probability of an event is given by the ratio of favorable outcomes to the total number of possible outcomes.

However, this interpretation faces a problem of circularity: .the notion of "equally likely" often assumes a symmetry in the outcomes, but in formal contexts this can be criticized for relying implicitly on the very concept of probability it seeks to define. An alternative approach is the *principle of indifference*, which holds that in the absence of any relevant evidence, all outcomes should be assigned equal probability. This principle, however, breaks down when there is evidence suggesting that the outcomes are not equally probable. This principle, however, only applies in the absence of evidence. When information is available, such as knowing the die is loaded, it cannot be justifiably used, and the assumption of equally likely outcomes breaks down.

The *frequentist interpretation* of probability posits that one should roll the die multiple times and compare the frequency of even outcomes to the total number of rolls. The fundamental idea is to repeat the experiment under similar conditions and assign to each outcome a probability equal to its relative frequency.

This interpretation, however, faces two major limitations. First, the notion of "similar conditions" is vague and lacks a precise definition; after all, if conditions were exactly identical in a deterministic system, the outcomes would also be identical. In practice, the assumption is that conditions are similar enough to allow statistical regularities to emerge. Second, the concept of a "large number of repetitions" is ill-defined—technically, the experiment must be repeated an infinite number of times.

From a practical standpoint, implementing the frequentist interpretation presents significant challenges. Some experiments, such as estimating the probability of a candidate winning an election, cannot be repeated. Moreover, probability is defined only in the context of a sequence of trials, which makes it impossible to compute the probability of a single, non-repeatable event. Finally, the interpretation assumes the existence of a limiting relative frequency, a condition that is not always satisfied, as illustrated by certain financial time series.

The *subjective interpretation*, representing a third approach to the concept of probability, proposes assigning probabilities to events based on our degree of belief: the stronger our conviction that an event will occur, the higher the probability we assign to it. However, not all possible probability assignments are acceptable; certain coherence conditions must be met. For example, assigning probabilities in a way that guarantees a loss in a betting system, a scenario known as a *Dutch book*, violates these conditions.

It turns out that the conditions necessary and sufficient to avoid such inconsistencies align precisely with the axioms of probability that will be introduced later. Thus, we are free to assign probabilities according to our beliefs, as long as these assignments remain consistent with those axioms.

A key limitation of the subjective interpretation is that degrees of belief can vary widely between individuals. The *Bayesian interpretation* offers a refinement: we begin with an initial (prior) assignment of probabilities and update them as new evidence becomes available. As more evidence is accumulated, revised probabilities tend to converge to values that are more consistent with observed data, and under certain conditions, may approximate the long-run frequencies or objective probabilities (if such exist). Nevertheless, assigning probabilities to an infinite number of events is generally infeasible for humans.

Currently, the notion of probability is defined axiomatically through the *axiomatic interpretation*. This approach abandons the attempt to define probability explicitly, and instead accepts certain fundamental properties as given.

Mathematically, probability is defined as a real number between 0 and 1, where a probability of 0 corresponds to an impossible event, and a probability of 1 corresponds to an event that is certain to occur. Intuitively, however, we often express probabilities as percentages, for example, saying that it will rain tomorrow with a 70% probability, which is also valid interpretation of the concept of probability.

Additional properties are also required. For example, if two events A and B, with probabilities $P(A)$ and $P(B)$ respectively, are disjoint, then the probability of either A or B occurring should be $P(A)+P(B)$. If A and B can occur simultaneously and are independent (independence being a concept that is mathematically well-defined but often conceptually subtle), then the probability of both occurring together should be $P(A)P(B)$. Furthermore, the probability of A occurring given that B has already occurred should equal the fraction of the probability of A that also lies within B.

B.2 Foundations of Probability Theory

Probability theory is fundamentally concerned with assigning numerical values to specific events drawn from a sample space [1].

Definition B.2.1 Given $(\Omega, \mathcal{A})$ as a field over a non-empty discrete set, Ω is called the *sample space*, its elements are called *outcomes*, and the elements of $\mathcal{A}$ are referred to as *events*. Specifically, Ω is known as the *certain event*, while the empty set $\varnothing$ is called the *impossible event*.

As discussed in Section A.1, since $(\Omega, \mathcal{A})$ is a field, it follows that $\Omega \in \mathcal{A}$ and $\varnothing \in \mathcal{A}$. Moreover, the union of a finite collection of events is also an event: $A_1 \cup A_2 \cup \ldots \cup A_n \in \mathcal{A}$, and likewise, the intersection of a finite collection of events is an event: $A_1 \cap A_2 \cap \ldots \cap A_n \in \mathcal{A}$.

As mentioned in the introduction to this chapter, our primary focus is

[1] The term "event" in this context may seem somewhat counterintuitive, as it typically suggests that something has happened, an implication not always applicable in the mathematical setting. For example, consider the sample space of all possible outcomes from tossing a fair coin. A subset of this sample space might be the empty set, which represents no outcome at all. From a conventional perspective, this does not correspond to anything "happening," which may confuse readers unfamiliar with the mathematical usage of the term. Nevertheless, for consistency and clarity, we will continue to use the term "events" to refer to subsets of the sample space.

on discrete mathematics. Accordingly, we will concentrate on probabilities defined over discrete sets, whether finite or countably infinite. Extending the concept of probability to continuous sets requires the use of σ-algebras of sets instead of fields, along with the tools of measure theory. On a philosophical level, one might argue that all sample spaces must be countable, since physical measurements cannot be made with infinite precision. In practice, this is indeed the case: any empirical observation is subject to finite resolution.

The standard axiomatization used in probability theory is encapsulated in the framework of the *Kolmogorov axioms*[2].

Definition B.2.2 (*Kolmogorov's Axioms*) A *probability* is a real number $P(A) \in \mathbb{R}$ assigned to each event $A \in \mathcal{A}$ in the field $(\Omega, \mathcal{A})$, subject to the following axioms:

Axiom 1 Non-negativity: For all events $A \in \mathcal{A}$, we have $P(A) \geq 0$.
Axiom 2 Normalization: The probability of the certain event is one, i.e., $P(\Omega) = 1$.
Axiom 3 Additivity: For any finite sequence of pairwise disjoint events $A_1, A_2, \ldots, A_n \in \mathcal{A}$, the probability of their union equals the sum of their individual probabilities:

$$P\left(\bigcup_{i=1}^{n} A_i\right) = \sum_{i=1}^{n} P(A_i).$$

The triplet $(\Omega, \mathcal{A}, P)$ is called a *probability space*.

Despite their foundational importance, the Kolmogorov axioms present certain limitations. While they establish essential constraints on any probability function (such as non-negativity, normalization, and additivity) they do not prescribe how to assign probabilities to specific events. In other words, the axioms define the formal rules that probabilities must satisfy but remain silent on how those probabilities should be determined in practice. This is a consequence of their high level of generality: any mathematical structure that satisfies these properties can be regarded as a valid probability model. As such, they are abstract enough to encompass not only probability measures but also other normalized physical measures such as mass, volume, or charge.

From an intuitive standpoint, it might seem more natural to assign probabilities directly to the individual elements of the sample space, especially in

[2] In discrete probability theory, the sample space consists of a finite or countably infinite set of distinct outcomes. As a result, events are typically made up of individual, separable outcomes. Since probabilities are assigned directly to these discrete events, only finite unions of disjoint events need to be considered in Axiom 3 to account for all practical cases.

the discrete case where each outcome is well, defined and countable. However, in the formal theory of probability, probabilities are assigned to events, which are subsets of the sample space. This approach, though less intuitive at first glance, ensures compatibility with the measure-theoretic framework that underlies modern probability theory. In the continuous case, individual outcomes (such as a specific real number) typically have probability zero, and probability must be defined directly over sets (e.g., intervals) rather than points.

■ **Example B.1** Consider a sample space Ω consisting of n equally probable outcomes. If an event $A \subset \Omega$ contains $d(A) = m$ elements, then the probability of event A is given by $P(A) = m/n$. ■

We now proceed to establish some fundamental results in probability theory, beginning with the calculation of the probability of the complement of an event, that is, the probability that the event does not occur.

Proposition B.2.1 For any event A, it holds that $P(A^c) = 1 - P(A)$.

Proof. The sets A and A^c are disjoint, and their union satisfies $A \cup A^c = \Omega$. By Axiom 3 (additivity), we have $P(A \cup A^c) = P(A) + P(A^c)$. By Axiom 2 (normalization), we know that $P(A \cup A^c) = P(\Omega) = 1$. Combining both equations, we obtain $P(A) + P(A^c) = 1$, which completes the proof. ■

As a direct consequence of the previous proposition, we can deduce the probability of the impossible event.

Proposition B.2.2 The probability of the impossible event is zero; that is, $P(\varnothing) = 0$.

Proof. Since $\varnothing = \Omega^c$, we apply the complement rule:

$$P(\varnothing) = P(\Omega^c) = 1 - P(\Omega) = 1 - 1 = 0.$$

■

As expected, sub-events (i.e., subsets) are associated with probabilities no greater than those of the events containing them.

Proposition B.2.3 If $A \subset B$, then $P(A) \leq P(B)$.

Proof. The event B can be written as the disjoint union of A and $B \cap A^c$. By Axiom 3: $P(B) = P(A) + P(B \cap A^c)$. Since $P(B \cap A^c) \geq 0$, it follows that $P(A) \leq P(B)$. ■

With these basic properties established, we can now confirm that all probabilities lie between zero and one.

Proposition B.2.4 For any event A, we have $0 \le P(A) \le 1$.

Proof. By Axiom 1, $P(A) \ge 0$. Since $A \subset \Omega$, the previous proposition implies $P(A) \le P(\Omega) = 1$. ■

Axiom 3 allows us to compute the probability of the union of disjoint events. However, it does not directly apply to cases involving non-disjoint events. The following proposition provides a formula for computing the probability of the union of two events that may overlap.

Proposition B.2.5 For any two events A and B, we have:

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

Proof. The union of A and B can be expressed as $A \cup B = (A \setminus B) \cup B$. Since $A \setminus B$ and B are disjoint, by Axiom 3 we obtain:

$$P(A \cup B) = P(B) + P(A \setminus B).$$

Now, observe that $P(A) = P(A \setminus B) + P(A \cap B)$, which implies:

$$P(A \setminus B) = P(A) - P(A \cap B).$$

Substituting this into the previous expression yields:

$$P(A \cup B) = P(B) + P(A) - P(A \cap B),$$

as required. ■

This result generalizes to any finite number of events via the *principle of inclusion-exclusion* (see Section A.3):

$$\begin{aligned} P\left(\bigcup_{i=1}^{n} A_i\right) = \sum_{i=1}^{n} P(A_i) - \sum_{i<j} P(A_i \cap A_j) + \sum_{i<j<k} P(A_i \cap A_j \cap A_k) - \\ \sum_{i<j<k<l} P(A_i \cap A_j \cap A_k \cap A_l) + \ldots + (-1)^{n+1} P(A_1 \cap \ldots \cap A_n) \end{aligned}$$

To ensure that a probability function satisfies Kolmogorov's axioms, we must define it using methods that are guaranteed to produce valid probability measures. One such method involves assigning probabilities to individual elements of a finite or countable sample space and extending this assignment to subsets via summation.

Proposition B.2.6 Let $(\Omega, \mathcal{A})$ be a field over a non-empty discrete set, and let $p_1, p_2, \ldots$ be a sequence of nonnegative real numbers such that $\sum_{i=1}^{\infty} p_i = 1$. Define a function $P : \mathcal{A} \to [0,1]$ by $P(A) = \sum_{\{i: s_i \in A\}} p_i$, with the convention that the sum over an empty index set is 0. Then P is a probability on $(\Omega, \mathcal{A})$.

Proof. We must verify that the function P satisfies the three Kolmogorov axioms:

Axiom 1 (Nonnegativity): Let $A \in \mathcal{B}$. Since each $p_i \geq 0$, the sum

$$P(A) = \sum_{\{i: s_i \in A\}} p_i$$

is a (possibly infinite) sum of nonnegative terms. Hence, $P(A) \geq 0$.

Axiom 2 (Normalization): We have that

$$P(\Omega) = \sum_{\{i: s_i \in \Omega\}} p_i = \sum_{i=1}^{\infty} p_i = 1,$$

by assumption. Hence, $P(\Omega) = 1$.

Axiom 3 (Finite Additivity): Let $A_1, \ldots, A_n \in \mathcal{B}$ be pairwise disjoint events. Define $A = \bigcup_{j=1}^{n} A_j$. Then the sets $\{i : s_i \in A_j\}$ are disjoint for distinct j, and we have:

$$P(A) = \sum_{\{i: s_i \in A\}} p_i = \sum_{j=1}^{n} \sum_{\{i: s_i \in A_j\}} p_i = \sum_{j=1}^{n} P(A_j),$$

where we used the disjointness of the A_j's and associativity of finite sums.

Hence, P satisfies all three axioms of probability (with finite additivity), and is therefore a valid probability function on $(\Omega, \mathcal{A})$. ■

Finally, we introduce the concept of a probability mass function[3]. A probability mass function assigns a probability to each event in a discrete sample space.

Definition B.2.3 Let $(\Omega, \mathcal{A}, P)$ be a discrete probability space. A *probability mass function* is a real-valued function $f : \mathcal{A} \to [0, 1]$ such that $f(A) = P(A)$ for every $A \in \mathcal{A}$.

In Example B.1, we introduced a discrete probability space $(\Omega, \mathcal{A}, P)$ consisting of n equally probable elements. The corresponding probability mass function is defined as $f : \mathcal{A} \to [0, 1]$, with

$$f(A) = \frac{d(A)}{n}, \quad \text{for all } A \in \mathcal{A},$$

[3]Most probability textbooks define the probability mass function as a real-valued function of the form $f : \mathbb{R} \to [0, 1]$. However, this definition requires the prior introduction of the concept of a random variable. Since random variables play a more secondary role in the context of discrete probability, we have postponed their introduction to a later subsection. For this reason, we have provided a definition of the probability mass function based directly on events.

where $d(A)$ denotes the number of elements in the event A.

In many discrete settings, it is common to treat each individual element $\omega \in \Omega$ as an elementary event. That is, we assume that every set $\{\omega\}$ belongs to $\mathcal{A}$. In this case, we can define the probability mass function as a function $f : \Omega \to [0,1]$, where $f(\omega) = P(\{\omega\})$ for each $\omega \in \Omega$. This formulation is often more natural, as it allows us to specify probabilities at the level of individual outcomes.

The following proposition shows that, under this assumption, the probability of any event $A \in \mathcal{A}$ can be computed by summing the probabilities of the individual outcomes that make up the event.

Proposition B.2.7 Let $(\Omega, \mathcal{A}, P)$ be a discrete probability space such that $\{\omega\} \in \mathcal{A}$ for every $\omega \in \Omega$. Define the function $f : \Omega \to [0,1]$ by $f(\omega) = P(\{\omega\})$. Then for any event $A \in \mathcal{A}$, the probability of A is given by:

$$P(A) = \sum_{\omega \in A} f(\omega).$$

Proof. Since $A \in \mathcal{A}$, and $\{\omega\} \in \mathcal{A}$ for each $\omega \in \Omega$, it follows that every singleton $\{\omega\} \subseteq A$ is a measurable event. Furthermore, the singletons $\{\omega\}$ for $\omega \in A$ are pairwise disjoint and their union is exactly A. Thus, by Axiom 3 (finite additivity),

$$P(A) = P\left(\bigcup_{\omega \in A} \{\omega\}\right) = \sum_{\omega \in A} P(\{\omega\}) = \sum_{\omega \in A} f(\omega).$$

■

B.3 Conditional Probability

The concept of conditional probability plays a fundamental role in statistical learning. Conditional probability allows us to refine the probability of an event based on new information or imposed conditions. Within the axiomatic framework established by Kolmogorov, conditional probability is introduced as a definition.

Definition B.3.1 Let A and B be two events such that $P(B) > 0$. The *conditional probability* of A given B, denoted by $P(A \mid B)$, is defined as:

$$P(A \mid B) = \frac{P(A \cap B)}{P(B)}.$$

Because it satisfies the Kolmogorov axioms, a conditional probability is itself a valid probability. Note that $P(A \mid B)$ is undefined when $P(B) = 0$.

Some scholars argue that, given its central role in probability theory, conditional probability should be a property logically deduced from the foundational axioms, rather than introduced as a definition. This viewpoint naturally calls for an extension of Definition B.2.2 to include additional properties. Unfortunately, there is no consensus among mathematicians or philosophers on how such an extension should be formalized.

The standard interpretation of conditional probability views it as the updated probability of event A given that event B has occurred. This interpretation, however, may implicitly suggest a temporal or even causal relationship between B and A, a suggestion that is not necessarily valid.

■ **Example B.2** Suppose we are playing a game with a standard deck of 52 cards and we draw two cards. Let event A be "drawing at least one heart," and event B be "drawing at least one queen." These two events are dependent, as the occurrence of B affects the probability of A. However, the events are not temporally related, since both cards are drawn simultaneously, one does not occur before the other. This example illustrates that dependency in probability theory does not require a temporal sequence between the events involved. ■

The probability of two events occurring together (though not necessarily in a temporal sequence, as discussed in Example B.2), given their conditional relationship, is captured by the formula $P(A \cap B) = P(A \mid B)P(B)$. This equation often provides a more intuitive understanding of the concept of conditional probability. In fact, several authors have argued that this formulation should serve as the primary definition of conditional probability, rather than the quotient-based approach.

This formula generalizes to any finite number of events through what is known as the *multiplication rule*, which is expressed as:

$$P(A_1 \cap A_2 \cap \ldots \cap A_n) = P(A_1)P(A_2 \mid A_1) \ldots P(A_n \mid A_1 \cap A_2 \cap \ldots \cap A_{n-1}) \tag{B.1}$$

The concept of event independence plays a central role in probability theory and statistical learning.

Definition B.3.2 Two events A and B are declared to be *independent* if $P(A \cap B) = P(A)P(B)$.

Intuitively, events A and B are considered independent if knowing that event B has occurred does not affect the probability of event A. This property follows logically from the definition of independence.

Proposition B.3.1 Let A and B be two events such that $P(A) > 0$ and $P(B) > 0$. Then A and B are independent if and only if $P(A \mid B) = P(A)$.

Proof. Assume A and B are independent, i.e., $P(A \cap B) = P(A)P(B)$. Then,

$$P(A \mid B) = \frac{P(A \cap B)}{P(B)} = \frac{P(A)P(B)}{P(B)} = P(A).$$

Conversely, assume that $P(A \mid B) = P(A)$. Then by the multiplication rule,

$$P(A \cap B) = P(A \mid B)P(B) = P(A)P(B),$$

which confirms independence. ■

Note that if $P(A \mid B) = P(A)$, then it also follows that $P(B \mid A) = P(B)$. This is a direct consequence of the fact that the joint probability $P(A \cap B)$ can be expressed as $P(A)P(B)$.

As in the case of conditional probability, some scholars have argued that independence should not be treated merely as a definition, but rather as a logical consequence of the foundational axioms of probability. However, incorporating independence as a derived property would require extending or modifying the axiomatic system, a topic for which no universally accepted approach currently exists.

The concept of independence can be generalized to collections of more than two events. The events $A_1, \ldots, A_n$ are said to be *mutually independent* if, for every subset of events $A_{i_1}, \ldots, A_{i_j}$ with $j \in 2, 3, \ldots, n$, the following condition holds:

$$P\left(A_{i_1} \cap \ldots \cap A_{i_j}\right) = P(A_{i_1}) \cdots P\left(A_{i_j}\right).$$

It is important to emphasize that *pairwise independence*, that is, the condition $P(A_i \cap A_j) = P(A_i)P(A_j)$ for all $i \neq j$, is not sufficient to guarantee mutual independence. Mutual independence requires that the product rule holds for *every* subset of two or more events, not just for pairs.

■ **Example B.3** Confusion often arises when distinguishing between mutually exclusive (or disjoint) events and independent events. For two mutually exclusive events A and B, the expression for the conditional probability $P(A \mid B)$ becomes problematic: if B occurs, then A cannot occur by definition, making $P(A \mid B)$ either undefined (if $P(B) = 0$) or equal to zero (if $P(B) > 0$). Similarly, computing the conditional probability of A given B when $P(B) = 0$ is not well-defined.

Although Definition B.3.2 does not explicitly prohibit A and B from being mutually exclusive, the two concepts are fundamentally incompatible unless one (or both) of the events has probability zero. In fact, two mutually exclusive events A and B are independent if and only if $P(A) = 0$, $P(B) = 0$, or both. ■

An interesting situation occurs when two events A and B are not independent in general, but become independent when conditioned on the occurrence of a third event C.

Definition B.3.3 Let A, B, and C be events such that $P(B \cap C) > 0$. We say that A and B are *conditionally independent* given C if $P(A \mid B \cap C) = P(A \mid C)$.

Next example illustrates that two events may be independent but fail to remain conditionally independent given a third event.

■ **Example B.4** Consider the experiment of rolling two fair dice. The outcomes of the two dice are independent, since knowing the result of one die does not provide any information about the result of the other. Now suppose we observe that the first die shows a four, and we are also given that the sum of the two dice is an odd number (event C). This additional condition restricts the possible outcomes of the second die: it must now show an odd number to make the total odd. As a result, the outcome of the second die is no longer independent of the first, once we condition on the sum being odd. ■

The following theorem presents Bayes' rule, a fundamental result that underpins an important statistical learning technique known as Bayesian inference (see Section F.1.2)[4].

Theorem B.3.2 — Bayes' Theorem. Let A and B be two events such that $P(B) \neq 0$. Then we have that

$$P(A \mid B) = \frac{P(B \mid A)\,P(A)}{P(B)}$$

In this context, $P(A)$ is called the *prior probability*, while $P(A \mid B)$ is known as the *posterior probability*.

Proof. From the definition of conditional probability, we have:

$$P(A \mid B) = \frac{P(A \cap B)}{P(B)} \quad \text{(provided } P(B) \neq 0\text{)},$$

[4] As shown in the proof, Bayes' theorem follows directly from the definition of conditional probability. However, despite its practical utility, this derivation raises important philosophical questions regarding its foundational status. If conditional probability is taken as a definition rather than a derived consequence of more fundamental axioms, then Bayes' theorem rests on the same definitional foundation. As such, it functions effectively within this framework, but its theoretical justification depends on accepting conditional probability as a primitive notion rather than as something logically deduced.

and

$$P(B \mid A) = \frac{P(A \cap B)}{P(A)} \quad \text{(provided } P(A) \neq 0\text{)}.$$

Solving the second equation for $P(A \cap B)$ and substituting into the first yields the desired result. ■

Bayesian inference allows us to update our degree of belief in the occurrence of an event A, initially represented by the prior probability $P(A)$, in light of new evidence, represented by the occurrence of another event B. The result is the posterior probability $P(A \mid B)$, which reflects our revised belief after considering the new information.

■ **Example B.5** Let E represent a rare disease that affects one in every million people, so that $P(E) = 1 \times 10^{-6}$. Let $+$ denote a diagnostic test designed to detect the disease, with a failure rate of one in a thousand tests; that is, $P(+ \mid E) = 999/1000$. We wish to compute the probability that a person has the disease given a positive test result, i.e., $P(E \mid +)$. Applying Bayes' theorem, we get:

$$P(E \mid +) = \frac{P(+ \mid E)P(E)}{P(+)} = \frac{P(+ \mid E)P(E)}{P(+ \mid E)P(E) + P(+ \mid E^c)P(E^c)} = 0.001$$

This result shows that, despite the test failing only once in a thousand applications, the probability of actually having the disease after a positive result remains extremely low. This seemingly paradoxical outcome arises because the probability of a false positive (10^{-3}) is much higher than the prior probability of having the disease (10^{-6}).

In practical settings, this problem is often addressed by administering a second, independent test to individuals who test positive. Under the assumption of test independence, the probability of disease given two positive results increases substantially, to approximately 0.5. ■

Bayes' theorem is particularly useful when the events involved are dependent, allowing new information about one event to revise our assessment of the probability of another.

■ **Example B.6** Suppose you draw a single card from a standard 52-card deck. Let event A be "drawing a red card," and let event B be "drawing a queen." In this case, applying Bayes' theorem to compute $P(A \mid B)$, the probability of having drawn a red card given that a queen has been drawn, yields little insight. This is because knowing that a queen was drawn does not significantly alter the probability of the card being red: two of the four queens are red and two are black, mirroring the overall color distribution in the deck. Thus, event B provides no relevant new information about event A. ■

Bayes' theorem can be generalized to accommodate multiple events. Let $A_1, \ldots, A_k$ be a finite collection of events with $P(A_j) > 0$ for all $j = 1, \ldots, k$, and assume that these events form a partition of the sample space Ω. Let B be an event such that $P(B) > 0$. Then, for each $i = 1, \ldots, k$, the conditional probability $P(A\_i \mid B)$ is given by:

$$P(A_i \mid B) = \frac{P(B \mid A_i)P(A_i)}{\sum_{j=1}^{k} P(B \mid A_j)P(A_j)}$$

This expression demonstrates the applicability of Bayes' theorem to a wider range of inference problems involving multiple events.

B.4 Random Variables

A random variable[5] is a function that assigns a real number to each possible outcome of an experiment, thus providing a quantitative representation of the results. Although the Kolmogorov framework assigns probabilities to events, random variables offer a more direct approach by associating numerical values with outcomes. This not only simplifies the representation of probabilistic phenomena but also facilitates the analysis of their properties. Owing to their effectiveness, most statisticians conduct their investigations primarily within the framework of random variables rather than working directly with probability spaces.

Definition B.4.1 Let $(\Omega, \mathcal{A}, P)$ be a discrete probability space. A *random variable* is a function $X : \Omega \to \mathbb{R}$ mapping from the set of the sample space Ω to the real numbers $\mathbb{R}$. A random variable is discrete if its range $\{x_1, x_2, \ldots, x_i, \ldots\}$ is finite or countably infinite.

Our focus here is on discrete random variables defined on discrete probability spaces. Although it is possible to define a discrete random variable on a non-discrete probability space by restricting it to a discrete range, this case is not considered in this book.

Random variables are particularly useful when they represent specific characteristics of the experiment. For example, if the sample space consists of a school's student body, a random variable could assign to each student their respective height. Random variables also allow us to transform the

[5]The term "random variable" can be somewhat misleading. First, a random variable is not a variable in the usual algebraic sense, but rather a function. Second, it is not the random variable itself that is random; the randomness lies in the experiment it represents. Despite this potential for confusion, we follow the standard terminology.

original outcomes of the sample space into new events. For instance, if two dice are rolled, a random variable could represent the sum of the two outcomes.

It is important to note that we are free to define a random variable on any sample space, even if the assignment does not appear intuitively meaningful. For example, one might assign a numerical value to each color in a deck of cards, draw two cards at random, and take the sum of the assigned numbers. While such a construction may have little practical interpretation, it nonetheless defines a valid random variable, and probabilities can be computed accordingly.

Definition B.4.2 Let $X : \Omega \to \mathbb{R}$ be a discrete random variable, and let $C \subset \mathbb{R}$ be a set such that $\{\omega \in \Omega : X(\omega) \in C\}$ is an event. The probability of X taking a value in C, denoted $P(X \in C)$, is defined by $P(X \in C) = P(\{\omega \in \Omega : X(\omega) \in C\})$.

The probability associated with a random variable X effectively defines a probability space on the real line, specifically over the range of X.

■ **Example B.7** Let $\Omega = \{1,2,3,4,5,6\}$ be the sample space for a single toss of a fair die, and P a probability that assigns $1/6$ to each single outcome in Ω. Let $X : \Omega \to \mathbb{R}$ be a discrete random variable defined as:

$$X(\omega) = \begin{cases} 0 & \text{if } \omega \text{ is even (2, 4, 6),} \\ 1 & \text{if } \omega \text{ is odd (1, 3, 5).} \end{cases}$$

This random variable maps each outcome of the die toss to either 0 (if the result is even) or 1 (if the result is odd). For $C = \{0\}$, the probability $P(X \in C) = P(X = 0) = P(\{2,4,6\}) = 1/2$. For $C = \{1\}$ the probability $P(X \in C) = P(X = 1) = P(\{1,3,5\}) = 1/2$. Through this transformation, the original discrete probability space has been mapped to the real numbers using the discrete random variable X, establishing a new probability over X's range. ■

Unless stated otherwise, we will assume that $\{\omega \in \Omega, :, X(\omega) = x_i\}$ is an event for every point x_i in the range of X. The following example shows a case were this assumption does not hold.

■ **Example B.8** Let $(\Omega, \mathcal{A}, P)$ be a discrete probability space, where $\Omega = \{1,2\}$, $\mathcal{A} = \{\varnothing, \Omega\}$, $P(\varnothing) = 0$ and $P(\Omega) = 1$. Let $X : \Omega \to \mathbb{R}$ be a discrete random variable defined as $X(1) = 1$ and $X(2) = 2$. We are interested in the probability $P(X = 1)$, however since $\{\omega \in \Omega : X(\omega) = 1\} = \{1\}$ is not an event (because $\{1\} \notin \mathcal{A}$), such probability cannot be determined. ■

Definition B.2.3 introduced the concept of probability mass function for probability spaces, based on the probabilities of the events. The following definition extends this concept to random variables.

Definition B.4.3 Let X be a discrete random variable over a discrete probability space, and let $\{x_1, x_2, \ldots\}$ be the range of X. The *probability mass function* of the discrete random variable X, abbreviated as p.m.f., is the function $f : \text{range}(X) \to [0,1]$ defined by $f(x_i) = P(X = x_i)$.

The set of values for which the probability mass function is positive, $\{x : f(x) > 0\}$, is called the *support* of the distribution of X.

It is possible for two random variables to share the same probability mass function while differing in other significant respects.

■ **Example B.9** Let $\Omega = \{H, T\}$ be the sample space for a single toss of a fair coin, and let P be a probability that assigns $1/2$ to each outcome in Ω. Define a discrete random variable $X : \Omega \to \mathbb{R}$ by setting $X = 1$ if the coin shows Head and $X = 0$ if coin shows Tail. The distribution of X is given by $P(X = 0) = P(X = 1) = 0.5$. This distribution is identical to that of the random variable in Example B.7, even though the two random variables are defined on different sample spaces and represent different experiments. ■

Given the probability mass function of a random variable, we can determine the probability of any subset of the real line.

Proposition B.4.1 Let X be a discrete random variable with probability mass function f. For any subset C of the real line, the probability $P(X \in C)$ is given by $\sum_{x_i \in C} f(x_i)$.

Proof. Since each outcome in the sample space corresponds to exactly one value in the range $x_1, x_2, \ldots$ of X, we have

$$P(X \in C) = P\big(\{\omega \in \Omega : X(\omega) \in C\}\big) = \sum_{x_i \in C} P(X = x_i) = \sum_{x_i \in C} f(x_i).$$

■

This result shows that the probability mass function completely determines the probability distribution of a discrete random variable, since the probability of any event involving X can be computed from it.

The following proposition states a fundamental property: the total probability over all possible values of a random variable is equal to 1.

Proposition B.4.2 Let X be a discrete random variable with probability mass function f. If $\{x_1, x_2, \ldots,\}$ is the range of X, then $\sum_{i=1}^{\infty} f(x_i) = 1$.

Proof. Since X is a total function, each outcome in the sample space is associated with exactly one value in the range $\{x_1, x_2, \ldots\}$. By the axioms of probability,

$$\sum_{i=1}^{\infty} f(x_i) = \sum_{i=1}^{\infty} P(X = x_i) = \sum_{i=1}^{\infty} P\big(\{\omega \in \Omega : X(\omega) = x_i\}\big) = P(\Omega) = 1.$$

■

The values $\{x_1, x_2, \ldots\}$ represent all the possible outcomes of X. Since these outcomes are mutually exclusive and collectively exhaustive, their probabilities must sum to the total probability of the entire sample space, which is 1.

A fundamental characterization of discrete distributions is that they are completely determined by a nonnegative function on the real line whose total mass is 1. The next proposition states this precisely.

Proposition B.4.3 A function $f(x)$ is a probability mass function of a random variable X if, and only if, i) $f(x) \geq 0$ for all x, ii) $\sum_{i=1}^{\infty} f(x_i) = 1$.

Proof. Suppose f is the probability mass function of a discrete random variable X with range $\{x_1, x_2, \ldots\}$. Then $f(x_i) = P(X = x_i) \geq 0$ for all i, and

$$\sum_{i=1}^{\infty} f(x_i) = \sum_{i=1}^{\infty} P(X = x_i) = P(\Omega) = 1,$$

so (i)-(ii) hold.

Conversely, assume $f(x) \geq 0$ for all x and $\sum_{i=1}^{\infty} f(x_i) = 1$ for some countable set $\{x_1, x_2, \ldots\}$ (the points where f may be positive). Define a discrete sample space $\Omega = \{x_1, x_2, \ldots\}$, set $P(x_i) = f(x_i)$, and define $X : \Omega \to \mathbb{R}$ by $X(\omega) = \omega$. Then for each i,

$$P(X = x_i) = P(\{\omega \in \Omega : X(\omega) = x_i\}) = P(\{x_i\}) = f(x_i),$$

so f is the probability mass function of X. ■

The proposition shows that a discrete distribution is fully specified by any function that is everywhere nonnegative and sums to 1 over its (countable) support; values of f outside the support are irrelevant.

The cumulative distribution function expresses the probability that a random variable takes a value less than or equal to a given point.

Definition B.4.4 The *cumulative distribution function* (c.d.f.) F of a discrete random variable X is defined by $F(x) = P(X \leq x)$ for all $-\infty < x < \infty$

If X has a distribution characterized by the probability mass function $f(x)$, its cumulative distribution function $F(x)$ behaves as follows: at each distinct value x_i in the range of X, $F(x)$ increases by $f(x_i)$; between these values, $F(x)$ remains constant.

The cumulative distribution function shows how probabilities accumulate over the range of a random variable, providing insight into the overall distribution of the data. It can be viewed as the running total of the probabilities given by the probability mass function.

■ **Example B.10** Let X be a discrete random variable representing the grades of students in a class, where each grade is between 0 and 10. The probability that a student receives a grade of x is given by the probability mass function $p(x)$. The cumulative distribution function $F(x)$ gives the probability that a randomly selected student scores x or less. For example, if $F(7) = 0.6$, this means there is a 60% chance that a randomly chosen student scored 7 or below. ■

The cumulative distribution function of a random variable is always non-decreasing.

Proposition B.4.4 Let F be the cumulative distribution function of a discrete random variable X. If $x_1 < x_2$, then $F(x_1) \leq F(x_2)$.

Proof. For $x_1 < x_2$, the event $X \leq x_1$ is a subset of the event $X \leq x_2$. By the monotonicity property of probability, $P(X \leq x_1) \leq P(X \leq x_2)$. Since $F(x) = P(X \leq x)$, it follows that $F(x_1) \leq F(x_2)$. ■

The following proposition states the asymptotic properties of the cumulative distribution function of a random variable, showing its limits as x approaches negative and positive infinity.

Proposition B.4.5 Let F be the cumulative distribution function of a discrete random variable X. Then $\lim_{x\to-\infty} F(x) = 0$ and $\lim_{x\to\infty} F(x) = 1$.

Proof. As $x \to -\infty$, the event $X \leq x$ eventually becomes empty, because there are no values in the range of X smaller than sufficiently negative x. The probability of this event is therefore 0, so

$$\lim_{x\to-\infty} F(x) = \lim_{x\to-\infty} P(X \leq x) = 0.$$

As $x \to \infty$, the event $X \leq x$ eventually contains the entire sample space Ω, since all possible values of X are less than or equal to sufficiently large x. The probability of this event is therefore 1, so

$$\lim_{x\to\infty} F(x) = \lim_{x\to\infty} P(X \leq x) = 1.$$

■

The probability that X exceeds x is the complement of the cumulative distribution function at that point.

Proposition B.4.6 Let F be the cumulative distribution function of a discrete random variable X. Then, for every $x \in \mathbb{R}$, $P(X > x) = 1 - F(x)$.

Proof. The events $X > x$ and $X \leq x$ are complementary, so their probabilities sum to 1 $P(X > x) + P(X \leq x) = 1$. Therefore, $P(X > x) = 1 - P(X \leq x)$. By the definition of the cumulative distribution function, $P(X \leq x) = F(x)$, and thus $P(X > x) = 1 - F(x)$. ■

The following proposition relates the probability of a random variable X taking a value between two points to the difference in its cumulative distribution function at those points.

Proposition B.4.7 Let F be the cumulative distribution function of a discrete random variable X. Then, for all $x_1, x_2 \in \mathbb{R}$ with $x_1 < x_2$, $P(x_1 < X \leq x_2) = F(x_2) - F(x_1)$.

Proof. The probability that $X \leq x_2$ is $F(x_2)$. Subtracting from this the probability that $X \leq x_1$, which is $F(x_1)$, leaves exactly the probability that X falls strictly between x_1 and x_2:

$$P(x_1 < X \leq x_2) = F(x_2) - F(x_1).$$

■

B.4.1 Multivariate Distributions

A multivariate probability distribution extends the concept of a probability distribution to multiple random variables, each with its own set of possible outcomes. While univariate distributions describe phenomena involving a single random variable, multivariate distributions capture the relationships and dependencies between two or more variables. This allows for the analysis of complex phenomena in which the outcome of interest is influenced by several factors simultaneously, providing insight into how these variables interact and affect the probabilities of different outcomes.

Definition B.4.5 Let $X_1, X_2, \ldots, X_n$ be n discrete random variables on a common discrete probability space $(\Omega, \mathcal{A}, P)$, where $X_i : \Omega \to \mathbb{R}$ for $i = 1, \ldots, n$. The *joint probability distribution* of $X_1, \ldots, X_n$ assigns probabilities to events involving all variables simultaneously. Formally, for any set $C \subset \mathbb{R}^n$, the joint probability is

$$P\big((X_1, X_2, \ldots, X_n) \in C\big),$$

where

$$\{\omega \in \Omega \,:\, (X_1(\omega), X_2(\omega), \ldots, X_n(\omega)) \in C\}$$

is an event in the sample space.

The joint probability distribution of the random variables $X_1, X_2, \ldots, X_n$ defines a probability distribution on $\mathbb{R}^n$. If the random variables $X_1, X_2, \ldots, X_n$ each have a discrete distribution, then the joint distribution is also a discrete distribution.

Definition B.4.6 Let $X_1, \ldots, X_n$ be n discrete random variables over a common discrete probability space. The *joint probability mass function* of $X_1, \ldots, X_n$ is the function

$$f : \text{range}(X_1) \times \ldots \times \text{range}(X_n) \to [0, 1]$$

defined by

$$f(x_1, \ldots, x_n) = P(X_1 = x_1, \ldots, X_n = x_n).$$

■ **Example B.11** A classic example of a bivariate discrete joint distribution involves rolling two six-sided dice. Define two discrete random variables: X_1 is the outcome of the first die, and X_2 is the outcome of the second die. Both X_1 and X_2 follow a discrete uniform distribution over $1, 2, 3, 4, 5, 6$. The joint distribution of X_1 and X_2 describes the probability of each possible pair of outcomes when the dice are rolled. The joint probability mass function $f(x_1, x_2)$ is:

$$f(x_1, x_2) = P(X_1 = x_1, X_2 = x_2) = \frac{1}{36}, \quad x_1, x_2 \in \{1, 2, 3, 4, 5, 6\}.$$

The joint distribution allows us to answer questions such as the probability that the sum of the two dice equals a certain value, or that one die shows a higher number than the other. ■

Before exploring the properties of multivariate random variables, we introduce the concept of a random vector. This simplifies notation and improves clarity by grouping multiple random variables into a single object.

Definition B.4.7 A *discrete random vector* $\mathbf{X}$ is an ordered collection of n discrete random variables $X_1, X_2, \ldots, X_n$, where $X_i : \Omega \to \mathbb{R}$ for all

$i = 1, \ldots, n$. Equivalently, $\mathbf{X} = (X_1, \ldots, X_n) : \Omega \to \mathbb{R}^n$.

Given the joint probability mass function of a random vector, we can determine the probability of any subset of the n-dimensional real space.

Proposition B.4.8 Let $\mathbf{X} = (X_1, \ldots, X_n)$ be a discrete random vector with joint probability mass function f. For any subset C of $\mathbb{R}^n$,

$$P(\mathbf{X} \in C) = \sum_{\mathbf{x} \in C} f(\mathbf{x}),$$

where $\mathbf{x} = (x_1, \ldots, x_n)$.

Proof. Since each outcome in the sample space corresponds to exactly one value in the range of $\mathbf{X}$, we have:

$$P(\mathbf{X} \in C) = P(\{\omega \in \Omega : \mathbf{X}(\omega) \in C\}) = \sum_{\mathbf{x} \in C} P(\mathbf{X} = \mathbf{x}) = \sum_{\mathbf{x} \in C} f(\mathbf{x}).$$

■

The following proposition states a fundamental property, that the total probability over all possible outcomes of a discrete random vector is 1.

Proposition B.4.9 Let $\mathbf{X} = (X_1, \ldots, X_n)$ be a discrete random vector with a joint probability mass function f. If the range of $\mathbf{X}$ is $\mathbf{x} = (x_1, \ldots, x_n)$, then $\sum_{\mathbf{x}} f(\mathbf{x}) = 1$.

Proof. Since $\mathbf{X}$ is a total function and each outcome in the sample space corresponds to exactly one value in the range of $\mathbf{X}$, the axioms of probability imply:

$$\sum_{\mathbf{x}} f(\mathbf{x}) = \sum_{\mathbf{x}} P(\mathbf{X} = \mathbf{x}) = P(\Omega) = 1.$$

■

A particularly important multivariate construction is the distribution of the sum of n random variables. The notation $X_1 + \cdots + X_n$ refers to the sum of the random variables (applied pointwise on outcomes), not a sum of n probability distributions. There are two standard ways to formalize this, depending on how the random variables are defined.

The first one refers to a sum on a commom sample space.

Definition B.4.8 Let $X_1, X_2, \ldots, X_n$ be discrete random variables on a common probability space $(\Omega, \mathcal{A}, P)$, with $X\_i : \Omega \to \mathbb{R}$. The sum is the discrete random variable

$$S = X_1 + \cdots + X_n : \Omega \to \mathbb{R}, \qquad S(\omega) = X_1(\omega) + \cdots + X_n(\omega).$$

The *distribution of the sum* is the distribution of S.

The second one refers to a sum on product space (independent relations).

Definition B.4.9 Let $X : \Omega \to \mathbb{R}$ model a single trial. To model n repetitions, consider the product sample space Ω^n (each n-tuple of outcomes is a sample point, and in the i.i.d. case all n-tuples are equally likely when Ω is finite). Define

$$X_i(\omega_1, \ldots, \omega_n) = X(\omega_i), \quad i = 1, \ldots, n,$$

and the sum

$$S(\omega_1, \ldots, \omega_n) = X(\omega_1) + \cdots + X(\omega_n), \qquad S : \Omega^n \to \mathbb{R}.$$

Again, the *distribution of the sum* is the distribution of S.

In both setups, the distribution of S depends on the joint distribution of $(X_1, \ldots, X_n)$. Independence is not assumed unless explicitly stated.

■ **Example B.12** Let $X : \Omega \to \mathbb{R}$ be the outcome of rolling a six-sided die (values $1, \ldots, 6$, each with probability $1/6$). For three rolls, use the product space Ω^3 with each triple equally likely. Define

$$X_1(\omega_1, \omega_2, \omega_3) = X(\omega_1), X_2(\omega_1, \omega_2, \omega_3) = X(\omega_2), X_3(\omega_1, \omega_2, \omega_3) = X(\omega_3),$$

and

$$S(\omega_1, \omega_2, \omega_3) = X(\omega_1) + X(\omega_2) + X(\omega_3).$$

Then $S : \Omega^3 \to \mathbb{R}$ is the sum of three (independent) die rolls. ■

B.4.2 Marginal Probability Mass Function

Given a multivariate discrete probability mass function, the marginal probability mass function of a subset of variables is derived by summing the joint probability mass function over all possible values of the remaining variables. This process "marginalizes" out the variables not of interest, allowing us focus on the probability mass function of a single variable or a subset of variables within the multivariate context.

Definition B.4.10 Let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ be an n-dimensional discrete random vector with joint probability mass function $f_{\mathbf{X}}(x_1, x_2, \ldots, x_n)$, partition $\mathbf{X}$ into two subvectors: $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_k)$, a k-dimensional random vector consisting of k discrete random variables selected from $\mathbf{X}$, and $\mathbf{Z} = (Z_1, Z_2, \ldots, Z_{n-k})$, the remaining $(n-k)$ discrete random variables of $\mathbf{X}$. The *marginal probability mass function* $f_{\mathbf{Y}}$ of $\mathbf{Y}$ is obtained by summing $f_{\mathbf{X}}$ over all possible values of the variables in $\mathbf{Z}$. That is, for any specific values $(y_1, y_2, \ldots, y_k)$ of $\mathbf{Y}$,

$$f_{\mathbf{Y}}(y_1, y_2, \ldots, y_k) = \sum_{z_1} \sum_{z_2} \cdots \sum_{z_{n-k}} f_{\mathbf{X}}(x_1, x_2, \ldots, x_n),$$

where in each term of the sum, $x_i = y_i$ for i corresponding to variables in $\mathbf{Y}$, and $x_j = z_j$ for j corresponding to variables in $\mathbf{Z}$.

This definition captures the marginalization process in the discrete setting, which is key to understanding and analyzing the behavior of specific variables within a larger multivariate framework.

■ **Example B.13** Consider two discrete random variables X and Y, each taking values in $0, 1$, with joint probability mass function:

$X \backslash Y$	0	1
0	0.1	0.3
1	0.2	0.4

To find the marginal probability mass function of X, sum over all possible values of Y:

$$f_X(0) = f_{X,Y}(0,0) + f_{X,Y}(0,1) = 0.1 + 0.3 = 0.4,$$
$$f_X(1) = f_{X,Y}(1,0) + f_{X,Y}(1,1) = 0.2 + 0.4 = 0.6.$$

■

While the marginal probability mass functions of $X_1, \ldots, X_n$ can be obtained from their joint probability mass function by summing over the range of the other variables, the reverse process is not possible without additional information about the dependence structure among the variables. Marginal probability mass functions describe only the individual behavior of each variable and do not capture interactions between them.

■ **Example B.14** Let X and Y be discrete random variables, each taking values in $0, 1$, with marginal probability mass functions:

$$f_X(0) = 0.5, \quad f_X(1) = 0.5,$$
$$f_Y(0) = 0.5, \quad f_Y(1) = 0.5.$$

Without additional information about the relationship between X and Y, the joint probability mass function cannot be reconstructed from the marginals alone. ■

A random vector $\mathbf{X}$ is said to have independent components if knowing the outcome of one component provides no information about the others.

In this case, events defined by different components occur independently, and the joint probability mass function factorizes into the product of the marginals.

Definition B.4.11 Let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ be an n-dimensional discrete random vector with joint probability mass function $f_{\mathbf{X}}$ and marginal probability mass functions $f_{X_1}, f_{X_2}, \ldots, f_{X_n}$. The components $X_1, \ldots, X_n$ are *independent* if, for all $(x_1, \ldots, x_n)$ in the support of $\mathbf{X}$,

$$f_{\mathbf{X}}(x_1, \ldots, x_n) = \prod_{i=1}^{n} f_{X_i}(x_i).$$

The concept of independence for a random vector $\mathbf{X}$ simplifies the computation and understanding of joint probability distributions, particularly in complex problems involving multiple variables. It allows the joint probability distribution of the vector $\mathbf{X}$ to be expressed as the product of the individual marginal distributions of $X_1, X_2, \ldots, X_n$.

Proposition B.4.10 Let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ be an n-dimensional random vector with joint probability mass function $f_{\mathbf{X}}$ and marginal probability mass functions $f_{X_1}, f_{X_2}, \ldots, f_{X_n}$. The random variables $X_1, X_2, \ldots, X_n$ are independent if and only if for every $(x_1, x_2, \ldots, x_n)$ in the support of $\mathbf{X}$, we have:

$$f_{\mathbf{X}}(x_1, x_2, \ldots, x_n) = f_{X_1}(x_1) f_{X_2}(x_2) \ldots f_{X_n}(x_n).$$

Proof. Assume that $X_1, X_2, \ldots, X_n$ are independent. Then, for any values $x_1, x_2, \ldots, x_n$, we have:

$$\begin{aligned} f_{\mathbf{X}}(x_1, x_2, \ldots, x_n) &= P(X_1 = x_1, X_2 = x_2, \ldots, X_n = x_n) \\ &= P(X_1 = x_1) P(X_2 = x_2) \ldots P(X_n = x_n) \\ &= f_{X_1}(x_1) f_{X_2}(x_2) \ldots f_{X_n}(x_n). \end{aligned}$$

Conversely, assume that for all $x_1, x_2, \ldots, x_n$,

$$f_{\mathbf{X}}(x_1, x_2, \ldots, x_n) = f_{X_1}(x_1) f_{X_2}(x_2) \ldots f_{X_n}(x_n).$$

Then, for any subsets $A_1, \ldots, A_n$ of $\mathbb{R}$, we have:

$$\begin{aligned} P(X_1 \in A_1, \ldots, X_n \in A_n) &= \sum_{(x_1, \ldots, x_n) \in A_1 \times \ldots \times A_n} f_{\mathbf{X}}(x_1, \ldots, x_n) \\ &= \sum_{x_1 \in A_1} \cdots \sum_{x_n \in A_n} f_{X_1}(x_1) \ldots f_{X_n}(x_n) \\ &= \left(\sum_{x_1 \in A_1} f_{X_1}(x_1) \right) \cdots \left(\sum_{x_n \in A_n} f_{X_n}(x_n) \right) \\ &= P(X_1 \in A_1) \ldots P(X_n \in A_n). \end{aligned}$$

This equality holds for all subsets $A_1, \dots, A_n$, which implies that $X_1, \dots, X_n$ are independent. ■

B.4.3 Conditional Probability Mass Function

The concept of the conditional probability mass function provides a way to quantify the probability of an event given that another event has occurred. In the case of discrete random variables, the conditional probability mass function of Y given $X = x$ describes the probability mass function of Y under the condition that X takes a specific value x. This concept is essential for analyzing dependencies between discrete random variables, allowing us to refine probability assessments based on new information.

Definition B.4.12 Let $\mathbf{X} = (X_1, X_2, \dots, X_n)$ be an n-dimensional random vector with joint probability mass function $f_{\mathbf{X}}(x_1, x_2, \dots, x_n)$. Partition $\mathbf{X}$ into two subvectors: $\mathbf{Y} = (Y_1, Y_2, \dots, Y_k)$, a k-dimensional random vector consisting of k discrete random variables selected from $\mathbf{X}$, and $\mathbf{Z} = (Z_1, Z_2, \dots, Z_{n-k})$, the remaining $n-k$ discrete random variables of $\mathbf{X}$. Let $f_{\mathbf{Z}}$ be the marginal probability mass function of $\mathbf{Z}$ across its $n-k$ dimensions. Provided that $f_{\mathbf{Z}}(\mathbf{z}) > 0$ for any vector $\mathbf{z} \in \mathbb{R}^{n-k}$, the *conditional probability mass function* $f_{\mathbf{Y}|\mathbf{Z}}$ of $\mathbf{Y}$ given $\mathbf{Z} = \mathbf{z}$ is defined as:

$$f_{\mathbf{Y}|\mathbf{Z}}(\mathbf{y} \mid \mathbf{z}) = \frac{f_{\mathbf{X}}(\mathbf{y}, \mathbf{z})}{f_{\mathbf{Z}}(\mathbf{z})}.$$

The following example illustrates how to compute the conditional probability mass function of Y given X.

■ **Example B.15** Consider two discrete random variables X and Y, each taking values in $\{0, 1\}$, with the joint probability mass function:

$X \backslash Y$	0	1
0	0.3	0.2
1	0.1	0.4

The conditional probability mass function of Y given $X = 0$ is:

$$f_{Y|X}(0 \mid 0) = \frac{f_{X,Y}(0,0)}{f_X(0)} = \frac{0.3}{0.5} = 0.6,$$
$$f_{Y|X}(1 \mid 0) = \frac{f_{X,Y}(0,1)}{f_X(0)} = \frac{0.2}{0.5} = 0.4.$$

Similarly, for $X = 1$:

$$f_{Y|X}(0 \mid 1) = \frac{f_{X,Y}(1,0)}{f_X(1)} = \frac{0.1}{0.5} = 0.2,$$
$$f_{Y|X}(1 \mid 1) = \frac{f_{X,Y}(1,1)}{f_X(1)} = \frac{0.4}{0.5} = 0.8.$$

■

The next proposition generalizes the multiplication rule (see Equation B.1) by combining marginal and conditional probability mass functions to recover the joint probability mass function for any configuration of discrete random variables within a random vector.

Proposition B.4.11 Let $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$, $f_{\mathbf{X}}(\mathbf{x})$, $f_{\mathbf{Z}}(\mathbf{z})$, and $f_{\mathbf{Y}|\mathbf{Z}}(\mathbf{y} \mid \mathbf{z})$ be as in Definition B.4.12. Then, for each $\mathbf{z}$ such that $f_{\mathbf{Z}}(\mathbf{z}) > 0$ and each possible value of $\mathbf{y}$, the joint probability mass function is:

$$f_{\mathbf{X}}(\mathbf{x}) = f_{\mathbf{Y}|\mathbf{Z}}(\mathbf{y} \mid \mathbf{z}) f_{\mathbf{Z}}(\mathbf{z}),$$

where $\mathbf{x} = (\mathbf{y}, \mathbf{z})$.

Proof. By the definition of the conditional probability mass function:

$$f_{\mathbf{Y}|\mathbf{Z}}(\mathbf{y} \mid \mathbf{z}) = \frac{f_{\mathbf{X}}(\mathbf{y},\mathbf{z})}{f_{\mathbf{Z}}(\mathbf{z})}, \quad \text{for } f_{\mathbf{Z}}(\mathbf{z}) > 0.$$

Rearranging yields:

$$f_{\mathbf{X}}(\mathbf{y},\mathbf{z}) = f_{\mathbf{Y}|\mathbf{Z}}(\mathbf{y} \mid \mathbf{z}) f_{\mathbf{Z}}(\mathbf{z}),$$

and since $\mathbf{x} = (\mathbf{y}, \mathbf{z})$, the result follows. ■

Similarly, the conditional probability mass function of $\mathbf{Z}$ given $\mathbf{Y} = \mathbf{y}$, denoted $f_{\mathbf{Z}|\mathbf{Y}}(\mathbf{z} \mid \mathbf{y})$, satisfies:

$$f_{\mathbf{X}}(\mathbf{x}) = f_{\mathbf{Z}|\mathbf{Y}}(\mathbf{z} \mid \mathbf{y}) f_{\mathbf{Y}}(\mathbf{y}).$$

Bayes' theorem (see Theorem B.3.2) provides a way to update probability estimates for a hypothesis given new evidence. For random vectors, the theorem extends naturally to the multidimensional case.

Theorem B.4.12 — Bayes' Theorem for Random Vectors. Let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ and $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_m)$ be two random vectors representing distinct sets of discrete random variables. The generalized Bayes' theorem states:

$$P(\mathbf{X} = \mathbf{x} \mid \mathbf{Y} = \mathbf{y}) = \frac{P(\mathbf{Y} = \mathbf{y} \mid \mathbf{X} = \mathbf{x})\, P(\mathbf{X} = \mathbf{x})}{P(\mathbf{Y} = \mathbf{y})},$$

where $P(\mathbf{Y}=\mathbf{y})$ is the marginal probability of $\mathbf{Y}$, given by:

$$P(\mathbf{Y}=\mathbf{y}) = \sum_{\mathbf{x}} P(\mathbf{Y}=\mathbf{y} \mid \mathbf{X}=\mathbf{x})\, P(\mathbf{X}=\mathbf{x}).$$

Proof. From the definition of conditional probability:

$$P(\mathbf{X}=\mathbf{x} \mid \mathbf{Y}=\mathbf{y}) = \frac{P(\mathbf{X}=\mathbf{x}, \mathbf{Y}=\mathbf{y})}{P(\mathbf{Y}=\mathbf{y})}.$$

Since

$$P(\mathbf{X}=\mathbf{x}, \mathbf{Y}=\mathbf{y}) = P(\mathbf{Y}=\mathbf{y} \mid \mathbf{X}=\mathbf{x})\, P(\mathbf{X}=\mathbf{x}),$$

substitution gives the stated result. ■

This generalized Bayes' theorem updates beliefs about $\mathbf{X}$ based on new evidence from $\mathbf{Y}$. It links the prior information we have about $\mathbf{X}$, the likelihood of observing $\mathbf{Y}=\mathbf{y}$ given $\mathbf{X}=\mathbf{x}$, and the evidence provided by the actual observation of $\mathbf{Y}=\mathbf{y}$.

Finally, building on the concept of independence between discrete random variables (see Definition B.4.11), we define conditional independence. This concept comes into play when the independence of a set of discrete random variables is considered in the context of being conditioned on another set of variables.

Definition B.4.13 Let $\mathbf{Z}$ be a random vector with joint probability mass function $f_{\mathbf{Z}}(\mathbf{z})$. The variables of the random vector $\mathbf{X} = (X_1, \ldots, X_n)$ are *conditionally independent* given $\mathbf{Z}$ if, for all $\mathbf{z}$ such that $f_{\mathbf{Z}}(\mathbf{z}) > 0$:

$$f_{\mathbf{X}|\mathbf{Z}}(\mathbf{x} \mid \mathbf{z}) = \prod_{i=1}^{n} f_{X_i|\mathbf{Z}}(x_i \mid \mathbf{z}),$$

where $f_{\mathbf{X}|\mathbf{Z}}(\mathbf{x} \mid \mathbf{z})$ is the conditional probability mass function of $\mathbf{X}$ given $\mathbf{Z}=\mathbf{z}$, and $f_{X_i|\mathbf{Z}}(x_i \mid \mathbf{z})$ is the conditional probability mass function of X_i given $\mathbf{Z}=\mathbf{z}$.

B.5 Characterizing Distributions

A *measure of central tendency* is a number derived from a probability distribution that summarizes its typical or central value. The two most commonly used measures are the *expected value* and the *median*, each offering a different perspective for characterizing a distribution.

In addition to central tendency, it is often useful to describe how much the distribution varies around its center. For this purpose, *measures of* *dispersion* are employed, the most common being the *variance* and the *standard deviation*. These quantify the spread of a distribution around its central measure.

In the case of bivariate distributions, analogous measures of dispersion are the *covariance* and the *correlation*, which capture the strength and direction of the statistical relationship between two discrete random variables.

Together, these measures—central tendency and dispersion—allow us to summarize, compare, and analyze probability distributions in a concise and meaningful way.

B.5.1 Measures of Central Tendency

The most common measures of central tendency used to characterize probability distributions are the expected value and the median.

Expeced Value

The expected value of a discrete random variable is computed as the weighted average of all its possible values, where the weights are the probabilities of the corresponding outcomes[6].

Definition B.5.1 Let X be a discrete random variable with probability mass function f. The *expected value* of X, denoted by $E(X)$, is defined as:

$$E(X) = \sum_x x f(x).$$

This definition depends only on the distribution of X, not on the original sample space. Consequently, two different random variables with the same distribution will have the same expected value, even if their underlying probability spaces are different.

A drawback of the expected value is that it can be heavily influenced by small changes in the probability assigned to large values of X.

▪ **Example B.16** Consider a company with 100 employees, and define a discrete random variable X based on their salaries. Suppose X takes the value 300 with probability $99/100$ and 6000 with probability $1/100$. The expected salary is:

$$E(X) = (300 \times 99/100) + (6000 \times 1/100) = 357.$$

[6]The term "expected value" can be misleading, because it does not necessarily coincide with one of the possible values of the random variable. For example, the expected value of a fair six-sided die is 3.5, which is not itself an attainable outcome. This counterintuitive aspect has often caused confusion in applications of probability.

Now suppose that one additional employee earns 6000 instead of 300. The expected salary becomes:

$$E(X) = (300 \times 98/100) + (6000 \times 2/100) = 414.$$

Thus, changing the salary of a single employee increases the expected salary of the company by more than 13%. ■

The expected value operator is linear: the expected value of a linear combination of discrete random variables equals the same linear combination of their expectations.

Proposition B.5.1 Let $X_1, \ldots, X_n$ be discrete random variables with expectations $E(X_i)$. For constants $a_1, \ldots, a_n$ and b,

$$E(a_1 X_1 + \ldots + a_n X_n + b) = a_1 E(X_1) + \ldots + a_n E(X_n) + b.$$

Proof. By definition,

$$E(a_1 X_1 + \ldots + a_n X_n + b) = \sum_{x_1,\ldots,x_n} (a_1 x_1 + \ldots + a_n x_n + b) f(x_1, \ldots, x_n) =$$

$$a_1 \sum_{x_1} x_1 f(x_1) + \ldots + a_n \sum_{x_n} x_n f(x_n) + b \; = a_1 E(X_1) + \ldots + a_n E(X_n) + b.$$

■

Note that independence is not required for linearity of expectation. Linearity holds for all discrete random variables as long as the expectations exist.

The expected value of the product of independent random variables equals the product of their expected values.

Proposition B.5.2 Let $X_1, \ldots, X_n$ be independent discrete random variables with expectations $E(X_i)$. Then:

$$E\left(\prod_{i=1}^{n} X_i\right) = \prod_{i=1}^{n} E(X_i).$$

Proof. By independence of $X_1, \ldots, X_n$, their joint probability mass function factorizes:

$$f(x_1, \ldots, x_n) = f_{X_1}(x_1) \cdots f_{X_n}(x_n).$$

Thus,

$$\begin{aligned} E(X_1 \cdots X_n) &= \sum_{x_1,\ldots,x_n} (x_1 \cdots x_n) f(x_1, \ldots, x_n) \\ &= \prod_{i=1}^{n} \left(\sum_{x_i} x_i f_{X_i}(x_i) \right) = \prod_{i=1}^{n} E(X_i). \end{aligned}$$

■

If the random variables are not independent, the equality above does not necessarily hold.

The Median

The median of a discrete random variable is a measure of central tendency that identifies a point dividing the probability distribution so that at least half of the probability mass lies on each side.

Definition B.5.2 Let X be a discrete random variable. A *median* of X, denoted by m, is any value satisfying:

$$P(X \leq m) \geq \tfrac{1}{2} \quad \text{and} \quad P(X \geq m) \geq \tfrac{1}{2}.$$

This definition guarantees that at least half of the probability mass lies at or below m, and at least half lies at or above m. In general, the median of a discrete distribution need not be unique; any value satisfying the inequalities is considered a valid median. In applications, it is common to select the smallest such m.

The median is often more intuitive than the expected value, since it always corresponds to an actual value of the random variable. It is also a robust measure of central tendency, particularly when the distribution is skewed or contains outliers.

■ **Example B.17** Consider the company from Example B.16. The median of the salaries is the value m for which $P(X \leq m) \geq \frac{1}{2}$. In this case, $m = 300$. Now suppose that one of the base employees is promoted to the executive level with a salary of 6000. The recalculated median remains $m = 300$. This illustrates that the median is more robust than the expected value in the presence of outliers. ■

B.5.2 Measures of Dispersion

The most common measures of dispersion in use to characterize probability distributions are the variance and its squared root, called standard deviation.

The Variance

The variance of a discrete random variable is a measure of the spread or dispersion of its possible values around the expected value.

Definition B.5.3 Let X be a discrete random variable with expected value $E(X)$ and probability mass function f. The *variance* of X, denoted by

$Var(X)$, is defined as:

$$Var(X) = E[(X - E(X))^2] = \sum_x (x - E(X))^2 f(x)$$

Variance depends only on the distribution of the random variable and quantifies how much the values typically differ from the expected value. For example, if all possible values of a random variable are identical, the variance is zero.

■ **Example B.18** Suppose the daily commuting time (in minutes) of an employee is modeled by a random variable X that takes values $20, 30, 40, 50$ with probabilities

$$P(X = 20) = 0.1,\ P(X = 30) = 0.4,\ P(X = 40) = 0.4,\ P(X = 50) = 0.1.$$

The expected value is

$$E(X) = 20(0.1) + 30(0.4) + 40(0.4) + 50(0.1) = 35.$$

The variance is

$$Var(X) = (20 - 35)^2(0.1) + (30 - 35)^2(0.4) + \\ (40 - 35)^2(0.4) + (50 - 35)^2(0.1) = 50.$$

Thus, the variance of commuting times is 50 (measured in squared minutes).
■

The following proposition shows how the variance behaves under linear combinations of independent random variables.

Proposition B.5.3 Let $X_1, \ldots, X_n$ be independent discrete random variables with finite expected values, and let $a_1, \ldots, a_n$ and b be constants. Then:

$$Var\left(a_1X_1 + \ldots + a_nX_n + b\right) = a_1^2 Var(X_1) + \ldots + a_n^2 Var(X_n).$$

Proof. Let $Y = a_1X_1 + \ldots + a_nX_n + b$. Since adding a constant does not affect variance,

$$Var(Y) = Var(a_1X_1 + \ldots + a_nX_n).$$

For independent random variables, variance is additive:

$$Var(a_1X_1 + \ldots + a_nX_n) = Var(a_1X_1) + \ldots + Var(a_nX_n).$$

Finally, for any constant a_i, $Var(a_iX_i) = a_i^2 Var(X_i)$, so

$$Var(a_1X_1 + \ldots + a_nX_n + b) = a_1^2 Var(X_1) + \ldots + a_n^2 Var(X_n).$$

■

A particularly useful identity expresses variance in terms of expected values. This formulation often simplifies calculations and highlights the connection between variance and variability.

Proposition B.5.4 Let X be a discrete random variable with expected value $E(X)$. Then:

$$Var(X) = E(X^2) - [E(X)]^2.$$

Proof. By definition,

$$Var(X) = E[(X - E(X))^2].$$

Expanding the square gives:

$$Var(X) = E[X^2 - 2XE(X) + (E(X))^2].$$

By linearity of expectation,

$$Var(X) = E(X^2) - 2E(X)E(X) + E((E(X))^2).$$

Since $E(X)$ is a constant, $E((E(X))^2) = (E(X))^2$, hence

$$Var(X) = E(X^2) - (E(X))^2.$$

■

Standard Deviation

The standard deviation is a measure of the dispersion of a distribution, closely related to the variance. Unlike variance, which squares the deviations from the mean and therefore uses squared units, the standard deviation is defined as the square root of the variance. This restores the measure to the same units as the original variable, making it easier to interpret.

Definition B.5.4 Let X be a discrete random variable with expected value $E(X)$ and finite variance $Var(X)$, and let f be its probability mass function. The *standard deviation* of X, denoted by σ, is defined as:

$$\sigma = \sqrt{Var(X)} = \sqrt{\sum_x (x - E(X))^2 f(x)}.$$

The standard deviation summarizes how far the values of X typically lie from the mean. A smaller standard deviation indicates that the values are concentrated near the mean, while a larger standard deviation indicates greater spread.

The following proposition describes how the standard deviation transforms under linear changes of a random variable.

Proposition B.5.5 Let X be a discrete random variable with standard deviation σ_X, and let a and b be constants. Then the standard deviation σ_Y of the random variable $Y = aX + b$ is

$$\sigma_Y = |a|\,\sigma_X.$$

Proof. The variance of Y is

$$Var(Y) = \sum_x (ax+b-(aE(X)+b))^2 f(x) = a^2 \sum_x (x-E(X))^2 f(x) = a^2\sigma_X^2.$$

Taking square roots gives

$$\sigma_Y = |a|\,\sigma_X.$$

■

In practice, variance is often more convenient for theoretical derivations because of its algebraic properties, while standard deviation is usually preferred for interpretation, since it is expressed in the same units as the original data.

■ **Example B.19** Continuing from Example B.18 the standard deviation is

$$\sigma = \sqrt{Var(X)} = \sqrt{50} \approx 7.07.$$

Unlike variance, which is expressed in squared minutes, the standard deviation is measured in minutes, the same units as the commuting times themselves. This means that the typical commuting time deviates from the average of 35 minutes by about 7 minutes. ■

B.5.3 Measures of Statistical Relationship

Covariance and correlation are measures that describe the relationship between two variables. Covariance quantifies the direction of their linear association, indicating whether the variables tend to increase or decrease together. However, covariance is expressed in the product of the units of the two variables, making its magnitude difficult to interpret. Correlation, in contrast, standardizes this measure to a dimensionless quantity between -1 and 1: a value of -1 indicates a perfect negative linear relationship, 1 a perfect positive linear relationship, and 0 the absence of a linear relationship.

Covariance

Covariance is a measure of the joint variability of two discrete random variables X and Y. It indicates the direction of their linear relationship: whether they tend to increase together, decrease together, or vary independently.

Definition B.5.5 Let X and Y be two discrete random variables with finite expected values $E(X)$ and $E(Y)$. The *covariance* of X and Y, denoted by $\mathrm{Cov}(X,Y)$, is defined as

$$\mathrm{Cov}(X,Y) = E[(X - E(X))(Y - E(Y))].$$

The sign of the covariance reveals the direction of the relationship: a positive value means that as X increases, Y tends to increase; a negative value means that as X increases, Y tends to decrease. A covariance of zero indicates no linear relationship, though nonlinear dependencies may still exist and are not captured by covariance.

The following result provides a useful formula for computing covariance.

Proposition B.5.6 For any two discrete random variables X and Y with finite expectations,

$$\mathrm{Cov}(X,Y) = E(XY) - E(X)E(Y).$$

Proof. By definition,

$$\mathrm{Cov}(X,Y) = E\left[(X - E(X))(Y - E(Y))\right].$$

Expanding the product inside the expectation,

$$E[XY - XE(Y) - YE(X) + E(X)E(Y)].$$

Using linearity of expectation and the fact that $E(X)$ and $E(Y)$ are constants,

$$E(XY) - E(X)E(Y) - E(X)E(Y) + E(X)E(Y) = E(XY) - E(X)E(Y).$$

■

The following proposition shows the connection between independence and covariance.

Proposition B.5.7 If X and Y are independent discrete random variables, then

$$\mathrm{Cov}(X,Y) = 0.$$

Proof. From the identity above,

$$\mathrm{Cov}(X,Y) = E(XY) - E(X)E(Y).$$

If X and Y are independent, then $E(XY) = E(X)E(Y)$. Substituting,

$$\mathrm{Cov}(X,Y) = E(X)E(Y) - E(X)E(Y) = 0.$$

■

The converse does not hold in general: a covariance of zero does not imply independence. Two random variables may be dependent yet uncorrelated.

Correlation

The magnitude of covariance depends on the scale of the variables, making it difficult to compare across different contexts. To address this, correlation standardizes covariance by dividing by the product of the standard deviations of the variables. This yields a dimensionless measure of the strength and direction of their linear relationship.

Definition B.5.6 Let X and Y be two discrete random variables with finite, nonzero variances $\mathrm{Var}(X)$ and $\mathrm{Var}(Y)$. The *correlation* of X and Y, denoted by $\mathrm{Cor}(X,Y)$ is defined as

$$\mathrm{Cor}(X,Y) = \frac{\mathrm{Cov}(X,Y)}{\sqrt{\mathrm{Var}(X)}\sqrt{\mathrm{Var}(Y)}}.$$

Correlation takes values in the interval $[-1,1]$.

Proposition B.5.8 For any pair of random variables X and Y with finite nonzero variances,

$$-1 \leq \mathrm{Cor}(X,Y) \leq 1.$$

Proof. Let $U = X - E(X)$ and $V = Y - E(Y)$. Then

$$\mathrm{Cov}(X,Y) = E[UV].$$

By the Cauchy–Schwarz inequality,

$$|E[UV]|^2 \leq E[U^2]\,E[V^2].$$

Noting that $E[U^2] = \mathrm{Var}(X)$ and $E[V^2] = \mathrm{Var}(Y)$, we obtain

$$|\mathrm{Cov}(X,Y)| \leq \sqrt{\mathrm{Var}(X)}\sqrt{\mathrm{Var}(Y)}.$$

Dividing both sides by the product of the standard deviations gives

$$-1 \leq \mathrm{Cor}(X,Y) \leq 1.$$

■

A value of $\mathrm{Cor}(X,Y) = 1$ indicates a perfect positive linear relationship, $\mathrm{Cor}(X,Y) = -1$ indicates a perfect negative linear relationship, and $\mathrm{Cor}(X,Y) = 0$ indicates no linear relationship.

■ **Example B.20** Consider two variables: weekly hours of exercise (X) and monthly weight loss in kilograms (Y). Suppose the following data are observed:

Person	X	Y
1	5	1
2	10	2
3	15	3
4	20	3.5
5	25	4

Computing the correlation coefficient yields ≈ 0.98, indicating a very strong positive linear relationship. This means that individuals who exercise more hours per week tend to lose more weight. However, it is important to note that correlation measures association, not causation. ■

The following proposition establishes that if two discrete random variables are independent and have finite variances, their correlation must be zero.

Proposition B.5.9 If X and Y are independent discrete random variables with finite, nonzero variances, then

$$\mathrm{Cor}(X,Y) = 0.$$

Proof. From the definition,

$$\mathrm{Cor}(X,Y) = \frac{\mathrm{Cov}(X,Y)}{\sqrt{\mathrm{Var}(X)}\sqrt{\mathrm{Var}(Y)}}.$$

If X and Y are independent, then $E(XY) = E(X)E(Y)$, so $\mathrm{Cov}(X,Y) = 0$. Substituting into the formula above gives $\mathrm{Cor}(X,Y) = 0$. ■

Note, however, that the converse is not true: correlation equal to zero does not imply independence, since variables can be dependent in nonlinear ways.

B.6 Common Distributions

In this section, we define and discuss several important families of distributions that are widely used in applications of probability theory. Specifically, we introduce the following families of discrete distributions: uniform, Bernoulli, binomial, and discrete normal. For each family, we briefly describe how it arises in practical problems and why it provides a suitable probability model for certain types of experiments. We also present the explicit form of the probability mass function and highlight some of the fundamental properties of the distributions in each family.

B.6.1 Uniform Distribution

The uniform distribution is the simplest probability distribution in probability theory. It models situations in which all outcomes are equally likely.

Definition B.6.1 A discrete random variable X is said to follow a *uniform distribution* if all outcomes have the same probability. Specifically, if X takes values in the set $x_1, x_2, \dots, x_n$, the probability mass function is

$$P(X = x_i) = \frac{1}{n}, \quad i = 1, 2, \dots, n.$$

A classic example of the discrete uniform distribution is the outcome of rolling a fair die, where each face has probability $1/6$. Unlike other distributions introduced in this section, the uniform distribution is determined solely by its set of possible values, with no additional parameters required.

For a discrete uniform random variable X taking values $x_1, x_2, \dots, x_n$, the expected value and variance are given by

$$E(X) = \frac{x_1 + x_2 + \cdots + x_n}{n}, \qquad \mathrm{Var}(X) = \frac{1}{n}\sum_{i=1}^{n}(x_i - E(X))^2.$$

B.6.2 Bernoulli Distribution

The Bernoulli distribution is one of the simplest and most fundamental in probability theory. It models experiments with only two possible outcomes, commonly referred to as "success" and "failure."

Definition B.6.2 A discrete random variable X is said to follow a *Bernoulli distribution* with parameter $p \in [0, 1]$, written $X \sim \mathrm{Bernoulli}(p)$, if it takes the value 1 (success) with probability p and the value 0 (failure) with probability $1 - p$. Its probability mass function is

$$P(X = x) = \begin{cases} p & \text{if } x = 1, \\ 1 - p & \text{if } x = 0. \end{cases}$$

The Bernoulli distribution arises naturally in many applied settings, especially those involving binary outcomes. For example, in medical studies, the result of a treatment can be modeled as a Bernoulli random variable, with "success" representing recovery and "failure" representing no improvement.

The expected value of $X \sim \mathrm{Bernoulli}(p)$ is $E(X) = p$. Intuitively, this reflects the long-run average outcome of many trials. The variance is

$$\mathrm{Var}(X) = E(X^2) - [E(X)]^2 = p - p^2 = p(1 - p).$$

This variance is maximized when $p = 0.5$, corresponding to maximum uncertainty when success and failure are equally likely.

Definition B.6.3 A sequence of independent and identically distributed random variables $X_1, X_2, \ldots$, each with $X_i \sim \text{Bernoulli}(p)$, is called a sequence of *Bernoulli trials* with parameter p. An infinite sequence of Bernoulli trials is called a *Bernoulli process*.

The Bernoulli process serves as the foundation for more complex stochastic processes and underlies many important models, including the binomial distribution.

B.6.3 Binomial Distribution

The binomial distribution is a discrete probability distribution that models the number of successes in a fixed number of independent Bernoulli trials, each with the same probability of success. It is one of the most widely used distributions in probability theory for problems involving repeated binary outcomes.

Definition B.6.4 A discrete random variable X is said to follow a *binomial distribution* with parameters n and p if it represents the number of successes in n independent Bernoulli trials, each with success probability p. The probability mass function is given by:

$$P(X = k) = \binom{n}{k} p^k (1-p)^{n-k} \quad k = 0, 1, 2, \ldots, n.$$

Here, n is the number of trials, and p is the probability of success on each trial. The coefficient $\binom{n}{k}$ counts the number of ways to obtain exactly k successes in n trials.

The binomial distribution arises naturally in many applications where outcomes can be classified as either "success" or "failure."

■ **Example B.21** Suppose a company produces light bulbs, and historically, 95% of them are functional (success) while 5% are defective (failure). The company tests a random sample of 20 bulbs. Let X be the number of functional bulbs. Then $X \sim \text{Binomial}(n = 20, p = 0.95)$. For example, the probability that exactly 18 bulbs are functional is:

$$P(X = 18) = \binom{20}{18} (0.95)^{18} (0.05)^2.$$

■

The expected value of a binomial random variable X with parameters n

and p is

$$E(X) = np,$$

representing the average number of successes in n trials. Its variance is

$$\mathrm{Var}(X) = np(1-p),$$

which measures the variability of the number of successes around the expected value.

B.6.4 Discrete Normal Distribution

The normal distribution is a continuous probability distribution that frequently appears in natural and social sciences, primarily due to the Central Limit Theorem (see Theorem B.7.5). However, many real-world situations involve discrete outcomes, such as counts of events or integer-valued random variables. In these cases, it is desirable to have a discrete analog of the normal distribution. This is not a limitation, but rather a reflection of the fact that continuous distributions often arise as limiting abstractions of underlying discrete processes.

In this section, we introduce the *discrete normal distribution*, which serves as a discrete counterpart to the normal distribution for integer-valued random variables. Although not as standardized as other families such as the Bernoulli or binomial distributions, the discrete normal can provide a useful tool in applications where outcomes must remain integer-valued. propositions.

To define the discrete normal distribution, we first introduce the concept of a standardized discrete random variable.

Definition B.6.5 Let X be a discrete random variable with expected value $E(X)$ and variance $\mathrm{Var}(X)$. The *standardized discrete random variable* of X, denoted by Z, is defined as:

$$Z = \frac{X - E(X)}{\sqrt{\mathrm{Var}(X)}}.$$

This transformation centers the distribution around 0 and rescales it so that the variance is 1.

■ **Example B.22** If $X \sim \mathrm{Bin}(n, p)$, then its standardized version is

$$Z = \frac{X - np}{\sqrt{np(1-p)}}.$$

The random variable Z takes values in the set

$$\left\{\frac{k-np}{\sqrt{np(1-p)}} : k=0,1,\ldots,n\right\},$$

with probability mass function

$$P\left(Z=\frac{k-np}{\sqrt{np(1-p)}}\right)=\binom{n}{k}p^k(1-p)^{n-k}.$$

■

The normal distribution arises as the limit of the standardized binomial distribution as $n\to\infty$. However, because the binomial is discrete and the normal is continuous, it is natural to consider a discrete distribution whose probabilities are proportional to the normal density evaluated at integer points.

Definition B.6.6 A discrete random variable X is said to follow a *discrete normal distribution* with parameters μ and σ^2 if it has probability mass function:

$$P(X=k)=\frac{1}{Z}\exp\left(-\frac{(k-\mu)^2}{2\sigma^2}\right), \quad k\in\mathbb{Z},$$

where Z is the normalization constant:

$$Z=\sum_{k=-\infty}^{\infty}\exp\left(-\frac{(k-\mu)^2}{2\sigma^2}\right).$$

This distribution retains the discrete nature of integer-valued random variables while exhibiting the bell-shaped curve characteristic of the continuous normal distribution.

Proposition B.6.1 The normalization constant Z in the discrete normal distribution satisfies:

$$Z\approx\sqrt{2\pi\sigma^2},$$

for large σ, and thus the probability mass function can be approximated by:

$$P(X=k)\approx\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(k-\mu)^2}{2\sigma^2}\right).$$

Proof. For large σ, the sum in Z can be approximated by an integral:

$$Z=\sum_{k=-\infty}^{\infty}\exp\left(-\frac{(k-\mu)^2}{2\sigma^2}\right)\approx\int_{-\infty}^{\infty}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)dx=\sqrt{2\pi\sigma^2}.$$

■

For large σ, the discrete normal approaches the continuous normal probability den evaluated at integer points.

■ **Example B.23** Suppose we model the number of defective items in a production run of 100 units, where each item is defective with probability $p = 0.1$ independently. Then $X \sim \text{Bin}(100, 0.1)$, with

$$E(X) = 100 \times 0.1 = 10, \quad \text{Var}(X) = 100 \times 0.1 \times 0.9 = 9.$$

For large n, X may be approximated by the discrete normal distribution with parameters $\mu = 10$ and $\sigma^2 = 9$. The probability of exactly 12 defective items is approximated by

$$P(X = 12) \approx \frac{1}{Z} \exp\left(-\frac{(12-10)^2}{2 \times 9}\right).$$

This provides an alternative to the usual continuous normal approximation, avoiding the need for continuity corrections and keeping the support discrete.
■

The following proposition highlights an important property of the discrete normal distribution, specifically its symmetry around the mean.

Proposition B.6.2 The discrete normal distribution is symmetric about its mean μ. Formally, for any integer k,

$$P(X = \mu + k) = P(X = \mu - k).$$

Proof. From the definition,

$$P(X = \mu + k) = \frac{1}{Z} \exp\left(-\frac{k^2}{2\sigma^2}\right),$$

and similarly,

$$P(X = \mu - k) = \frac{1}{Z} \exp\left(-\frac{(-k)^2}{2\sigma^2}\right) = \frac{1}{Z} \exp\left(-\frac{k^2}{2\sigma^2}\right).$$

Thus the distribution is symmetric about μ. ■

The discrete normal distribution serves as a bridge between discrete and continuous probability models. It inherits key properties of the normal distribution—such as symmetry and centrality—while remaining defined on the integers. This makes it particularly useful in contexts such as manufacturing, epidemiology, or educational testing, where outcomes are integer-valued but approximately normal in shape.

B.7 Large Random Samples

A random sample is a collection of independent and identically distributed random variables. Random samples are fundamental in probability theory, providing the foundation for making inferences about an unknown probability distribution. Two key results that arise from random samples are the law of large numbers, which ensures that the sample mean converges to the expected value of the distribution as the sample size increases, and the central limit theorem, which states that the distribution of the sample mean approaches a normal distribution as the sample size grows, regardless of the original population's distribution.

Random sampling assumes that every member of the population has an equal probability of being selected and that selections are independent of one another. In this sense, the sample is an idealized representation of how real-world data might be generated. Perfect random sampling is rarely achievable in practice, but it provides a baseline against which deviations can be evaluated. This framework allows us to construct probability distributions describing the expected behavior of sample statistics (e.g., sample mean, variance), making it possible to quantify uncertainty and to draw principled conclusions about the population.

The random sampling model is therefore a powerful representation of how data might be collected, though it is not identical to reality. Like all models, it works well in specific contexts, but its assumptions do not universally hold. The practical usefulness of random sampling depends on how closely the model aligns with the real-world situation under study.

B.7.1 Random Sample

The concept of a random sample is pivotal in the field of statistical learning, since assuming that a set of discrete random variables forms a random sample greatly simplifies the mathematical foundations of inference. However, the criteria required for a collection of variables to be considered a random sample are not always satisfied in real-world scenarios.

Definition B.7.1 Let f be a probability mass function, and let $X_1, X_2, \ldots, X_n$ be a collection of discrete random variables. The variables $X_1, X_2, \ldots, X_n$ form a *random sample* from the distribution f if each X_i follows the probability mass function f and the variables $X_1, X_2, \ldots, X_n$ are mutually independent. Such variables are called *independent and identically distributed (i.i.d.)*. The number n of variables is called the *sample size*.

The joint probability mass function g of a random sample $X_1, X_2, \ldots, X_n$

is

$$g(x_1,x_2,\dots,x_n) = f(x_1)f(x_2)\dots f(x_n).$$

■ **Example B.24** A factory produces light bulbs, and the quality control department is interested in estimating the proportion of defective bulbs. The number of defectives in a batch of 100 bulbs is modeled by a binomial distribution with parameter p, the probability of a bulb being defective. Suppose the department randomly selects 5 batches, each of 100 bulbs. Let $X_1,\dots,X_5$ denote the number of defectives in each batch. Each $X_i \sim \text{Binomial}(100, p)$, and assuming the batches are independent, the variables $X_1,\dots,X_5$ form a random sample. ■

In statistical inference, it is convenient to compute the sample mean, as the average of n random variables.

Definition B.7.2 Let $X_1,X_2,\dots,X_n$ be n discrete random variables. The *sample mean*, denoted by $\bar{X}_n$, is:

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

Do not confuse the random variable $\bar{X}_n = \frac{1}{n}(X_1 + \cdots + X_n)$ with the population mean $E(X_i)$, which is a fixed real number. Recall that $X_1+\cdots+X_n$ defines a new random variable on the Cartesian product of the original sample spaces, not a sum of probability distributions.

The following proposition shows that the sample mean provides an unbiased estimate of the population mean, and that its variance decreases as the sample size increases.

Proposition B.7.1 Let $X_1,\dots,X_n$ be a random sample with finite mean $E(X_i) = \mu$ and variance $\text{Var}(X_i) = \sigma^2$. Then

$$E(\bar{X}_n) = \mu, \qquad \text{Var}(\bar{X}_n) = \frac{\sigma^2}{n}.$$

Proof. By linearity of expectation,

$$E(\bar{X}_n) = E\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right) = \frac{1}{n}\sum_{i=1}^{n} E(X_i) = \mu.$$

For the variance,

$$\text{Var}(\bar{X}_n) = \text{Var}\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right) = \frac{1}{n^2}\text{Var}\left(\sum_{i=1}^{n} X_i\right).$$

Since the X_i are independent,

$$\mathrm{Var}\left(\sum_{i=1}^{n} X_i\right) = \sum_{i=1}^{n} \mathrm{Var}(X_i) = n\sigma^2,$$

so

$$\mathrm{Var}(\bar{X}_n) = \frac{1}{n^2} \cdot n\sigma^2 = \frac{\sigma^2}{n}.$$

■

Thus, the sample mean is unbiased, and its variance shrinks at rate $1/n$. As n grows, the distribution of $\bar{X}_n$ becomes more concentrated around the population mean μ.

In statistical inference, it is also convenient to compute the sample variance as a measure of the dispersion of the sample values.

Definition B.7.3 Let $X_1, X_2, \ldots, X_n$ be a set of discrete random variables with sample mean $\bar{X}_n$. The *sample variance*, denoted by S^2, is:

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

The factor $1/(n-1)$ ensures that S^2 is an unbiased estimator of the population variance when the X_i are i.i.d. Do not confuse the sample variance, which is computed from observed data, with the theoretical variance of the underlying distribution.

■ **Example B.25** Suppose we observe $X_1 = 6$, $X_2 = 4$, $X_3 = 5$, $X_4 = 7$, $X_5 = 3$. Then

$$\bar{X}_5 = \frac{6+4+5+7+3}{5} = 5,$$

and

$$S^2 = \frac{1}{4}\left[(6-5)^2 + (4-5)^2 + (5-5)^2 + (7-5)^2 + (3-5)^2\right] = \frac{10}{4} = 2.5.$$

■

The sample standard deviation is used to estimate the standard deviation of a population based on a sample taken from it. Unlike the population standard deviation, which uses the true mean of the entire population, the sample standard deviation uses the mean of the sample as an estimate of the true mean.

Definition B.7.4 Let $X_1, X_2, \ldots, X_n$ be n discrete random variables with sample mean $\bar{X}_n$ and sample variance S^2. The *sample standard deviation*, denoted by S, is:

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

■ **Example B.26** Using the variance from the previous example, the sample standard deviation is

$$S = \sqrt{2.5} \approx 1.58.$$

■

Finally, when two variables are sampled together, the sample covariance estimates the covariance between their populations.

Definition B.7.5 Let $X_1, X_2, \ldots, X_n$ and $Y_1, Y_2, \ldots, Y_n$ be two sets of discrete random variables with sample means $\bar{X}$ and $\bar{Y}$ respectively. The *sample covariance* is:

$$s_{XY} = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})$$

■ **Example B.27** Suppose we observe the paired data

i	1	2	3	4	5
X_i	2	4	6	8	10
Y_i	1	3	5	7	9

Then

$$\bar{X} = 6, \quad \bar{Y} = 5,$$

and

$$s_{XY} = \frac{1}{4}\left[(-4)(-4) + (-2)(-2) + (0)(0) + (2)(2) + (4)(4)\right] = \frac{40}{4} = 10.$$

■

B.7.2 Law of Large Numbers

The law of large numbers states that the sample mean of a large random sample, i.e., a large number of independent and identically distributed (i.i.d.) discrete random variables, will be close to the expected value of the distribution, and that as we increase the sample size, the sample mean gets closer (in a precise probabilistic sense) to that value. Before proving this theorem, we establish two related propositions: Markov's inequality and Chebyshev's inequality.

Markov's inequality provides a simple bound on how unlikely it is for a nonnegative discrete random variable to take a large value, given its expected value. Intuitively, if the average value of a nonnegative random variable X is small, then X is unlikely to be very large (recall Example B.16). Markov's inequality is particularly useful because it requires no assumptions on the distribution of X beyond nonnegativity and finiteness of the mean.

Proposition B.7.2 — Markov's Inequality. Let X be a nonnegative discrete random variable, i.e. $P(X \geq 0) = 1$, with expected value $E(X)$. Then for every real number $t > 0$ we have that

$$P(X \geq t) \leq \frac{E(X)}{t}$$

Proof. Let f be the probability mass function of X. Since X is non-negative we have that $E(X) = \sum_{x>0} xf(x)$. Then

$$E(X) = \sum_{x>0} xf(x) = \sum_{x=0}^{t} xf(x) + \sum_{x=t}^{\infty} xf(x) \geq$$
$$\sum_{x=t}^{\infty} xf(x) \geq \sum_{x=t}^{\infty} tf(x) = t\sum_{x=t}^{\infty} f(x) = tP(X \geq t)$$

that is, $E(X) \geq tP(X \geq t)$. ■

For example, if $E(X) = 10$ and we ask for $P(X \geq 50)$, Markov's inequality gives $P(X \geq 50) \leq 10/50 = 0.2$. While Markov's inequality is very general and easy to use, its bound is often not tight because it uses only the mean of X.

Chebyshev's inequality bounds the probability that a random variable deviates from its expected value by more than a specified number of standard deviations. Unlike Markov's inequality, which only requires non-negativity, it does not require X to be nonnegative, but it requires knowledge of both the mean and variance.

Corollary B.7.3 — Chebyshev's Inequality. Let X be a discrete random variable with finite mean $E(X)$ and finite variance $\mathrm{Var}(X)$. Then for every $t > 0$,

$$P\big(|X - E(X)| \geq t\big) \leq \frac{\mathrm{Var}(X)}{t^2}.$$

Proof. Apply Markov's inequality to the nonnegative random variable $(X - E(X))^2$:

$$P\big(|X-E(X)|\geq t\big) = P\big((X-E(X))^2 \geq t^2\big) \leq \frac{E\left[(X-E(X))^2\right]}{t^2} = \frac{\mathrm{Var}(X)}{t^2}.$$

■

Chebyshev's inequality formalizes the idea that most of the probability mass of a distribution lies near its mean: the probability of being several standard deviations away decays at least on the order of $1/t^2$.

The last notion we need for the law of large numbers is convergence in probability. Intuitively, a sequence of random variables converges in probability to b if the values X_n concentrate around b as n increases.

Definition B.7.6 Let $X_1, X_2, \ldots$ be a sequence of discrete random variables. It is said that the sequence $X_1, X_2, \ldots$ *converges in probability* to b , denoted by $X_n \xrightarrow{p} b$, if for every positive real number $\varepsilon > 0$,

$$\lim_{n\to\infty} P\left(|X_n - b| < \varepsilon\right) = 1$$

Given these elements, we can state and prove the (weak) law of large numbers.

Theorem B.7.4 — Law of Large Numbers. Let $X_1, X_2, \ldots$ be i.i.d. random variables with finite mean $E(X_i) = \mu$ and finite variance $\mathrm{Var}(X_i) = \sigma^2$. Let $\overline{X}_n = \frac{1}{n}(X_1 + \cdots + X_n)$ be the sample mean. Then

$$\overline{X}_n \xrightarrow{p} \mu.$$

Proof. By Proposition B.7.1, $E(\overline{X}_n) = \mu$ and $\mathrm{Var}(\overline{X}_n) = \sigma^2/n$. Applying Chebyshev's inequality,

$$P\left(\left|\overline{X}_n - \mu\right| \geq \varepsilon\right) \leq \frac{\sigma^2}{n\varepsilon^2}.$$

From there we can obtain

$$P\left(\left|\overline{X}_n - \mu\right| < \varepsilon\right) = 1 - P\left(\left|\overline{X}_n - \mu\right| \geq \varepsilon\right) \geq 1 - \frac{\sigma^2}{n\varepsilon^2}.$$

As n approaches infinity, the above expression approaches 1. Thus,

$$\overline{X}_n \xrightarrow{p} \mu$$

■

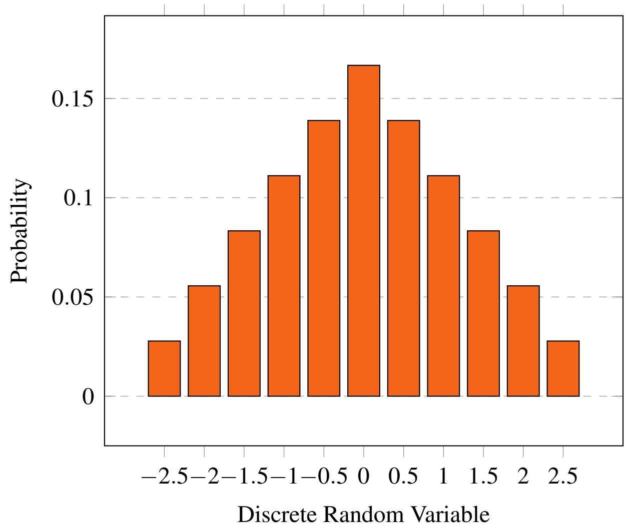


Figure B.1: Probability mass function of the discrete random variable $\frac{X_1+X_2}{2} - \mathbb{E}(X)$.

It is important to note that the assumptions (independence and identical distribution, with finite variance) are essential. The theorem is an asymptotic statement: for a finite sample, the sample mean is typically close to the population mean, but not necessarily equal to it.

■ **Example B.28** Consider rolling a fair six-sided die with sample space $\Omega = \{1,2,3,4,5,6\}$ and $P(\omega) = 1/6$ for each outcome. Let $X : \Omega \to \mathbb{R}$ map each side to its face value, so $E(X) = 3.5$.

First take a random sample of size two: roll the die twice (in sequence, so the rolls are distinguishable) and let X_1 and X_2 be the outcomes. The sample mean is the random variable

$$\frac{X_1+X_2}{2} : \Omega \times \Omega \to \mathbb{R}, \quad (\omega_1, \omega_2) \mapsto \frac{X_1(\omega_1)+X_2(\omega_2)}{2}.$$

whose probability mass function is depicted in Figure B.1. A direct calculation shows

$$\begin{aligned} P\left(\left|\frac{X_1+X_2}{2} - E(X)\right| < 1\right) &= P\big(|X_1+X_2-7| < 2\big) \\ &= P\big(X_1+X_2 \in \{6,7,8\}\big) = \frac{16}{36} \approx 0.444. \end{aligned}$$

Now consider a random sample of size ten. The distribution of

$$\frac{X_1+\cdots+X_{10}}{10} - E(X)$$

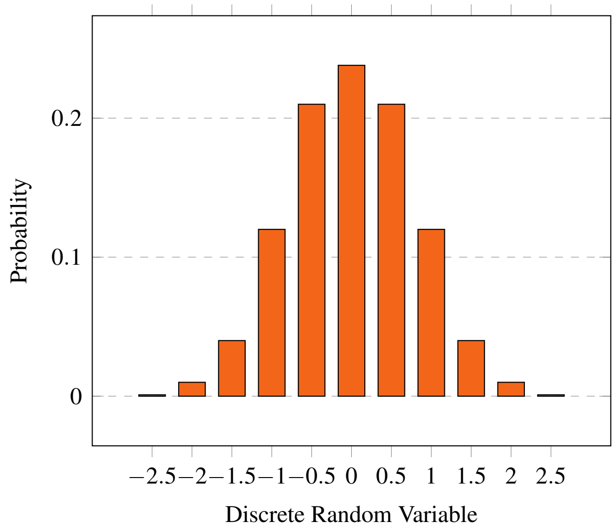


Figure B.2: Probability mass function of the discrete random variable $\frac{X_1+X_2+\ldots+X_{10}}{10} - E(X)$.

is much more concentrated around 0 (see Figure B.2); numerically,

$$P\left(\left|\frac{X_1+\cdots+X_{10}}{10} - 3.5\right| < 1\right) \approx 0.97,$$

illustrating the sharpening concentration predicted by the law of large numbers.

■

Finally, the law of large numbers concerns the *sample mean* $\frac{1}{n}\sum_{i=1}^{n} X_i$, not other aggregates. For instance, the deviation from the expected total,

$$\sum_{i=1}^{n} X_i \; - \; nE(X),$$

does not converge to 0; in fact, its typical size grows on the order of $\sqrt{n}$ (see Example B.29). Confusing these statements underlies a common misconception.

■ **Example B.29** If we toss a fair coin, the probability of heads is $1/2$. By the law of large numbers, the *proportion* of heads in many tosses is close to $1/2$. However, the *difference* between the number of heads and tails need not be close to 0; in fact, its typical magnitude grows like a constant multiple of $\sqrt{n}$ as the number of tosses n increases. The belief that the counts of heads and tails should stay nearly equal as n grows is a form of the gambler's fallacy. ■

B.7.3 Central Limit Theorem

Let $X_1, \ldots, X_n$ be a sample of n independent and identically distributed random variables with mean μ and variance σ^2. As we saw in the previous section, the law of large numbers states that the sample average $\overline{X}_n$ converges in probability to μ as n increases. The central limit theorem strengthens this by describing the distribution of the centered and scaled sample mean: the quantity $\sqrt{n}(\overline{X}_n - \mu)$ converges in distribution to a normal random variable with mean 0 and variance σ^2. Equivalently, the standardized statistic

$$Z_n = \frac{\overline{X}_n - \mu}{\sigma/\sqrt{n}}$$

converges in distribution to the standard normal distribution $N(0,1)$. This result holds regardless of the shape of the underlying distribution, provided it has finite variance.

Theorem B.7.5 — Central Limit Theorem. Let $X_1, \ldots, X_n$ be i.i.d. random variables with mean μ and finite variance σ^2. Define

$$Z_n = \frac{\overline{X}_n - \mu}{\sigma/\sqrt{n}}, \quad \text{where} \quad \overline{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i.$$

Then, as $n \to \infty$,

$$Z_n \Rightarrow N(0,1),$$

i.e., Z_n converges in distribution to the standard normal law with density $\phi(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)$. Equivalently,

$$\sqrt{n}\,(\overline{X}_n - \mu) \Rightarrow N(0, \sigma^2).$$

Proof sketch. We first consider the special case of Bernoulli random variables. Let $X_i \sim \text{Bernoulli}(p)$ and $S_n = \sum_{i=1}^{n} X_i$. The standardized sum is

$$Z_n = \frac{S_n - np}{\sqrt{np(1-p)}}.$$

Using Stirling's approximation for factorials in the binomial formula, one shows that for integers k close to np (within order $\sqrt{n}$),

$$P(S_n = k) \approx \frac{1}{\sqrt{2\pi np(1-p)}} \exp\left(-\frac{(k-np)^2}{2np(1-p)}\right).$$

This is exactly the probability mass function of a discretized normal distribution. Summing over such k produces a Riemann sum converging to the normal distribution function, proving the result for Bernoulli variables.

For general i.i.d. random variables with finite mean and variance, one reduces to the Bernoulli case by truncating the variables to control large deviations and matching means and variances. The same approximation then applies, and the limiting distribution is again standard normal. ■

The central limit theorem is a cornerstone of probability and statistics. It justifies normal approximations for sampling distributions of means and enables approximate inference. The basic conditions used here are i.i.d. observations with finite variance.

■ **Example B.30** Suppose a factory produces light bulbs and the lifetime of each bulb (measured, say, in hours) has mean $\mu = 1000$ and standard deviation $\sigma = 50$. A random sample of $n = 36$ bulbs is tested. What is the probability that the sample mean lifetime lies between 990 and 1010 hours?

By the CLT, for $n = 36$ the sample mean $\overline{X}_n$ is approximately normal with mean μ and standard deviation $\sigma/\sqrt{n} = 50/6 \approx 8.33$:

$$\overline{X}_n \approx N\left(1000,\ \left(\frac{50}{\sqrt{36}}\right)^2\right).$$

Standardizing,

$$z_{990} = \frac{990 - 1000}{8.33} \approx -1.20, \qquad z_{1010} = \frac{1010 - 1000}{8.33} \approx 1.20.$$

Thus

$$\begin{aligned} P(990 \le \overline{X}_n \le 1010) &\approx P(-1.20 \le Z \le 1.20) = \Phi(1.20) - \Phi(-1.20) \\ &\approx 0.8849 - 0.1151 = 0.7698. \end{aligned}$$

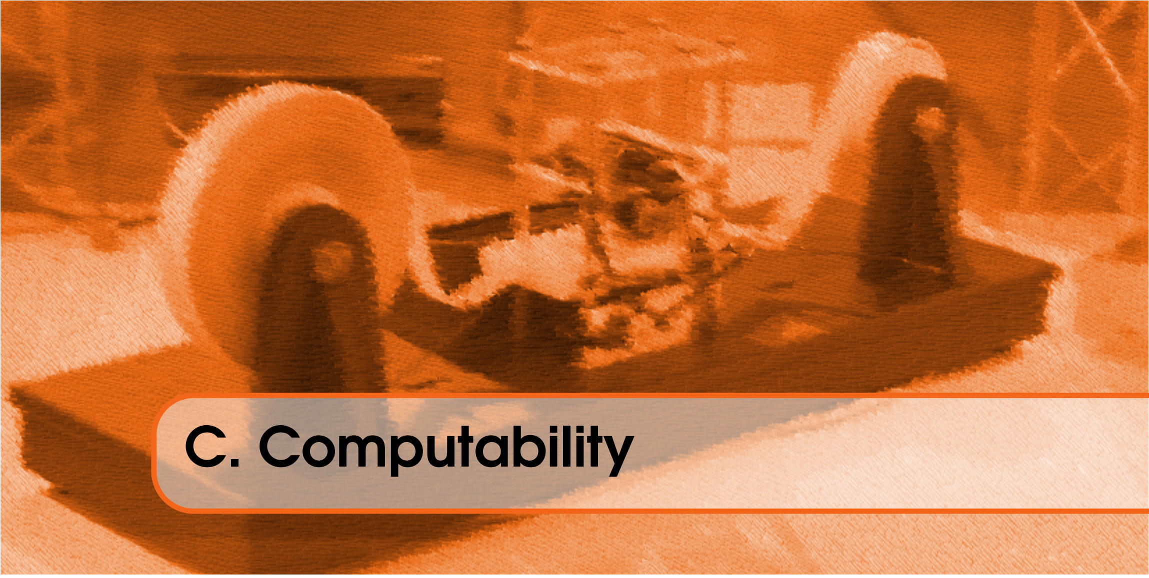
So the probability is about 76.98%. ■

References

[DeG+86] is a widely respected textbook in the fields of statistics and probability theory. First published in 1975, this book is known for its clear exposition of the fundamental concepts of probability and statistics, making it suitable for both beginners and those with some background in the subject. The book's approach balances theory and application, making it useful both for learning theoretical underpinnings and for applying probability and statistics to real-world problems.

[Chi13] offers a comprehensive introduction to the foundational aspects of probability, with a focus on the philosophical questions it raises. Childers explores various interpretations of probability, including frequentist, propensity, classical, Bayesian, and objective Bayesian, and presents these complex ideas in a way that is accessible even to those without a strong background in probability or mathematics.

An example of the problems associated with the misinterpretation of expected value is the St. Petersburg Paradox. Introduced by Nicholas Bernoulli in 1713, this paradox involves a gambling game with an infinite expected payoff, yet no reasonable person would pay more than $25 to play it. Despite being three centuries old, the paradox continues to inspire new arguments and solutions in recent years (see [Hua13] for a historical review of the main proposed solutions).



C. Computability

Wanderer, there is no road,
the road is made by walking.
Antonio Machado

We continue our review of the background required to understand the theory of nescience by providing a mathematical formalization of the concept of a *computable procedure*. Intuitively, a computable procedure is a method consisting of a finite sequence of instructions that, when applied to a problem, produces the correct answer after a finite number of steps. This informal notion rests on the requirement that the instructions be clear and precise enough for any human to follow without additional guidance. We may strengthen this requirement further by demanding that the instructions be so unambiguous that a machine could execute them.

In 1936, the British mathematician Alan Turing introduced a formal model of a family of hypothetical machines and argued that, for every intuitively computable procedure, there exists a *Turing machine* capable of carrying it out. The model is not only simple enough to allow precise mathematical analysis but also sufficiently general to capture the intuitive concept of effective computation.

Over the years, many alternative approaches have been proposed to formalize the notion of computability. Some of these are technically intricate, yet all have been shown to be equivalent in expressive power to Turing machines; in other words, they characterize the same class of effectively computable functions. Two notable examples are Alonzo Church's *lambda calculus* and the *theory of recursive functions* developed by Kurt Gödel and Stephen Kleene. The *Church-Turing thesis* asserts that any reasonable formalization of a computable procedure (subject to minimal requirements, such as performing only a finite amount of work in a single step) coincides with the Turing machine model. While not a theorem, this thesis has become a widely accepted working principle, providing a stable and shared notion of computability that is independent of any specific formalism.

The concept of the Turing machine, originally conceived as a model of a mechanical device designed to solve a particular problem, was later extended and generalized. A *universal Turing machine* can simulate the behavior of any other Turing machine and thereby compute any function that is computable in the intuitive sense. This is analogous to modern digital computers, which can execute algorithms expressed in diverse programming languages. This universality raises a natural question: Are there problems that no Turing machine can solve? The answer is yes. Certain well-defined problems, such as the Halting problem, lie beyond the reach of computation, and such problems are more common than one might initially expect. The existence of uncomputable functions will play a central role in our theory of nescience.

Given the abstract character of many entities studied in science, we employ the concept of the *oracle Turing machine* to formalize our framework. An oracle Turing machine resembles an ordinary Turing machine but is augmented with the ability to query an external oracle. The oracle, whose internal mechanism is unspecified, provides answers to questions that may be uncomputable for standard machines. Different oracles yield different computational powers, giving rise to a hierarchy of relative computability. For our purposes, the oracle can be viewed as a theoretical construct that models access to sources of information beyond the limits of mechanical computation. It should be emphasized that the oracle is not a physical device but an abstract tool for reasoning about the boundaries of computation.

Turing machines reveal the intrinsic limitations of computation. Exploring these limitations is not merely a philosophical exercise; it has profound implications for the field of *computational complexity*. Situated at the intersection of computer science and mathematics, computational complexity studies the resources (most notably time and space) required to solve problems. Problems are classified into *complexity classes* according to the

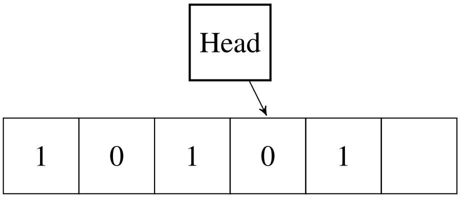


Figure C.1: Turing Machine

asymptotic resources needed by the best algorithms known for their solution. One of the most famous open problems in this field is the $P \stackrel{?}{=} NP$ question, which asks whether the class P of problems solvable in polynomial time coincides with the class NP of problems for which proposed solutions can be verified in polynomial time. In this book, our interest extends beyond the epistemological issue of determining which problems can be solved in principle, given unlimited resources, to the more practical question of which problems can be solved efficiently with respect to time.

C.1 Turing Machines

A Turing machine is an extremely simplified model of a general-purpose computer, yet it is powerful enough to capture the notion of effective computation. Intuitively, the machine consists of a head that operates on a two-way infinite tape divided into cells, each containing a symbol. At each time step, the machine reads the symbol under the head and, according to a fixed set of rules, either writes a new symbol, moves the head one cell to the left or right, or performs both actions. The rules are encoded in a finite control table. The input to the computation is written on the tape at the start, and once the machine enters a designated halting state, the output can be read from the tape. Figure C.1 illustrates a machine in its initial configuration, with the head positioned at the beginning of the input string.

Definition C.1.1 — Turing Machine. A *Turing machine* is a 7-tuple

$(Q, \Gamma, \sqcup, \Sigma, q_0, q_f, \tau)$ where:

Q is a finite, non-empty set of *states*,

Γ is a finite, non-empty set of *tape symbols*,

$\sqcup \in \Gamma$ is the *blank symbol*,

$\Sigma \subseteq \Gamma \setminus \{\sqcup\}$ is the set of *input symbols*,

$q_0 \in Q$ is the *initial state*,

$q_f \in Q \setminus \{q_0\}$ is the designated *halting state*,

$\tau : (Q \setminus \{q_f\}) \times \Gamma \rightharpoonup Q \times \Gamma \times \{L, R, S\}$ is a *transition function*.

The algorithm executed by the machine is defined by the (partial) transition function τ. This function dictates the machine's actions based on its current state and the tape symbol currently under the head. According to τ, the machine transitions to a new state, writes a new symbol on the tape (or retains the existing one), and moves the head left, right, or keeps it stationary (L, R, or S respectively). The machine follows a finite, uniquely determined sequence of steps until it reaches the final state q_f[1] and *halts*, making no subsequent moves. The algorithm's output is the string of symbols $s \in \Gamma^*$ remaining on the tape after halting. Some machines, however, may enter an infinite loop, never reaching a halting state. If a machine encounters an undefined transition, it will enter an infinite loop, never halting. We assume that the head of the machine is initially positioned at the first symbol of the input string.

■ **Example C.1** The following Turing machine is designed to solve the problem of adding two natural numbers. It consists of the set of states $Q = \{q_o, q_1, q_f\}$, the set of tape symbols $\Gamma = \{0, 1, \sqcup\}$, and the set of input symbols $\Sigma = \{0, 1\}$. The transition function is defined in the table below, where rows are indexed by machine states, and columns by tape symbols:

	0	1	$\sqcup$
q_o	$(q_f, \sqcup, R)$	$(q_1, \sqcup, R)$	$\uparrow$
q_1	$(q_f, 1, S)$	$(q_1, 1, R)$	$\uparrow$

Table C.1: Transition Rules

For natural numbers n and m, the input string is composed of n occurrences of the symbol '1', followed by a '0', and then followed by m occurrences of '1'. The machine's output will be a string of $n+m$ consecutive '1's. For instance, to add the numbers 2 and 3, the input string should be

[1] Some authors allow multiple halting states in the definition of Turing machines.

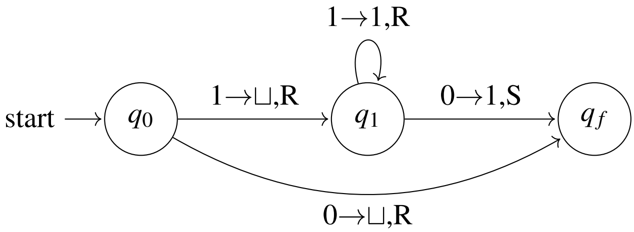


Figure C.2: State diagram of the addition machine

⊔110111⊔, resulting in the output string ⊔11111⊔. ■

A Turing machine can also be represented by a *state diagram*. A state diagram is similar to a labeled directed graph[2] where the vertices represent the states of the machine. The edges signify transitions from one state to another, and the edge labels indicate the symbol under the head that leads to the new state, the symbol that gets written on the tape, and the direction in which the head moves. Following these conventions, the state diagram for the Turing machine in Example C.1 is depicted in Figure C.2.

It is a remarkable fact that minor alterations to the definition of a Turing machine do not change its computational power. In other words, the definition is highly robust. In Example C.2, it's demonstrated that adding more tapes to the machine doesn't expand the range of problems it can solve. Similar arguments can be made when adding finite storage to the control, allowing for parallel processing with multiple control heads, and so on.

■ **Example C.2** A *multitape Turing machine* is a Turing machine equipped with multiple heads and their respective tapes. In the initial configuration, the input string resides in tape 1, while the other tapes are blank. The transition function for a multitape Turing machine is:

$$\tau : (Q \setminus q_f) \times \Gamma^k \to Q \times \Gamma^k \times \{L, R, S\}^k,$$

where k denotes the number of tapes. Multitape Turing machines are equivalent in power to standard Turing machines. We can validate this claim by devising a method for a standard Turing machine to mimic a multitape machine's behavior. This requires encoding the content of multiple tapes onto a single tape, introducing a new symbol as a tape separator, and encoding the positions of the heads across the tapes with a distinct head location symbol. If we designate the tape separation symbol as $|$ and the head location symbol as h, a simulation tape for a machine with 3 tapes might appear as

[2]In this particular case, we allow loops and multiple edges originating from vertices.

$\sqcup 01h00|000h1|h0101\sqcup$. The standard machine's operation would involve scanning the subtapes one by one, pinpointing the head's location, and executing the necessary transition. If the computation on one subtape necessitates writing a new symbol beyond its boundary, we'd need to shift subsequent symbols to accommodate the new one. While the simulation might operate at a slower pace than the original multitape machine, both machine types can solve an identical set of problems. ■

For the remainder of this book, without any loss of generality, we'll assume that the set of input symbols is $\Sigma = \mathcal{B}$ and the set of tape symbols is $\Gamma = \{0, 1, \sqcup\}$.

In addition to providing a formal definition of a Turing machine, it's essential to formally outline its computational process. This entails detailing how the machine reads the input string, produces the output string, and transitions between states during computation. We will start by defining the concept of the machine's internal configuration. This configuration captures the machine's current state and position, as well as the present state of the tape.

Definition C.1.2 A *configuration* of a Turing machine T is the 3-tuple (q, s, i), where $q \in Q$ represents a state of the machine, $s \in \Gamma^+$ denotes a string containing the tape's content (excluding the blank symbols), and $1 \leq i \leq n$ is the index of the symbol s_i beneath the head. Here, s_1 is the first symbol on the tape, and $n = l(s)$.

Configurations enable us to describe the current state of a Turing machine without any loss of information. At any stage of computation, one could halt the machine, record its configuration, and later resume the computation from the exact point of interruption using this configuration.

The following definition explains how we transition from one configuration to the next during computation.

Definition C.1.3 A configuration $C = (q, s, i)$ *yields* another configuration $C' = (r, s', j)$ if there exists a transition $\tau : (q, s_i) = (r, s'_i, a)$, where $s = s_1 \ldots s_{i-1} s_i s_{i+1} \ldots s_n$, $s' = s_1 \ldots s_{i-1} s'_i s_{i+1} \ldots s_n$, and

$$j = \begin{cases} i+1 & \text{if } a = R \\ i-1 & \text{if } a = L \\ i & \text{if } a = S \end{cases} \tag{C.1}$$

If $a = L$ and $i = 1$, we extend s on the left by a blank and keep the head at position 1 (now on $\sqcup$); if $a = R$ and $i = n$, we extend s on the right by a blank and set the head to position $n+1$.

Building on the concepts of configuration and one configuration yielding another, we can now formally articulate the notion of computation.

Definition C.1.4 — Computation. Let T be a Turing machine, C_0 its initial configuration, and C_n a configuration encompassing the final state q_f. A *computation* under machine T refers to a finite sequence of $n+1$ configurations $(C_0, C_1, \ldots, C_n)$ wherein each configuration C_k yields the subsequent configuration C_{k+1}, for all $0 \leq k < n$.

Computations are deterministic; meaning, for a given Turing machine T and an input string s, the configuration sequence is uniquely determined.. If machine T neither halts nor progresses with input s, we deduce the absence of computation.

■ **Example C.3** The computation of the Turing machine described in Example C.1 using the input string 110111 results in the following sequence of configurations:

1 $(q_0, 110111, 1)$
2 $(q_1, 10111, 1)$
3 $(q_1, 10111, 2)$
4 $(q_f, 11111, 2)$

■

Intuitively, a procedure is deemed computable by a human if it can be delineated through specific steps, executed systematically, without relying on intuition or ingenuity. This intuitive grasp aligns with the formalized concept of a Turing machine, bridging informal comprehension and the machine's rigorous definition—a cornerstone in the theory of computation. However, this alignment presents an intriguing challenge. Affirming that our grasp of computability mirrors a Turing machine's capabilities cannot be proven traditionally, as 'computability' lacks a well-defined interpretation. Consequently, some researchers categorize this as a *thesis*, avoiding the formal 'theorem' label. Turing himself opted to term it a *definition*, steering clear of denoting it as a theorem.

Theorem C.1.1 — Turing's Thesis. A procedure is computable if, and only if, it can be executed by a Turing machine.

To further underscore the significance and robustness of the Turing machine as a model of computation, it's worth noting, as mentioned earlier in this chapter, that all alternative formalizations of computability proposed to date align in terms of their computational capabilities with that of the Turing machine. This universality underscores the Turing machine's central position in the realm of theoretical computer science.

C.2 Universal Turing Machines

In Section C.1, we explored storing the current state of a Turing machine, its configuration, to pause and later resume computation. In Example C.4, we will delve into a similar procedure, not for storing the machine's current state, but for saving a comprehensive description of the machine itself. This methodology facilitates the enumeration, or listing, of all possible Turing machines. Such enumeration is instrumental in demonstrating the existence of problems that cannot be solved by any Turing machine (refer to Section C.3) and unveiling the pivotal concept of the *Universal Turing Machine*.

■ **Example C.4** To describe a Turing machine concisely, we need to encode the transition function $\tau : (Q \setminus \{q_f\}) \times \Gamma \to Q \times \Gamma \times \{L,R,S\}$. This function can be represented as a collection of quintuples (q,s,r,t,a), where $q \in (Q \setminus \{q_f\})$, $r \in Q$, $s,t \in \Gamma$, and $a \in \{L,R,S\}$. In this manner, any Turing machine T is fully described by a collection of quintuples:

$$(q_1,s_1,r_1,t_1,a_1),(q_2,s_2,r_2,t_2,a_2),\ldots,(q_m,s_m,r_m,t_m,a_m)$$

where $m \le d\,(Q \setminus \{q_f\}) \times d(\Gamma)$, with the stipulation that the first quintuple refers to the initial state and the second one to the final state; i.e., $q_1 = q_o$ and $r_2 = q_f$. A possible approach to describe these quintuples is to encode the elements of the set $Q \cup \Gamma \cup \{L,R,S\}$ using a fixed-length binary code (refer to Definition D.1.6 for more details), encoding the quintuple (q,s,r,t,a) as $\langle q,s,r,t,a \rangle$. The length of an encoded quintuple is $5l$, where $l = \lceil \log\left(d\left(Q \cup \Gamma \cup \{L,R,S\}\right)\right) \rceil$. Following this convention, machine T is encoded as the binary string:

$$\langle T \rangle = \left\langle \bar{l}, \langle q_1,s_1,r_1,t_1,a_1 \rangle, \ldots, \langle q_r,r_r,s_r,t_r,a_r \rangle \right\rangle$$

The length of the encoded machine, following this schema, would be $l(\langle T \rangle) \le 5lm + \log l + 1$. ■

Since each Turing machine is composed by a finite set of quintuples, we can encode and list all the machines using a shortlex ordering. We associate each machine T with the index i corresponding to its position in this list, and we denote by T_i the i-th Turing machine. Each positive integer i encodes one, and only one, Turing machine. However, as Proposition C.2.1 shows, all Turing machines have an infinite number of indexes. We associate each Turing machine with its smallest index.

Proposition C.2.1 — Padding Lemma. Each Turing machine has infinitely many indexes.

Proof. Consider a Turing machine T_i encoded by the string $\langle T_i \rangle$. We can create a new encoding $\langle T_j \rangle$ by appending a finite number of 0's to $\langle T_i \rangle$, such that $\langle T_j \rangle = \langle T_i \rangle 0^n$ for some positive integer n. Since n can take on any positive integer value, there are infinitely many possible encodings $\langle T_j \rangle$ for the same Turing machine T_i. ■

A universal Turing machine is a machine that can simulate the behavior of any other Turing machine on arbitrary input. The universal machine achieves this by reading both the description of the machine to be simulated (for instance, using the coding schema described in Example C.4) and the input string for the computation from its own tape.

Definition C.2.1 — Universal Turing Machine. A *Universal Turing Machine* is a Turing machine U such that $U(\langle\langle T_i \rangle, s\rangle) = T_i(s)$ for all Turing machines T_i and all input strings $s \in \mathcal{B}$.

Naturally, we must prove that such a machine exists before we can utilize it. One could argue that a human being could decode the machine T_i and simulate its behavior with the input string s, and then refer to Theorem C.1.1. A more rigorous approach would be to explicitly construct a universal Turing machine. However, providing a detailed description of one of these machines is beyond the scope of this book. Instead, we direct the reader to the references included at the end of the chapter for further exploration.

C.3 Non-Computable Problems

Turing machines enable us to delineate the set of problems that can be resolved through effective procedures or, in other words, by computers. It may be surprising to learn that numerous problems cannot be addressed using algorithms; such challenges lie beyond the computational capabilities of machines. We are not alluding to speculative queries like whether a computer can be intelligent or self-aware but to concrete, well-defined mathematical problems. We are also not referring to complex problems that demand a substantial amount of time to solve, as those, irrespective of their time consumption, remain computable.

One classic exemplar of non-computability is the *halting problem*. As illustrated in Algorithm C.1, it involves a program or algorithm tasked with determining whether any given program (including itself) and input will eventually halt or continue to run indefinitely. Alan Turing proved that no algorithm can exist to solve this problem for all possible program-input pairs. This revelation wasn't a reflection on the limitations of technology or processing power but highlighted a profound theoretical limit intrinsic to computation.

The proposition below proves that the halting problem is non-computable.

Algorithm C.1 HALT function

```
procedure HALT(A, I)
    if A(I) halts then
        return 1
    else
        return 0
    end if
end procedure
```

Proposition C.3.1 — Halting Problem. Define HALT as in Algorithm C.1. There does not exist a Turing machine that computes the HALT function for all possible pairs (A,I), where A is a Turing machine and I is the input string to that machine.

Proof. The proof is by contradiction. Assume that the machine $HALT$ exists, and define a new Turing machine TC such that $TC(A) = 1$ if $HALT(A,A) = 0$, and $TC(A)$ will never stop if $HALT(A,A) = 1$. Then the contradiction arises when we ask about the result of $TC(TC)$: if $TC(TC)$ stops we have that $HALT(TC,TC) = 0$ and that $TC(TC)$ should not stop, and if $TC(TC)$ does not stop then we have that $H(TC,TC) = 1$ and thus $TC(TC)$ should stop. ■

The existence of such non-computable problems underscores the boundaries of mechanical computation. It illustrates that while Turing machines, and by extension, computers are profoundly powerful tools capable of solving an extensive array of problems, they are not omnipotent. A frontier of unsolvable problems exists, necessitating deeper exploration into the realms of mathematics, logic, and perhaps even philosophy to understand the inherent limits of computation.

The Halting Problem also has significant practical consequences in computer programming. For instance, it is impossible to write a program that can guarantee any other arbitrary program is bug-free or that all infinite loops with conditional exits will eventually halt for all possible inputs.

The next example introduces a well-defined, practical problem involving simple string manipulation that cannot be solved using computers.

■ **Example C.5** Given two finite lists $(\alpha_1,\ldots,\alpha_n)$ and $(\beta_1,\ldots,\beta_n)$ of strings over some alphabet Σ, where $d(\Sigma) \geq 2$, the *Post Correspondence Problem* (PCP) asks to determine if there exists a sequence of $K \geq 1$ indices (i_k), with $1 \leq i_k \leq n$ for all $1 \leq k \leq K$, such that $\alpha_{i_1}\ldots\alpha_{i_K} = \beta_{i_1}\ldots\beta_{i_K}$. For instance, given the sequences (a,ab,bba) and (baa,aa,bb), a solution would be $\alpha_3\alpha_2\alpha_3\alpha_1 = \beta_3\beta_2\beta_3\beta_1$. No algorithm exists to solve PCP. Like many proofs of incomputability, the proof proceeds by showing that HALT can be reduced to PCP, meaning if PCP is decidable, then the Halting Problem should be decidable as well. We will not detail the proof in this section; for interested readers, we refer to the references at the end of this chapter. ■

Non-computable problems are generally not derived directly from natural phenomena but from logical and mathematical constructs. To date, there are no known examples of non-computable problems manifesting plainly in natural phenomena. It's essential to distinguish between non-computability and unpredictability. Non-computable problems are those for which no algorithm can ever be created to solve them. In contrast, unpredictable systems (such as chaotic or complex systems) are theoretically computable but are unpredictable in practice due to factors like sensitivity to initial conditions or measurement precision.

C.4 Computable Functions and Sets

Each Turing machine T defines a function $f_T : \mathcal{B}^* \to \mathcal{B}^*$ that assigns to each input string $s \in \mathcal{B}^*$ an output string $T(s) \in \mathcal{B}^*$. The relationship between Turing machines and functions forms the basis for introducing the concept of a *computable function*.

Definition C.4.1 A function $f : \mathcal{B}^* \to \mathcal{B}^*$ is *computable* if there exists a Turing machine T that defines the function f and halts for all the values of $\mathcal{B}^*$.

The terminology in computational theory can vary. While computable functions are occasionally referred to as *recursive functions*, this book opts for the term computable functions for consistency.

■ **Example C.6** The function that assigns to each pair of natural numbers x and y their sum $x+y$ is computable, as demonstrated in Example C.1. ■

In real-world scenarios, certain functions don't provide a defined output for all possible inputs. Partial computable functions, characterized by Turing machines that don't halt for specific inputs, model these cases.

Definition C.4.2 A partial function $f : \mathcal{B}^* \to \mathcal{B}^*$ is *partial computable* if there exists a Turing machine T that defines f for defined values and does not halt for undefined values.

The distinction between total computable functions and partial computable functions is significant in computability theory because it reflects the difference between problems that are always solvable by an algorithm (total) and those that are only solvable in some cases (partial).

■ **Example C.7** The function $f : \mathbb{N} \times \mathbb{N} \to \mathbb{N}$ that assigns to each pair of natural numbers x and y the number $x-y$ is a partial computable function, since it is not defined in the case that $x<y$. Recall that according to our definition of Turing machine (see Definition C.1.1), when the machine reaches an undefined configuration enters an infinite loop without ever halting. ■

We can expand the application of the principles of computability and partial computability to the domain of sets. We characterize sets through the lens of theirs characteristic functions that discern the membership of elements within the sets.

Definition C.4.3 A set $A \in \mathcal{B}^*$ is *computable* if its characteristic function $\mathcal{X}_A$ is a total computable function. A set $A \in \mathcal{B}^*$ is *computably enumerable* if its characteristic function $\mathcal{X}_A$ is a partial computable function, that is, $\mathcal{X}_A(a) = 1$ if $a \in A$, but $\mathcal{X}_A(a)$ is undefined if $a \notin A$.

The application of these concepts is illustrated through the example of the set of all Turing machines that halt for all inputs.

■ **Example C.8** The set of all Turing machines that halt on all inputs, as demonstrated in C.3.1, is not computable but is computably enumerable. ■

Next proposition provides an alternative characterization of computable sets.

Proposition C.4.1 A set $A \in \mathcal{B}^*$ is computable if and only if A and its complement A^c are computably enumerable.

Proof. If A is computable, by definition, there exists a Turing machine that decides for any input $x \in \mathcal{B}^*$ whether $x \in A$ or $x \notin A$, halting in both cases. This implies that both A and its complement A^c can be enumerated by Turing machines. Thus, both A and A^c are computably enumerable.

Conversely, suppose A and A^c are computably enumerable. This means there exist two Turing machines, T_A and T_{A^c}, that enumerate the elements of A and A^c, respectively. To show that A is computable, construct a Turing machine T that, given an input $x \in \mathcal{B}^*$, simulates T_A and T_{A^c} in parallel to search for x. If x appears in the enumeration produced by T_A, T halts and accepts x as an element of A. If x appears in the enumeration produced by T_{A^c}, T halts and accpts x, indicating $x \notin A$. Since every element of $\mathcal{B}^*$ must be in either A or A^c and both sets are computably enumerable, T will eventually halt for every input x, proving that A is computable. ■

C.5 Oracle Turing Machine

An oracle Turing machine (see Figure C.3) is a theoretical model of computation that extends the capabilities of a standard Turing machine by providing

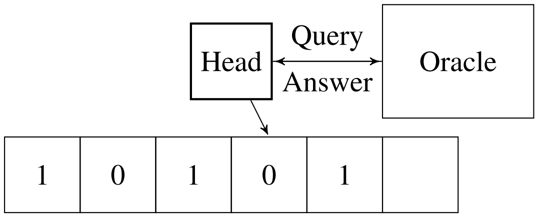


Figure C.3: Oracle Turing Machine

it with an oracle. The oracle is a black box that can instantly compute certain answers, even for problems that are unsolvable or would take an impractical amount of time for a standard Turing machine to process. This model helps computer scientists and mathematicians explore the implications and boundaries of computational theory, including questions about complexity classes and the limits of what is computationally possible. The oracle Turing machine isn't a physical or implementable machine but rather a conceptual tool used in theoretical studies.

Definition C.5.1 — Oracle Turing Machine. An *oracle Turing machine* with oracle set $\mathcal{O}$ is a 8-tuple $(Q, \Gamma, \sqcup, \Sigma, q_i, q_f, \tau, \mathcal{O})$ where:

Q is a finite, non-empty, set of *states*,

Γ is a finite, non-empty, set of *tape symbols*,

$\sqcup \in \Gamma$ is the *blank symbol*,

$\Sigma \subseteq \Gamma \setminus \sqcup$ is the set of *input symbols*,

$q_o \in Q$ is the *initial state*,

$q_f \in Q \setminus \{q_0\}$ is the *final state*,

$\tau : (Q \setminus \{q_f\}) \times \Gamma \times \{0,1\} \to Q \times \Gamma \times \{L, R, S\}$ is the *transition function*,

$\mathcal{O} \subseteq \Sigma^*$ is the *oracle set*.

Building on the concept of a regular Turing machine (refer to Definition C.1.1), an oracle Turing machine introduces the unique feature of an oracle set $\mathcal{O}$. This set comprises a subset of strings for which the oracle can instantly provide answers. The true strength of an oracle machine emerges when the set $\mathcal{O}$ is non-computable; in cases where $\mathcal{O}$ is computable, a regular Turing machine would be sufficient.

The transition function τ for the oracle Turing machine is nuanced. At each step the machine will query the oracle. Specifically, it sends the current string w —starting under the head and extending to the rightmost non-empty cell of the input tape—to the oracle. The oracle then responds with a binary answer: '1' if w is in $\mathcal{O}$ or '0' if it isn't. The machine doesn't always utilize this response. There are steps where, despite receiving an answer, the computation proceeds unaffected by the oracle's response—essentially ignoring it. However, when the oracle's answer is pivotal, the machine makes a decision based on it. This decision could affect the next state, the next symbol to be written, or the next move (left, right, or stay). In essence, while the machine has the capability to continuously consult the oracle, it strategically chooses when to act on the information received. We could have modified the τ funcion in such a way that the oracle is queried only when the answer is relevant for the computation, but that would require making important changes to the behaviour of the function, such as the introduction of new control states.

■ **Example C.9** In the realm of theoretical computer science, an oracle can be invoked to "solve" the halting problem (refer to Theorem C.3.1). The oracle is a hypothetical device or black box that, as if by magic, provides an instantaneous answer to a specific problem instance. The oracle set $\mathcal{O}$ would consist of a collection of strings in the form $\langle P, I \rangle$, where P represents a program encoded as a string and I denotes its input. Given a program and its input, this oracle would instantly inform us whether the program halts on that input. Naturally, this concept is purely theoretical. No such oracle exists in reality, and the halting problem remains unsolvable in practical terms. ■

A standard Turing machine can be viewed as an oracle machine that simply *ignores* its oracle or, equivalently, uses any fixed oracle set and never branches on the oracle bit. Thus ordinary Turing machines embed as a subclass of oracle Turing machines.

Proposition C.5.1 For every (ordinary) Turing machine $T = (Q, \Gamma, \sqcup, \Sigma, q_0, q_f, \tau)$ and every oracle set $\mathcal{O} \subseteq \Sigma^*$, there exists an oracle Turing machine $T^{\mathcal{O}}$ such that for all inputs $x \in \Sigma^*$, the computation of T on x and the computation of $T^{\mathcal{O}}$ on x (with oracle $\mathcal{O}$) produce the same outcome.

Proof. Define $T^{\mathcal{O}} = (Q, \Gamma, \sqcup, \Sigma, q_0, q_f, \tau', \mathcal{O})$ with the same components as T and transition function τ' given by

$$\tau'(q,s,b) = \tau(q,s) \qquad \text{for all } (q,s) \in (Q \setminus \{q_f\}) \times \Gamma \text{ and } b \in \{0,1\}.$$

That is, $T^{\mathcal{O}}$ ignores the oracle bit. A step-by-step induction on the unique computation of T on x shows that T and $T^{\mathcal{O}}$ visit identical configurations (up to the presence of the unused oracle bit) and therefore have the same outcome and output. ■

An oracle machine is specified by two pieces of data: the *machine component* $(Q, \Gamma, \sqcup, \Sigma, q_0, q_f, \tau)$ and the *oracle set* $\mathcal{O}$. The former is defined syntactically and does not depend on which $\mathcal{O}$ is chosen. Semantically, the behavior of a fixed machine component on a given input depends only on the answers to the queries it actually makes (i.e., on the restriction of $\mathcal{O}$ to those queries).

Proposition C.5.2 Let $M = (Q, \Gamma, \sqcup, \Sigma, q_0, q_f, \tau)$ be a fixed machine component. For any two oracle sets $\mathcal{O}_1, \mathcal{O}_2 \subseteq \Sigma^*$ and any input x, if $\mathcal{O}_1$ and $\mathcal{O}_2$ give the same answers to all oracle queries made during the run of M on input x (with either oracle), then the computations $M^{\mathcal{O}_1}(x)$ and $M^{\mathcal{O}_2}(x)$ are identical (same sequence of configurations, hence same outcome and output).

Proof. Consider the (unique) run of $M^{\mathcal{O}_1}$ on input x. By hypothesis, $\mathcal{O}_2$ agrees with $\mathcal{O}_1$ on precisely the queried strings that arise along this run. Since τ is deterministic given the current state, scanned symbol, and oracle bit, and the oracle bit provided by $\mathcal{O}_2$ matches that from $\mathcal{O}_1$ at every step, both computations take the same transition at each step. Thus the configuration sequences coincide, yielding identical outcomes. ■

A (partial) function is *computable relative to* $\mathcal{O}$ if some oracle machine with oracle $\mathcal{O}$ computes it. Two useful facts: (i) ordinary computable functions are $\mathcal{O}$-computable for any oracle (by ignoring the oracle); (ii) if $\mathcal{O}$ is itself computable, then $\mathcal{O}$-computability coincides with ordinary computability.

Definition C.5.2 — Oracle computability. Given $\mathcal{O} \subseteq \Sigma^*$, a partial function $f : \Sigma^* \rightharpoonup \Sigma^*$ is $\mathcal{O}$-*computable* if there exists an oracle Turing machine $M^{\mathcal{O}}$ such that, for every $x \in \Sigma^*$:
- if $f(x)$ is defined, then $M^{\mathcal{O}}$ halts on input x and outputs $f(x)$ (under the chosen output convention);
- if $f(x)$ is undefined, then $M^{\mathcal{O}}$ does not halt on input x.

Proposition C.5.3 If $\mathcal{O}$ is (ordinarily) computable, then a partial function f is $\mathcal{O}$-computable if and only if f is computable by an ordinary Turing machine.

Proof. Suppose f is $\mathcal{O}$-computable via $M^{\mathcal{O}}$. Since $\mathcal{O}$ is computable, there exists an ordinary machine D deciding membership in $\mathcal{O}$. Simulate $M^{\mathcal{O}}$ step by step on an ordinary machine; whenever $M^{\mathcal{O}}$ needs the oracle bit, call D on the current query string to obtain the bit and continue the simulation. This yields an ordinary machine computing f.

If f is computable by an ordinary machine T, then by Proposition C.5.1 there is an oracle machine $T^{\mathcal{O}}$ that ignores the oracle and computes f for any $\mathcal{O}$. Hence f is $\mathcal{O}$-computable. ■

More generally, if $\mathcal{O}$ is *Turing reducible* to $\mathcal{O}'$ (i.e., decidable by some $\mathcal{O}'$-oracle machine), then every $\mathcal{O}$-computable function is $\mathcal{O}'$-computable. This captures the standard notion of *relative computability*.

■ Example C.10 — Toy oracle machine that outputs the oracle's answer. Let $\Sigma = 0,1$ and $\Gamma = 0,1,\sqcup$. Fix the oracle set $\mathcal{O} = 11,101$ (finite for concreteness). Consider the oracle machine $M^{\mathcal{O}}$ that, on any input $w \in \Sigma^*$, writes a single symbol indicating the oracle's answer and halts:

- If the queried string (as per your convention) is in $\mathcal{O}$, write 1 and halt.
- Otherwise, write 0 and halt.

Use states $Q = q_0, q_f$, with q_0 initial and q_f halting. Define τ independently of the scanned symbol $s \in \Gamma$ by the sextuples

$$(q_0,0,1,q_f,1,S), \quad (q_0,1,1,q_f,1,S), \quad (q_0,\sqcup,1,q_f,1,S),$$

$$(q_0,0,0,q_f,0,S), \quad (q_0,1,0,q_f,0,S), \quad (q_0,\sqcup,0,q_f,0,S),$$

and leave all other transitions undefined (so the machine halts after one step). Then $\langle M \rangle$ is obtained by concatenating the fixed-length codes of these six sextuples after the header. The oracle's finite code is, for example,

$$\langle \mathcal{O} \rangle = \big\langle 2, \langle 11 \rangle, \langle 101 \rangle \big\rangle,$$

using any self-delimiting code for strings. The full encoding is the pairing $\big\langle \langle M \rangle, \langle \mathcal{O} \rangle \big\rangle$. ■

These additions make explicit (i) how ordinary computation embeds into oracle computation, (ii) in what precise sense the machine component is independent of the oracle set, (iii) that an oracle machine is exactly a pair $(M, \mathcal{O})$, and (iv) what it means for a function to be computable *relative* to an oracle. The encoding example matches your earlier quintuple-based scheme with a minimal extension to handle the oracle bit.

References

The original paper form Alan Turing where the concepts of Turing machine, universal Turing machine, and non-computable problems were introduced is [Tur36], however it is a difficult to read paper for the contemporary reader. An easier to read introduction to computability theory, from the point of view of languages, can be found in [Sip12], and a more advanced introductions in [Coo03] and [Soa16]. In [Fer09] we can find a description of the most important computability models proposed so far. The Post Correspondence Problem was introduced by Emil Post in [Pos46]; for the details of the proof sketched in Example C.5 please refer to [Sip12].

D. Coding

Information is the resolution of uncertainty.
Claude Shannon

In this section, we are going to review the conceptual ideas and main results behind coding theory and the related area of information theory.

Coding is the process of describing a sequence of symbols from some alphabet by a sequence of symbols from another alphabet. Coding has many practical applications, such as error detection, cryptography, and telecommunications. Here, our interest is in data compression, that is, encoding a message using fewer symbols than its original representation, without losing any information. Compression algorithms reduce the size of messages by identifying unnecessary elements and removing them, usually by means of computing and eliminating statistical redundancies. For example, data compression can be achieved by assigning shorter descriptions to the most frequent symbols from the source, and longer descriptions to the less frequent symbols. A particular type of codes, the prefix-free codes, will be discussed as playing a central role in this book. Prefix-free codes allow us to link coding theory with probability theory, a link that will be very useful in the context of the theory of nescience.

Information theory proposes that the amount of information we receive when some event happens is the negative logarithm of the probability of that event. In this sense, the theory assumes that information is equivalent to surprise: the more unlikely an event is, the more information we receive when the event occurs. We are not going to use that interpretation of information in our theory of nescience, but we will extensively use another concept from information theory: entropy. Entropy quantifies the amount of uncertainty involved in the value of a random variable or the outcome of a random process. Entropy is important to us because it establishes a limit to the compression of texts: it is not possible to find a code with an average word length smaller than the entropy of the source alphabet.

There exist many interesting concepts derived from entropy, like joint entropy, conditional entropy, or mutual information. However, these concepts are more relevant in the context of communication because they allow us to solve the problem of how to transmit information in a reliable manner over a noisy channel. Here, they are introduced for completeness purposes, and to compare them with our own definitions of joint nescience and conditional nescience.

D.1 Coding

Intuitively, coding refers to the process of losslessly describing a sequence of symbols (a message) coming from some alphabet by other sequences of symbols coming from a (potentially) different alphabet. There is no general agreement about what exactly a code is, as different authors propose different definitions in the literature. Fortunately, the definition of a prefix-free code, the kind of codes used in the theory of nescience, is a standard one.

Let $\mathcal{S} = \left\{s_1, s_2, \ldots, s_q\right\}$ be a finite set called *source alphabet*, and $\mathcal{X} = \{x_1, x_2, \ldots, x_r\}$ a finite set called *code alphabet*.

Definition D.1.1 — Code. A *code* for $\mathcal{S}$ is a total function $C : \mathcal{S} \rightarrow \mathcal{X}^+$. If $(s, x) \in C$ we say that s is the *source symbol* and x is the *code word*. If C is an injective function we say that the code is *nonsingular*.

Nonsingularity allows us to unambiguously describe the individual symbols of the source alphabet. For the rest of this book, whenever we talk about a code we mean a nonsingular code. Moreover, without any loss of generality, we will restrict ourselves to *binary codes*, that is, $\mathcal{X} = \mathcal{B} = \{0, 1\}$.

The property of nonsingularity can also be applied to strings of symbols. In order to do that, we have to extend the concept of code from symbols to strings.

Definition D.1.2 The *extension of order n* of a code C is a function $C^n : \mathcal{S}^n \to \mathcal{B}^+$ defined as $C^n(s_{i_1} \dots s_{i_n}) = C(s_{i_1}) \dots C(s_{i_n})$, where $C(s_{i_1}) \dots C(s_{i_n})$ is the concatenation of the code words corresponding to the symbols of the string $s_{i_1} \dots s_{i_n} \in \mathcal{S}^n$. An extension of order n of a code C is *nonsingular* if the function C^n is injective.

If it is clear from the context, we will also use the word *code* to refer to a nonsingular extension of order n of a code, and the elements of $\mathcal{S}^n$ will be called *source words*.

■ **Example D.1** The code $C(a) = 0$, $C(b) = 00$, $C(c) = 01$, and $C(d) = 11$ is a nonsingular code, but its extension of order 2 is singular, since, for example, $C^2(ab) = C^2(ba) = 000$. ■

As we have seen in Example D.1 not all nonsingular codes have nonsingular extensions, that is, it might happen that we are not able to decode the original messages given their encoded versions. Unique decodability is a highly desirable property of codes.

Definition D.1.3 A code C is called *uniquely decodable* if its order n extension C^n is nonsingular for all n.

Next proposition provides a characterization of the unique decodability of codes.

Proposition D.1.1 A code C is uniquely decodable if, and only if, the function $C^+ : \mathcal{S}^+ \to \mathcal{B}^+$ is injective.

Proof. If the function C^+ is injective, then the restriction to C^n must be injective for all n. Now, let us assume that C^n is nonsingular for all n and let's prove that C^+ must be nonsingular by contradiction: select two source words $s_1 \in \mathcal{S}^n$ and $s_2 \in \mathcal{S}^m$, $n \neq m$, and assume that they have the same code word $C^+(s_1) = C^+(s_2)$. Then construct the words $s_3 = s_1 s_2$ and $s_4 = s_2 s_1$, both s_3 and s_4 have the same length, and $C^+(s_3) = C^+(s_4)$, which is a contradiction with the fact that C^{n+m} must be nonsingular. ■

■ **Example D.2** The code $C(a) = 0$, $C(b) = 01$, $C(c) = 011$, and $C(d) = 0111$ is a uniquely decodable code. For example, the code word 0010011 uniquely corresponds to the source word *abac*. Unique decodability is achieved because the 0 symbol plays the role of a delimiter, separating code words. ■

The Sardinas-Patterson theorem provides a necessary and sufficient condition for a code to be uniquely decodable. The theorem is based on an algorithmic approach, enabling the examination of a code's unique decodability through a sequence of iterative steps. Let C_0 denote the set of code words of a code C. We define the set C_n as

$$C_n = C^{-1}C_{n-1} \cup C_{n-1}^{-1}C$$

for all $n \in \mathbb{N}$ and where $C^{-1}C_{n-1}$ represents the left quotient of C and C_{n-1}. And let C_∞ be defined as

$$C_\infty = \bigcup_{n=1}^{\infty} C_n$$

Proposition D.1.2 — Sardinas-Patterson. A code C is uniquely decodable if and only if the sets C_0 and C_∞ are disjoint.

Proof. TODO: Pending ■

■ **Example D.3** Given the code of Example D.1 we have that

$$C_0 = \{0, 00, 01, 11\}$$
$$C_1 = \{0, 1\}$$

And since $C_0 \cap C_1 \neq \varnothing$ we can conclude that the code is not uniquely decodable.

Given the code of Example D.2 we have that

$$C_0 = \{0, 01, 011, 0111\}$$
$$C_1 = \{1, 11, 111\}$$
$$C_2 = \varnothing$$

And since $C_0 \cap C_\infty = C_0 \cap \bigcup_{n=1}^{\infty} C_n = C_0 \cap C_1 = \varnothing$ we can conclude that the code is uniquely decodable. ■

Next definition introduces the concept of prefix-free codes. Prefix-free codes will play a critical role in the computation of the amount of algorithmic information of an arbitrary string (described in Chapter E), and in our own theory of nescience. Prefix-free codes also allow us to link coding theory and probability theory through the Kraft inequality (Theorem D.2.1). Note that we prefer the name *prefix-free code* over the more standard *prefix code*, since the former more accurately describes the concept.

Definition D.1.4 — Prefix-free Code. A code C is *prefix-free* if for all i, j where $1 \leq i, j \leq q$ and $i \neq j$, $C(s_i)$ is not a prefix of $C(s_j)$.

Note that the fact that a string is a prefix of itself does not violate the prefix-free property because the condition specifically excludes considering a string as a prefix of itself ($i \neq j$) for the purpose of determining whether a set of code words is prefix-free.

■ **Example D.4** The code $C(a) = 0$, $C(b) = 10$, $C(c) = 110$ and $C(d) = 1110$ is a prefix-free code. Here, the 0 symbol plays the role of a comma as it was the case of Example D.2, but its new position at the end of the code words is what makes the code prefix-free. ■

Prefix-free codes are uniquely decodable, as the next proposition proves.

Proposition D.1.3 Let C be a prefix-free code, then C is uniquely decodable.

Proof. Let C be a prefix-free code, and assume that C is not uniquely decodable. This implies there exist two different sequences of source symbols, say r and s, such that they encode to the same sequence of code words: $C(r) = C(s)$. Since C is prefix-free, the start of any code word sequence uniquely determines the first code word, as no other code word can be a prefix. Therefore, the first symbols in r and s must be the same, as they are encoded into the same first code word. However, this leads to the conclusion that $r = s$, contradicting our initial assumption that r and s are different. Therefore, our assumption must be false, and the code C must be uniquely decodable. ■

From an engineering point of view it is highly convenient to have codes whose source symbols can be decoded as soon as the corresponding code words are received, that is, it is not necessary to wait for the next code word in order to decode the current symbol, this is why some authors refer to these codes as *instantaneous codes*.

Definition D.1.5 A code C is *instantaneous* if, for any order n and for any sequence of code words $C(s_{i_1}), C(s_{i_2}), \ldots, C(s_{i_n})$, each sequence of code words $\mathbf{t} = C(s_{i_1})C(s_{i_2})\ldots C(s_{i_m})\ldots$ can be uniquely decoded as $\mathbf{s} = s_{i_1}s_{i_2}\ldots s_{i_m}\ldots$ without ambiguity, regardless of the continuation of $\mathbf{t}$.

■ **Example D.5** The code described in Example D.2 is not instantaneous. For example, after receiving the sequence 011 the source symbol could be a c if the next symbol is a 0 or a d if it is a 1. ■

Prefix-free codes and instantaneous codes are essentially two terms for the same concept. A prefix-free code is one in which no code word is a prefix of any other code word. This property ensures that there is a clear demarcation between code words when they are concatenated in a sequence, allowing each code word to be decoded immediately upon receipt without the need to look ahead to subsequent code words for context.

Proposition D.1.4 A code C is instantaneous if, and only if, it is a prefix code.

Proof. Assume C is an instantaneous code, and suppose that C is not a prefix-free code. This means there exists at least a pair of code words, say $C(s_i)$ and $C(s_j)$, such that $C(s_i)$ is a prefix of $C(s_j)$. Consider a sequence where $C(s_j)$ is transmitted. Since $C(s_i)$ is a prefix of $C(s_j)$, the decoder would decode $C(s_i)$ from the initial part of $C(s_j)$, leading to ambiguity, as the rest of $C(s_j)$ could be seen as another code or part of the next code. This contradicts the assumption that C is instantaneous.

Assume C is a prefix code. This property ensures that once a code word is identified in a sequence, there can be no confusion as to where it ends, and the next code word begins. There is no need to look ahead to determine the boundary between code words, as the end of one code word cannot be mistaken for the beginning of another. Hence, a prefix code allows for instantaneous decoding. ■

The last type of codes we are going to review are fixed length codes. We will use fixed length codes to compute the length of a text when there are no regularities we can exploit to compress it.

Definition D.1.6 If all the code words of a code have the same length we say that the code is a *fixed length code*.

Fixed length codes have the property of being prefix-free (or instantaneous).

Proposition D.1.5 Let C be a fixed-length code, then C is prefix-free.

Proof. Let C be a fixed length code, and $C(s_i)$ and $C(s_j)$ the code words of two arbitrary source words s_i and s_j. Assume that $C(s_i) <_p C(s_j)$, given the fact that $l(C(s_i)) = l(C(s_j))$ we have that $C(s_i) = C(s_j)$ and so, the code C is prefix-free. ■

Of course, the converse of the previous proposition does not hold; not all prefix-free codes are of fixed length. The code described in Example D.4 is prefix-free but it is not fixed-length.

Figure D.1 provides a graphical representation of the relation among the different types of codes that have been introduced in this section.

D.2 Kraft Inequality

The Kraft inequality provides a condition for the existence of a prefix-free code given a set of code word lengths. Kraft's inequality states that for a given set of code word lengths in a binary code, the sum of the reciprocals of the powers of two corresponding to the code word lengths must be less than or equal to one. This condition is both necessary and sufficient; not only

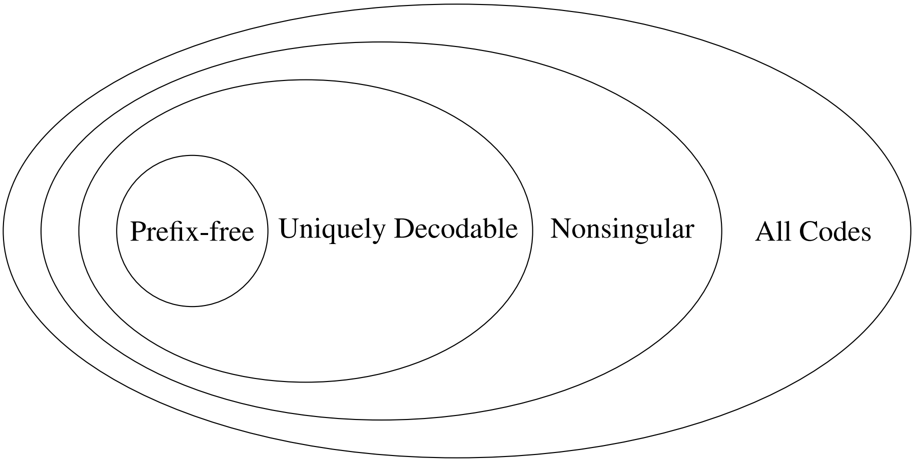


Figure D.1: Classification of Codes

must any prefix-free code satisfy this inequality, but given a set of lengths that meets this condition, it is always possible to construct a corresponding prefix-free code. The elegance and utility of Kraft's inequality lie in its ability to link the lengths of code words with the mathematical properties of probability.

Theorem D.2.1 — Kraft Inequality. Let $\mathcal{L} = \{l_1, l_2, \ldots, l_q\}$ be a set of lengths, where $l_i \in \mathbb{N}$, then there exists a binary prefix-free code C whose code words have the lengths of $\mathcal{L}$ if, and only if,

$$\sum_{l_i \in \mathcal{L}} 2^{-l_i} \leq 1$$

Proof. Consider a binary tree whose branches are labeled with the symbols of the code alphabet, in such a way that the path from the root to the leaves traces out the symbols of a code word. The prefix-free condition implies that nodes representing complete code words cannot have descendants. An example of such a tree, for the code described in Example D.4, is shown in Figure D.2.

Let $l_{max} = \max\{l_1, l_2, \ldots, l_q\}$, that is, the length of the longest code word from the set of lengths. There will be at most $2^{l_{max}}$ leaf nodes in the tree, but at level l_i we have to prune $2^{l_{max}-l_i}$ leaves, since the code is prefix-free. Summing over all the code words' lengths, we have that the total number of pruned leaves must be less than or equal to the maximum number of leaves,

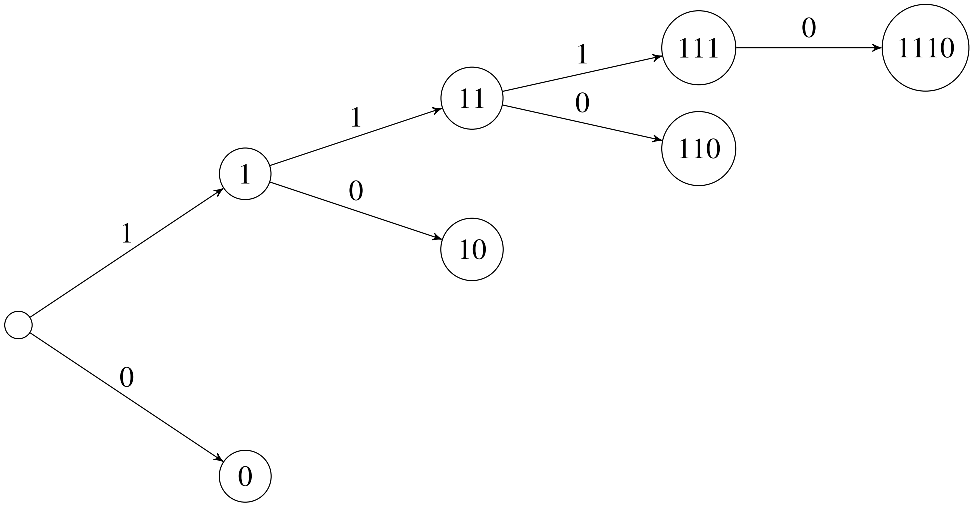


Figure D.2: Prefix-free Tree

that is

$$\sum_{l_i \in \mathcal{L}} 2^{l_{max}-l_i} \leq 2^{l_{max}}$$

or, equivalently,

$$\sum_{l_i \in \mathcal{L}} 2^{-l_i} \leq 1$$

which is exactly the inequality we are trying to prove.

Conversely, given any set of code words' lengths $\mathcal{L} = \left\{l_1, l_2, \ldots, l_q\right\}$ that satisfy the Kraft inequality, we can always construct a binary tree, like the one in the Figure D.2. Label the first node (lexicographically) of depth l_1 as code word 1, and remove its descendants from the tree. Then label the first remaining node of depth l_2 as code word 2, and so on. Proceeding this way, we construct a prefix code with the specified lengths. ■

Given a code C whose code word lengths $\mathcal{L}$ satisfy the Kraft inequality does not necessarily mean that the code is prefix-free, since what the inequality states is that there exists a prefix-free code with those word lengths, not that all codes with those word lengths are prefix-free.

■ **Example D.6** The code $C(a) = 0, C(b) = 111, C(c) = 110$ and $C(d) = 100$ satisfies the Kraft inequality, but it is not prefix-free. ■

McMillan's Inequality enriches our understanding of coding theory by establishing a crucial link between the lengths of code words in uniquely decodable codes. This inequality mirrors Kraft's Inequality, yet it broadens the scope to encompass all uniquely decodable codes, not just those that are prefix-free. By demonstrating that the sum of the reciprocals of the powers of two for code word lengths must be less than or equal to one for a code to be uniquely decodable, McMillan's Inequality ensures that such codes can be constructed with a given set of lengths.

Theorem D.2.2 — McMillan's Inequality. Let $\mathcal{L} = \{l_1, l_2, \ldots, l_q\}$ be a set of lengths, where $l_i \in \mathbb{N}$, then there exists a uniquely decodable code C whose code words have the lengths of $\mathcal{L}$ if, and only if,

$$\sum_{l_i \in \mathcal{L}} 2^{-l_i} \leq 1$$

Proof. TODO: review

We must show that if there exists a uniquely decodable code with code word lengths $l_1, l_2, \ldots, l_q$, then the inequality holds.

Suppose C is a uniquely decodable code with code word lengths $l_1, l_2, \ldots, l_q$. Consider a sequence of code words produced by C that is long enough to contain any possible concatenation of n code words (for some n large enough). Let's denote the set of all such sequences as S_n.

Because C is uniquely decodable, each sequence in S_n corresponds to a unique sequence of source symbols. The number of different sequences in S_n is at least 2^{nl}, where l is the smallest length among all l_i. This is because, for the shortest code word, we can consider a sequence of length nl and all possible fillings with the shortest code word. Since the code is uniquely decodable, none of these sequences can be the same as any sequence containing longer code words.

The total number of bits required to represent all sequences in S_n can indeed be calculated as $(2^{-l_1} + 2^{-l_2} + \ldots + 2^{-l_q})^n$, considering the combinatorial possibilities of all code word concatenations.

Since each sequence in S_n must be different (uniquely decodable) and can be represented in a binary tree (where each leaf corresponds to a code word and the length of the path to the leaf corresponds to the length of the code word), the number of sequences in S_n cannot exceed $2^{nl_{max}}$, where l_{max} is the length of the longest code word.

Therefore, we have:

$$(2^{-l_1} + 2^{-l_2} + \ldots + 2^{-l_q})^n \leq 2^{nl_{max}}$$

Taking the nth root of both sides, we have:

$$2^{-l_1} + 2^{-l_2} + \ldots + 2^{-l_q} \leq 2^{l_{max}}$$

Since $2^{l_{max}}$ is always less than or equal to 1 (because there must be at least one code word of the maximum length and thus occupying the "full" length of the binary tree), we obtain:

$$2^{-l_1} + 2^{-l_2} + \ldots + 2^{-l_q} \leq 1$$

To prove sufficiency, we must show that if the inequality holds, then there exists a uniquely decodable code with those lengths.

If the inequality holds, we can use the Kraft construction to build a prefix-free code, which is always uniquely decodable, with code word lengths $l_1, l_2, \ldots, l_q$. The construction starts by assigning the shortest code word first and ensuring no other code word is a prefix of any other. Since prefix-free codes are a subset of uniquely decodable codes, we have constructed the required code.

Therefore, by satisfying the inequality, we can construct a uniquely decodable code, proving that the condition is sufficient.

■

In the theory of nescience, we are primarily interested in prefix-free codes. This preference may seem to impose a limitation, as it appears more rational to consider the broader category of uniquely decodable codes. However, this perceived limitation does not actually exist. As the following theorem demonstrates, uniquely decodable codes also satisfy Kraft's inequality. This means that for any uniquely decodable code, there exists a prefix-free code with exactly the same code word lengths, ensuring no compromise in the generality of our analysis when focusing on prefix-free codes.

Corollary D.2.3 There is an instantaneous (prefix-free) code with word lengths $l_1, \ldots, l_q$ if and only if there is a uniquely decodable code with these word lengths.

Proof. TODO: Review This corollary is a direct consequence of McMillan's Inequality, which is a counterpart to Kraft's Inequality for uniquely decodable codes. McMillan's Inequality states that for a set of code word lengths $\{l_1, l_2, \ldots, l_q\}$, a uniquely decodable code exists if and only if the sum of 2^{-l_i} for all i is less than or equal to one. Given that prefix-free codes are a subset of uniquely decodable codes and also satisfy this condition, the existence of a uniquely decodable code with given word lengths implies the possibility of constructing a prefix-free code with the same lengths. The reverse is inherently true by the definition of prefix-free codes, which are always uniquely decodable. ■

In the context of nescience, our interest lies not in the specific codes themselves but in the lengths of the code words. This emphasis allows us to abstract away from the details of code construction to concentrate on the mathematical properties and implications of these lengths, which are central to understanding and applying the principles of nescience.

D.3 Optimal Codes

In coding theory, a compact code is an optimal encoding strategy that minimizes the expected length of code words, a concept central to evaluating a code's efficiency. The expected length of a code is determined by the weighted average of the lengths of its code words, with weights corresponding to the probability distribution of the source symbols. By designing code words so that more frequent symbols are assigned shorter lengths and less frequent ones longer lengths, compact codes effectively reduce the average size needed to encode information. This principle is pivotal in data compression, as it allows for a significant reduction in the space required for storage or the bandwidth needed for transmission.

Let's establish $\mathcal{S} = \{s_1, s_2, \dots, s_q\}$ as a finite source alphabet, with P denoting a probability distribution defined over the elements of $\mathcal{S}$.

Definition D.3.1 The *expected length* of a code C, denoted by L_C, is the weighted sum of the lengths of the code words, calculated as

$$L_C = \sum_{i=1}^{q} P(s_i) l_i,$$

where $\mathcal{L} = \{l_1, l_2, \dots, l_q\}$ represents the lengths of the code words of C. We may simply use L to denote L_C when the code C is understood from the context.

Our goal is to identify a code C that minimizes the expected length L of the codewords $\mathcal{L}$ under the given probability distribution P. Such an optimal code C would enable us to compress messages composed of the source alphabet $\mathcal{S}$ effectively, reducing the number of symbols required to encode these messages.

Next, the following definition formalizes what it means for a code to be compact, which is a desirable attribute for efficient data encoding.

Definition D.3.2 A code C is *compact* if its average length L is less than or equal to the average length of all the other codes for the same source alphabet and code alphabet.

Definition D.3.3 A code C is *compact* if, for a given source alphabet $\mathcal{S}$ and a corresponding probability distribution, its expected length L_C is minimized among all possible codes that can be constructed for $\mathcal{S}$.

This means C achieves the lowest possible weighted average codeword length, where each codeword length is weighted by the probability of its corresponding source symbol.

The existence of compact codes for all possible source alphabets is a foundational aspect of coding theory, suggesting that for every finite source alphabet, an optimally efficient encoding scheme can be devised. It is not entirely clear that compact codes exist for all possible source alphabets, so the following proposition must be proven.

Proposition D.3.1 For every finite source alphabet $\mathcal{S} = \left\{s_1, s_2, \ldots, s_q\right\}$ with a defined probability distribution over its symbols, there exists at least one code C that is compact.

Proof. The proof of this proposition involves constructing or identifying a code C for the source alphabet $\mathcal{S}$ that achieves the minimum possible expected length L_C. This can be demonstrated through the use of Huffman's algorithm, which is designed to produce an optimal prefix code based on the probabilities of the source symbols. By definition, the Huffman code for a given probability distribution over $\mathcal{S}$ minimizes the expected length of the codewords, thereby proving the existence of a compact code for any finite source alphabet with a given probability distribution. ∎

This clarification not only completes the explanation but also aligns the definition of compactness with established principles in coding theory. It provides a more rigorous basis for discussing the efficiency of encoding schemes and underscores the role of probability distributions in determining the compactness of a code.

TODO: Introduce this concept

Definition D.3.4 The redundancy of a code is defined as

$$\eta = \frac{H((S))}{L}$$

Of course, our goal is to minimize the redundancy of codes.

Next theorem states that the entropy of the probability distibution P poses a limit to the average length of prefix-free codes.

Theorem D.3.2 The expected length L_C of any prefix-free r-ary code, given the probability distribution P, is greater than or equal to the entropy of P, that is

$$H_r(P) \leq L_C$$

with equality if, and only if, $r^{-l_i} = P_i$ for all $0 \leq i \leq q$.

Proof. ■

Definition D.3.5 A probability distribution is called *D-adic* if each of the probabilities is equal to D^n for some n.

Corollary D.3.3 We have the equality in the theorem if, and only if, the distribution of X is D-adic.

Proof. TODO ■

Mention that in practice we will non-integer code word lengths. Show that, on average, the length of the encoded string will be less than 1 bit than usind a code with code words with integer lengths

Kraft's inequality allows us to compare how efficient different codes are for the same source alphabet.

Definition D.3.6 Let $C_1 : \mathcal{S} \to \mathcal{X}^+$ and $C_2 : \mathcal{S} \to \mathcal{X}^+$ be two different codes. We say that code C_1 is *more efficient* than code C_2 if for all $s \in \mathcal{S}$ we have that $l(C_1(s)) \leq l(C_2(s))$, and there exists at least one $s' \in \mathcal{S}$ such that $l(C_1(s')) < l(C_2(s'))$.

■ **Example D.7** The code described in Example D.6 is more efficient than the code of Example D.4. Of course, the problem with the code described in Example D.6 is that it is not prefix-free, but since it satisfies Kraft's inequality, we know that there must exist another code with the same code word lengths that is prefix-free. For example, $C(a) = 0$, $C(b) = 10$, $C(c) = 110$ and $C(d) = 111$. ■

We are interested in the most efficient possible codes.

TODO: This definition is wrong

Definition D.3.7 A code C is *complete* if there does not exist a code C' that is more efficient than C.

It turns out that Kraft's inequality provides a very useful characterization of complete codes.

Proposition D.3.4 A code C is complete if, and only if, its code word lengths $\mathcal{L} = \left\{l_1, l_2, \ldots, l_q\right\}$ satisfy the property:

$$\sum_{l_i \in \mathcal{L}} 2^{-l_i} = 1$$

Proof. Suppose the sum of the exponentiated inverses of the code word lengths equals 1:

$$\sum_{l_i \in \mathcal{L}} 2^{-l_i} = 1$$

This implies that the code utilizes the full capacity of the coding space. In other words, there is no redundancy or additional space in the code that could be used to encode a symbol with a shorter length. This is because each term in the sum 2^{-l_i} represents the proportion of the coding space taken up by the code word of length l_i. If these proportions sum up to 1, then all possible code words of the given lengths are used, and there's no space left to introduce any new code word without increasing the length of at least one existing code word. Therefore, the code is as efficient as possible, hence complete.

Now suppose that the code C is complete. This means that there is no other code C' with the same source alphabet and the same or shorter code word lengths that is more efficient than C.

Assume for contradiction that the sum of the exponentiated inverses is less than 1:

$$\sum_{l_i \in \mathcal{L}} 2^{-l_i} < 1$$

This would imply that there is still unused coding space, meaning that it would be possible to construct a more efficient code by using this unused space to represent at least one symbol with a shorter code word, contradicting the assumption that C is complete. Therefore, the sum cannot be less than 1.

Since C is complete and cannot be less efficient, the only alternative left is that the sum is exactly 1:

$$\sum_{l_i \in \mathcal{L}} 2^{-l_i} = 1$$

Combining both directions, we have shown that a code C is complete if and only if the sum of the exponentiated inverses of its code word lengths equals 1, as stated in the proposition.

■

D.4 Entropy

In this section we are going to introduce the concept of *entropy*, as a measure of the uncertainty of a random variable. Entropy is a very difficult to grasp concept that can be applied in many different contexts, such as communications, statistics, finance, etc. Here we are interested in entropy because it will allow us to identify codes with the shortest possible average length.

Let $A = \{a_1, a_2, \ldots, a_n\}$ a finite set, and X a random variable defined over the set A with probability mass function $p(a)$.

Definition D.4.1 — Entropy. The *entropy* of the random variable X, denoted by $H(X)$ and measured in *bits*, is defined as:

$$H(X) = \sum_{a \in A} p(a) \log \frac{1}{p(a)}$$

Note that the entropy of X does not depend on the individual elements of A, but on their probabilities. It is easy to show that $H(X) \geq 0$ since $0 \leq p(a) \leq 1$ implies that $-\log p(a) \geq 0$. In case of $p(a_i) = 0$ for some i, the value of the corresponding summand $0 \log 0$ is taken to be 0, which is consistent with the limit $\lim_{p \to 0^+} p \log p = 0$. If we change the base of the logarithm to u, entropy will be scaled by a factor of $\log_u 2$ (see Equation **??**).

■ **Example D.8** Let X a random variable defined over the set $A = \{a_1, a_2\}$, with values $p(a_1) = q$ and $p(a_2) = 1 - q$. Then, the entropy of X is given by:

$$H(X) = q \log \frac{1}{q} + (1-q) \log \frac{1}{1-q}$$

Figure D.3 shows the entropy of X for different values of q. If $q = 0$ or $q = 1$ the entropy is 0, that is, there is no uncertainty about which value of A we will get. The maximum value of H is 1, and it is reached when $q = 1/2$; that is, we could say that 1 bit is the uncertainty associated to two equally probable symbols. ■

Next proposition shows that the maximum value for entropy is the logarithm of the number of symbols of A, and that this value is reached when all the symbols have the same probability.

Proposition D.4.1 Given the random variable X we have that $H(X) \leq \log n$, and $H(X) = \log n$ if, and only if, $p(a_1) = p(a_2) = \ldots = p(a_n)$.

Proof. Consider the expression:

$$\log n - H(X) = \sum_{i=1}^{n} p(a_i) \log n - \sum_{i=1}^{n} p(a_i) log \frac{1}{p(a_i)} = \sum_{i=1}^{n} p(a_i) \log n p(a_i)$$

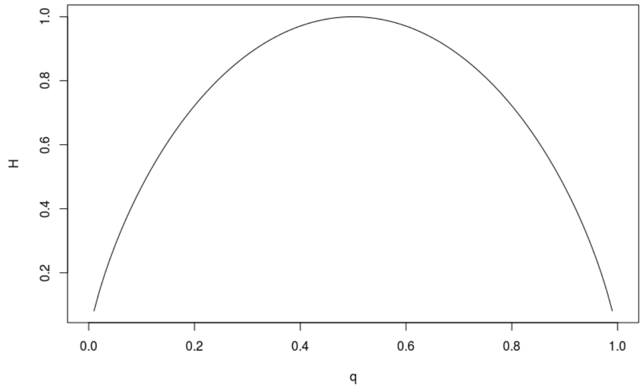


Figure D.3: Binary Entropy Function

Applying property **??** we have that:

$$\log n - H(X) = \log e \sum_{i=1}^{n} p(a_i) \ln np(a_i)$$

And applying property **??** (equalling $x = 1/np(a_i)$):

$$\log n - H(X) \geq \log e \sum_{i=1}^{n} p(a_i) \left(1 - \frac{1}{np(a_i)}\right) \geq \log e \left(\sum_{i=1}^{n} p(a_i) - \frac{1}{n} \sum_{i=1}^{n} \frac{p(a_i)}{p(a_i)}\right) \geq 0$$

Which proves that $H(X) \leq \log n$.

The inequality becomes an equality if, and only if, $p(a_i) = 1/n$ (given that the inequality **??** becomes an equality if, and only if, $x = 1$).

■

■ **Example D.9** If we choose a random symbol from A according to the probability mass function p, entropy would be the minimum expected number of binary questions (Yes/No questions) required to identify the selected symbol. If the symbols of A are equiprobable, the expected number of questions is maximal and equal to $\log d(A)$. ■

We can extend the concept of entropy to a pair of random variables by means of using the joint probability mass function. In this way, the joint entropy will be a measure of the uncertainty associated to both variables. Let $A = \{a_1, a_2, \ldots, a_n\}$ and $B = \{b_1, b_2, \ldots, b_m\}$ two finite sets, and X and Y two random variables defined over the sets A and B respectively, with probability mass function $p(a)$ and $p(b)$, and joint probability mass function $p(a,b)$.

Definition D.4.2 The *joint entropy* of the random variables A and B, denoted by $H(A,B)$, is defined as:

$$H(A,B) = \sum_{a\in A}\sum_{b\in B} p(a,b)\log\frac{1}{p(a,b)}$$

Since $p(a,b) = p(b,a)$ we have that the joint entropy does not depend of the order in which the random variables are selected, that is $H(A,B) = H(B,A)$. We can provide a similar definition for the joint entropy of a set of n random variables $A_1, A_2, \ldots, A_n$ using the joint probability mass function $p(a_1, a_2, \ldots, a_n)$.

Adding a second random variable whose outcome is not know might increase the entropy, as following proposition proves.

Proposition D.4.2 We have that

$$H(A,B) \geq \max\left(H(A), H(B)\right)$$

Proof.

$$H(A,B) = \sum_{a\in A}\sum_{b\in B} p(a,b)\log\frac{1}{p(a,b)} \geq \sum_{a\in A}\sum_{b\in B} p(a,b)\log\frac{1}{p(a)} = \sum_{a\in A} p(a)\log\frac{1}{p(a)} = H$$

In the same way we can prove that $H(A,B) \geq H(B)$. Combining both inequalities we get the desired result. ■

The joint entropy of two random variables cannot be greater that the sum of their individual entropies.

Proposition D.4.3 We have that $H(A,B) \leq H(A) + H(B)$ and $H(A,B) = H(A) + H(B)$ if, and only if, $p(a)$ and $p(b)$ are statistically independent.

Proof. TODO: Prove without using the concept of conditional entropy nor mutual information. ■

The next derived concept from entropy that we are going to introduce is conditional entropy. Conditional entropy measures the uncertainty of a random variable given that the value of another random variable is known.

Definition D.4.3 The *conditional entropy* of the random variable B given the random variable A, denoted by $H(B \mid A)$, is defined as:

$$H(B \mid A) = \sum_{a\in A}\sum_{b\in B} p(a,b)\log\frac{1}{p(b \mid a)}$$

Since $p(b \mid a) \neq p(a \mid b)$ we have that $H(B \mid A) \neq H(A \mid B)$. If $H(B \mid A) = 0$ we have that the value of B is completely determined by the value of A.

Next proposition proves that knowing the value of a second random variable can never increase the uncertainty of a random variable.

Proposition D.4.4 Given the random variables X and Y, we have that $H(Y \mid X) \leq H(Y)$, and $H(Y \mid X) = H(Y)$ if, and only if, $p(a)$ and $p(b)$ are independent.

Proof.

$$H(Y \mid X) = \sum_{a \in A} \sum_{y \in B} p(a,b) \log \frac{1}{p(b \mid a)} = \sum_{a \in A} \sum_{b \in B} p(a,b) \log \frac{p(a)}{p(a,b)}$$
$$= \sum_{a \in A} \sum_{b \in B} p(a,b) \log p(a) - \sum_{a \in A} \sum_{b \in B} p(a,b) \log p(a,b) = -H(X) + H(X,Y)$$

Applying Propositon D.4.3 we have that $H(Y \mid X) = H(X,Y) - H(X) \leq H(X) + H(Y) - H(X) = H(Y)$. The iff equality is also proved by applying Proposition D.4.3. ■

From an intuitive point of view we could expect that the uncertainty associated to a pair of random variables must be equal to the uncertainty of one of them plus the uncertainty of the second given that we know the outcome of the first one.

Proposition D.4.5 — Chain rule. Given the random variables X and Y we have that $H(X,Y) = H(X) + H(Y \mid X)$.

Proof.

$$H(Y,X) = \sum_{a \in A} \sum_{b \in B} p(a,b) \log \frac{1}{p(a,b)} = \sum_{a \in A} \sum_{b \in B} p(a,b) \log \frac{1}{p(a)p(a \mid b)}$$
$$= \sum_{a \in A} \sum_{b \in B} p(a,b) \log \frac{1}{p(a)} + \sum_{a \in A} \sum_{b \in B} p(a,b) \log \frac{1}{p(a \mid b)} = H(X) + H(Y \mid X)$$

■

The last derived concept of entropy we are going to see is mutual information. Intuitively, the mutual information of two random variables X and Y measures the information that X and Y share, that is, how much knowing one of these variables reduces the uncertainty about the other.

Definition D.4.4 The *mutual information* of the random variable X and Y, denoted by $I(X;Y)$, is defined as:

$$I(X;Y) = \sum_{a \in A} \sum_{b \in B} p(a,b) \log \frac{p(a,b)}{p(a)p(b)}$$

Since $p(a,b) = p(b,a)$ we have that $I(X;Y) = I(Y;X)$, that is, the order of the random variables does not affect the concept of mutual information.

Next proposition shows that mutual information is a positive quantity, and it is equal to 0 if, and only if, the random variables are independent.

Proposition D.4.6 Given the random variables X and Y we have that $I(X;Y) \geq 0$, and $I(X;Y) = 0$ if, and only if, the variables X and Y are independent.

Proof. TODO: to be done ■

Introduce this proposition

Proposition D.4.7 Given the random variables X and Y, we have that:

$$I(X;Y) = H(X) - H(X \mid Y) = H(Y) - H(Y \mid X)$$

Proof. TODO: to be done ■

Introduce this proposition

Proposition D.4.8 Given the random variables X and Y, we have that:

$$I(X;Y) = H(X) + H(Y) - H(X,Y)$$

Proof. TODO: to be done ■

Prove that $I(\mathcal{S};\mathcal{S}) = H(\mathcal{S})$
Use the Venn diagrams in this example

■ **Example D.10** ■

D.5 Huffman Algorithm

This section should be about compression algorithms. Not sure if only about algorithms based on information theory, or generic compression algorithms. Depends of what we need in practice

Mention that Huffman is not necessarily the optimal compression algorithm

From a practical point of view, there exists an algorithm, called *Huffman algorithm*, that provides a method to build compact prefix-free codes given a probability distribution. For simplicity, we will study first the particular case of constructing binary prefix-free codes, and later I will provide its generalization to the case of D-ary prefix-free codes.

Algorithm D.1 Huffman Algorithm

```
procedure HUFFMAN(Q)
    T ← empty tree
    for i ← 1, d(Q) − 1 do
        allocate a new node z
        z.left = x = EXTRACT-MIN(Q)
        z.rigth = y = EXTRACT-MIN(Q)
        z.freq = x.freq + y.freq
        INSERT(Q, z)
    end for
    return T
end procedure
```

The algorithm (see Algorithm D.1) expects as input a source alphabet $\mathcal{S} = \{s_1, s_2, \ldots, s_q\}$ and their corresponding probabilities $P = \{p_1, p_2, \ldots, p_q\}$. For simplicity, we will merge both sets into a single one $Q = \{(s_1, p_1), (s_2, p_2), \ldots, (s_q, p_q)\}$. The algorithm works by constructing a binary tree T, similar to the one used in the proof of Theorem D.2.1. The algorithm requires $d(Q) - 1$ iterations to finish. During each iteration, the two elements with the lowest probability are selected and removed from set Q, and a new tree node z is created, with the addition of the removed values, and added to the set Q. Once the tree has been constructed, we have to perform a tree transversal assigning a 0 to each left branch, and a 1 to each right branch, until we reach a leaf.

■ **Example D.11** Assume we have the source alphabet $\mathcal{S} = \{a, b, c, d, e, f\}$ with the associated probabilities $P = \{0.35, 0.16, 0.08, 0.12, 0.06, 0.23\}$. In Figure are depicted the contents of the set Q and the tree T for each iteration of the algorithm. At the end of the algorithm, if we perform a traversal of the T tree, we will get the following prefix-free compact code for the source alphabet S:

Source Word	Code Word
a	11
b	00
c	1011
d	100
e	1010
f	01

The expected length of the code is $L = 2.4$, and its entropy is $\mathcal{H} \approx 2.34$. Since the set of probabilities is not D-adic ...

■

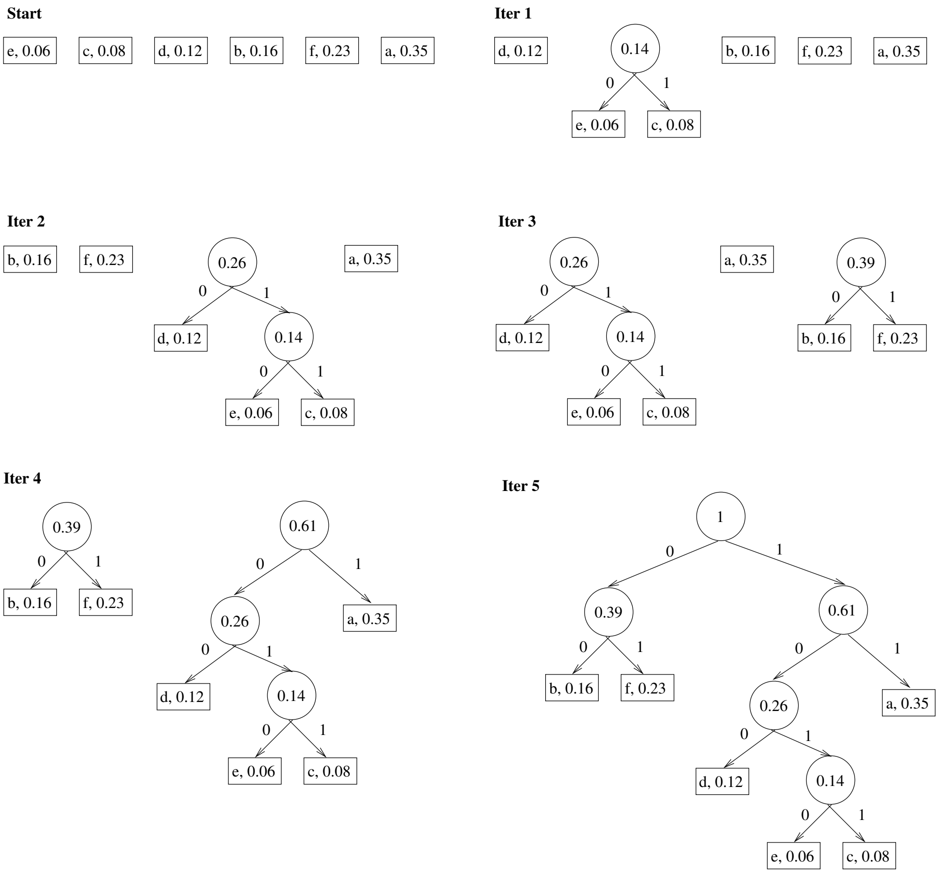


Figure D.4: Huffman Algorithm

This order is arbitrary; switching the left and rigth child of any node yields a different code of the same cost

Proposition D.5.1 Given the probability is ...

Proof. TODO ■

The next theorem shows the optimality of the Huffman coding.

Theorem D.5.2 If C is a Huffman code then C is compact.

Proof. TODO ■

TODO: Rewrite the following paragraphs

So not only is this code optimal in the sense that no other feasible code performs better, but it is very close to the theoretical limit established by the entropy

Although we have proved the theorem for a binary alphabet, the proof can be extended to establishing optimality of the Huffam coding algorithm for a D-ary alphabet as well.

TODO: show how to extend the algorithm to D-ary codes

Then -ary Huffman algorithm uses the 0, 1, ..., n-1 alphabet to encode message and build an n-ary tree [...] the same algorithm applies as for binary codes, except that the n least probable symbols are taken together , instead of just the 2 least probable. Note that for n greater than 2, not all sets of source words can properly form an n-ary tree for Huffman coding. In this case, additional 0-probability place holders must be added. This is because the tree must form and n to 1 contractor; for binary coding, this is a 2 to 1 contractor, and any sized set can form such a contractor. If the number fo source words is congruent to 1 module n-1, then the set of source words will form a proper Huffman tree.

Mention arithmetic coding

D.6 Discretization of Continuous Variables

When summarizing large masses of raw data, it is often useful to distribute the data into classes, or categories, and to determine the number of individuals belonging to each class, called absolute frequency. The following definition formally introduces this concept.

Definition D.6.1 Let $\mathcal{S}$ be a population consisting of n individuals, and let a variable $X : \mathcal{S} \to \mathcal{D}$ represent the mapping of individuals in $\mathcal{S}$ to values in the set $\mathcal{D}$, where k is the cardinality of $\mathcal{D}$. The *absolute frequency*, also known simply as *frequency*, denoted by n_i for $1 \leq i \leq k$, quantifies the number of individuals in $\mathcal{S}$ for which X assigns the value corresponding to the i-th category of $\mathcal{D}$.

The sum of the frequencies must be equal to population size, that is, $\sum_{i=1}^{k} n_i = n$.

If the variable X is continuous, the elements of $\mathcal{D}$ are referred to as *class intervals*. The endpoints of these intervals are known as *class limits*; the smaller number is termed the *lower class limit*, and the larger number, the *upper class limit*. A *class interval* that lacks either an upper or a lower class limit is known as an *open class interval*. The *width* of a class interval is defined as the difference between the upper and lower class boundaries, denoted by $a_i = e_i - e_{i-1}$. The *class mark*, or the midpoint of a class interval, is calculated as $a_i = \frac{e_i + e_{i-1}}{2}$. It is assumed that all observations within a specific class interval are equivalent concerning their categorical assignment. Refer to Section **??** for more information about how to discretize a continous variable into discrete intervals.

■ **Example D.12** In a study measuring adult heights within a community, researchers record heights ranging from 150 cm to 200 cm and organize them into 10 cm class intervals: 150-159 cm, 160-169 cm, 170-179 cm, 180-189 cm, and 190-199 cm. Each interval's lower and upper class limits are respectively the start and end points, such as 150 cm and 159 cm for the first interval. If the last interval had no specified upper limit, it would be considered an open class interval. The class width, typically 10 cm, is the operational span between boundaries, and the class mark, calculated as the midpoint of each interval (e.g., 154.5 cm for the first interval), provides a central value for summarizing data within that range. ■

A tabular arrangement of data by classes together with the corresponding class frequencies is called a frequency distribution, or frequency table.

Definition D.6.2 Let $\mathcal{S}$ be a population consisting of n individuals, and let $X : \mathcal{S} \rightarrow \mathcal{D}$ be a variable that maps individuals in $\mathcal{S}$ to k distinct values of the set $\mathcal{D}$. A *frequency distribution* is represented the set of pairs $\{(d_i, n_i) : 1 \leq i \leq k\}$, where d_i denotes the i-th interval and n_i represents the number of individuals from $\mathcal{S}$ whose value under X falls within the interval d_i.

Frequency distributions are useful for statistical analysis and helps in visualizing data by grouping values, which simplifies the understanding of distribution and central tendencies within the data.

The relative frequency of a class is the frequency of the class divided by the total frequency of all classes

Definition D.6.3 Let $\mathcal{S}$ be a population consisting of n individuals, and let a variable $X : \mathcal{S} \rightarrow \mathcal{D}$ represent the mapping of individuals in $\mathcal{S}$ to values in the set $\mathcal{D}$, where k is the cardinality of $\mathcal{D}$. The *relative frequency*, denoted by f_i, is the ratio $f_i = \frac{n_i}{n}$ for $1 \leq i \leq k$.

The sum of the relative frequencies is equal to one, that is, $\sum_{i=1}^{k} f_i = 1$.

The total frequency of all values less than the upper class boundary of a given class interval is called the cumulative frequency up to and including that class interval.

Definition D.6.4 Let $\mathcal{S}$ be a population consisting of n individuals, and let a variable $X : \mathcal{S} \to \mathcal{D}$ represent the mapping of individuals in $\mathcal{S}$ to values in the set $\mathcal{D}$, where k is the cardinality of $\mathcal{D}$. The *cumulative frequency*, denoted by N_i for $1 \leq i \leq k$, represents the total number of individuals in $\mathcal{S}$ for which X assigns a value less than or equal to the upper limit of the i-th category of $\mathcal{D}$. This is mathematically expressed as $N_i = \sum_{j=1}^{i} n_j$, where n_j is the absolute frequency of the j-th category.

By accumulating the frequencies up to each category or interval, cumulative frequencies provides a running total that shows how many data points fall below a certain value.

Discretization Algorithms

TODO: Rewrite this section.

Let $\mathcal{X}$ a continuous random variable that follows a probability density function $P_{\mathcal{X}}$, and assume we have collected n independent and identically distributed samples $\mathbf{x} = \{x_1, \ldots, x_n\}$ from $\mathcal{X}$. We are interested in computing the length of a compressed version of $\mathbf{x}$ using an optimal compressor. Unfortunately, and except for some degenerate distributions, there is no lossless compression algorithm that produces a string with fewer bits than encoding directly the elements $\mathbf{x}$. Compression algorithms for continuous data only work in case that the elements of $\mathbf{x}$ are not independent, as it is the case with images or sound. But, if this is not the case, the only option available to compress $\mathbf{x}$ is to use a lossy compression algorithm, where some information is lost.

We are looking for an algorithm to produce a finite non-overlapping partition of m discrete intervals $D = \{[d_o, d_1], (d_1, d_2], \ldots, (d_{m-1}, d_m]\}$, where $d_o = \min \mathbf{x}_j$, and $d_m = \max \mathbf{x}_j$, and $d_i < d_{i+1}$ for $i = 0, 1, \ldots, m-1$, assign a unique label to each interval, and encode the elements of $\mathbf{x}$ using this labeling schema. As compression algorithm we will use an optimal length code given the relative frequencies of the labels in the encoded vector. In this sense, our goal is to have a collection of intervals with sufficiently number of samples (so they are statistically significant) and that the distribution of frequencies resembles the original probability distribution $P_{\mathcal{X}}$.

A discretization algorithm is a mapping between a (possibly huge) number of numeric values and a reduced set of discrete values, and so, it is a process in which some information is potentially lost. The choice of discretization algorithm is something that could have a high impact in the practical computation of the nescience. We are interested in a discretization algorithm that produces a large number of intervals (low bias), with a large number of number of observations per interval (low variance). Common techniques include *equal width discretization*, *equal frequency discretization* and *fixed frequency discretization*. However, these techniques require the optimization of an hyperparameter, and so, they are not suitable for our purposes.

In a *proportional discretization approach* the number of intervals m and the number of observations per interval s are equally proportional to the number of observations n. The algorithm starts by sorting the values of $\mathbf{x}_j$ in ascending order and then discretizing them into m intervals of approximately s (possibly identical) values each. In this way, as the number of training observations increases, both interval frequency and number of intervals increases, taking advantage of the larger number of observations. In the same way, when the number of observations decreases, we reduce both.

Our approach begins by selecting the number of bins according to *Rice's rule*, which is asymptotically motivated in the context of histogram density estimation and offers a good balance between resolution and robustness. This rule avoids the excessive granularity of the square-root heuristic (which can result in too few samples per bin when building joint encodings), while remaining less conservative than Sturges' logarithmic rule.

Trimmed core range and minimum occupancy threshold

Instead of relying on the naive plug-in estimator $p_i = c_i/n$, we adopt the Krichevsky-Trofimov (or Jeffreys) smoothing. This Bayesian correction eliminates zero-probability events, stabilizes the estimation of code length, and achieves minimax-optimal redundancy in universal coding.

Mixed-radix encoding

References

TODO: write this section

In 1948, Claude E. Shannon published a paper entitled "A Mathematical Theory of Communication", where he established the foundations of a new discipline, later called *information theory*.

Paper of Shannon ... Harley

Huffman -> D. A. Huffman. A method for the construction of minimum redundancy codes. Proc. IRE, 40:1098-1101, 1952.

The algorithm of huffman has been adapted from Cover. Here also you can find a proof that the algorithm is of order XX.

Kraft's inequality was published by Leon G. Kraft in 1949 as part of his Master Thesis [Kra49]. The inequality was independently rediscovered and proved for the general case of uniquely decodable codes by Brockway McMillan in 1956 [McM56]. The proofs contained in this book have been adapted from [CT12].

The proof of proposition D.4.1 has been adapted from [Abr63]. The proof of proposition 4.3.1 has been adapted from Abramson.

In the area of *digital signal processing* [GG12] it is common to apply a pre-processing step called *quantization*, in which a large number of samples from a continuous signal are mapped into a finite number of representative values. It can be a *scalar quantization* when the signal is one dimensional, or *vector quantization* in case of a multidemensional signal. The optimization goal is to identify a (pre-defined) number of quantizied values such that the mean squared error between the selected values and the original signal is minimized. The problem is solved using the Lloyd-max algorithm [Llo82] (closely relted to the kmeans clustering algorithm [**<empty citation>**] used in machine learning) in which the search space is paritioned in a collection of convex regions and their centroids used as quant, and then, are continously adapted until some stopping criteria is reached. Although it can be shown that the algorithm converges to the optimal solution that minimizes the mean squared error, the selected intervals cannot be used as estimation of the original probability distribution.

An excellent survey of the available discretization methods can be found in [Gar+13]; in the paper the authors also propose a taxonomy to classify existing methods based in their properties and they conduct an extensive comparative experimental study. The proportional discretization method used to compute miscoding is introduced in [YW09], where there is also a theoretical justification of why this method reduces the bias and the variance of the discretized variable.

```
% Rice's rule

A common rule of thumb for determining the number of bins in a histog

Freedman, D., Pisani, R., & Purves, R. (1978). Statistics (2nd ed.).

@book{freedman1978statistics,
  title={Statistics},
  author={Freedman, David and Pisani, Robert and Purves, Roger},
  year={1978},
  publisher={W. W. Norton \& Company}
}

% Jeffreys smoothing
```

```
@article{krichevsky1981performance,
  title={The performance of universal encoding},
  author={Krichevsky, R. E. and Trofimov, V. K.},
  journal={IEEE Transactions on Information Theory},
  volume={27},
  number={2},
  pages={199--207},
  year={1981},
  publisher={IEEE}
}
```

To avoid degenerate estimates when computing code lengths from fini

% Trimmed core range

```
@book{huber1981robust,
  title={Robust Statistics},
  author={Huber, Peter J.},
  year={1981},
  publisher={John Wiley \& Sons}
}
```

When discretizing continuous variables, extreme outliers can distor

E. Complexity

Everything should be made as simple as possible,
but not simpler.
Albert Einstein

In Appendix D, the concept of the complexity of a string based on the lengths of the codewords of a prefix-free code was introduced. This definition is limited by two main factors: first, it necessitates prior knowledge of the set of possible strings, and second, it requires the definition of a probability distribution over this set a priori. It would be highly desirable to expand the set of strings to encompass all strings (that is, $\mathcal{B}^*$) without requiring a probability distribution, thereby providing an absolute notion of string complexity. Unfortunately, even if these issues are resolved, a more fundamental limitation arises when studying the complexity of strings using codes: certain strings that we intuitively expect to be simple cannot be compressed. For instance, the binary expansion of the constant π is widely conjectured to behave like a uniform distribution over the set $\{0,1\}$ and, as such, cannot be compressed. Yet it can be fully and effectively described by a very short mathematical formula. This motivates the need for an alternative definition of string complexity.

Kolmogorov complexity, also known as *algorithmic information theory*, offers a definition of the complexity of a string that directly addresses these issues. Intuitively, the amount of information in a finite string is measured by the length of the shortest computer program capable of producing the string. This approach does not require prior knowledge of the set of valid strings or their probability distribution. Furthermore, objects like π are appropriately classified as having low complexity. We may argue that Kolmogorov complexity provides a universal definition of the amount of information that closely aligns with our intuitive understanding. To compute the Kolmogorov complexity of a string, it is necessary to fix a universal description method or computer language, together with a universal computer. One might question whether, in doing so, the complexity of a string becomes dependent on the chosen language. Fortunately, it has been shown that this is not the case: all reasonable (and sufficiently powerful) languages yield the same description length, up to a fixed constant that depends on the choice of languages but not on the string itself. Unfortunately, Kolmogorov complexity also introduces a significant challenge: it is a non-computable quantity and, as such, must be approximated in practice.

At this point, one might ask whether it is possible to define the complexity of arbitrary objects, not just strings. The answer is yes, at least in theory. Given an object x, the task is to provide an encoding method that represents the object as a string. This encoding is useful only if we can losslessly and effectively reconstruct the original object from its description. However, providing such encodings is not always feasible, either because the objects in question are abstract (as in much of mathematics) or because practical reconstruction of the object from its description is currently impossible (for example, with living organisms[1]).

E.1 Strings Complexity

In Section C.1, the concept of the Turing machine, an idealized model of computation, was introduced. We saw that Turing machines can be represented as partial computable functions $T : \mathcal{B}^* \to \mathcal{B}^*$, which assign to each input string $s \in \mathcal{B}^*$ an output string $T(s) \in \mathcal{B}^*$ (Definition C.4.1). We also introduced the concept of a universal Turing machine $U : \mathcal{B}^* \times \mathcal{B}^* \to \mathcal{B}^*$ (Definition C.2.1), a machine that can simulate the behavior of any other Turing machine; that is, for all $(x,v) \in \mathcal{B}^* \times \mathcal{B}^*$, we have that $U(x,v) = T_x(v)$. Later, in Section D.1, the concept of a code, and in particular, the notion of a prefix-free code, was introduced (Definition D.1.4). We saw that this kind of code presents important properties (Theorem D.2.1). The next definition

[1] As of now, it is not possible to recreate an animal solely based on its DNA.

merges the best of both worlds, Turing machines and prefix-free codes, and introduces a new type of universal Turing machine.

Definition E.1.1 A *prefix-free universal Turing machine* is a universal Turing machine $U : \mathcal{B}^* \times \mathcal{B}^* \to \mathcal{B}^*$ such that, for every $v \in \mathcal{B}^*$, the domain U_v is prefix-free, where $U_v : \mathcal{B}^* \to \mathcal{B}^*$ and $U_v(p) = U(p, v)$ for all $p \in \mathcal{B}^*$.

Using modern computer science terminology we could say that U is the computer, p is the program, and v is the input to the program. Intuitively, the above definition requires that no computer program can be a prefix of any other program. This is not a limitation from the point of view of string lengths, since, by applying McMillan's theorem (Theorem D.2.1), given a uniquely decodable program, we could always find a prefix-free one that computes exactly the same function and has the same length. In practice, programming languages enforce syntactic rules that make programs effectively self-delimiting (for example, programs or functions must terminate with specific delimiters).

Fixing the input v allows us to regard the set of valid programs $\{p : U(p, v) \downarrow\}$ as prefix-free. This ensures that descriptions can be uniquely parsed and avoids ambiguity when concatenating programs.

The concept of a prefix-free universal Turing machine allows us to introduce a new definition of the complexity of a string that aligns more closely with our intuitive understanding of the amount of computational information contained in an object (encoded as a string).

Definition E.1.2 — Kolmogorov Complexity. Fix a prefix-free universal Turing machine $U : \mathcal{B}^* \times \mathcal{B}^* \to \mathcal{B}^*$. The *Kolmogorov complexity* of a string $s \in \mathcal{B}^*$, denoted by $K(s)$, is defined as:

$$K(s) = \min_{p,v \in \mathcal{B}^*} \{l(p) + l(v) : U(p, v) = s\}.$$

Intuitively, the shortest description of a string s is given by two elements: a program p (a self-delimiting program) that captures all the regular patterns of the string, and a new string v that comprises those parts of s that do not present any regularity. We have to find the optimum balance between increasing the complexity of the program, trying to grasp more regularities, or increasing the size of the non-compressible part.[2]

■ **Example E.1** Consider the string composed of one thousand repetitions

[2]In the literature, the Kolmogorov complexity of the string s is defined as $K(s) = \min_{p \in \mathcal{B}^*} \{l(p) : U(p, \lambda) = s\}$, that is, the length of the shortest computer program that, without any additional input, can print the string s. We prefer to use the two-part definition $l(p) + l(v)$ because it is more in line with the requirements of the theory of nescience.

of the substring "10", that is "$\underbrace{1010\ldots1010}_{1.000\,\text{times}}$". We could write the following program:

```
example(char *v) {
    for (int i=1; i<=1000; i++)
        printf("%s", v);
}
```

and then run it with:

```
example("10");
```

in order to print it. The length of the original string is 2,000 bits, but suppose the program length is approximately 480 bits (assuming that every symbol is encoded using a uniform code of 8 bits), and the input length is 2 bits. We can then conclude that the string has a low complexity. Of course, in order to compute the actual Kolmogorov complexity of the string we would need to find the shortest Turing machine that prints that string.

On the contrary, a string composed of two thousand random bits would, with overwhelming probability, have high complexity, since no program significantly shorter than the string itself can generate it. ■

As we mentioned in the preface of this chapter, Kolmogorov complexity would not be particularly useful if the complexity of strings depended on the choice of universal Turing machine. The following theorem demonstrates that this concern is unfounded, up to a constant that depends on the choice of machines, but not on the strings themselves. This establishes Kolmogorov complexity as an inherent property of strings.

Theorem E.1.1 — Invariance theorem. Let U and U' be two universal Turing machines. Then, there exists a constant $C_{U,U'}$, depending only on U and U', such that for each string $s \in \mathcal{B}^*$ we have:

$$K_U(s) \leq K_{U'}(s) + C_{U,U'}.$$

Proof. Let p, v be the shortest strings such that $U'(p,v) = s$. Then we can encode the pair (U', p) and simulate it on U, obtaining $U(\langle U', p, v\rangle, \lambda) = U'(p,v) = s$. Encoding the pair (U', p) requires a fixed description of U' plus the description of p. Thus, $K_U(s) \leq K_{U'}(s) + C_{U,U'}$, where $C_{U,U'}$ is the length of an interpreter for U' on U. ■

■ **Example E.2** Consider a universal programming language, such as Java, and an alternative language, such as Python. We can write a Python interpreter in Java, that is, a Java program that takes a Python script as input and executes it. Then, to compute the complexity of a string $s \in \mathcal{B}^*$ using Java, $C_J(s)$, it would be no greater than the complexity of the string using Python, $C_P(s)$, plus the length of the Python interpreter written in Java, $C_{J,P}$. Importantly, the length of the interpreter, $C_{J,P}$, does not depend on the string s. ■

Although we have proved that Kolmogorov complexity does not depend on the selected universal Turing machine, the size of the constant $C_{U,U'}$ could pose a limitation in practical applications, especially when computing the complexity of short strings where the constant might significantly exceed the complexity of the string itself. This challenge is addressed by the Minimum Description Length principle, as described in Section F.3.

Notation E.1. *We denote by s^* the shortest program that outputs the string s on the universal Turing machine U, that is, $s^* = \langle p, v \rangle$, $U(s^*) = s$, and $l(s^*) = K(s)$. If more than one program satisfies these properties, we select the first one using a lexicographical order induced by* $0 < 1$.

The size of the constant $C_{U,U'}$ is not the only challenge presented by Kolmogorov complexity; another issue is its non-computability, that is, there is no algorithm capable of determining the shortest program that generates an arbitrary string. The following theorem on the uncomputability of Kolmogorov complexity marks a pivotal insight into the intrinsic limits of complexity theory.

Theorem E.1.2 The function $K : \mathcal{B}^* \to \mathbb{N}$ that assigns to each string s its Kolmogorov complexity $K(s)$ is not computable.

Proof. Assume, for contradiction, that K is computable. Then we could construct a function that, for any n, finds the first string s such that $K(s) > n$. This function would produce such an s by a program of length $O(\log n)$, thereby giving a description of s much shorter than n. This contradicts the definition of Kolmogorov complexity. Therefore, K is not computable. ■

If K were computable, we could also solve the Halting Problem by constructing a program that, for any input program and input, computes whether the program halts by checking if its Kolmogorov complexity is finite. Since the Halting Problem is known to be undecidable, this provides an alternative contradiction.

In practice, we approximate Kolmogorov complexity using compression algorithms, such as the Huffman algorithm described in Section D.5, or more sophisticated schemes like Lempel-Ziv, which provide practical upper bounds on $K(s)$ relative to their model class.

E.2 Properties of Complexity

In this section, we delve into the properties of Kolmogorov complexity. We will explore the foundational principles that govern this complexity measure, including its invariance, symmetry, and non-computability. Through examining these properties, we gain deeper insights into the interplay between information, computation, and randomness.

Kolmogorov complexity is always a finite positive natural number.

Proposition E.2.1 For all $s \in \mathcal{B}^*$ we have that $0 < K(s) < \infty$.

Proof. Since $K(s)$ is defined as the length of a program-input pair, it is a non-negative integer. For non-empty strings s, we have $K(s) > 0$. The property $K(s) < \infty$ is a consequence of Proposition E.2.2 and the fact that we are only dealing with finite strings. ■

The Kolmogorov complexity of a string cannot surpass the sum of its own length and a constant.

Proposition E.2.2 There is a constant c such that for all $s \in \mathcal{B}^*$ we have that $K(s) \leq l(s) + c$.

Proof. Let $s \in \mathcal{B}^*$ be an arbitrary string, and consider the encoding of a Turing machine p such that for any input $v = s$, it halts and outputs s. The program p is designed to simply reproduce its input. Given this setup, when p is executed on a universal Turing machine U with s as input, it satisfies the condition $U(p, s) = s$. The length of p is a constant c across all strings s. There exists a fixed program p_{id} that outputs its input; its length is constant and independent of s. By the definition of Kolmogorov Complexity $K(s)$, which seeks the minimum length of a program-input pair that generates s, the combination of p and s presents a feasible solution. Therefore, we have $K(s) \leq l(s) + l(p) = l(s) + c$. ■

The size of the constant c depends on the specific encoding schema used by the selected universal Turing machine U, but it is independent of the string s. In Section E.6, we will explore the characteristics of random strings, which are defined as strings that cannot be compressed. Such strings exhibit a Kolmogorov complexity close to their own length, that is, $K(s) \geq l(s) - c$ for some constant c.

The absolute difference in Kolmogorov complexity between any string x and its transformed counterpart $f(x)$, via a computable bijection, is bounded by a constant c. That is, not only does f not increase the complexity of x by more than a constant, but also f does not decrease the complexity by more than a constant.

Proposition E.2.3 Let $f : \mathcal{B}^* \to \mathcal{B}^*$ is a computable bijection, then there exists a constant c such that $|K(f(x)) - K(x)| < c$.

Proof. Let P_f be the program that computes f and $P_{f^{-1}}$ the program that computes the inverse of f. For any string x, let P_x be the shortest program that generates x. Then, a program $P_{f(x)}$ that generates $f(x)$ can be constructed by concatenating P_x with P_f. The length of this program is $|P_{f(x)}| = |P_f| + |P_x|$. Since $|P_f|$ is a constant that does not depend on x, we can say that $K(f(x)) \leq K(x) + |P_f|$. Similarly, given $f(x)$, we can construct a program P'_x to generate x by applying $P_{f^{-1}}$ to $f(x)$. The length of this program is $|P'_x| = |P_{f^{-1}}| + |P_{f(x)}|$. Thus, $K(x) \leq K(f(x)) + |P_{f^{-1}}|$. The two inequalities combined imply that $|K(f(x)) - K(x)| \leq \max(|P_f|, |P_{f^{-1}}|) = c$, where c is a constant that represents the maximum of the lengths of the programs that compute f and f^{-1}. This constant c does not depend on x, but rather on the complexity of the functions f and f^{-1}. ■

This proposition shows a remarkable stability of informational content under computable bijections, underscoring the intrinsic robustness of Kolmogorov complexity in the face of such transformations.

■ **Example E.3** Consider the function $f : \mathcal{B}^* \to \mathcal{B}^*$ that reverses the order of the bits in a string, i.e., $f(x_1x_2 \ldots x_n) = x_n \ldots x_2x_1$. This function is a computable bijection, since both f and its inverse (which is itself) can be computed by a fixed, finite program. If x is a highly compressible string, such as $x = 1010\ldots10$ repeated 1,000 times, then $f(x)$ is also highly compressible (it is the same pattern written backwards). If x is an incompressible random string, then $f(x)$ is also incompressible. The difference in Kolmogorov complexity between x and $f(x)$ is bounded by the length of the fixed program that reverses the bits, a constant independent of x. ■

Finally, it is worth emphasizing that some strings are very compressible, and this phenomenon occurs at every string length. For instance, the string of n zeros,

$$0^n = \underbrace{00\ldots0}_{n \text{ times}},$$

has a description of length $O(\log n)$: a program that prints "0" exactly n times. Therefore, $K(0^n) \leq c + \log n$, which is which is asymptotically much smaller than n. Similarly, strings with simple patterns, such as alternating zeros and ones, or repetitions of short substrings, can always be described concisely regardless of their total length.

E.3 Joint Kolmogorov Complexity

The joint Kolmogorov complexity of two strings s and t is defined as the length of the shortest program p that, when executed on a universal Turing machine U, outputs the pair $\langle s,t\rangle$, in such a way that both strings can be unambiguously retrieved. Here, $\langle s,t\rangle$ denotes a computable pairing function that encodes two strings into a single string in such a way that both components can be effectively recovered. The pairing function $\langle s,t\rangle$ is assumed to be a fixed, computable bijection with computable inverse, so that both s and t can be effectively recovered. Different choices of pairing function affect $K(s,t)$ by at most an additive constant.

Definition E.3.1 — Joint Kolmogorov Complexity. The *Joint Kolmogorov complexity* of the strings $s,t \in \mathcal{B}^*$, denoted by $K(s,t)$, is defined as:

$$K(s,t) = \min_{p,v\in\mathcal{B}^*} \{l(p)+l(v) : U(p,v) = \langle s,t\rangle\}$$

The notation $K(s,t)$ and $K(st)$ represent two different concepts in the context of Kolmogorov complexity. $K(s,t)$ refers to the joint Kolmogorov complexity of two strings s and t as per Definition E.3.1, meanwhile $K(st)$ represents the Kolmogorov complexity of the concatenation of s and t, without any additional structure to distinguish between them, and so, Defintion E.1.2 is applied. The choice between $K(s,t)$ and $K(st)$ depends on whether it's important to preserve and utilize the distinction and relationship between s and t. If analyzing the interplay or the shared characteristics of s and t is relevant, $K(s,t)$ is more appropriate. If the focus is on the information content of the combined sequence without regard to its origin from two separate strings, $K(st)$ is used.

■ **Example E.4** Consider the strings $s = 0000$ and $t = 1111$. The concatenation $st = 00001111$ can be described by a short program that prints this eight-bit string directly, so $K(st)$ is roughly the length of that description. However, the joint description $\langle s,t\rangle$ requires that the decoding procedure be able to recover the boundary between s and t. Thus $K(s,t)$ and $K(st)$ differ by at most a fixed constant, reflecting the extra information required to separate s and t. ■

Our first proposition highlights a fundamental symmetry in Kolmogorov complexity, illustrating that the complexity of describing a pair of strings in either order differs by at most a constant. This reflects the intrinsic property that the information content is independent of the specific arrangement of the strings being described. The constant c encapsulates the overhead associated with the operations needed to reverse the order of the strings.

Proposition E.3.1 There is a constant c such that for all $x, y \in \mathcal{B}^*$ we have that $|K(x,y) - K(y,x)| \leq c$.

Proof. Let U be a universal Turing machine, and let p_{yx} be the shortest program that outputs $\langle y, x \rangle$ when executed on U. To obtain a program that outputs $\langle x, y \rangle$, we can prepend p_{yx} with a fixed program that swaps the order of the two components in the decoded pair. This additional program has a constant length c, independent of x and y. Therefore, $K(x,y) \leq K(y,x) + c$. ■

Next proposition underscores the subadditive nature of Kolmogorov complexity, proving that the total complexity of describing two strings jointly cannot exceed the sum of their individual complexities by more than a fixed constant, irrespective of the strings' content.

Proposition E.3.2 There is a constant c such that for all $s, t \in \mathcal{B}^*$ we have that $K(s,t) \leq K(s) + K(t) + c$.

Proof. Let s^* and t^* be the shortest self-delimiting programs that generate s and t, respectively. Since s^* and t^* are prefix-free, their concatenation can be parsed unambiguously by a universal Turing machine U. A fixed wrapper program of length c instructs U to run both s^* and t^* in sequence and output the pair $\langle s, t \rangle$. Therefore, $K(s,t) \leq K(s) + K(t) + c$. ■

The final proposition establishes a lower bound on the joint complexity of two strings relative to their individual complexities.

Proposition E.3.3 There is a constant c such that for all $s, t \in \mathcal{B}^*$ we have

$$K(s,t) \geq \max(K(s), K(t)) - c.$$

Proof. Let p be the shortest program that outputs the pair $\langle s, t \rangle$, so $K(s,t) = l(p)$. From $\langle s, t \rangle$, both s and t can be effectively recovered using a fixed decoding program of length c. Thus $K(s) \leq K(s,t) + c$ and $K(t) \leq K(s,t) + c$. Rearranging gives $K(s,t) \geq K(s) - c$ and $K(s,t) \geq K(t) - c$, which together imply $K(s,t) \geq \max(K(s), K(t)) - c$. ■

E.4 Conditional Kolmogorov complexity

In this section, we explore the concept of *conditional Kolmogorov complexity*, which measures how the description length of a string s may decrease when prior knowledge of another string t is available. This notion highlights the impact of background information on the compressibility of a description. Here, $\langle v, t \rangle$ denotes a computable pairing function with computable inverse, ensuring both v and t can be recovered unambiguously. Different choices of pairing function affect $K(s|t)$ by at most an additive constant.

Definition E.4.1 — Conditional Kolmogorov Complexity. The *conditional Kolmogorov complexity* of a string $s \in \mathcal{B}^*$ given the string $t \in \mathcal{B}^*$ is defined as:

$$K(s|t) = \min_{p,v \in \mathcal{B}^*} \{l(p) + l(v) \, : \, U(p, \langle v,t \rangle) = s\}$$

This definition is equivalent up to a constant to the standard formulation $K(s|t) = \min_p\{|p| : U(p,t) = s\}$, since the encoding $\langle v,t \rangle$ can be replaced by t alone with at most constant overhead. As with unconditional Kolmogorov complexity, the conditional complexity is machine-independent: for any two universal Turing machines U and U', there exists a constant $C_{U,U'}$ such that for all $s,t \in \mathcal{B}^*$,

$$K_U(s|t) \leq K_{U'}(s|t) + C_{U,U'}.$$

■ **Example E.5** Let $s = 1010101010$ and $t = 10$. The unconditional complexity $K(s)$ is proportional to the length of s, since it is a ten-bit string. However, given t, we can describe s succinctly by a short program: "print t five times." Thus $K(s|t)$ is only $O(\log 5)$, far smaller than $K(s)$. This illustrates how prior knowledge reduces the description length. ■

As with the unconditional Kolmogorov complexity, the conditional Kolmogorov complexity is a finite non-negative integer.

Proposition E.4.1 For all $s,t \in \mathcal{B}^*$ we have that $0 \leq K(s|t) < \infty$.

Proof. $K(s|t)$ is the length of a program-input pair, so it is non-negative. The property $K(s|t) < \infty$ is a consequence of Proposition E.2.2 and the fact that we are only dealing with finite strings. ■

Next proposition posits that when a string s is conditioned upon itself, its complexity reduces to at most a universal constant.

Proposition E.4.2 There is a constant c such that for all $s \in \mathcal{B}^*$ we have that $K(s|s) \leq c$.

Proof. When a string s is conditioned on itself, the information needed to generate s from s can be encapsulated in a Turing machine that simply copies its input to its output. This machine, being independent of the specific content of s, has a fixed length c. ■

This proposition explores the relationship between unconditional and conditional Kolmogorov complexities, establishing an upper bound for the latter. It asserts that for any strings s and t, the complexity of s given t is at most the complexity of s alone, plus a constant c. This highlights the intuitive notion that having additional information can only reduce the complexity of describing a string, or in the worst case, add a constant overhead, but does not increase it beyond this bound.

Proposition E.4.3 There is a constant c such that for all $s,t \in \mathcal{B}^*$ we have that $K(s|t) \leq K(s) + c$.

Proof. Let p_s be the shortest program that generates s without any auxiliary input, so $|p_s| = K(s)$. Construct a new program p' that ignores the conditional input t and executes p_s. The additional instructions have fixed length c, independent of s or t. Therefore $K(s|t) \leq K(s) + c$. ■

Conditional complexity is not symmetric. In general, $K(s|t) \neq K(t|s)$.

Proposition E.4.4 There exist strings $s,t \in \mathcal{B}^*$ such that $K(s|t) \neq K(t|s)$.

Proof. Consider s as a random n-bit string, and let t be a shortest description of s. Then $K(s|t) = O(1)$, since given t one can directly reconstruct s. On the other hand, $K(t|s) \geq n - O(1)$, since otherwise we would obtain a shorter description of s, contradicting minimality. Thus, in general, conditional Kolmogorov complexity is asymmetric. ■

The relationship between conditional, unconditional, and joint Kolmogorov complexities offers a comprehensive perspective on the informational interdependencies of binary strings. It posits that the complexity of a string s given another string t is at most the complexity of s alone, which in turn is no greater than the joint complexity of both s and t.

Proposition E.4.5 For all $s,t \in \mathcal{B}^*$ we have that $K(s|t) \leq K(s) \leq K(s,t)$.

Proof. The first inequality follows from Proposition E.4.3. The second inequality follows from Proposition E.3.3, since from $\langle s,t \rangle$ we can recover s with constant overhead. ■

The Kolmogorov complexity chain rule is a fundamental principle that connects the joint complexity of two strings with their individual and conditional complexities. It asserts that the total complexity of a pair of strings s and t can be decomposed into the complexity of s plus the complexity of t given s, up to a logarithmic additive term. This relationship mirrors the additive property of entropy in information theory and provides a powerful tool for understanding the interplay between information content and conditional information in the context of Kolmogorov complexity.

Proposition E.4.6 — Kolmogorov chain rule. For all $s,t \in \mathcal{B}^*$ we have

$$K(s,t) = K(s) + K(t \mid s) + O(\log(K(s,t))).$$

Proof. The upper bound follows by concatenating a shortest program p_s that generates s with a shortest program $p_{t|s}$ that generates t given s, plus a fixed wrapper program that runs them in sequence. The overhead is logarithmic, due to the need for self-delimiting encodings of program lengths.

For the lower bound, note that from $\langle s,t \rangle$ one can reconstruct s, and then from s and a decoding procedure reconstruct t. This yields $K(s,t) \geq K(s) + K(t|s) - O(\log(K(s,t)))$. Together, these inequalities establish the claim. ■

▪ **Example E.6** Let $s = 0000$ and $t = 1111$. The joint description $\langle s,t \rangle$ can be generated by first describing s (a short program "print four zeros") and then describing t given s (a short program "print four ones"). Hence $K(s,t) \approx K(s) + K(t|s)$ up to logarithmic overhead, illustrating the chain rule in practice. ▪

E.5 Information Distance

In this section, we aim to introduce a universal metric for quantifying the absolute information distance between two or more individual entities encoded as strings of symbols. Intuitively, the information distance between two strings s and t can be understood as the length of the shortest computer program for a universal computer that enables the generation of s given t and vice versa.

Definition E.5.1 The *information distance* between two strings $s,t \in \mathcal{B}^*$ with respect to a universal Turing machine U, denoted by $ID_U(s,t)$, is defined as

$$ID_U(s,t) = \min\{l(p) : U(p,s) = t, U(p,t) = s\}$$

For any two universal Turing machines U_1 and U_2, the information distance between two strings differs by at most an additive constant c, which depends only on the choice of machines and not on the specific strings. It is also important to note that despite its theoretical significance, information distance is non-computable: there does not exist an algorithm that can compute it exactly for arbitrary strings.

One might consider using the conditional Kolmogorov complexity $K(s \mid t)$ as a measure of information distance. However, this quantity is asymmetric (see Proposition E.4.2), making it unsuitable as a distance. Similarly, the sum $K(s \mid t) + K(t \mid s)$ is also inadequate, as it double-counts the overlapping information needed to transform s into t and vice versa.

The following result shows how information distance can be expressed in terms of conditional Kolmogorov complexities.

Proposition E.5.1 Let $s,t \in \mathcal{B}^*$ be two binary strings. Then

$$ID_U(s,t) = \max\{K(s \mid t), K(t \mid s)\} + O(\log \max\{K(s \mid t), K(t \mid s)\}).$$

Proof sketch. Suppose without loss of generality that $K(s|t) \geq K(t|s)$. A shortest program p of length $K(s|t)$ transforms t into s. To also transform s into t, we append a fixed routine that, given s, reconstructs t by inverting the transformation. This requires at most logarithmic overhead to encode program lengths in a self-delimiting way. Thus one program of length $K(s|t) + O(\log K(s|t))$ suffices in both directions. Therefore,

$$ID_U(s,t) = \max\{K(s|t), K(t|s)\} + O(\log \max\{K(s|t), K(t|s)\}).$$

∎

■ **Example E.7** Let $s = 0011$ and $t = 1100$. The bitwise exclusive-or $s \oplus t = 1111$ captures the difference between the two strings. Given s and the xor-mask $s \oplus t$, one can reconstruct t by $t = s \oplus (s \oplus t)$, and conversely obtain s from t and the mask. Hence, the information distance between s and t is essentially the Kolmogorov complexity of the xor-mask, $K(s \oplus t)$, up to logarithmic overhead. If the mask is simple (all ones), the distance is small; if it is random, the distance is close to the full length of the strings. ■

It is convenient to introduce the following function, which captures the essence of information distance:

$$E(x,y) = \max\{K(x \mid y), K(y \mid x)\}.$$

Proposition E.5.2 $E(x,y)$ is a metric up to logarithmic additive terms.

Proof sketch. Non-negativity and symmetry are immediate from the definition. Identity holds since $E(x,x) = O(1)$, while if $x \neq y$, at least one of $K(x|y)$ or $K(y|x)$ is large, so $E(x,y) > 0$. For the triangle inequality, let x,y,z be strings. From x one can compute y using a program of length $K(y|x)$, and from y one can compute z using a program of length $K(z|y)$. Composing these programs, from x we can compute z using a program of length $K(y|x) + K(z|y) + O(\log)$. Hence

$$K(z|x) \leq K(y|x) + K(z|y) + O(\log).$$

A similar argument applies symmetrically, establishing the triangle inequality for $E(x,y)$ up to logarithmic additive terms. ∎

The information distance $E(x,y)$ admits an alternative characterization in terms of the joint and individual Kolmogorov complexities, as follows.

Proposition E.5.3

$$E(x,y) = \max\{K(x \mid y), K(y \mid x)\} = K(xy) - \min\{K(x), K(y)\} + O(\log K(xy)).$$

Proof sketch. Assume without loss of generality that $K(x) \leq K(y)$. By the chain rule,

$$K(xy) = K(x) + K(y \mid x) + O(\log K(xy)).$$

Thus

$$K(y|x) = K(xy) - K(x) + O(\log K(xy)).$$

Since $E(x,y) = \max\{K(x|y), K(y|x)\}$, the dominant term is $K(y|x)$ in this case. Hence

$$E(x,y) = K(xy) - \min\{K(x), K(y)\} + O(\log K(xy)).$$

■

We now introduce the notion of *admissible information distances*.

Definition E.5.2 An *admissible information distance* $d(x,y)$ is a total function mapping pairs of strings to non-negative integers such that: (1) $d(x,y)$ is upper semicomputable, (2) it satisfies the metric properties up to $O(1)$, and (3) it is normalized in the sense that $\sum_y 2^{-d(x,y)} \leq 1$ for all x.

Among all admissible information distances, $E(x,y)$ plays a distinguished role by being the smallest one up to an additive constant, as stated next.

Proposition E.5.4 $E(x,y)$ is an admissible information distance, and moreover it is minimal: for every other admissible information distance $d(x,y)$, we have

$$E(x,y) \leq d(x,y) + O(1).$$

Proof idea. $E(x,y)$ is upper semicomputable because conditional complexities are. It satisfies the metric axioms up to logarithmic additive terms, as shown earlier. Normalization follows because conditional Kolmogorov complexities induce a semimeasure. Minimality holds because any admissible distance can be simulated by conditional descriptions, while $E(x,y)$ already captures the maximal overlap of descriptions. Thus $E(x,y)$ is universal among admissible information distances. ■

This universality means that $E(x,y)$ encompasses all other admissible information distances: it is the minimal such function up to additive constants. Therefore, $E(x,y)$ provides a canonical, universal measure of information distance.

Normalized Information Distance

Information distance is an absolute measure; however, when assessing similarity, we are often more concerned with relative measures. For instance, two strings of length 1,000,000 differing by 1000 bits are perceived as relatively more similar than two strings of length 1000 that differ by the same number of bits. This motivates the introduction of a normalized version of information distance: the size of the description required for transformation should be evaluated relative to the sizes of the objects being compared.

Definition E.5.3 The *normalized information distance* between two binary strings $s,t \in \mathcal{B}^*$, denoted by $NID(s,t)$, is defined as:

$$NID(s,t) = \frac{\max\{K(s \mid t), K(t \mid s)\}}{\max\{K(s), K(t)\}}.$$

As expected, the normalized information distance takes values between 0 and 1, up to negligible additive terms.

Proposition E.5.5 The normalized information distance $NID(s,t)$ takes values in the range $[0,1]$ up to vanishing additive terms.

Proof. Non-negativity follows because Kolmogorov complexities are non-negative, so $NID(s,t) \geq 0$. For the upper bound, we use the fact that $K(s|t) \leq K(s) + O(1)$ and $K(t|s) \leq K(t) + O(1)$. Therefore

$$\max\{K(s|t), K(t|s)\} \leq \max\{K(s), K(t)\} + O(1).$$

Dividing by $\max\{K(s), K(t)\}$ gives

$$NID(s,t) \leq 1 + O\left(\frac{1}{\max\{K(s),K(t)\}}\right).$$

Hence, up to negligible terms, $NID(s,t) \in [0,1]$. ■

The normalized information distance not only captures relative similarity but also inherits the essential structure of a metric space, satisfying the axioms of a metric up to vanishing additive terms.

Proposition E.5.6 The normalized information distance $NID(x,y)$ is a metric, up to negligible errors.

Proof sketch. Non-negativity and symmetry are immediate from the definition. For identity, $NID(x,y) = O(1/\max\{K(x),K(y)\})$ when $x = y$, while if $x \neq y$ at least one of the conditional complexities is large, so $NID(x,y) > 0$. For the triangle inequality, let x,y,z be strings. From the inequality

$$K(z|x) \leq K(y|x) + K(z|y) + O(\log),$$

we obtain

$$E(x,z) \leq E(x,y) + E(y,z) + O(\log),$$

where $E(\cdot,\cdot)$ is the (unnormalized) information distance. Normalizing by $\max\{K(x),K(z)\}$ introduces at most a vanishing additive error. Thus *NID* satisfies the metric axioms up to negligible terms. ■

The normalized information distance can also be expressed directly in terms of the joint and individual Kolmogorov complexities, as shown below.

Proposition E.5.7

$$NID(x,y) = \frac{K(xy) - \min\{K(x),K(y)\} + O(\log K(xy))}{\max\{K(x),K(y)\}}.$$

Proof sketch. From the earlier result for information distance we know

$$E(x,y) = \max\{K(x|y),K(y|x)\} = K(xy) - \min\{K(x),K(y)\} + O(\log K(xy)).$$

Dividing both sides by $\max\{K(x),K(y)\}$ yields the stated expression for $NID(x,y)$. ■

Normalized Compression Distance

Although the normalized information distance is not computable, it has a wide range of potential applications. By approximating Kolmogorov complexity with practical compressors, we can obtain a computable surrogate of *NID*. Let $Z(s)$ denote the length in bits of the string s compressed using a compressor Z (such as `gzip`, `bzip2`, or `PPMZ`). Similarly, $Z(s \mid t)$ denotes the compressed size of s when the compressor is given t as auxiliary input. This motivates the following definition.

Definition E.5.4 The *normalized compression distance* between two strings $s,t \in \mathcal{B}^*$, given the compressor Z, and denoted by $NCD_Z(s,t)$, is defined as:

$$NCD_Z(s,t) = \frac{\max\{Z(s \mid t),Z(t \mid s)\}}{\max\{Z(s),Z(t)\}}$$

In practice, most compressors do not support conditional compression, making $Z(s \mid t)$ difficult to compute directly. Fortunately, the definition can be reformulated in terms of concatenated compression, which avoids this issue.

Proposition E.5.8 The normalized compression distance between two strings $s,t \in \mathcal{B}^*$, given the compressor Z, satisfies:

$$NCD_Z(s,t) = \frac{Z(st) - \min\{Z(s), Z(t)\}}{\max\{Z(s), Z(t)\}}.$$

Proof sketch. From the definition of NCD_Z, we have

$$NCD_Z(s,t) = \frac{\max\{Z(s|t), Z(t|s)\}}{\max\{Z(s), Z(t)\}}.$$

For real-world compressors, the conditional compression $Z(s|t)$ can be approximated by

$$Z(s|t) \approx Z(st) - Z(t),$$

since compressing the concatenation st encodes s with t as a prefix, effectively using t as context. Similarly,

$$Z(t|s) \approx Z(st) - Z(s).$$

Therefore,

$$\max\{Z(s|t), Z(t|s)\} \approx Z(st) - \min\{Z(s), Z(t)\}.$$

Substituting this into the definition yields

$$NCD_Z(s,t) = \frac{Z(st) - \min\{Z(s), Z(t)\}}{\max\{Z(s), Z(t)\}}.$$

This equality holds up to negligible additive errors, which vanish for ideal compressors. ■

The normalized compression distance constitutes a family of distances, each defined by the choice of compressor Z. The effectiveness of Z determines how closely the normalized compression distance mirrors the normalized information distance, ultimately influencing how well NCD approximates NID in practical applications.

E.6 Incompressibility and Randomness

A string is considered incompressible if its Kolmogorov complexity is approximately equal to its length; in other words, there is no significantly shorter description or program that can produce it.

Definition E.6.1 For each constant c we say that a string $s \in \mathcal{B}^*$ is *c-incompressible* if $K(s) \geq l(s) - c$.

The next proposition shows that incompressible strings exist for every string length.

Proposition E.6.1 For every length n, there exists a string of length n that is incompressible.

Proof. By a counting argument, the number of programs of length less than n is at most $2^n - 1$, while the number of binary strings of length n is exactly 2^n. Therefore, at least one string of length n cannot be generated by any program shorter than n, and is thus incompressible. ■

We extend the term *incompressible string* to include all c-incompressible strings with c small. In this sense, most strings are incompressible.

Proposition E.6.2 For any n and constant $c > 0$, at least a fraction $1 - 2^{-(c-1)}$ of the strings of length n are c-incompressible.

Proof. Consider the number of programs of length at most $n - c$. There are at most

$$\sum_{i=0}^{n-c} 2^i = 2^{n-c+1} - 1$$

such programs. Since there are 2^n strings of length n, at least $2^n - (2^{n-c+1} - 1)$ strings must be c-incompressible. Thus the fraction of c-incompressible strings of length n is at least

$$1 - \frac{2^{n-c+1} - 1}{2^n} = 1 - 2^{-(c-1)} + \frac{1}{2^n}.$$

For large n, this tends to $1 - 2^{-(c-1)}$. ■

The notion of randomness, especially in the context of sequences or strings, is often associated with unpredictability, lack of pattern, or absence of structure. Kolmogorov complexity formalizes this intuition by linking randomness to incompressibility: a string is random if it cannot be generated by any program significantly shorter than the string itself.

Definition E.6.2 We say that a string $s \in \mathcal{B}^*$ is *random* if it is c-incompressible for some fixed small constant c.

Random strings are characterized by high Kolmogorov complexity, meaning they are incompressible. The shortest program that can generate a random string is essentially the string itself. Such strings contain the maximum amount of information possible.

■ **Example E.8** Consider a string generated by flipping a fair coin for each bit, such as 1011010110110101. With overwhelming probability, this string will be incompressible, since no shorter program or pattern can generate it. Any attempted compression would yield a program of length comparable to the string itself. ■

The unpredictability of random strings stems from their incompressibility. Because no algorithm can exploit patterns in such strings, predicting their bits is no better than random guessing.

Random strings are typical in the space of all strings. In the sense of Kolmogorov complexity, almost all strings are random, while only a vanishing fraction admit significantly shorter descriptions.

■ **Example E.9** Consider the set of all conceivable high-resolution digital photographs, each represented as a binary string encoding pixel colors and intensities. Only a tiny fraction of these images exhibit recognizable regularities, such as a uniform blue sky or a solid monochromatic background, which can be compressed into shorter binary descriptions. By contrast, the overwhelming majority of possible images resemble random strings: they lack compressible patterns and are essentially incompressible. ■

References

Kolmogorov complexity, named after the Soviet mathematician Andrey Kolmogorov, is a measure of the complexity of a string of text or other data. It is defined as the length of the shortest possible description of the string in some fixed universal description language. This measure is inherently uncomputable in general, as proven by the halting problem's undecidability, but it provides a powerful theoretical tool for understanding data complexity. Beyond theoretical interest, Kolmogorov complexity has applications in pattern recognition, data compression, and the study of randomness. It offers a framework for understanding the limits of compressibility and the nature of information.

The concept of Kolmogorov complexity emerged independently in the works of several researchers in the early 1960s. Andrey Kolmogorov introduced it in 1965 [Kol65], motivated by trying to formalize the concept of randomness and complexity through the lens of information theory. Ray Solomonoff laid the groundwork for algorithmic information theory, introducing a related concept that would later be recognized as a form of Kolmogorov complexity [Sol64]. His work focused on the idea of describing data compactly using probabilistic models. Almost simultaneously with Kolmogorov, Gregory Chaitin developed similar ideas [Cha69]. Chaitin is known for introducing the concept of algorithmic randomness and for his work on the incompleteness theorem, which relates to the limits of formal systems in proving the complexity of sequences. The motivations behind the development of Kolmogorov Complexity were multifaceted, encompassing the desire to better understand the nature of information, randomness, and the limits of computation and prediction, thus laying the groundwork for numerous applications in theoretical computer science, mathematics, and beyond.

For those readers interested in delving into the details of Kolmogorov complexity, a variety of foundational texts and advanced treatments are available. [LV13] provides a comprehensive coverage to the concepts and applications of Kolmogorov complexity, and it's widely regarded as the definitive textbook on the subject, although it is not recommended for beginners. [Cal02] delves deeply into the foundations of algorithmic information theory, focusing on the rigorous mathematical exploration of randomness and complexity through Kolmogorov complexity. [CT12] broader in scope, this book provides an excellent foundation in information theory, including discussions relevant to Kolmogorov complexity. It's a great resource for understanding the context in which Kolmogorov complexity operates within information theory.

F. Learning

Some mathematical statements are true for no reason,
they're true by accident.
Gregory Chaitin

Warning: This section still requires a significant amount of work!

Machine learning refers to a large collection of algorithms designed to automatically build mathematical models based on sample data sets, usually with the aim of making predictions, classifying objects, or simply to better understand the structure of the data. In the past decade, machine learning algorithms have been highly successful in areas like self-driving cars, practical speech recognition, effective web search, and purchase recommendations.

In this chapter we are going to see how the problem of learning from data is formally formulated in the area of machine learning. In this sense, the chapter is a continuation of the introduction to discrete probability included in Section **??**. Also, we are going to study in detail two particular approaches to machine learning that are highly related to our theory of nescience: the Minimum Description Length principle and the Minimum Message Length principle.

Most of the learning algorithms used today in practice are known since forty years ago. The high success of current machine learning applications is largely due to the availability of huge, high-quality, training datasets, and to the advance of computing power, and in particular, thanks to the powerful graphical processing units (GPU) used in video-games. In Chapter 8 we will introduce a collection of new machine learning algorithms based on the theory of nescience, and we will compare them with the current, state of the art, algorithms.

F.1 Statistical Inference

Statistical inference has traditionally been presented as the way to make sense of reality through data. It applies probabilistic models to relate finite observations to broader populations, aiming to offer predictions and structured conclusions. However, statistical inference is not a direct reflection of reality but rather a tool that depends heavily on assumptions and idealized models. These models simplify complex phenomena, and the validity of their conclusions relies on how well these assumptions align with the underlying data-generating processes.

The random sampling model serves as a stepwise framework in statistical inference, guiding how we connect finite samples to broader populations:

Step 1.- Defining the Population and Collecting Data: The first step is to define the population of interest and determine how data will be collected. This involves specifying the sampling process and ensuring that each data point is drawn independently and identically distributed (iid) from the same population, with every unit having a nonzero probability of selection. Once the sampling process is defined, data is collected as a sample from the population, and each observation is treated as a realization of a random variable following the specified distribution.

Step 2.- Constructing and Checking the Random Sampling Model: Based on the assumptions about how the data was generated, the random sampling model is mathematically expressed. For example, , where is the unknown population distribution with parameter . This step formalizes the relationship between the data and the population. Real-world data rarely fits these idealized assumptions perfectly, so it is essential to check for deviations such as selection biases or lack of independence and address them appropriately.

Step 3.- Applying the Likelihood Function and Estimating Parameters: The likelihood function plays a central role in parameter estimation by quantifying how plausible different parameter values are given the observed data . Methods such as maximum likelihood estimation (MLE) or Bayesian inference refine these estimates, translating raw data into structured knowledge about the population. For example, the sample mean is often used as an estimate of the population mean .

Step 4.- Quantifying Uncertainty and Generalizing to the Population: Recognizing that the sample is just one realization of a random process, uncertainty must be quantified to understand how sample statistics behave across repeated samples. Sampling distributions, confidence intervals, and hypothesis tests help describe this variability. The Central Limit Theorem ensures that for large samples, the sample mean approximates a normal distribution, making inference more reliable. Finally, results are generalized from the sample to the population using frequentist methods such as confidence intervals and p-values or Bayesian methods that update beliefs about by incorporating prior knowledge.

The random sampling model provides a structured, step-by-step approach for making inferences from data. However, each step depends on assumptions that rarely hold perfectly in practice. As such, conclusions drawn from statistical inference should be viewed as tentative and context-dependent, subject to revision when new data or insights become available.

Definition F.1.1 A *statistical model* is a random variable, together with a specification of its probability distribution, and the identification of the parameters, denoted by θ, of that distribution.

A statistic is a function of the observable data. A statistic is used to summarize or describe some aspect of the sample. For example, the sample mean and the sample variance are statistics because they summarize data drawn from a sample.

Definition F.1.2 Let $\mathbf{X} = (X_1, \ldots, X_n)$ be a random sample. A *statistic* is a random variable $T = r(X_1, \ldots, X_n)$, where $r()$ is an arbitrary real-valued function of n variables.

A *parametric random variable* is a random variable X that belongs to a family of functions parameterized by θ. The parameter θ can either be a single scalar or a vector of values, and it is treated itself as a random variable that follows a probability distribution. The set $\Theta = \{\theta_1, \theta_2, \ldots\}$, consisting of all possible values of θ, is called the *parameter space*, and its elements are referred to as *parameters*. When the parameter θ is unknown, the distribution of the random variable X is said to be conditional on θ, denoted by $f(X \mid \theta)$.

As was the case in Chapter B, in this section, we are only considering parametric discrete random variables defined over discrete probability spaces.

■ **Example F.1** We have seen in Definition B.6.4 that a binomial distribution with parameters n and p is a model for a family of experiments in which we are interested in knowing the number of successes in a sequence of n independent binary trials, where the probability of success is p. If X is a random variable following a binomial distribution, the probability of getting exactly k successes is given by:

$$Pr(X=k)=\binom{n}{k}p^k(1-p)^{n-k}$$

In statistical inference, we are usually interested in the inverse problem. That is, we have the actual result of an experiment composed of n trials, in which we know how many successes k we have obtained, and we would like to estimate the parameter p, that is, the probability of success. ■

We assume that the true value of the unknown parameter θ can be inferred, typically by analyzing a collection of data samples. The observable data $\mathbf{X}=(X_1,\ldots,X_n)$ is modeled as a random sample from the distribution $f(X \mid \theta)$ conditional on θ.

An estimator of a parameter θ is a function of the random sample $\mathbf{X}$ that we hope provides a value close to the unknown parameter θ.

Definition F.1.3 Let $\mathbf{X}=(X_1,\ldots,X_n)$ be a random sample from a discrete random variable X with parameter θ. An *estimator* of the parameter θ is a real-valued function $\delta(X_1,\ldots,X_n)$. If $X_1=x_1,\ldots,X_n=x_n$ are observed, then $\delta(x_1,\ldots,x_n)$ is called the *estimate* of θ.

The estimator itself is a random variable, and its probability distribution can be derived from the joint distribution of $X_1,\ldots,X_n$. Every estimator is a statistic, but not every statistic is an estimator. The estimate is a real number.

Estimators help us estimate the quantities of interest in statistical inference and quantitatively assess the quality of the results. A good estimator is one where it is highly likely that the error $\delta(\mathbf{X})-\theta$ will be close to zero.

In practice, we begin our analysis by deriving a distribution for the parameter θ based on theoretical assumptions and our current knowledge of the experiment.

When selecting an estimator, it is important to measure how "good" an estimate is. One common approach is to quantify the loss or cost associated with choosing an estimate that deviates from the true parameter value. This is done using a loss function, which assigns a numerical penalty to the difference between the estimate and the actual parameter.

Definition F.1.4 A loss function is a real-valued function of two variables, $L(\theta,a)$, where $\theta \in \Theta$ and a is a real number.

The loss function represents the cost incurred when the true parameter value is θ and the estimate is a. In other words, $L(\theta,a)$ quantifies the loss when there is a discrepancy between the estimate and the true value.

Let $\xi(\theta)$ denote the prior probability mass function (p.m.f.) of θ on the set Θ. Given a particular estimate a, the expected loss for discrete random variables is computed as:

$$E\left[L(\theta,a)\right] = \sum_{\theta \in \Theta} L(\theta,a)\,\xi(\theta)$$

The expected loss is the weighted average of the losses, where the weights are the probabilities $\xi(\theta)$ assigned to each possible value of θ. The goal is to choose an estimate a that minimizes this expected loss.

The loss function $L(\theta,a) = (\theta - a)^2$ is called squared error loss. Let θ be a real-valued parameter. Suppose that the squared error loss function is used and that the posterior mean of θ, $E(\theta \mid \mathbf{X})$, is finite. Then, a Bayes estimator of θ is $\delta^*(\mathbf{X}) = E(\theta \mid \mathbf{X})$.

The loss function $L(\theta,a) = |\theta - a|$ is called absolute error loss. When the absolute error loss function is used, a Bayes estimator of a real-valued parameter $\delta^*(\mathbf{X})$ equal to a median of the posterior distribution of θ.

F.1.1 Maximum Likelihood Estimator

The Maximum Likelihood Estimator (abreviated MLE) is a method of estimating the parameters of a probability model. It is one of the most commonly used techniques in statistics for fitting model parameters to observed data. The core idea behind MLE is to find the parameter values that maximize a likelihood function, which represents the probability of observing the given data under the model. MLE is widely used due to its desirable properties for large samples, but its effectiveness relies on correct model specification and may struggle with small sample sizes or computational difficulties.

The likelihood represents the probability (or likelihood) of observing the data as a function of the parameters of the model.

Definition F.1.5 Let $X_1, X_2, \ldots, X_n$ be n independent and identically distributed discrete random variables, and let $P(X_i = x_i \mid \theta)$ be the probability mass function of X_i, where $\theta \in \Theta$ is an unknown parameter, and Θ is the parameter space. The *likelihood function* is then defined as:

$$L(\theta \mid X_1, X_2, \ldots, X_n) = \prod_{i=1}^{n} P(X_i = x_i \mid \theta)$$

where $x_1, x_2, \ldots, x_n$ are the observed data points.

The likelihood function is a product of probabilities. Taking the logarithm of the likelihoodm, what it is called the *log-likelihood function*, simplifies this product into a sum:

$$\ell(\theta \mid X_1, X_2, \ldots, X_n) = \log L(\theta \mid X_1, X_2, \ldots, X_n) = \sum_{i=1}^{n} \log f(X_i \mid \theta)$$

Sums are generally much easier to work with than products, particularly when performing differentiation for optimization purposes. This transformation makes it more straightforward to compute derivatives and apply optimization algorithms.

Maximum likelihood estimation is a method that determines values for the parameters of a model. The parameter values are found such that they maximise the likelihood that the process described by the model produced the data that were actually observed.

Definition F.1.6 The *Maximum Likelihood Estimator*, abreviated as MLE, for discrete random variables is defined as the parameter value that maximizes the likelihood function, i.e.,

$$\hat{\theta}_n = \arg\max_{\theta \in \Theta} L(\theta \mid X_1, X_2, \ldots, X_n)$$

Equivalently, the MLE can also be found by maximizing the log-likelihood function:

$$\hat{\theta}_n = \arg\max_{\theta \in \Theta} \ell(\theta \mid X_1, X_2, \ldots, X_n)$$

■ **Example F.2** Consider $X_1, X_2, \ldots, X_n$ i.i.d. random variables from a Bernoulli distribution with parameter p. The probability mass function is:

$$P(X_i = x_i \mid p) = p^{x_i}(1-p)^{1-x_i}$$

where $X_i \in \{0, 1\}$. The likelihood function for this sample is:

$$L(p \mid X_1, X_2, \ldots, X_n) = \prod_{i=1}^{n} p^{X_i}(1-p)^{1-X_i}$$

Which can be rewritten as:

$$L(p) = p^S(1-p)^{n-S}$$

where $S = \sum_{i=1}^{n} X_i$ is the total number of successes (number of times $X_i = 1$). The function $f(p) = p^a(1-p)^b$ attains its maximum at $p = \dfrac{a}{a+b}$. In our case, $a = S$ and $b = n - S$, so the likelihood function $L(p)$ reaches its maximum at:

$$\hat{p} = \frac{S}{S + (n-S)} = \frac{S}{n}$$

Therefore, the maximum likelihood estimator for p is:

$$\hat{p} = \frac{1}{n}\sum_{i=1}^{n} X_i$$

which is simply the sample mean of the Bernoulli trials (the proportion of successes). ■

The maximun likelihood estimator is consitant.

Proposition F.1.1 Let $\hat{\theta}_n$ be the MLE for θ when the random variables are discrete. Under regularity conditions (such as identifiability of the model and the existence of a unique maximizer of the likelihood function), the MLE is consistent, i.e.,

$$\hat{\theta}_n \xrightarrow{\mathrm{P}} \theta_0 \quad \text{as} \quad n \to \infty$$

where θ_0 is the true value of the parameter.

Proof. TODO: Finish 1. Show that the expected log-likelihood is maximized at the true parameter θ_0. 2. Prove that the empirical likelihood function converges uniformly to the expected log-likelihood as the sample size increases. 3. Establish that $\hat{\theta}_n$ converges to θ_0 as $n \to \infty$. ■

The MLE has several notable disadvantages. Firstly, it is highly dependent on sample size; for small samples, MLE may exhibit bias or high variance, as its desirable asymptotic properties, such as consistency, are guaranteed only for large datasets. Additionally, MLE requires correct model specification. It is sensitive to assumptions about the underlying model, and if the model is misspecified, the resulting estimates can be misleading. From a computational perspective, maximizing the likelihood function can pose numerical challenges, often necessitating complex optimization techniques that are computationally demanding and may result in convergence to local rather than global maxima. Furthermore, MLE is sensitive to outliers; since it seeks to maximize the likelihood based on observed data, extreme values can disproportionately affect the estimates, leading to distortions.

■ **Example F.3** Consider a situation where we are dealing with a uniform distribution $U(0,\theta)$, where θ is the unknown upper bound of the distribution. We have a sample $X_1, X_2, \ldots, X_n$ of i.i.d. observations from this distribution, and we wish to estimate the parameter θ using the maximum likelihood estimator. The log-likelihood function is:

$$\ell(\theta \mid X_1, X_2, \ldots, X_n) = -n \log \theta, \quad \text{subject to} \quad \theta \geq \max(X_1, X_2, \ldots, X_n)$$

To maximize the log-likelihood, observe that $\ell(\theta)$ is a decreasing function of θ. Therefore, the maximum likelihood occurs when θ is minimized, subject to the constraint $\theta \geq \max(X_1, X_2, \ldots, X_n)$. Hence, the MLE for θ is:

$$\hat{\theta} = \max(X_1, X_2, \ldots, X_n)$$

The MLE $\hat{\theta}$ tends to underestimate the true value of θ when the sample size is small. This is because the maximum observation in a sample is unlikely to exactly reach the true upper bound, leading to a systematic bias. For example, if $\theta = 10$ and we take a sample of size 5, the expected value of $\hat{\theta}$ is $\frac{5}{6} \cdot 10 = 8.33$, meaning we systematically underestimate the true parameter.

Since the MLE depends only on the maximum observed value, the estimate $\hat{\theta}$ is highly sensitive to outliers. If an unusually large value appears in the sample, it can drastically inflate the estimate of θ, even if the rest of the data suggests a much smaller upper bound. This makes the MLE fragile in the presence of anomalous observations.

Another issue with the MLE in this case is that it ignores most of the data. The MLE is solely determined by the largest value in the sample, meaning the other $n-1$ data points do not contribute to the estimate. This seems inefficient because the estimator does not use all available information, which could be helpful in producing a more reliable estimate. ■

F.1.2 Bayesian Inference

Unlike the Maximum Likelihood Estimator (MLE), which selects the parameter values that maximize the probability of the observed data, *Bayesian inference* takes a fundamentally different approach by treating parameters as probability distributions rather than fixed values. Bayesian inference also incorporates prior knowledge, allowing for an informed estimation process even before observing data. This approach enables Bayesian methods to dynamically update beliefs as new data becomes available. Bayes' theorem (see Theorem B.3.2)) formalizes this process by combining a prior probability mass function with the likelihood of the observed data to produce a posterior probability mass function, which represents the updated belief about the parameter.

Definition F.1.7 Let $f(X \mid \theta)$ be the probability mass function of a discrete random variable X with parameter θ. The probability distribution of the parameter θ, denoted by $\xi(\theta)$, is called the *prior distribution*.

The prior distribution must be defined over the parameter space Θ. It is called the prior distribution because it represents our knowledge or belief about the parameter θ before observing any data.

Definition F.1.8 Let $f(X \mid \theta)$ be the probability mass function of a discrete random variable X with parameter θ, and let $\mathbf{X} = (X_1, \ldots, X_n)$ be a random sample from X. The conditional probability mass function of the parameter θ given the observed values $X_1 = x_1, \ldots, X_n = x_n$, denoted $\xi(\theta \mid x_1, \ldots, x_n)$, is called the *posterior distribution*.

The posterior distribution represents our updated knowledge of the parameter θ after taking into account the observed data. A strongly informative prior will dominate the posterior, while a weak or uniform prior will let the data speak for itself.

The posterior pmf is computed using Bayes' theorem:

$$\xi(\theta \mid \mathbf{X}) = \frac{L(\mathbf{X} \mid \theta)\xi(\theta)}{P(\mathbf{X})}$$

where:

- $\xi(\theta)$ is the prior distribution, which encodes our belief about θ before seeing the data.
- $L(\mathbf{X} \mid \theta)$ is the likelihood function, representing the probability of observing the data given a particular value of θ.
- $P(\mathbf{X})$ is the marginal probability, ensuring the posterior pmf is a valid probability mass function, computed as:

$$P(\mathbf{X}) = \sum_{\theta \in \Theta} L(\mathbf{X} \mid \theta)\xi(\theta)$$

Thus, the posterior pmf $\xi(\theta \mid \mathbf{X})$ represents an updated belief about θ after incorporating the observed data.

■ **Example F.4** Suppose we have a biased coin with an unknown probability θ of landing heads. We want to estimate θ using Bayesian inference after observing a few coin flips. Before flipping the coin, we assume a prior belief about θ. Let's say we assume a uniform prior:

$$\xi(\theta) = \begin{cases} \frac{1}{3}, & \theta \in \{0.2, 0.5, 0.8\} \\ 0, & \text{otherwise} \end{cases}$$

This prior suggests we believe θ is equally likely to be 0.2, 0.5, or 0.8 before any data is observed. Now, we flip the coin $n = 3$ times and observe $x = 2$ heads. Assuming independent flips, the likelihood function is given by:

$$p(X = x \mid \theta) = \binom{3}{2}\theta^2(1-\theta)^1$$

For the possible values of θ:

$$p(2 \mid 0.2) = \binom{3}{2}(0.2)^2(0.8)^1 = 3(0.04)(0.8) = 0.096$$

$$p(2 \mid 0.5) = \binom{3}{2}(0.5)^2(0.5)^1 = 3(0.25)(0.5) = 0.375$$

$$p(2 \mid 0.8) = \binom{3}{2}(0.8)^2(0.2)^1 = 3(0.64)(0.2) = 0.384$$

Using Bayes' rule:

$$\xi(\theta \mid X = 2) = \frac{p(X = 2 \mid \theta)\xi(\theta)}{P(X = 2)}$$

where the denominator is the marginal probability:

$$P(X = 2) = \sum_{\theta} p(X = 2 \mid \theta)\xi(\theta)$$

$$P(X = 2) = (0.096 \times \frac{1}{3}) + (0.375 \times \frac{1}{3}) + (0.384 \times \frac{1}{3})$$

$$P(X = 2) = 0.032 + 0.125 + 0.128 = 0.285$$

Now, calculating the posterior probabilities:

$$\xi(0.2 \mid X = 2) = \frac{0.096 \times \frac{1}{3}}{0.285} = \frac{0.032}{0.285} \approx 0.112$$

$$\xi(0.5 \mid X = 2) = \frac{0.375 \times \frac{1}{3}}{0.285} = \frac{0.125}{0.285} \approx 0.439$$

$$\xi(0.8 \mid X = 2) = \frac{0.384 \times \frac{1}{3}}{0.285} = \frac{0.128}{0.285} \approx 0.449$$

Before observing the data, we believed θ was equally likely to be 0.2, 0.5, or 0.8. After observing 2 heads in 3 flips, our belief has shifted: the most probable value for θ is now 0.8 (44.9% probability), followed by 0.5 (43.9% probability). The probability that $\theta = 0.2$ has dropped significantly to 11.2%.

■

A Bayes estimator is a point estimate derived from the posterior distribution in Bayesian inference, similar to the Maximum Likelihood Estimator (MLE), which selects the parameter values that maximize the likelihood function. However, while MLE relies solely on observed data, the Bayes estimator incorporates both prior knowledge and observed data through the posterior distribution. It is a single value that represents the "best guess" for the unknown parameter by minimizing the expected loss under a given loss function.

Suppose we can observe the value $\mathbf{x}$ of the random vector $\mathbf{X}$ before estimating θ, and let $\xi(\theta \mid \mathbf{x})$ denote the posterior pmf of θ on Ω. For each estimate a the expected loss will be

$$E[L(\theta, a) \mid \mathbf{x}] = \sum_{\theta \in \Theta} L(\theta, a)\,\xi(\theta \mid \mathbf{x})$$

Definition F.1.9 Let $L(\theta, a)$ be a loss function. For each possible value $\mathbf{x}$ of $\mathbf{X}$, let $\delta^*(\mathbf{x})$ be a value of a such that $E[L(\theta,a) \mid \mathbf{x}]$ is minimized. Then δ^* is called a *Bayes estimator* of θ. Once $\mathbf{X} = \mathbf{x}$ is observed, $\delta^*(\mathbf{x})$ is called a *Bayes estimate* of θ.

Another way to describe a Bayes estimator δ^* is to note that, for each possible value $\mathbf{x}$ of $\mathbf{X}$, the value $\delta^*(\mathbf{x})$ is chosen so that

$$E[L(\theta, \delta^*(\mathbf{x})) \mid \mathbf{x}] = \min_{\forall a} E[L(\theta,a) \mid \mathbf{x}]$$

The theory of Bayes estimators provides a satisfactory and coherent theory for the estimation of parameters. To apply the theory, it is necessary to specify a particular loss function, and also a prior distribution for the parameter. Specifying a meaningful prior distribution in a multidimensional parameter space Ω is particularly challenging because it requires incorporating dependencies between multiple parameters, which may not be well understood. Additionally, computational complexity increases significantly as the number of parameters grows, making posterior calculations more difficult.

F.2 Machine Learning

Machine learning is the study of algorithms that, given a finite sample of individuals from a population, learn a rule to make predictions about new, previously unseen individuals. Each individual is represented by a vector of attributes, one of which is designated as the target. Since the true relationship between the predictors and the target is unknown, the algorithm must approximate it. The primary objective is to construct a function, called a model, that uses the observed attributes to predict the target with minimal error, both on the training examples and on future individuals drawn from the same population.

Although statistical inference and machine learning share the goal of using data to draw conclusions about unseen cases, they tend to emphasise different aspects of this task. Classical statistical inference often begins with a probabilistic model and seeks estimators that maximise likelihood, yield interpretable parameters, and satisfy theoretical properties such as consistency, efficiency, or convergence. In contrast, machine learning typically starts with a flexible class of functions, often implemented as large-scale software artefacts such as neural networks, and focuses on minimising an empirical loss that reflects predictive accuracy, even in the absence of formal guarantees. In practice, however, the boundary is fluid: statisticians often minimise risk functions, and many machine learning methods are grounded in statistical theory.

In this book, we present machine learning as a distinct discipline, adopting a fully deterministic approach. We introduce models, residuals, and optimization criteria without relying on probability theory or its results. This choice is deliberate: by avoiding probabilistic assumptions, we align the theoretical foundations of machine learning with the framework of the theory of nescience, facilitating the integration and reuse of results across both domains.

We begin by defining the basic mathematical objects that will underpin the rest of the discussion: populations and their individuals.

Definition F.2.1 A *population* is a non-empty, well-defined set $\mathcal{S}$. The elements $\mathbf{x} \in \mathcal{S}$ are called *individuals*.

Throughout this book, we restrict our attention to countable populations. Both finite and countably infinite cases are permitted.

Each individual is described by a fixed list of attributes (also called features), and each attribute has a domain that specifies its set of admissible values.

Definition F.2.2 Each individual $\mathbf{x}$ in the population $\mathcal{S}$ is characterized by p *attributes* ($p \geq 1$), such that $\mathbf{x} = (x_1, x_2, \ldots, x_p) \in \mathcal{S}$. For each $i \in 1, \ldots, p$, the *domain* of the i-th attribute is defined as $\mathcal{D}_i = \{x_i : \mathbf{x} \in \mathcal{S}\}$.

The set $\mathcal{D}_i$ may be any type of set—for example, the real numbers $\mathcal{D}_i = \mathbb{R}$, a set of integers such as $0, 1, \ldots, k$, or a collection of categorical labels like $\mathrm{red}, \mathrm{green}, \mathrm{blue}$. An attribute is called *quantitative* if the elements of $\mathcal{D}$_*i* can be measured numerically. Quantitative attributes can be further classified as *discrete* if they take a countable number of distinct values, or *continuous* if they can take any value within a given range or interval.

An attribute is called *qualitative* or *categorical* if it represents characteristics that cannot be measured numerically. A qualitative attribute is said to be *nominal* if there is no natural order among its categories, and *ordinal* if such an order exists.

■ **Example F.5** Consider a population consisting of the inhabitants of a small village, where we are interested in studying three attributes: age, gender, and daily water consumption. The attribute representing age, mapping individuals to their age in years, is a quantitative discrete attribute, as it takes integer values. Gender, mapping individuals to categories like "Male" or "Female," is a qualitative nominal attribute, since the categories have no inherent order. Daily water consumption, mapping individuals to the number of liters they drink per day, is a quantitative continuous attribute, as it can take any real value within a measurable range. ■

Broadly speaking, machine learning algorithms can be classified into two main categories: supervised and unsupervised. In *supervised* learning, we are given a collection of training samples (also called *predictors*) along with their corresponding observed target values (or *labels*), and our goal is to predict the target for new, previously unseen observations. In contrast, in *unsupervised* learning, no target values are provided; we are given only training samples, and the objective is to uncover the underlying structure of the data. We postpone the discussion of unsupervised learning to Section XX.

Definition F.2.3 Let $\mathcal{S}$ be a population whose individuals $\mathbf{x}$ are characterized by p *attributes*, with $\mathbf{x} = (x\_1, x\_2, \ldots, x\_p) \in \mathcal{S}$. A *target variable*, denoted by $\mathbf{y}$, is a vector corresponding to another attribute of the individuals in $\mathcal{S}$, distinct from the p attributes used as predictors. The *domain* of the target variable is $\mathcal{D}_y = y_i$.

We typically choose statistical learning methods based on whether the target attribute is quantitative or qualitative. (Whether the predictors are qualitative or quantitative is generally considered less critical.) Supervised learning algorithms are applied to *regression problems* when the target attribute is quantitative, and to *classification problems* when the target attribute is qualitative.

We assume the existence of an underlying function, or model, that relates the predictors to the target.

Definition F.2.4 Let $\mathcal{S}$ be a population and $\mathbf{y}$ a target attribute. A *model* is a function $f : \mathcal{S} \to \mathbf{y}$ such that, for every individual $\mathbf{x} \in \mathcal{S}$, we have $y = f(\mathbf{x})$.

In practice, and for most of the populations, the set of attributes measured is not sufficient to fully characterize the target variable, meaning that $f(\mathbf{x})$ do not maps to y_k, but to something approximated. This fact is modeled in the discipline of mahcine lerning using a random variable, and saying that $y_k = f(\mathbf{x}) + \varepsilon_k$ where the errors $\varepsilon_1, \ldots, \varepsilon_n$ are independent, $\mathbb{E}[\varepsilon_k] = 0$, and $\mathrm{Var}[\varepsilon_k] < \infty$.

In practice, for most populations, the measured attributes are not sufficient to fully determine the target variable. This means that $f(\mathbf{x})$ does not exactly map to the observed value $\mathbf{y}$, but rather to an approximation. In the traditional formulation of machine learning, this uncertainty is modeled using a random variable, assuming that

$$y_k = f(\mathbf{x}) + \varepsilon_k,$$

where the errors $\varepsilon_1, \ldots, \varepsilon_n$ are independent random variables, with $\mathbb{E}[\varepsilon_k] = 0$ and $\mathrm{Var}[\varepsilon_k] < \infty$.

Learning algorithms operate on a finite sample of data, called the *training set*, from which they infer an approximation to the unknown function f.

Definition F.2.5 A *training data set*, is a finite subset of the population $\mathcal{S}$, consisting of a collection of predictor $\mathbf{X}$ and the corresponding target $\mathbf{y}$.

Let x_{ij} represent the value of the j-th predictor for the i-th observation, where $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, p$. Correspondingly, let y_i represent the target value for the i-th observation. Then, the training data consist of the pairs $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, where each $x_i = (x_{i1}, x_{i2}, \ldots, x_{ip})$.

The objective of supervised learning is to construct a model $\hat{f} : \mathcal{S} \to \mathbf{y}$ such that the predicted value $\hat{y}$ is as close as possible to the true value $y(\mathbf{x})$.

Definition F.2.6 Given a training set $\mathcal{T}$, a learning procedure returns an *estimator*

$$\hat{f} : \prod_{i \neq j} \mathcal{D}_i \longrightarrow \mathcal{D}_j.$$

For a new individual $\mathbf{x} \notin \mathbf{x}_1, \ldots, \mathbf{x}_n$, the predicted target value is

$$\hat{y} = \hat{f}\left(\mathbf{x}_{-j}\right),$$

where $\mathbf{x}\_-j$ denotes the vector of predictor values, excluding the target.

The challenge for the machine learning algorithms is to ensure that the estimator $\hat{f}$ generalizes well to the entire population $\mathcal{S}$, even though it was constructed using only the training data $\mathbf{X}$.

F.2.1 Parametric vs. Non-parametric Models

Most of the statistical learning methods can be characterize as either parametric or non-parametric. With *parametric* methods we select a priori a functional for, and the we fit the free parameters of this functional form. In contrast, with *non-parametric* models we do not make any assumption about the form of the mmodels. Given their flexibility, non-parametric methods ususally require more traing data to train, and they are more difficult to interpret by human.

Parametric methods involve a two-step model-based approach: 1) First, we make an assumption abut the functional form, or shape, of f; 2) After a model has been selected, we need a procedure that uses the training data to fit or train the model. Parametric methods reduce the problem of estimating f down to one of estimating a set of parameters. The potential disadvantage of a parametric approach is that the model we choose will usually not match the true unknown form of f. More flexible models can fit may different possible functional forms for f. But fitting a more flexible model requires estimating a greater number of parameters. More complex models can lead to a phenomenon known as overfitting the data, which essentially means they follow the errors, or noise, too closely.

TODO: Provide an example, like linear regression.

Non-parametric methods do not make explicit assumption about the functional form of f. By avoiding the assumption of a particular functional form for f, they have the potential to accurately fit a wider range of possible shapes for f. However, with non-parametric methods, a very large number of observations is required in order to obtain an accurate estimate for f.

TODO: Provide an example.

Concept of regularization to control model complexity. Ridge and Lasso: definitions and intuition. Regularized objective: Effect on optimization and generalization. Practical considerations: choosing.

TODO: Talk about the overfitting problem

There exists a trade-off between flexibility and interpretability of the machine learning methods. If we are interested in inference, then restrictive models are much more interpretable. If we are only interested in prediction, the interpretability of the predictive model is simply not of interest.

F.2.2 Model Accuracy

The error term ε introduced in Equation **??** correspond to variables that have not been taken into account in our study, and other effects that can not be measured. This kind of error is called *irreducible*, since there is nothing we can do to reduced it. A second type of error, called *reducible*, refers t the fact that our estimate $\hat{f}$ of the function f might not be perfect. It is called reducible because with better estimates the error will decrease.

Derive this property

We are interested in the average error made by our model. Assuming that both $\hat{f}$ and X are fixed, it can be shown that

$$E\left(Y-\hat{Y}\right)^2 = E\left[f\left(X\right)+\varepsilon-\hat{f}\left(X\right)\right]^2 = \left[f\left(X\right)-\hat{f}\left(X\right)\right]^2 + Var\left(\varepsilon\right)$$

The irreducible error is an upper bound to the accuracy of our predictions. Unfortunately, in practice, this bound is almost always unknown.

Mean Squared Error

A common metric used to quantitatively evaluate and compare the performance of the different machine learning algorithms is to compute the mean square error (MSE) of the predictions made,

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(Y_i-\hat{f}(X_i)\right)^2$$

where Y_i is the ith observed value, and the $\hat{f}(X_i)$ is the prediction that $\hat{f}$ gives for the ith vector of predictors.

Explain how MSR relates to MLE

We are interested in the capability of the model $\hat{f}$ to generalize to previously unseen data, that is, to correctly make predictions based on input vectors not included in the training dataset $\mathcal{X}$. In this sense, out goal should be to select that method with the lowest MSE over a test dataset, that is, over a collection of input vectors that have not been used for the training of the algorithm. When a model $\hat{f}$ has a very low train MSE but very high test MSE we say that the model overfits the training data.

If the response variable is qualitative the quantity we seek to minimize is the average number of misclassification made by the model, that is,

$$\frac{1}{n}\sum_{i=1}^{n} I\left(Y_i \neq \hat{f}(X_i)\right)$$

where $\hat{f}(X_i)$ is the predicted class for the ith observation, and I is a function that equals 1 if $Y_i \neq \hat{f}(X_i)$ and zero otherwise.

F.2.3 No free lunch theorem

Inductive Bias and the Role of Assumptions. Why learning is not possible without assumptions. Inductive bias: choosing H, priors, constraints. Examples: smoothness, sparsity, linearity. The No Free Lunch Theorem (informal statement)

There is no free lunch in statistics: no one method dominates all others over all possible data sets. On a particular data set, one specific method may work best, but some other method may work better on a similar but different data set

F.2.4 The bias-variance trade-off

It is possible to show that the expected test MSE, for a given value x_0, can be always decomposed into the sum of tree fundamental quantities: the variance of $\hat{f}(x_0)$, the squared ed bias of $\hat{f}(x_0)$ and the variance of the error term ε:

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = Var\left(\hat{f}(x_0)\right)\left[Bias\left(\hat{f}(x_0)\right)\right]^2 + Var(\varepsilon)$$

where $E\left(y_0 - \hat{f}(x_0)\right)^2$ defines the expected test MSE, and refers to the average test MSE that would obtain if we repeatedly estimated f using a large number of training sets, and tested each at x_0.

In order to minimize the expected test error, we need to select a statistical learning method that simultaneously achieves low variance and low bias.

The expected test MSE can never lie below $Var(\varepsilon)$, the irreducible error. Variance refers to the amount by which $\hat{f}$ would change if we estimated it using a different training data set. In general, more flexible statistical methods have higher variance. Bias refers to the error that is introduced by approximating a real-life problem, which may be extremely complicated, by a much more simpler model. Generally, more flexible methods result in less bias. As a general rule, as we use more flexible methods, the variance will increase and the bias will decrease. The relative rate of change of these two quantities determines whether the test MSE increases or decreases.

The relationship between bias, variance, and test set MSE is referred to as the bias-variance trade-off. It is easy to obtain a method with extremely low bias but high variance, or a method with very low variance but high bias. The challenge lies in finding a method fro which both the variance and the squared bias are low. In a real-life situation in which f is unobserved, it is generally not possible to explicitly compute the test MSE, bias, or variance for a statistical learning methods. Alternative approaches, like for example cross-validation, are used to estimate the test MSE using the training data.

F.2.5 Generative vs. discriminative models

TODO: Pending

F.2.6 k-means Clustering

K-means clustering is an algorithms that partitions n observations into k clusters in such a way that each observation belongs to the cluster with the nearest mean. In this way, we can replace the observation that belong to a cluster by its means, as a discretization. The optimization criteria in k-means is to minize the within-cluster variance. Given the fact that the problem is NP-Complete, some approximation algorithms are used instead.

TODO: Define the concept of Voronoi diagram / Voronoi cell

F.2.7 Decision Trees

A decision tree is a mathematical model f that predicts the value of a target variable $\mathbf{y}$ by learning simple `if-else` decision rules inferred from the training set $(\mathbf{X}, \mathbf{y})$ (see Example F.6). Trees are simple and easy to interpret, but they do not give good accuracy.

The nodes of the tree contain pairs of values (j, w), where $1 \leq j \leq p$ is a feature index and $w \in \mathbb{R}$ is a threshold, and the tree leafs contain labels of $\mathcal{G}$ in case of a classification problem, or numbers in case of a regression problem. Given a vector $\mathbf{x} \in \mathbb{R}^p$ we perform a tree traversal checking at each node if $x_j \leq w$ to decide if we continue with the left or right branch of the

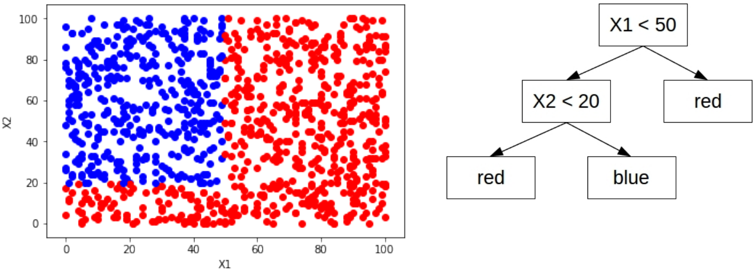


Table F.1: Example of Decision Tree

node, until a leaf is reached. We associate the value $\hat{y}$ of the reached leaf with the vector $\mathbf{x}$.

■ **Example F.6** In Figure F.1, left side, it is shown an example of a dataset composed by two classes, red dots and blue dots. We want to find a decision tree such that given the features $X1$ and $X2$, it returns if the corresponding dot is blue or red. A possible solution to this problem is depicted in the right side of the figure. This decision tree can be also encoded as a function in a programming language, for example in Python, as next code shows.

```
def tree(X1, X2):
    if X1 < 50:
        if X2 < 20:
            return "red"
        else:
            return "blue"
    else:
        return "red"
```

■

The algorithms for the construction of decision trees usually work by recursively partitioning the training set $\mathbf{X}$ in such a way that the values of the target vector $\mathbf{y}$ are grouped together, until all partitions are composed by a single label. The problem with these building methods is that they produce very complex trees that overfit the training data. Overfitted trees not only lead to poor predictive capabilities on non-training data, but also produce models that can be exceedingly difficult to interpret. A common approach to avoid overfitting in decision trees is to force an early stopping of the algorithm before the tree becomes too complex. Popular stopping criteria include limiting the maximum depth of the tree, requiring a minimum number of sample points at leaf nodes, or computing the accuracy gain yielded by adding new nodes. However, those heuristics demand the optimization of hyperparameters which makes the training process computationally expensive.

TODO: briefly describe bagging, random forests, and boosting [...] produce multiple trees which are then combined to yield a single consensus prediction [...] combining a large number of trees can often result in dramatic improvement in prediction accuracy, at the expense of some loss of interpretability [...]

F.2.8 Time Series Analysis

A time series is a sequence of measurements taken at successively equally spaced points in time, so there exists a natural ordering of the observations. Examples of time series include the daily closing prices of the Standard and Poor's 500 index, the monthly number of passengers of an airline, or the yearly gross domestic product of a country.

Definition F.2.7 A *time series* of length $n \in \mathbb{N}$, denoted by $\{x_t : t = 1, \dots, n\}$ or $\{x_t\}$, is a sequence $\{x_1, x_2, \dots, x_n\}$ of *observed values*.

The elements x_i of the series correspond to values sampled at fixed time intervals $1, 2, \dots, n$. The sampling interval must be short enough to provide a very close approximation to the original continuous signal. Observed values could be continuous, discrete or even categorical.

In statistics, a time series is usually represented as a sequence of n random variables, and a particular time series is a realization of this representation. In this sense, $\{x_t\}$ would denote a collection of random variables. In this book, we do not follow this approach for time series formalization.

Time series forecasting refers to the process of building a model to predict future values of the series based on the previously observed values. Time series forecasting is based on identifying the mean features in data and the random variation, and it is generally based on the assumption that present characteristics will continue in the near future, something that cannot be validated in practice.

Notation F.1. *Given the time time series $\{x_t : t = 1, \dots, n\}$ we denote $\hat{x}_{t+k|t}$ the forecast made at time t for a future value at time $t + k$, where k is the number of steps in the future.*

Trends and Seasons

Many time series ... and a repeating seasonal component.

a systematic change in a time series that does not appear to be periodic is known as a trend. [...] A repeating pattern [...] within any fixed period [...] is known as seasonal variation [...] cycles [...] do not correspond to some fixed natural period. [...]

trend [...] change direction in unpredictable times [...] stochastic trend [...]

The main features of many time series are trends and seasonal variations that can be modelled deterministically with mathematical functions of time.

it is usually appropiate to remove trends and seasonal effects before comparing multiple series.

Definition F.2.8 Let $\{x_t\}$ be a time series, a *simple additive model* is defined as

$$x_t = m_t + s_t + z_t$$

where m_t is called the *trend component*, s_t is the *seasonal component*, and z_t is the *error term*.

If the time series presents the property that the seasonal component increases as the trend increases, it might be better to use a multiplicative model.

Definition F.2.9 Let $\{x_t\}$ be a time series, a *simple multiplicative model* is defined as

$$x_t = m_t \dot{s}_t + z_t$$

where m_t is called the *trend component*, s_t is the *seasonal component*, and z_t is the *error term*.

In practice, a simple approach of estimating the trend of a tiem series is to compute a moving average.

Definition F.2.10 Let $\{x_t\}$ be a time series, a *simple moving average* of lenth l is

The best results are achieved when the length l of the moving average is equal to the length of the seasonal component. The seasonal componet can be estimated by

Definition F.2.11 Additive

$$\hat{s}_t = x_t - \hat{m}_t$$

Multiplicative

$$\hat{s}_t = \frac{x_t}{\hat{m}_t}$$

[...] many series are dominated by a trend and/or a seasonal effect [...] A simple additve decomposition model is given by

$$x_t = m_t + s_t + z_t$$

where, a time t, x_t is the observed series, m_t is the trend, $_t$ is the seasonal effect, and z_t is an error terms that is, in general, a sequence of correlated random variables with mean zero.

If the seasonal effect tends to increase as the trend increases, a multiplicative model may be more appropriate

$$x_t = m_t \dot{s}_t + z_t$$

Definition F.2.12

Once we have identired any trend and seasonal effects, we can deseasonalise the time series and remove the trend. If we use the additive decomposition method, we first calculate the seasonality adjusted time series and then remove the trend by substraction. This leaves the random component, but the random component is not necessarily well modelled by independent random variables. In many cases, consecutive variables will be correlated. If we identify such correlations, we can improve our forecast, quite dramatically if the correlations are high.

Second Order Properties

A possible approach to forecas future values of a time-series based variable is to extrapolate the current trend and to apply some adaptative estimations.

Exponential Smoothing

Definition F.2.13 Let's x and y two time series. The cross covariance function of x and y as a function of a lag k, denoted $\gamma(x,y)$, is defined as:

$$\gamma(x,y) = E$$

Definition F.2.14

Autocorrelation, Cross-correlation and Partial Autocorrelation

Another important feature of most time series is that observations close toghether in time tend to be correlated (serially dependent)

two unrelated time series will be correlated if they both contain a trend

Autocorrelation measures the (Pearson) correlation of a time series with a delayed version of itself, and as a function of that delay. Autocorrelation is intended to estimate the degree of similarity of an observation with respect to previous observations.

Definition F.2.15 Let $\{\mathbf{X}_t\}$ be a time series with mean μ and varianze σ^2. The *autocorrelation* function, denoted by ρ, is defined as:

$$\rho_x(k) = \frac{E\left[(x_t - \mu)(x_{t+k} - \mu)\right]}{\sigma^2}$$

The value k is called *lag*.

The autocorrelation function is not defined for all time series, because the mean may not exist (time series with a trend), or the variance may be zero (constant time series). A time series for which the autocorrelation is defined is called *second order stationary*.

The *sample autocorrelation* is computed in practice by:

$$\hat{\rho}_x(k) = \frac{\frac{1}{n}\sum_{t=1}^{n-k}(x_t - \bar{x})(x_{t+k} - \bar{x})}{\left(\frac{1}{n}\sum_{t=1}^{n}(x_t - \bar{x})\right)^2}$$

On the contrary of what happened with autocorrelation, sample autocorrelation is defined in case of time series with a trend. However, we must be carefull about the interpretation of the results. In general, sample autocorrelation is applied over the residuals of a time series once the trend and the seasonal components have been removed.

A correlogram is a plot of the sample autocorrelations $\hat{\rho}(k)$ versus time lags k (see Figure XXX). The dotted lines are drawn at $-\frac{1}{n} \pm \frac{2}{\sqrt{n}}$. If $\hat{\rho}(k)$ is outside these lines for a value of k we have evidence against the null hypothesis that $\hat{\rho}(k) = 0$ at the 5% level (See Section XXX). It is expected that 5% of the estimates $\hat{\rho}(k)$ fall outside these lines.

■ **Example F.7** TODO: Insert Figure. If the example is drawn using matplotlib.pyplot.acorr, the above paragraph is not true. Investigate how the shared areas in the correlogram used by matplotlib are computed. ■

Crosscorrelation measures ...

Definition F.2.16 Let $\{\mathbf{x}_t\}$ and $\{\mathbf{y}_t\}$ be time series with means μ_x and μ_y and variances σ_x^2 and σ_y^2. The *crosscorrelation* function, denoted by ρ, is defined as:

$$\rho_{x,y}(k) = \frac{E\left[(x_{t+k} - \mu_x)(y_t - \mu_y)\right]}{\sigma_x \sigma_y}$$

The value k is called *lag*.

If the crosscorrelation is defined it is said that the combined model is *second order stationary*.

The *sample crosscorrelation* is computed in practice by:

$$\hat{\rho}_{x,y}(k) = \frac{\frac{1}{n}\sum_{t=1}^{n-k}(x_t - \bar{x})(y_{t+k} - \bar{y})}{\frac{1}{n}\sum_{t=1}^{n}(x_t - \bar{x})\frac{1}{n}\sum_{t=1}^{n}(y_t - \bar{y})}$$

In general, sample crosscorrelation is applied over the residuals of both time series once trends and the seasonal components have been removed.

In the same way we draw a correlogram we can plot a crosscorrelogram of the crosscorrelation between to time series.

■ **Example F.8** TODO: Insert Figure. If the example is drawn using matplotlib.pyplot.acorr, the above paragraph is not true. Investigate how the shared areas in the correlogram used by matplotlib are computed. ■

Structural Time Series

A univariate structural time series model is one which is formulated in terms of components which, although unobservable, have a direct interpretation. It not only provides the basis for making predictions of future observations, but it also provides a description of the salient features of a time series.

Examples of structural components could be a trend, a seasonal effect, a cycle, an intervention, or the noise.

Definition F.2.17 Let $\mathbf{x}_t$ be a time series. The structural decomposition of $\mathbf{x}_t$ in given by

$$y_t = \mu_t + \psi_t + \gamma_t + \ldots + \varepsilon_t$$

where $\mu_t, \psi_t, \gamma_t, \ldots$ is a finite collection of additive stochastic terms, called structural components, and ε_t is a random term composed by independent and identically distributed samples with zero mean.

■ **Example F.9** dd ■

State Space Model

Definition F.2.18 Let y_t be a time series. The state space decomposition of y_t is given by

$$\begin{aligned} y_t &= \mathbf{Z}_t \alpha_t + \varepsilon_t \\ \alpha_{t+1} &= \mathbf{T}_t \alpha_t + \mathbf{R}_t \eta_t \end{aligned}$$

where

$$\begin{array}{ll} \alpha_t & \textit{explain} \\ \mathbf{Z}_t & \textit{explain} \\ \mathbf{T}_t & \textit{explain} \end{array}$$

$$\mathbf{y} = f(\mathbf{X}) + \varepsilon \tag{F.1}$$

measurement equation and transition equation

Mulivariate Time Series

TODO: Introduce this section.

A time series could be multivariate, where a dependant variable $\{x_{m+1}\}$ is sampled toghether with a collection of m independent variables $\{\mathbf{x}_i\}$.

Definition F.2.19 A *multivariate time series* of length $n \in \mathbb{N}$ composed by $m+1 \in \mathbb{N}$ variables, denoted by $\{\mathbf{x}_t^i : i = 1, \ldots, m+1 \text{ and } t = 1, \ldots, n\}$ or $\{\mathbf{x}_t\}$, is a sequence $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$ of *observed vector values*. The time series $\{\mathbf{x}^{m+1}\}$ is called the *independent variable*, and the time series $\{\mathbf{x}^i : i = 1, \ldots m\}$ the *dependant variables*.

TODO: cross-correlation and partial cross-correlation.

F.3 Minimum Message Length

The *Minimum Message Length* (MML) is based on the idea that a good theory, or explanation, for a dataset is a small collection of premises under which the data is not surprising. The best theories are those which are short, able to explain most of the data, and with a high accuracy. An *explanation message* is composed by two parts: the fist part comprises all the premises induced from the data, including numerical values; the second part contains all the data that cannot be derived from the premises. The message also assumes the existence of some already known and accepted premises (prior knowledge). Given the prior premises and the message it should be possible to recover the original dataset. According to the MML, theories are not rejected due to contradictory measurements, they only make the second part of the message longer.

In the MML principle, a message is a lossless encoded version of the original data. The first part of the message contains a probabilistic model about the data, and the second part is the data encoded using this model. We are interested in finding the shortest possible explanation message. If the length of the explanation message is longer than the original data, the theory is considered unacceptable.

Bayes' theorem (see Theorem **??**) states that the probability $P(H \mid E)$ of a hypothesis H given an evidence E is:

$$P(H \mid E) = \frac{P(E \mid H)P(H)}{P(E)}$$

We are interested in finding the hypothesis H with the highest posterior probability $P(H \mid E)$ of being true, assuming a fixed evidence E. That is, we are looking for maximize $P(E \mid H)P(H)$ or, equivalently, maximize $P(H \wedge E)$.

The *Minimum Message Length* principle (MML for short) is based on the idea that the length of encoding $H \wedge E$ as a binary string using an optimal code is equal to $-\log_2 P(H \wedge E)$ (see Theorem D.3.2). That is:

$$l(H \wedge E) = -\log_2 P(H \wedge E) = -\log_2 P(E \mid H)P(H) = -\log_2 P(E \mid H) - \log_2 P(H)$$

The most probable model H would be that model that allows us to encode $H \wedge E$ with the shortest possible string. The encoded string would be composed by two parts, a general assertion about the data, and a detailed description of the data assuming that the assertion is true.

Let $\mathbb{X}$ be a discrete set composed by all possible datasets, $\mathcal{X}$ a random variable taking values on $\mathbb{X}$, and $f(X \mid \theta)$ a probability distribution for $\mathcal{X}$ given the parameter θ.

Definition F.3.1 Let Θ be a discrete set of possibles parameters for f with probability distribution $h(\theta)\ \theta \in \Theta$, and let $\hat{\theta} \in \Theta$ be an inferred parameter. An *assertion* is the encoded version of $\hat{\theta}$ using an optimal code given the probability distribution h.

The length of the assertion given an optimal binary code is $-\log_2 h(\hat{\theta})$ (see Section D.3). Note that θ could be a single scalar or a vector of values. Moreover, θ could be related to more than one family of probability distributions f.

Definition F.3.2 Let $X \in \mathbb{X}$ be a dataset, and $\hat{\theta} \in \Theta$ an inferred value for the distribution f. A *detail* is the encoded version of X using an optimal code given the probability distribution $f(X \mid \hat{\theta})$.

The length of the detail given an optimal binary code is $-\log_2 f(X \mid \hat{\theta})$. That is, the length of the detail is the negative of the log-likelihood of X given $\hat{\theta}$.

Definition F.3.3 Let $X \in \mathbb{X}$ be a dataset, and $\hat{\theta} \in \Theta$ an inferred value for the distribution f A *message* for the dataset X given an inference $\hat{\theta} \in \Theta$ is the concatenation of the assertion for $\hat{\theta}$ and the corresponding detail for X given θ.

The length of a message given an optimal binary code is $-\log_2 h\left(\hat{\theta}\right) - \log_2 f\left(X \mid \hat{\theta}\right)$. The length of a message allow us, for example, to compare the posterior probabilities of two competing explanations or hypotheses $\hat{\theta}_1$ and $\hat{\theta}_2$.

Definition F.3.4 Let $X \in \mathbb{X}$ be a dataset. The *Minimum Message Length* of X, denoted by $MML(X)$, is given by:

$$MML(X) = \underset{\hat{\theta} \in \Theta}{\arg\min} \left(-\log_2 h\left(\hat{\theta}\right) - \log_2 f\left(X \mid \hat{\theta}\right)\right)$$

In practice, the actual messages will not be constructed, since our interest is in the length of the messages, not in their content. It is assumed that the sets $\mathbb{X}$ and Θ and the functions $f(X \mid \hat{\theta})$ and $h(\theta)$ are known a priori, and so, it is not necessary to include them as part of our encoding message.

■ **Example F.10** Consider an experiment in which we toss a weighted coin 100 times. Denote by 1 if we get a face and 0 a cross, so that each experiment is a binary string of length 100. Our collection of all possible datasets is $\mathbb{X} = \mathcal{B}^{100}$, θ is a number in the interval $[0,1]$, the likelihood $f(X \mid \theta)$ follows a binomial distribution (that is, $f(X \mid \theta)) = \theta^n (1-\theta)^{100-n}$ where n is the number of faces in X), and since we do not know anything about how the coin is weighted, we could assume that $h(\theta)$ is the uniform distribution in the interval $[0,1]$ (that is, $h(\theta) = 1$ for $\theta \in \Theta$). Under these assumptions, the length of a message for X given an inferred parameter $\hat{\theta}$ would be:

$$-\log_2 h\left(\hat{\theta}\right) - \log_2 f\left(X \mid \hat{\theta}\right) = -n \log_2 \hat{\theta} - (100-n)\log_2(1-\hat{\theta})$$

We are interested in finding the value of $\hat{\theta}$ that minimizes the length of the encoded version of X, that is, the minimum message length for X. ■

A Maximum A Posteriori analysis of the experiment in Example F.10 would provide the same inference for $\hat{\theta}$ than the Minimum Message Length approach. Moreover, given that $h(\theta)$ follows an uniform distribution, a Maximum Likelihood approach would reach exactly the same value for $\hat{\theta}$.

F.4 Minimum Description Length

The *Minimum Description Length* (MDL) principle is a reformulation of the Kolmogorov complexity with the goal to make it applicable to solve practical problems. MDL explicitly address the two most important practical limitations of the Kolmogorov complexity: its uncomputability (in general, the Kolmogorov complexity cannot be computed), and the large constants involved in the invariance theorem (that makes it inapplicable to short strings). The approach of MDL to these problems is to scale down Kolmogorov complexity until it does become applicable: instead of using general-purpose computer languages, MDL is based on fixed languages and coding functions.

In contrast to Kolmogorov that states that the complexity of a string is equal to the length of the shortest program that prints that string, MDL proposes that our capacity to learn about a string is equivalent to our ability to compress that string. The idea behind MDL is to describe a dataset with the help of an hypothesis: the more the hypothesis fits the data (and here good fit equals learning), the more we can compress the data given that hypothesis.

In our particular case, we are interested in MDL because it will allow us to compute the nescience of a topic given a dataset, instead of requiring a text describing the topic. Thus, given a topic t and a sample dataset $D = \{x_1, x_2, \ldots, x_n\}$, the nescience of a particular hypothesis H will be related to the capacity of that hypothesis to compress the dataset.

MDL comes into two versions, *simplified (two-part code) MDL* and *refined MDL*. Simplified MDL is easier to understand, and it will allows us to introduce some important concepts and notation. The extension of the concept of nescience to datasets will be based on the refined version of MDL.

TODO: Explain how this relates to cross entropy

In this section we are going to introduce the two-part code version of the minimum description length principle for probabilistic models.

Given a set of candidate models (a set of probability distributions (for example first-order Markov chains) or functions of the same functional form (for example the kth degree polynomials)) $\mathcal{H}^{(1)}, \mathcal{H}^{(2)}, \ldots$ *the simplified, two-part version, of the* Minimum Description Length Principle [**Gr=0000FC05**] *states that the best point hypothesis (a single probability distribution (e.g. a Markov chain will all parameters values specified)* $H \in \mathcal{H}^{(1)} \cup \mathcal{H}^{(2)} \cup \ldots$ *to explain the data* $D = (x_1, \ldots, x_n) \in \mathcal{X}^n$ *is the one that minimizes the sum* $L(M) + L(D \mid M)$*, where* $L(M)$ *is the length (in bits) of the model description, and* $L(D \mid M)$ *is the length (in bits) of the data encoded with the help of the hypothesis ... there is only one reasonable choice for this code ... the so-called Shannon-Fano code ... Each hypothesis* H *may be viewed as a probability distribution over* $\mathcal{X}^n$*. For each such distribution there exists a code with length function* L *such that for all* $x^n \in \mathcal{X}^n$ *we have that* $L(x^n) = -\log_2 P(x^n \mid H)$*. The quantity* $L(M)$ *depends on each model.*

A description of the data "with the help of" a hypothesis means that the better the hypothesis fits the data, the shorter the description will be. A *hypothesis that fits the data well gives us a lot of information about the data. Such information can always be used to compress the data. This is because we only have to code the errors the hypothesis makes on the data rather than the full data.*

The sum of the two description length will be minimized at a hypothesis that is quite (but not too) "simple", with a good (but not perfect) fit.

The length of the data given the model, that is, $L(D \mid M)$.

$$-\log P(D) = L_C(D)$$

This choice for C gives a short codelegth to sequences which have high probability according to (k, ttita) while it gives a high codelength to sequences with low probability. The codelength thus directly reflects the goodness-of-fit of the data with respect to (k,tita) measured in terms of the probability fo D according to (k,tita).

When we say we "code the data D with the help of probabilistic hypothesis P" we mean that we code D using the Shannon-Fano code corresponding to P.

$$L(D \mid P) := -\log P(D)$$

the code with these lengths is the only one that would be optimal if P where true. (mention we are only interested in code lengths, we are not interested in to find the code itself).

For $L(M)$ *we use the standard code for integers.*

■ **Example F.11** Markov Chain Hypothesis Selection: Suppose we are given data $DX\hat{}n$ where $X = \{0,1\}$. We seek a reasonable model for D that allows us to make good predictions of future data coming from the same source. We decide to model our data using the cass B o all Markov chains [...] we face the problem of overfitting: for a given sequence $D = (x1, ..., xn)$, there may be a Markov chain P of very high order that fits data D quite well but that will behave very badly when predicting future data from the same source. ■

F.4.1 Refined MDL

In refined MDL, we associate a code for encoding D not with a single $H \in \mathcal{H}$ but with the full model $\mathcal{H}$ ... we design a single one-part code with lengths $\bar{L}(D \mid H)$ (called the stochastic complexity of the data given the model). This code is designed such that whenever there is a member of (parameter in) $\mathcal{H}$ that fits the data well, in the sense the $L(D \mid H)$ is small, then the codelenth

$\bar{L}(D \mid H)$ will also be small. Codes with this property are called universal codes.

There are at least four types of universal codes:

1 *The normalized maximum likelihood (NML) code and its variations.*
2 *The Bayesian mixture code and its variations.*
3 *The prequential plug-in code.*
4 *The two-part code.*

Refined MDL is a general theory of inductive inference based on universal codes that are designed to be minimax, or close to minimax optimal. It has mostly been developed for model selection, estimation and prediction.

F.5 Multiobjective Optimization

Multiobjective optimization is the area of mathematics that deals with the problem of simultaneously optimizing two or more conflicting functions. Multiobjective optimization has been applied in many areas of science, including engineering, economics and logistics, where there is no single solution that simultaneously satisfies all objectives, so a decision must be made in the presence of trade-offs between the conflicting goals.

From a formal point of view, we are interested in solving the following *multiobjective optimization* problem:

$$\begin{array}{ll} \text{minimize} & \{f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_k(\mathbf{x})\} \\ \text{subject to} & \mathbf{x} \in \mathbf{S} \end{array}$$

where $f_i : \mathbb{R}^n \to \mathbb{R}$, $i = 1, \ldots, k$, are two or more objective *objective functions*, and the nonempty set $\mathbf{S} \subset \mathbb{R}^n$ is the *feasible region*, whose elements $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ are *decision vectors*. The image of the feasible region $f(\mathbf{S}) \subset \mathbb{R}^k$, denoted by $\mathbf{Z}$, is called *objective region*, and its elements $\mathbf{z} = (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_k(\mathbf{x}))$ *objective vectors*. In some applications, the feasible region is formed by a collection of inequality constraints $\mathbf{S} = \{\mathbf{x} \in \mathbb{R}^n \mid g(\mathbf{x}) = (g_1(\mathbf{x}), \ldots, g_m(\mathbf{x})) \leq 0\}$.

In this book we will be dealing with nonlinear multiobjective minimization problems, where at at least one of the objective functions, or the constraint functions, is not linear. Objective functions can be also incommensurable, that is, measured in different units or in different scales.

Since the objective functions are conflicting, it does not exist a single solution that is optimal with respect to every objective function (the objective region is partially ordered).

Definition F.5.1 A decision vector $\mathbf{x} \in \mathbf{S}$ *dominates* another decision vector $\mathbf{y} \in \mathbf{S}$ if $f_i(\mathbf{y}) \leq f_i(\mathbf{x})$ for all $i \in \{1,\ldots,k\}$ and $f_j(\mathbf{y}) < f_j(\mathbf{x})$ for at least one $j \in \{1,\ldots,k\}$. An objective vector $\mathbf{z} \in \mathbf{Z}$ *dominates* another objective vector $\mathbf{w} \in \mathbf{Z}$ if $w_i \leq z_i$ for all $i \in \{1,\ldots,k\}$ and $w_j < z_j$ for at least one $j \in \{1,\ldots,k\}$.

Dominance can be studied from the point of view of decision variable space or objective space. An objective vector dominates another objective vector if, and only if, its corresponding decision vector also dominates the other decision vector.

We are interested in those objective vectors for which none of its individual components can be improved without deteriorating at least one of the others.

Definition F.5.2 A decision vector $\mathbf{x} \in \mathbf{S}$ is *Pareto optimal* if there does not exists another decision vector $\mathbf{y} \in \mathbf{S}$ such that $\mathbf{y}$ dominates $\mathbf{x}$. An objective vector $\mathbf{z} \in \mathbf{Z}$ is Pareto optimal if there does not exits another objective vector $\mathbf{w} \in \mathbf{Z}$ such that $\mathbf{w}$ dominates $\mathbf{z}$.

Pareto optimality can be also studied from the point of view of decision variable space or objective space. An objective vector is Pareto optimal if, and only if, its corresponding decision vector is Pareto optimal.

Definition F.5.3 The set of Pareto optimal solutions, denoted by $\mathbf{P}_D$, is called the *Pareto optiomal set*. The set of Pareto optimal solutions in the space of objectives, denoted by $\mathbf{P}_O$, is called the *Pareto frontier*.

Sometimes, in practice, it is convenient to use a more restrictive definition of the concept of optimaily, in which we identify those vectors for which there does not exist any other vector that improves over all the components simultaneously.

Definition F.5.4 A decision vector $\mathbf{x} \in \mathbf{S}$ is *weakly Pareto optimal* if there does not exist another decision vector $\mathbf{y} \in \mathbf{S}$ such that $f_i(\mathbf{y}) < f_i(\mathbf{x})$ for all $i = 1,\ldots,k$. An objective vector $\mathbf{z} \in \mathbf{Z}$ is weakly Pareto optimal if there does not exists another objective vector $\mathbf{w} \in \mathbf{Z}$ such that $w_i < z_i$ for all $i = 1,\ldots,k$.

An objetive vector is weakly Pareto optimal if its corresponding decision vector is weakly Pareto optimal. Oviously, the Pareto optimal set is a subset of the weakly Pareto optimal set.

■ **Example F.12** TODO: Provide an example based on a multi-variable function. In figure F.1 we have depicted a sample of the objective region of a multiobjetive optimization problem composed by two real-valued objective

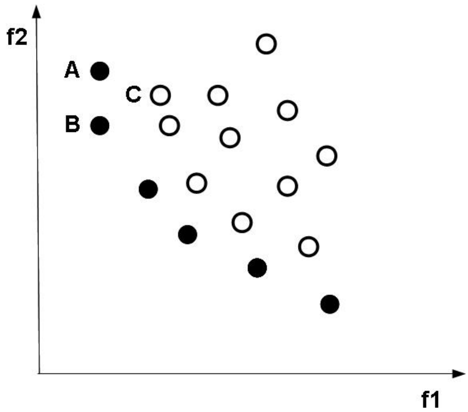


Figure F.1: Pareto optimality.

functions f_1 and f_2 that we are interested in minimizing. White points are not weakly Pareto optimal since there exist points that improve both components at the same time (for example, point **B** improves point **C** in both functions). Black points are weakly Pareto optimal since there is no point that improves both components at the same time. Point **A** is not Pareto optimal since point **B** improves one component without deteriorating the other. ■

Mathematically speaking all the solutions that compose the Pareto optimal set are equally good. However, for the majority of the practical applications, it is highly desirable to have a single solution. Finding this solution requires additional information not included in the definition of the optimization problem. The relation of preference between objective function values is expresed using a *decision maker*, that it is supposed to have additional insights about the problem to solve. In this sense, solving a multiobjective optimization problem would require to find those feasible decision vectors that it are Pareto optimal and that satisfy the additional requirements imposed by the decision maker.

In practice, we assume that the preferences of the decision maker can be expressed using a value function.

Definition F.5.5 A *value function* is a function $U : \mathbb{R}^k \rightarrow \mathbb{R}$ that assigns t each objective vector $\mathbf{z} = (z_1, \ldots, z_k)$ a single real value $U(\mathbf{z})$.

value functions are miximized

Value functions allow us to order the vectors of the objective region **Z**. We are interested in applying the value function to the Pareto optimal subset to find a unique solution to the multiobjective optimization problem.

F.5.1 Range of the Solutions

We are intersted in investigating the range of the solutions included in the Pareto optimal set. To do that, we have to find the lower and upper bounds of this set. In the rest of this section, we assume that the objective functions are bounded over the feasible region $\mathbf{S}$.

TODO: rewrite the concepts of nadir and ideal vector using the supremum and infimum.

An objective vector that minimizes all objective functions is called an ideal objective vector.

Definition F.5.6 A vector $\mathbf{z}^\star \in \mathbb{R}^k$ is called *ideal* if each of its components z_i, minimizes the objective funcion $f_i(\mathbf{x})$ subject that $\mathbf{x} \in \mathbf{S}$.

If there exits an ideal objective vector that belongs to the feasible region, that is $\mathbf{z}^\star \in \mathbf{Z}$, then that vector would be a solution of the optimization problem, and that solution would be unique. Ideal vectors are lower bounds to the Pareto set.

The upper bound of the Pareto optimal set is given by the nadir objective vector. The nadir vector can be estimated using the decision vectors calculated when obtaining the objective ideal vector.

Definition F.5.7 Let $\mathbf{z}^\star \in \mathbb{R}^k$ be an ideal objective vector. The set of decision vectors $\{\mathbf{x}_1^\star, \ldots, \mathbf{x}_k^\star\}$ used to compute $\mathbf{z}^\star$ is called the *payoff table* for $\mathbf{z}^\star$. That is, if $\mathbf{z}^\star = \{z_1^\star, \ldots, z_k^\star\}$, we have that $z_i^\star = f_i(\mathbf{x}_i^\star)$.

It turns out that $f_i(\mathbf{x}_i^\star)$ $(i = 1, \ldots, k)$ is minimal for all for all the elements of the payoff table.

Having the payoff table we can provide an estimation for the nadir vector. For simplicity, let's $f_{ij}^\star$ denote the value of the objective function f_i computed over the vector $\mathbf{x}_j^\star$, where $i, j = 1, \ldots, k$.

Definition F.5.8 Let $\mathbf{z}^\star \in \mathbb{R}^k$ be an ideal objective vector, and $\{\mathbf{x}_1^\star, \ldots, \mathbf{x}_k^\star\}$ its payoff table. The *nadir* objective vector $\mathbf{z}^{nad} = \{z_1^{nad}, \ldots, z_k^{nad}\}$ is given by $z_i^{nad} = \max_j f_{ij}^\star$.

The ideal objective vector and the nadir objective vector may, or may not, be feasible. In figure F.2 are depicted the ideal (vector $\mathbf{E}$) and nadir (vector $\mathbf{F}$) vectors of the multiobjective optimization problem of Example F.12.

For some applications, the range of values of the objective functions can differ by orders of magnitude. In those situations, it is advisable to normalize them, so the values are in the same scale. We can use the ideal and nadir vector for this normalization process, by replacing each objective function

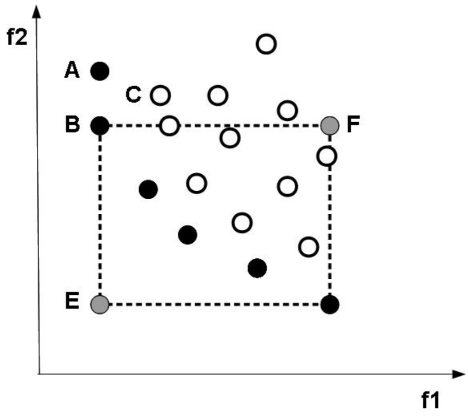


Figure F.2: Ideal and Nadir vectors.

$f_i(\mathbf{x})(i = 1, \ldots, k)$ by the normalized function

$$\frac{f_i(\mathbf{x}) - z_i^{\star}}{z_i^{nad} - z_i^{\star}}$$

F.5.2 Trade-offs

Since the functions we want to minimize are conflicting, sometimes we have to assume that the only way to gain a benefit in on aspect of the problem is to losse something in another aspect. How much we have to give up in one objective to improve a certain quantity in the other is called a trade-off.

Definition F.5.9 Let $\mathbf{x}^1, \mathbf{x}^2 \in \mathbf{S}$ be two decision vectors. The *ratio of change* between the functions f_i and f_j for the vectors $\mathbf{x}^1, \mathbf{x}^2$, denoted by Δ_{ij}, is defined as:

$$\Delta_{ij}(\mathbf{x}^1, \mathbf{x}^2) = \frac{f_i(\mathbf{x}^1) - f_i(\mathbf{x}^2)}{f_j(\mathbf{x}^1) - f_j(\mathbf{x}^2)}$$

for all $i, j = 1, \ldots, k$ such that $f_j(\mathbf{x}^1) - f_j(\mathbf{x}^2) \neq 0$.

Δ_{ij} is called a *partial trade-off*, involving f_i and f_j between $\mathbf{x}^1$ and $\mathbf{x}^2$ if $f_l(\mathbf{x}^1) = f_l(\mathbf{x}^2)$ for all $l = 1, \ldots, k$, $l \neq i, j$. If $f_l(\mathbf{x}^1) \neq f_l(\mathbf{x}^2)$ for at least one $l = 1, \ldots, k$, and $l \neq i, j$ then Δ_{ij} is called a *total trade-off*.

If the trade-off between two objective functions is very small or very large, that is, if a small change in one aspect of the optimization problem has a significant impact in another aspect, we have a case that is similar to having a weakly Pareto solution that it is not Pareto optimal. In some practical applications is convenient to filter out those solutions that present this undesirable behaviour.

Definition F.5.10 A decision vector $\mathbf{x} \in \mathbf{S}$ is *properly Pareto optimal* if it is Pareto optimal and if there exists a real number $M > 0$ such that for each f_i and $\mathbf{y} \in \mathbf{S}$ satisfying $f_i(\mathbf{y}) < f_i(\mathbf{x})$, there exists at least one f_j such that $f_j(\mathbf{x}) < f_j(\mathbf{y})$ and

$$\frac{f_i(\mathbf{x}) - f_i(\mathbf{y})}{f_j(\mathbf{y}) - f_j(\mathbf{x})} \leq M$$

An objective vector $\mathbf{z} \in \mathbf{Z}$ is properly Pareto optimal if the decision vector corresponding to it is properly Pareto optimal.

A solution is properly Pareto optimal if there is at least one pair of objectives functions for which a small decrement in one objective is possible only at the expense of a large increment in the other objective.

Note that the properly Pareto optimal set is a subset of the Pareto optimal set, and the Pareto optimal set is a subset of the weakly Pareto optimal set.

F.5.3 Optimization Methods

Generating Pareto optimal solutions plays an important role in multiobjective optimizatoin, and mathematically the problem is considered to be solved when the Pareto optimal set is found [...] However, this is not always enough. We want to obtain only one solution. This means that we must find a way to put the Pareto optimal solutions in a comple order. This is why we need a decision maker an his preference structure.

In general, multiobjective optimization problems are solved by scalarization [...] scalarization means converting the problem into a single or a family of single objective optimization problems with a real-valued objective function

three requirement are set for a scalarization function: 1) It can cover any Pareto optimal solution. 2) Every solution is Pareto optimal.

[...] classify the methods according to the participation of the decision maker in the solution process. The classes are: 1) methods where no articulation of preference information is used (no-preference methods) 2) methods where a posteriory articulation of preference is used (a posteriory methods) 3) methods whre a priori articulation of preference information is used (a priory methods), and 4) methods whre progressive articulation of preference information is used (interactive methods).

In no-preference methods, the knowledge of the decision maker is not taken into account, and the optimization problem is solved using a relatively simple method. In a posteriory methods, the set (or part of it) of Pareto optimal points is identified and then the decision maker select the preferred solution among the alternatives.

Global Criterion

The global criterion is a non-prefrence method in which the distance between some reference point and the fasible objective region is minimized. In this method, all the objective functions are considered to be equally important. As reference point it is usually used the ideal vector, and as metric it is common to use a L_p-metric. Under these assumptions, the goblal criterion method becomes the following minimization problem:

$$\begin{aligned} &\text{minimize} \quad \left(\sum_{i=1}^{k} (f_i(\mathbf{x}) - z_i^{\star})^p \right)^{\frac{1}{p}} \\ &\text{subject to} \quad \mathbf{x} \in \mathbf{S} \end{aligned}$$

Different values for p result in different solutions to the minimization problem. Common values for p are 1, 2 or ∞.

Proposition F.5.1 The solution of the L_p-based global criterion is Pareto optimal.

Proof. Let $\mathbf{x}$ be a solution of the L_p-based global criterion problem, with $1 \leq p < \infty$, and assume that $\mathbf{x}$ is not Pareto optimal. Then, according to Definition F.5.2 there must exists a point $\mathbf{y} \in \mathbf{S}$ such that $f_i(\mathbf{y}) \leq f_i(\mathbf{x})$ for all $i = 1, \ldots, k$, and $f_j(\mathbf{y}) < f_j(\mathbf{x})$ for at least one j. Then we have that $(f_i(\mathbf{y}) - z_i^{\star})^p \leq (f_i(\mathbf{x}) - z_i^{\star})^p$ for all $i \neq j$ and $(f_j(\mathbf{y}) - z_j^{\star})^p < (f_j(\mathbf{x}) - z^{\star})^p$. Adding all these terms and raising to the $1/p$ power, we obtain

$$\left(\sum_{i=1}^{k} (f_i(\mathbf{y}) - z_i^{\star})^p \right)^{\frac{1}{p}} < \left(\sum_{i=1}^{k} (f_i(\mathbf{x}) - z_i^{\star})^p \right)^{\frac{1}{p}}$$

which is a contradiction with the fact that $\mathbf{x}$ is a solution to the minimization problem. ■

Although all the solutions selected by the L_p-based global criterion are Pareto optimal, as we have proved in previous proposition, there are solutions of the optimal Pareto set are that will never be selected by this method. In practice it is convenient to normalize the range of the objective values, so that those points closer to the ideal vector do not receives more importance. A common normalization term used in practice is $z_i^{nad} - z_i^{\star}$.

Weighting Method

The weighting method is a simple way to generate different Pareto optimal solutions.

In the weighting method [...] the idea is to associate each objective function with a weighting coefficient and minimize the weighted sum of the objectives. In this way, the multiple objective functions are transformed into a single objective function. We suppose that the weighting coefficients w_i are real numbers such that $w_i \geq 0$ for all $i = 1, \ldots, k$. It is also usually supposed that the weights are normalized, that is $\sum_{i=1}^{k} w_i = 1$.

The multiobjective optimization problem is modified into the following problem, to be called a weighting problem:

$$\begin{aligned} \text{minimize} \quad & \sum_{i=1}^{k} w_i f_i(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{x} \in \mathbf{S} \end{aligned}$$

where $w_i \geq 0$ for all $i = 1, \ldots, k$ and $\sum_{i=1}^{k} w_i = 1$.

[...] weighting coefficient zero makes no sense. It means that we hae included in the problem some objective function that has no significance at all.

The objective functions should be normalized or scaled so that their objective values are approximately of the same magnitude [...] Only in this way can one control and manoeuvre the method to produce solutions of a desirable nature in proportion to the ranges of the objective functions. Otherwise the role of the weighting coefficients may be greatly misleading.

Proposition F.5.2 The solution of weighting problem is Pareto optimal i the weighting coefficients are positive, that is $w_i > 0$ for all $i = 1, \ldots, k$.

Proof. TODO ∎

the solution of the weighting method is always Pareto optimal if the weighting coefficients are all positie or if the solution is unique [...] The weakness of the weighting method is that not all of the Pareto optimal solutions can be found.

the weighting method is used to generate Pareto optimal solutions

in practical calculations the contion $w_i \geq \varepsilon$, where $\varepsilon > 0$, must be used instead of the condition $w_i > 0$ for all $i = 1, \ldots, k$. This necessitates a correct choice as to the value of ε.

The weighting method can be used so that the decision maker specifies a weighting vector representing his preference information [...] In this case, the weighting problem can be considered (a negative of) a value function (remember that value functions are maximized.

If the weighting method is used as an a prioriy method one can ask what the weighting coefficients in fact represent. Ofthen, they are said to reflect the relative importance of the objective functions. However, it is not all clear what underlies this notion [...] instead of relative importance, the weighting coefficients should represent the rate at which the decision maker is willing to trade off values of the objective functions

if some of the objective functions correlate with each other, then seemingly "good" weighting vectors may produce poor results and seemingly "bad" weighting vectors may produce useful results

Weighting coefficients are not easy to interpret and understand for average decision makers.

Employing the weighting method as an a priori method presumes that the decision maker's unerlying value function is or can be approximated by a linear function [...] it must be noted that altering the weighting vectors linearly does not have to mean that the values of the objective functions also change linearly. It is difficult to control the direction of the solutions by the weighting coefficients

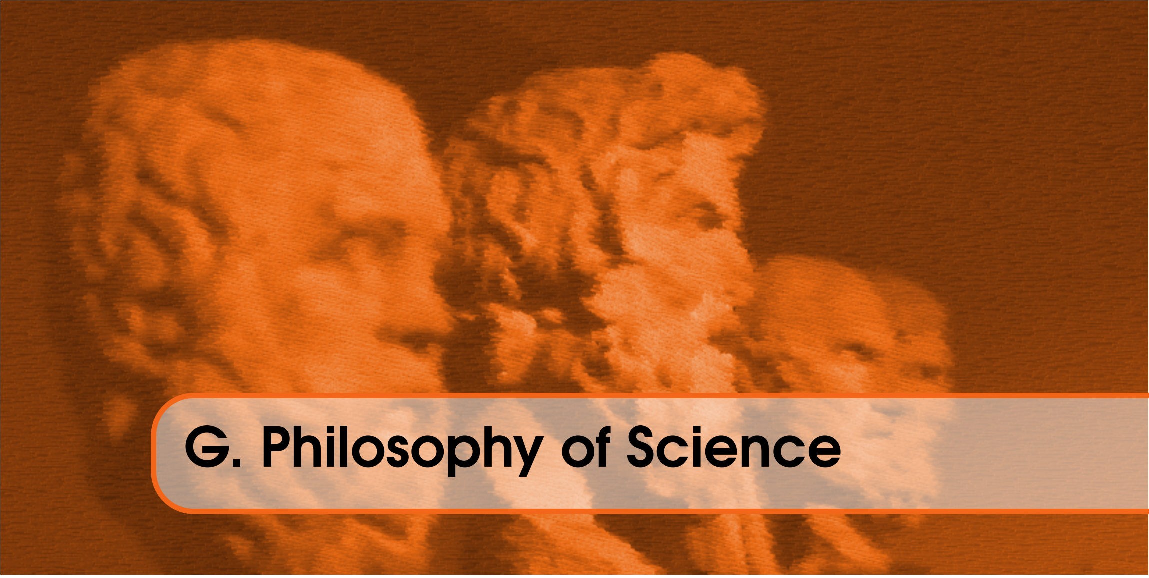
Shall I explain the ε-Constraint method?

References

TODO: Add paper of Turing about AI.

The minimum message length principle was developed by Chris Wallace, published for first time in 1968 in [WB68]. The book [Wal05], written by the same author, contains a detailed description of the principle.

A good introduction to the discipline of non-linear multiobjective optimization can be found in [Mie12]; Section F.5 is largely based on this book.



G. Philosophy of Science

To go where you don't know,
you have to go the way you don't know.
San Juan de la Cruz

The *philosophy of science* is the branch of philosophy that examines the foundations, methods, and implications of scientific inquiry. It explores how scientific knowledge is generated, the validity of scientific theories, the nature of scientific reasoning, and the role of values in science. By addressing fundamental questions about objectivity, reality, and the limits of scientific explanation, the philosophy of science helps us understand how science works and its impact on our understanding of the world.

The philosophy of science provides a theoretical framework for analyzing the core elements that constitute our theory of nescience. It enables us to critically examine the foundations and assumptions of our theory, guiding us toward the identification of the essential questions that we must address. Moreover, philosophical inquiry compels us to rigorously push the boundaries of our analysis, ensuring that our theory is explored to its ultimate consequences, both logically and conceptually. This approach strengthens the robustness of the theory, even if these results do not directly translate into practical applications.

A central theme in scientific methodology is the distinction between *discovery* and *justification*. Discovery refers to how new ideas or hypotheses emerge, often through creativity, intuition, or serendipity, while justification involves the use of evidence and logical reasoning to evaluate and validate these ideas. Philosophers of science have historically emphasized justification, focusing on methods to rigorously test and analyze scientific claims. However, both discovery and justification are critical to understanding scientific progress, and this chapter will address both aspects.

In this chapter, we provide a concise overview of key elements from the philosophy of science, as well as relevant concepts from other branches of philosophy, such as metaphysics, epistemology, and ontology, that are important to the theory of nescience. Certain other topics within the philosophy of science, such as the problem of objectivity (examining whether science can be truly objective or is influenced by social and personal values) or the role of values in science, including the relationship between ethical, social, and political values and scientific practices, are not included in this review, as they are not directly relevant to a mathematical theory of nescience.

The chapter begins with a brief introduction to the field and its importance in understanding scientific inquiry. We delve into the problem of which entities can be known, examining the scope of scientific knowledge and the nature of observable and unobservable phenomena. The chapter also addresses the concept of scientific representation, discussing how models, theories, and laws reflect aspects of reality. We examine how science discovers new knowledge, the principles behind the scientific method, and the various ways in which scientists formulate and test hypotheses. Finally, we explore the limits of science, considering the boundaries of what science can explain and where its explanatory power may fall short.

G.1 What is Science

Science is a systematic method of investigating the world around us, aimed at generating reliable knowledge through observation and reasoning. Unlike other forms of inquiry, science is rooted in the idea that knowledge must be based on evidence that can be tested and verified. By combining theoretical thinking with empirical data, science offers a powerful way to explain, predict, and understand natural phenomena. Sometimes science seeks explanations for practical purposes, but other times it is sought simply to satisfy our intellectual curiosity.

The *scientific method* is understood as the systematic process by which science acquires new knowledge. In schools, the scientific method is often taught as a series of steps: first observing and describing a phenomenon, then coming up with a hypothesis to explain it, testing that hypothesis through experiments, analyzing the results, and finally making a conclusion. However, the idea of a single, universal scientific method that can be applied to all sciences isn't widely accepted anymore. Instead, scientists and philosophers recognize that different scientific fields require different methods because each field faces its own challenges and complexities.

The following is a list of the key features that make science distinct and valuable as a way of knowing [as opposed to other kinds of knowledge].

- *Empiricism*: (Do no use the word "empiricism" since this is a philosophical school and might confuse the reader.) At its core, science is an empirical endeavor, meaning it relies on observation, experimentation, and measurable evidence to understand the natural world. Scientific knowledge is grounded in data that can be gathered through direct or indirect observation, ensuring that claims can be tested and verified by others. [Science is derived from facts]
- *Testability*: A key characteristic of science is its focus on developing testable hypotheses, that is, statements or predictions that can be empirically investigated. This means that scientific claims must be falsifiable, open to potential disproof if the evidence does not support them. This distinguishes science from fields that rely on unfalsifiable or speculative claims.
- *Theoretical Frameworks*: Science is not merely about collecting facts; it seeks to develop broader explanations through models, laws, and theories. Models offer simplified representations of complex systems, while theories are well-supported frameworks that explain the underlying mechanisms of phenomena. These frameworks help interpret data and guide further investigation, offering coherence to the body of scientific knowledge.
- *Self-Correction*: A defining feature of science is its self-correcting nature. Scientific theories are not static; they evolve as new evidence comes to light. When new data contradicts a theory, science adapts, modifies, refines, or sometimes discards the theory in favor of one that better fits the evidence. This continuous process of revision ensures that scientific knowledge becomes more accurate over time.
- *Generalizability*: Science strives to uncover universal principles that apply across various contexts, not just to isolated cases. While science begins with specific observations, its goal is to identify general laws and patterns that explain a broad range of phenomena. This pursuit of generalizable knowledge allows science to predict future occurrences and provide deeper insights into the workings of the natural world.

The main task of the philosophy of science is to understand how techniques such as experimentation, observation, and theory building enable scientists to discover the secrets of nature. The philosophy of science draws on other areas of philosophy, such as ontology, epistemology, metaphysics, and logic. *Ontology*, the branch of philosophy concerned with the nature of existence, addresses the question of which entities exist in the real world. It examines the types of entities that science can study, whether they are observable, abstract, or indeterminate, and engages with the philosophical debates surrounding their existence. Ontology provides the foundation for exploring the boundaries of scientific knowledge and the limits of inquiry. *Epistemology* is the branch of philosophy concerned with knowledge itself—how we acquire it, what justifies it, and what its limits are. While ontology deals with what exists, epistemology addresses how we come to know what exists. In the context of science, epistemology examines the methods, evidence, and reasoning that underpin scientific investigation, exploring how scientific knowledge is built, how reliable it is, and what counts as a justified belief in scientific practice. Both ontology and epistemology are part of the broader field of *metaphysics*, which deals with the fundamental nature of reality and existence. Metaphysics explores the most basic concepts and categories of being, such as time, space, causality, and possibility, as well as the relationship between mind and matter. *Logic*, the study of valid reasoning, underpins the entire scientific enterprise by providing the tools to analyze arguments, identify fallacies, and structure sound reasoning. In science, logic is used to ensure the coherence of theoretical frameworks, the validity of inferences drawn from data, and the consistency of explanations and predictions. Formal logic, including propositional and predicate logic, provides a systematic way to evaluate arguments and detect errors, while informal logic addresses reasoning in everyday scientific discourse. Together, ontology, epistemology, metaphysics, and logic provide a comprehensive philosophical foundation for understanding what science studies, how it builds knowledge, and the fundamental nature of the reality science seeks to explain.

This chapter on philosophy of science is structured around key components that illustrate how scientific knowledge is developed and justified (see Figure G.1). It begins with a discussion on *Entities*, which can be either concrete or abstract, representing the objects of scientific study. From these entities, knowledge is acquired through *Observation*, which involves gathering empirical data and facts. These observations are then transformed into *Representations*, such as recorded data, or facts, that scientists use to analyze and interpret phenomena. Through the process of *Discovery*, these representations lead to the formulation of *Explanations*, which take the form of scientific *theories and laws* that describe underlying principles governing the natural world. The chapter also explores how scientific explanations

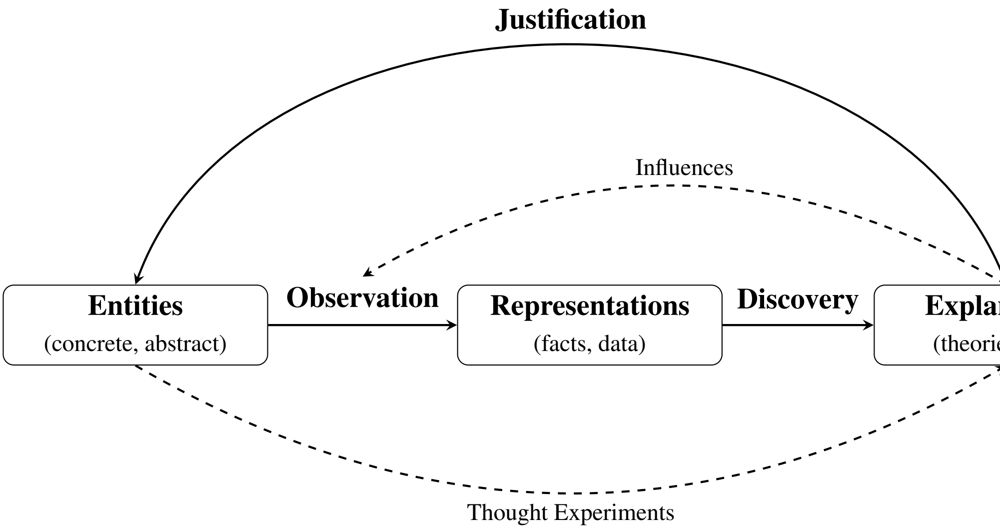


Figure G.1: Chapter Organization

influence future observations, shaping what is investigated and how data is interpreted. Additionally, thought Experiments provide an alternative way of reasoning about scientific problems beyond direct empirical observation. Finally, the chapter addresses *Justification*, emphasizing the criteria by which scientific claims are validated, ensuring that discoveries and explanations are robust, reliable, and well-supported by evidence. This structure provides a comprehensive view of the scientific process, from the identification of entities to the formation and justification of scientific theories.

G.2 What is an Entity

Perhaps cover in this section. [...] science is derived from facts [...] facts are presumed to be claims about the world that can be directly established by a careful unprejudiced observation [...] via senses, which may not be reliable [...] how facts relate to theories, or require previous knowledge [...] (refer to epistemology?, the application of epistemology to science) Perhaps I should cover here two competing schools: empiricism and logical positivism.

In this section, we focus on the fundamental problem of determining which kinds of entities can be known or investigated by science.

A *knowable entity* is an object, phenomenon, or concept that can be investigated, understood, or described through scientific or intellectual inquiry. Knowable entities are those that, either directly or indirectly, can be observed,

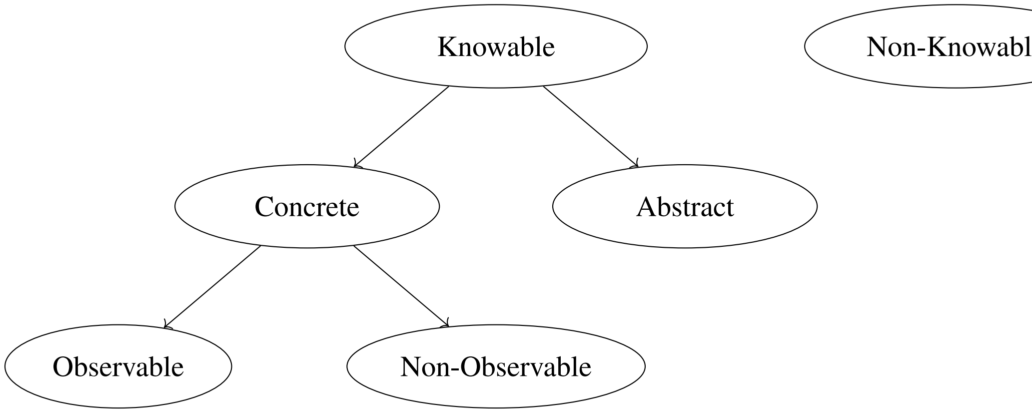


Figure G.2: Classification of Research Entities

measured, inferred, or modeled, using available tools, methods, or theories. They are within the scope of human knowledge, and their properties can be analyzed or explained. Examples of knowable entities include the stars and plantes, animals, or computer algorithms. A *non-knowable entity* refers to something that cannot be directly observed, measured, or understood using current scientific or intellectual methods. This could be due to limitations in technology, the abstract or metaphysical nature of the entity, or inherent epistemological boundaries. Non-knowable entities might remain beyond the reach of human understanding either temporarily (until methods evolve) or permanently (due to their nature). Examples of non-knowable entities include the nature of consciousness, the origin of the universe, or the existence of a deity. The distinction between knowable and non-knowable entities is not always fixed, but varies depending on the clarity and precision of the area of interest and the evolving nature of scientific understanding in each field.

Scientific research encompasses both *concrete entities* and *abstract entities*. Concrete entities refer to physical objects or phenomena that can be directly observed, measured, or interacted with, such as stars, cells, or chemical compounds. These entities form the basis of empirical research, where data is collected through direct observation or experimentation. In contrast, abstract entities are conceptual and do not have a physical presence, such as numbers, algorithms, or theoretical models. Abstract entities play a crucial role in scientific research, particularly in fields like mathematics and theoretical physics, where they provide the framework for understanding and modeling concrete phenomena. While abstract entities cannot be observed directly, they can be known through indirect methods. The inclusion of these abstract entities in scientific inquiry raises important philosophical questions about their ontological status: Are these abstract entities real in the same way that physical objects are, or are they simply conceptual tools? This question remains an open and debated issue in the philosophy of science.

Finally, in scientific inquiry, there is also a distinction between *observable entities*, which can be directly perceived or measured, and *non-observable entities*, which cannot be directly observed but can still be detected or inferred from empirical evidence. Observable entities include things like trees, planets, and bacteria, objects that can be seen or measured using scientific instruments. Non-observable, but still detectable, entities include things like subatomic particles and gravitational forces. These entities are often crucial for explaining observable phenomena and are identified through the use of scientific instruments and theoretical frameworks. For example, we cannot observe a quark in the same way we observe a tree, but through scientific theory, experimentation, and the detection of indirect evidence, we infer its existence.

A central debate within the scope of science is the tension between *reductionism* and *holism*. Reductionism is the view that complex systems can be fully understood by breaking them down into their simplest, most fundamental parts. For example, a reductionist might argue that biological processes can be explained entirely by chemistry, and chemistry by physics. This approach assumes that understanding the smallest components of a system will provide a complete explanation of the whole. In contrast, holism argues that some phenomena cannot be fully understood by reducing them to their components. Instead, the whole system exhibits properties that cannot be predicted or explained by analyzing its parts in isolation. For example, in ecology, the interactions within an ecosystem can produce emergent properties that are not reducible to the behavior of individual species.

Finally, the scope of science is shaped by the debate between *scientific realism* and *anti-realism*, which addresses the question of whether the entities posited by scientific theories are real or merely useful constructs. The contrast between realism and anti-realism is most marked for sciences which make claims about non-observable entities. Scientific realism holds that the entities described by scientific theories exist independently of our knowledge of them. According to this view, successful scientific theories reveal truths about the world. In contrast, anti-realism argues that scientific theories are useful tools for predicting and organizing observations, but we should not necessarily believe that non-observable entities like electrons or gravitational waves are real. For anti-realists, the purpose of science is not to describe an independent reality, but rather to provide models that help us navigate and predict phenomena.

Scientists often seek to classify the objects they study into general kinds or categories. A key goal of classification is to convey meaningful information, enabling us to better understand and navigate the complexities of the natural world. However, this process raises several intriguing philosophical questions. Do the categories used in science represent real, essential divisions in nature, or are they merely human-made constructs designed to impose order on a complex and often ambiguous reality (realism vs. anti-realism)? Since any set of objects can, in principle, be classified in various ways, how should we determine the most appropriate approach? Is there a 'correct' way to classify, or are all classification systems fundamentally arbitrary? Some philosophers argue that *natural kinds*, groups that correspond to divisions genuinely existing in the world, do exist, as opposed to merely reflecting human interests. Understanding whether and how such natural kinds exist can provide valuable insights into the structure of reality and inform scientific inquiry.

G.3 Observation

* Sientific knowledge has a special status in part because it is founded on a secure basis, solid facts firmly established by observation.

* Facts are claims about the world.

* Facts are directly given to careful, unprejudiced observers via the senses. * Facts are prior to and independent of theory * Facts constitute a firm and reliable foundation for scientific knowledge.

* There are reasons for doubting that facts acquired by observation and experiment are as straightforward and secure as has traditionally been assumed.

[...] what observers see, the subjective experience that they undergo, when viewing an object or scene is not determined solely by the images on their retinas, but depends also on the experience, knowledge and expectations of the observers [...] one has to learn to be a competent observer in science [...] The experienced and skilled observer does not have perceptual experiences identical to those of the untrained novice when the two confront the same situation. This clashes with a literal understanding of the claim that perception are given in a straightforward way via the senses. [...] observers viewing the same scene from the same place see the same thing but interpret wath they see differently.

* Before an observer can formulate and assent to an observation statement, he must be in possesion of the approprate conceptual framework and a knowlege of how to appropriately apply it. Facts, formulated as statements, presuppose quite a lot of knowledge.

Our search for relevant facts needs to be guided by our current state of knowledge [...] the formulation of observation statements presupposes significatn knowledge, and that the search for relevant observable facts in science is guided by that knowledge. [...] the fact that knowledge is neccesary for the formulation of significant observationstatements still leaves open the question of which of the statements so formulated are borne out by observation and which are not. The idea that knowledge should be based on facts that are confirmed by observation is not undermined by the recognition that the formulation of the satements describing those facts are knowledge-dependent.

The point is hat if the knowledge that provides the categories we use to describe out observations is defective, the observation statements that presopose those categories are similarly defective. [...] observation statemts depends on the knowledge that forms the backgroud against which the judment is made [...] scientific revolution involved not just a progressive transformation of scientific theore, but also a transformation in what were considered to be the observable facts.

* Facts are fallible and subjet to correction.

* Perception are influenced by the background and expectations of the observer, so that what appears to be an observable fact for one need not be for another.

* Judgments about the truth of observation statements depend on what is alerady known or assumed, thus rendering the observable facts as fallible as the presuppositions underlying them.

* Everyday observation is far from passive. Thre is a range of things that are done, many of them automatically and perhaps unconsciously, to establish the validity of a perception.

* Statements should be such that their validity can be tested in ways that involve routine, objective procedures that do not necessitate fine subjective judgement on the part of the observer.

* Observations suitable for constituting a basis for scientific knowledge are both objective and fallible. They are objective insofar as they can be publicly tested and straightforward procedures, and they are fallible insofar as they may be undermined by new kinds of test made possible by advances in science in technolgy.

* What is needed in science is not just facts but relevant facts. Which facts are relevant and which are not relevant to a science will be relative to the current state of development of that science.

Many kind of processes are at work in the world around us, and they are all superimposed on, and interact with, each other in complicated ways. [...] It is not possible to arrive at un undesrtanding of these various processes by careful observation of events as they typically are naturally occur. [...] To acquire factors relevant for the identification and specification of the various processes at work in nature it is, in general, necessary to practically intervene to try to isolate the process under investigation and eliminate the effects of others. In short, it is ncessary to do experiments. [...] If these are facts that constitute the basis for science, then those facts come in the form of experimental results rather than any old observable facts.

Experimental results are by no means straightforwardly given [...] the complexity of practical struggle involved in the production of an experimental result. [...] If experimental results constitute the facts on which sicence is based, then they are not straightforwardly given via the senses. They have to be worked for, and their establishment involves cosiderable know-how and practical trial and error as well as exploitation of the available technology. [...] Nor are judgments about the adequacy of experimental results straightforward. [...] Experimental results can be faulty if the knoledge informing them is deficient or faulty. [...] Experimental results are fallible, and can be updated or replaced for reasonably straightforward reasons. Experimental results can become outmoded because of advanced in technology, they can be rejected because of some advance in understanding (in the light of which an experimental set-up comes to be seen as inadequate) and they can be ignored as irrelevant in the light of some shift in theoretical understanding.

* Experimental results are required not only to be adequate, but also to be appropriate or significant. What is an adequate and significant experiment depends heavily on how the practical and theoretical situation is understood.

* Experimental results are theory-dependent: All experiments will presume the truth of some theories to help judge that the set-up is adequate and the instruments are reading what they are meant to read.

* Experimental results are fallible and revisable.

Two schools of thought that involve attempts to formalise [...] that scientific knowledge is derived from the fact, are empiricists and the positivism. Empiricists [...] held that all the knowledge should be derived from ideas implanted in the mind by way of sense perception. The positivist had a broader view of what fact amount to. [...] The logical positivist [...] attempted to formalise it, paying close attention to the logical form of the relationship between scientific knowledge and the facts.

G.4 Scientific Representation

Science helps us understand the natural world by using different kinds of representations of research entities. These representations include measurements from scientific instruments, descriptions of observations, digital images like X-rays or MRI scans, and more. Scientific practice also often considers mathematical equations, models, and theoretical constructs as valid forms of representation. The challenge of *scientific representation* is to identify the conditions that make a representation scientific and determine what makes an effective representation. The main issues discussed in this area of philosophy include:

Scientific Representation Problem: The scientific representation problem is about figuring out the necessary and sufficient conditions that make a representation valid in science. It explores whether these conditions are the same across all scientific fields or if they vary depending on the discipline or research context. For example, what qualifies as a valid representation in physics, which often uses mathematical models, might be different from what is used in biology, where visual and descriptive representations are common. This problem also questions whether scientific representations need to be adapted to specific research goals to be considered valid.

Representational Demarcation Problem: The representational demarcation problem looks at whether scientific representations are fundamentally different from other kinds of representations, like those found in art or everyday life. It examines what makes scientific representations unique, focusing on their purpose, accuracy, and the methods used to create them. Unlike artistic representations, which may emphasize subjective interpretation or aesthetic value, scientific representations are generally held to standards of precision, reliability, and empirical adequacy. Understanding these differences helps clarify the specific role that scientific representations play in knowledge production.

Problem of Style: The problem of style addresses the fact that the same entity can be represented in different ways, depending on the goals and methods of the research. Different styles of representation—such as diagrams, mathematical equations, physical models, or computer simulations—each have unique characteristics, including the intended audience, level of abstraction, and type of information conveyed. This issue also asks whether these styles are fixed or if new styles can be invented to meet emerging scientific needs. The flexibility of representation styles is crucial because it allows for new insights and different ways of understanding scientific phenomena.

Standard of Accuracy: The standard of accuracy problem is about determining what makes a scientific representation accurate. It involves figuring out how to distinguish between accurate and inaccurate representations by considering factors like how well the representation matches empirical data, captures important features of the phenomenon, and its ability to make predictions. This issue also explores whether accuracy should be seen as an objective standard or if it depends on the specific aims and context of the research. For example, a simplified model might still be considered accurate if it effectively serves its purpose, such as making predictions or providing explanations.

Problem of Ontology: The problem of ontology in scientific representation deals with the nature of the entities that can serve as representations. It asks whether representations need to be concrete, like physical models or graphs, or if they can also be abstract, like mathematical equations or theoretical constructs. This issue also questions whether representations must be realistic or if more abstract, idealized forms can still be effective in scientific inquiry. Understanding these ontological aspects helps define the types of entities that are allowed in scientific discourse and how they relate to the real-world phenomena they represent.

There are also five conditions of adequacy that a scientific representation should satisfy to be considered effective and reliable:

Requirement of Directionality: The requirement of directionality examines the relationship between representations and the real world. Representations are meant to describe entities in the real world, but this condition raises the question of how, if at all, real-world entities might describe their representations. It challenges us to think about the direction of influence between the representation and the entity it aims to depict.

Surrogative Reasoning: Surrogative reasoning addresses how scientific representations allow researchers to generate hypotheses about the entities they represent. This condition explores how using a representation as a surrogate can lead to new insights or predictions about the target, effectively using the representation to stand in for the real-world entity during reasoning and analysis.

Applicability of Mathematics: The applicability of mathematics condition is concerned with how mathematical models can be used to represent the real world. It questions how abstract mathematical constructs can effectively describe complex physical systems and whether the success of mathematical representation depends on any special features of the target phenomena. This condition highlights the central role of mathematics in developing and understanding scientific theories.

Possibility of Misrepresentation: The possibility of misrepresentation addresses whether representations that are not fully accurate can still be considered valid scientific representations. It considers situations where simplifications or approximations are necessary and whether these less-than-perfect representations can still contribute valuable understanding of a phenomenon. This condition is important for understanding how idealizations and abstractions function in scientific practice.

Targetless Models: The targetless models condition explores whether we can allow representations that do not have a direct real-world counterpart.

It questions if a model that does not represent any existing entity can still be useful in scientific inquiry, perhaps as a way to explore theoretical possibilities or to understand potential scenarios. This condition emphasizes the creative and exploratory aspects of scientific modeling.

There have been multiple proposals to formally define the concept of scientific representation. Unfortunately, none of these proposals can provide a convincing answer to the questions and conditions of adequacy described above. In the rest of this section, we describe some of these proposals, identifying their advantages and drawbacks. To compare these proposals, we will present them as: "A scientific model M represents a target system T if, and only if ...".

Stipulative Fiat: The stipulative fiat proposal states that "a scientific model M represents a target system T if, and only if, a scientist stipulates that M represents T." The main problem with this interpretation is that, since anything can be a representation if a scientist says so, it is difficult to guarantee the surrogative reasoning condition. If any model can be deemed a representation by simple stipulation, it becomes challenging to determine which representations are genuinely useful for making scientific inferences. Proponents of this theory acknowledge that while all representations may be stipulated, some are undeniably more useful than others.

Similarity Conception: The similarity conception proposes that "a scientific model M represents T if, and only if, M and T are similar." This conception addresses the surrogative reasoning condition since similarity between the model and the target allows us to derive similar properties. However, it introduces new challenges, particularly regarding the problem of style. The concept of similarity is often vague: in what sense are M and T similar? This vagueness can lead to issues with directionality and accuracy, as different aspects of similarity may not always align with what is relevant for scientific representation.

Structuralist Conception: The structuralist conception is based on the idea of isomorphism. According to this view, a scientific model M represents a target system T if the structure of M is isomorphic to the structure of T. In other words, there is a one-to-one correspondence between the elements and relationships in both M and T. This approach justifies surrogative reasoning because having the same structure implies that properties and relations in the model correspond to those in the target. Furthermore, since mathematics is fundamentally concerned with the study of structures, this conception also supports the applicability of mathematics in representing natural systems.

Inferential Conception: The inferential conception proposes that a model M is an epistemic representation of a target T if, and only if, the user adopts an interpretation of M in terms of T. This view emphasizes the role of the user in giving meaning to the model, suggesting that representation is not an inherent property of the model itself but arises through its use in making inferences about the target system. This conception underscores the importance of context and interpretation in determining whether a model effectively represents its target.

Fiction View of Models: According to the fiction view of models, M represents T if and only if M functions as a prop in a game of make-believe that prescribes imagining certain things about T. This view draws an analogy between scientific modeling and storytelling, where models are treated as fictional constructs that facilitate imaginative engagement with the target system. Although this approach highlights the creative aspects of modeling, it raises questions about how such fictional constructs can be rigorously linked to real-world entities.

Representation-As: The representation-as approach suggests that a scientific model represents a target system as something, emphasizing that representation involves highlighting certain features of the target while downplaying others. This conception focuses on the interpretive aspect of modeling, where the modeler selects specific attributes of the target to represent, depending on the research goals. This approach allows for a flexible understanding of representation that can accommodate different styles and purposes, but it also implies that the usefulness of a representation is contingent on how well the modeler captures the relevant aspects of the target.

Each proposal has its strengths and weaknesses, highlighting the complexity of what it means for a model to effectively represent a target in scientific inquiry. Understanding these various perspectives is crucial for advancing our comprehension of the role of representation in science.

G.5 Scientific Discovery

Scientific discovery refers to the process through which new knowledge, ideas, or principles are uncovered within science. Unlike the systematic procedures associated with justification, discovery often involves creativity, intuition, and inspiration. While some discoveries arise from planned experiments or systematic observation, others occur unexpectedly, challenging existing paradigms or opening new fields of inquiry. The general agreement among philosophers is that the creative process of conceiving a new idea is a non-rational process that cannot be formalized as a set of steps. Understanding discovery is crucial for appreciating how science evolves and adapts, as it reveals the dynamic and often unpredictable nature of scientific progress.

The following two proposals assume that a domain-neutral logic of discovery can be formalized, offering attempts to develop such a framework.

- *Discovery as abduction*: Abductive reasoning is a mode of discovery that begins with surprising or anomalous phenomena and seeks to generate plausible hypotheses to explain them. This process is conceptualized as follows: (i) some unexpected data, such as $p_1, p_2, \ldots, p_n$, is encountered; (ii) these data would be less surprising if a hypothesis of type H were true; and (iii) therefore, there is justification to develop a hypothesis of type H. Two types of abduction are distinguished: *selective abduction*, which involves choosing from known hypotheses, and *creative abduction*, which generates entirely new hypotheses. Abduction present some limitations. First, multiple hypotheses may explain the same phenomena, making additional criteria necessary to evaluate their merit. Second, the schema of abductive reasoning does not account for the act of conceiving a hypothesis itself.
- *Heuristic programming* is a computational approach designed to simulate and assist the creative aspects of human problem-solving. These programs operate as searches within a defined problem space, which includes all possible configurations for a given domain. Each configuration represents a specific state within the problem space, with two key states being the initial state, the starting point of the search, and the goal state, which represents the desired outcome. Operators define the moves that transition between states, while path constraints limit permissible moves within the problem space. Problem-solving in this context involves finding a sequence of operations that connects the initial state to the goal state. The core aim of this approach is to develop heuristics (practical rules or strategies) to efficiently navigate and solve complex problems. Heuristic programming has its limitations, scientific problem spaces are often ill-defined, and computer programs rely on experimental data, meaning that simulations frequently cover only specific aspects of scientific discovery.

Many philosophers argue that discovery is an important topic within the philosophy of science, even as they move away from the idea of a formal logic of discovery. A highly influential perspective is Thomas Kuhn's examination of how new facts and theories emerge in the so-called *paradigm shifts*. According to Kuhn, discovery is not a single event but rather a complex and prolonged process that often results in paradigm shifts. Paradigms consist of shared generalizations, theoretical commitments, values, and exemplars that unify a scientific community and shape its research practices. During periods of normal science, research focuses on expanding and refining the existing paradigm rather than pursuing novelty. Discovery typically begins with the recognition of anomalies—phenomena that defy the expectations established by the current paradigm. This process includes observing and conceptualizing the anomaly, followed by revising the paradigm to accommodate it. During paradigm crises, theory-driven discoveries may occur as scientists propose speculative theories, develop new expectations, and conduct experiments or observations to test these ideas. Ultimately, a new paradigm emerges, transforming the once-anomalous phenomena into standard expectations.

Scientific discovery can be also viewed as inherently tied to creativity, with philosophers drawing from cognitive science, neuroscience, computational research, and environmental and social psychology to better understand how new ideas emerge. This perspective aims to demystify the mental processes behind creative thought, emphasizing that scientific creativity can be analyzed and understood philosophically. Central to this analysis are two pivotal cognitive mechanisms: analogies and mental models, which serve as fundamental tools in the generation of innovative ideas and the advancement of knowledge.

- *Analogy*: Analogies play a crucial role in scientific discovery by enabling the transfer of ideas from one domain to another. Philosophers distinguish between three types of analogies: positive, negative, and neutral. Positive analogies involve properties that are shared by both the model (the well-understood domain) and the target domain (the new domain). Negative analogies include properties that belong solely to the model and do not apply to the target domain. Neutral analogies are the most intriguing because they consist of properties whose relevance to the target domain remains uncertain. These neutral analogies are significant as they often lead to new insights and hypotheses about the less familiar domain. Additionally, there is a distinction between horizontal and vertical analogies. Horizontal analogies connect two domains at the same level of abstraction, whereas vertical analogies involve relationships between different levels of abstraction within the same domain.
- *Model-based reasoning*: The concept of model-based reasoning suggests that much of human thought, including probabilistic and causal reasoning as well as problem-solving, relies on mental models rather than formal logic or strict methodological rules. In this approach, the mind constructs structural representations of real-world or imagined situations and manipulates these models to explore possibilities and generate insights. Conceptual structures are viewed as models, and conceptual innovation involves creating new models using various operations. Analogical reasoning, or analogical modeling, is one of the primary forms of model-based reasoning, alongside visual modeling and simulative modeling, such as through experiments.

G.6 Scientific Explanation

If the reasoning that takes us from this factual basis to the laws and theories that constitute scientific knoledge is sound, then the resulting knowledge can itself be taken to be securely established and objective

In philosophy of science it is often made the assumption that there exists a single, distinct type of explanation that qualifies as "scientific." The concept of "scientific explanation" suggests at least two key elements: first, a contrast between explanations characteristic of science and those that are not, and second, a contrast between "explanations" and other forms of discourse, such as mere "descriptions." It is important to note that a set of claims can be true, accurate, and supported by evidence while still failing to qualify as explanatory.

Good scientific explanations are typically evaluated based on several key characteristics. While different philosophical frameworks might emphasize different criteria, the following characteristics are broadly agreed upon:

Empirical Adequacy: A good explanation must align with observed and experimental evidence. It should accurately describe the phenomena being explained, providing a detailed account of how the observed data supports the explanation. Additionally, it should integrate well with existing empirical findings, ensuring reliability and fostering broader scientific understanding.

Logical Coherence: The explanation should be logically consistent and free of contradictions. Its components should interconnect in a structured and harmonious way, enabling clear and valid reasoning. This coherence ensures that the explanation aligns with established logical principles and provides a solid foundation for understanding the phenomena under investigation.

Causal Relevance: Good explanations often identify the causal mechanisms responsible for the phenomenon. They should clarify how and why the phenomenon occurs, detailing the specific interactions and processes involved. By establishing a clear causal link, these explanations provide a framework for understanding not just what happens, but the underlying reasons and mechanisms driving the event. This depth of causality enables predictions, interventions, and broader scientific application.

Generality: Explanations that apply to a broader range of phenomena are considered more valuable. They should transcend individual instances to reveal patterns or principles that connect seemingly disparate phenomena. By addressing a wider scope, such explanations enhance our ability to generalize knowledge, foster predictive accuracy, and provide a unifying perspective across different domains of inquiry.

Simplicity (Parsimony): A good explanation should not be unnecessarily complex. Among competing explanations, the one that makes the fewest assumptions while still accounting for the phenomena is often preferred

(Occam's Razor). This principle emphasizes clarity and efficiency in reasoning, ensuring that explanations avoid superfluous details or unwarranted complexity. Simpler explanations are easier to test, communicate, and apply, fostering a more practical and streamlined understanding of the phenomena.

Explanatory Depth: Good explanations go beyond surface descriptions to provide a deeper understanding of the underlying mechanisms, principles, or causes. They delve into the fundamental elements that drive the phenomenon, offering insights into its origins and interconnections with related concepts. By unraveling these deeper layers, such explanations help uncover not just the "how," but the "why," enriching our comprehension and enabling a more profound application of knowledge.

Testability: The explanation must allow for predictions that can be tested and potentially falsified. This criterion ensures that the explanation is scientifically meaningful and subject to empirical scrutiny. By being testable, the explanation invites rigorous examination and challenges, which help to confirm its validity or expose its weaknesses. Testability also connects scientific explanations to the broader experimental process, enabling continuous refinement and adaptation in light of new evidence, thereby fostering scientific progress and reliability.

Unification: A good explanation often unifies disparate phenomena under a single framework or theory, showing how they are related. It highlights the connections and underlying principles that bring coherence to seemingly unrelated phenomena. By doing so, unification not only simplifies our understanding but also enhances the explanatory power of a theory, allowing for a more integrated and comprehensive perspective on the natural world.

Use of Laws: Good explanations often incorporate established scientific laws or theories to provide a robust foundation for their claims. By grounding explanations in well-established principles, they ensure credibility and consistency with the broader scientific framework. This approach not only strengthens the explanatory power of the claims but also facilitates their integration into existing knowledge systems, thereby fostering coherence, predictability, and utility in advancing scientific understanding.

Practical Applicability: In some cases, the usefulness of an explanation in solving problems, guiding further research, or applying knowledge in practical ways adds to its value. An explanation with practical applicability not only enhances theoretical understanding but also bridges the gap between abstract knowledge and real-world implementation. It can inform decision-making, inspire technological innovations, and address pressing societal challenges. By demonstrating utility in diverse contexts, such explanations underscore the relevance of scientific inquiry to everyday life and future advancements.

Asymmetry: The requirement of asymmetry in scientific explanation is a widely discussed topic in the philosophy of science. According to most philosophical accounts, explanation is indeed considered to be an asymmetric relation, meaning that if X explains Y, it should not also be true that Y explains X under the same laws and additional facts. However, there are debates and complications surrounding this idea. Let's examine the arguments for and against asymmetry in scientific explanations.

Explanation as prediction: When we provide a covering law explanation for a phenomenon, the laws and specific facts we reference could have allowed us to predict the phenomenon's occurrence. This highlights that a scientific explanation is inherently a potential prediction. Conversely, every reliable prediction is inherently a potential explanation, illustrating that explanation and prediction are structurally symmetric in their foundational principles.

The following paragraphs briefly introduce the most relevant proposals to characterize what is a scientific explanation.

The *Deductive-Nomological model*, or DN model, emphasizes the importance of deductive reasoning and general laws. According to this model, a phenomenon is explained by demonstrating how it logically follows from a general law combined with specific initial conditions. This explanation comprises two main components: the *explanans*, which includes the general laws and initial conditions, and the *explanandum*, which is the phenomenon to be explained. For the explanation to be valid, the explanans must be true and logically entail (see logical deduction at Section G.7) the explanandum, meaning the phenomenon can be deduced from the laws and conditions provided. A DN model answers the question "Why did the explanandum occur?" by showing that the phenomenon resulted from specific circumstances $C_1, C_2, \ldots, C_i$, in conjunction with laws $L_1, L_2, \ldots, L_j$. For example, the motion of a particular pendulum can be explained by applying Newton's laws of motion (general laws) along with specific details such as the pendulum's length and initial displacement (specific initial conditions). Alternatively, the general behavior of pendulums can also be explained using the same laws and reasoning, since the DN model can be applied to both particular occurrences and general patterns.

The *Statistical-Relevance model*, or SR model focuses on explaining phenomena through statistical relationships rather than strict deductive reasoning. Unlike the Deductive-Nomological model, which requires logical entailment from general laws, the SR model emphasizes the identification of statistically relevant factors that significantly influence the likelihood of a phenomenon. In this model, given some class or population A, an attribute C is *statistically relevant* to another attribute B if and only if $P(B|A,C) \neq P(B|A)$. This means that C affects the probability of B within the context of A. An explanation involves identifying such statistically relevant factors and evaluating their impact within a reference class (a group of events or entities sharing common characteristics). For example, in explaining the likelihood of developing a particular disease, an SR explanation might highlight factors such as age, genetic predisposition, or lifestyle choices, showing how these variables alter the probability of the disease occurring. By uncovering these statistical relationships, the SR model provides a method for explaining probabilistic phenomena that cannot be addressed deterministically.

The *Causal-Mechanical model*, or CM model, of scientific explanation emphasizes understanding phenomena by uncovering the underlying causal mechanisms that produce them (see causality at Section G.7). This model asserts that explanations are not just about identifying laws or statistical relationships but about revealing the actual processes and interactions that link causes to effects. A causal-mechanical explanation requires tracing a continuous causal chain, often through detailed physical or biological processes, to show how an event is brought about. For example, explaining the boiling of water involves identifying the causal mechanism: heat energy transfers to the water molecules, increasing their kinetic energy until intermolecular bonds are overcome, leading to a phase change from liquid to gas. The CM model prioritizes clarity in how individual components interact and influence each other, providing a deeper understanding of the phenomenon by grounding it in observable and empirically testable mechanisms. This approach is particularly effective in fields like biology, physics, and engineering, where complex systems and their interactions play a central role in explanation.

The *unificationist account* of scientific explanation, emphasizes the power of explanation through the unification of diverse phenomena under a single, coherent framework of principles and patterns. According to this model, the primary aim of scientific explanation is to reduce the number of independent assumptions and derive a wide range of phenomena from a minimal, consistent set of explanatory patterns. An explanation is considered successful if it contributes to this unifying framework by connecting seemingly disparate observations through common principles. For instance, Newtonian mechanics unifies the motions of celestial bodies and terrestrial objects under the same laws of motion and gravitation. The unificationist approach highlights the importance of simplicity, generality, and coherence in scientific theories, proposing that the value of an explanation lies in its ability to integrate knowledge into an organized, explanatory schema. By offering a comprehensive understanding of diverse phenomena, this account showcases the interconnectedness and systematic nature of scientific inquiry.

The *pragmatic theories* of scientific explanation emphasize the context-dependent and audience-specific nature of explanations, focusing on their purpose and practical utility rather than strict formal structures. These theories argue that explanations are answers to "why" questions posed within a specific context, and their adequacy depends on how well they address the interests and background knowledge of the audience. A scientific explanation, therefore, is not inherently tied to a universal standard but varies depending on the explanatory goals, such as prediction, understanding, or control. For instance, explaining why a bridge collapsed might involve detailed structural analysis for engineers, whereas a simplified account focusing on the immediate cause, like high winds, might suffice for the general public. Pragmatic approaches recognize that explanatory demands can differ across disciplines, situations, and audiences, making the effectiveness of an explanation contingent on its relevance, clarity, and alignment with the inquirer's needs. This perspective underscores the interplay between scientific knowledge and its communication within varied practical contexts.

G.7 Scientific Justification

scientific knowledge can neither be conclusively proved nor conclusively disproved

Logicians make an important distinction between deductive and inductive inference [...] The two statements above the line are called the premises of the inference, while the statements below the line is called the conclusion. This is a deductive inference because it has the following property: if the premises are true, then the conclusion must be true too [...] This is sometimes expressed by saying that the premises of the inference entail the conclusion [...] In a typical inductive inference, we move from premises about objects that we have examined to conclusions about objects of the same sort that we haven't examined.

When we reason deductively, we can be certain that if we start with true premises we will end up with a true conclusion. By contrast, inductive reasoning is quite capable of taking us from true premises to a false conclusion [...] Scientists reason inductively whenever they move from limited data to a more general conclusion, which they do all the time.

Popper claimed that scientist only need to use deductive inferences.

Although a scientific theory (or hypothesis) can never be proved true by a finite amount of data, it can be proved false, or refuted.

Hume argued [Hume's problem of induction] that the use of induction cannot be rationally justified at all [...] whenever we make inductive inferences, we presuppose the 'uniformity of nature' [...] our reasoning depend on the assumption that objects fwe haven't examined will be similar, in relevant aspects, to object of the same sort we have examined [...] we cannot prove the uniformity assumption.

Inductive inferences have all the same structure, the premise has had the form 'all examined Fs have been G' and the conclusion the from 'other Fs are also G' [...] Reasoning of this sort is known as 'inference to the best explanation' (IBE) [...] The basic idea behind IBE – reasoning from one's data to a theory or hypothesis that explains the data – good explanation should be simple [...] Preferring a theory which explains the data in terms of the fewest number of causes seems sensible. But are there any objective grounds for thinking that such a theory is more likely to be true than a less simple rival?

Thomas Kuhn introduced the concept of scientific paradigms, which revolutionized the understanding of scientific progress. A paradigm encompasses the set of practices, theoretical frameworks, methodologies, and standards that define a scientific discipline during a specific period. According to Kuhn, normal science operates within the confines of a prevailing paradigm, solving puzzles and extending the framework. However, scientific revolutions occur when anomalies accumulate—phenomena that the existing paradigm cannot adequately explain—leading to a paradigm shift. This shift replaces the old framework with a new one that better accommodates the observed data, fundamentally altering the trajectory of scientific inquiry. Kuhn's insights emphasize the sociocultural and historical dimensions of science, challenging the notion of continuous, cumulative progress.

[...] scientific revolutions, periods of great upheaval when existing scientific ideas are replaced with radically new ones [...] these revolutions led to a fundamental change in the scientific worldview, the overthrow of an existing act of ideas by a completely different set [...] revolutions happen relatively infrequently [...] 'normal science' [...] the ordinary day-to-day activities that scientists engage in when their disciplines is not undergoing revolutionary change [...] A paradigm consists or two main components: first, a set of fundamental theoretical assumptions which all members of a scientific community accept; secondly, a set of 'examplars' or particular scientific problems which have been solved by means of those theoretical assumptions [...] When scientists share a paradigm [...] they agree on how future research in the field should proceed, on which problems are the pertinetn ones to tackle, on what the appropriate methods for solving those problems are, and on what an acceptable solution of the problems would look like [...] a paradigm is an entire scientific outlook, a constellation of shared assumptions, beliefs, and values which unite a scientific community and allow normal science to take place. [...] The job of the normal scientist is to try to eliminate these minor puzles while making a few changes as possible to the paradigms [...] normal scientists are not trying to test the paradigm. On the contrary, they accept the paradigm unquestioningly, and conduct their research within the limits it sets [...] as anomalies accumulate, a burgeoning sense of crisis envelops the scientific community. [...] A variety of alternatives to the old paradigm are proposed, and eventually a new paradigm becomes established [...] The essense of a scientific revolution is thus the shoft from an old paradigm to a new one. [...] Kuhn argued that adopting a new paradigm involves a certain act of faith on the part of the scientists. [...] if paradigm shifts work the way Kuhn says, it is hard to see how science can be regarded as a rational activity at all. [...] the facts about the world are paradigm-relative, and thus change when paradigms change [...] Kuhn espose a radical form of anti-realism about science.

[...] competing paradigms are typicallly 'incommensurable' with one another [...] Incommensurability is the idea that two paradigms may be so different as to render impossible any straightforward comparison of them with each other, there is no common language into which both can be translated [...] concepts cannot be explained independently of the theories in which they cannot be explained independently of the theories in which they are embedded. This idea, which is sometimes called 'holism' [...] replacement of 'wrong' iddeas by 'right' ones [...] later paradigms are not better than earlier, just different [...] old and new paradigms to be incompatible [...] lack of a common language [...] incommensurability of standars.

[...] theory-ladenness of data [...] the ideal of theory-neutrality is an ilusion, data are invariable contaminated by theoretical assumptions [...] a dispute between competing paradigms could not be resolved by simply appealing to 'the data' or 'the facts', for what a scientist counts as data, or facts, will depend on which paradigms they accept [...] To be objectively true, a theory must corespond to the facts, but the idea of such a correspondence makes little sense if the fact themselves are infected by our theories [...] perception is heavly conditioned by background beliefs [...] scientists' experimental and observational reports are often couched in highly theoretical language.

[...] there is 'no algorithm' for theory choice in science. [...] no one has ever succeeded in producing such an algorithm. [...] For one thing, there may be trade-offs: theory A maybe simpler than theory B, but B may fit the data more closely. So an element of subjective judment, or scientific common sense, will often be needed to decide between competing theories. [...] is not that paradigm shifts are irrational, but rather that a more relaxed, pragmatic concept of rationality is required to make sense of them.

[...] as did the idea of a sharp dicotomy between the context of discovery and justification. [...] His doctrines of paradigm shifts, normal and revolutionary science, incommesurability, and theory landenness.

Paul Feyerabend, in his provocative work "Against Method," argued that there is no universal scientific method that guarantees the success of science. He criticized the rigid methodological rules proposed by philosophers like Popper and Kuhn, suggesting that science has advanced precisely because of its methodological anarchy. Feyerabend contended that "anything goes" in science, meaning that historical scientific breakthroughs often occurred by defying established rules and norms. For example, Galileo's use of persuasive rhetoric and creative reasoning, rather than strict adherence to empirical observation, was crucial in advancing heliocentrism. Feyerabend's ideas challenge the assumption that scientific progress is orderly and rational, emphasizing instead the role of historical, cultural, and personal factors in shaping scientific practice. While his views remain controversial, they highlight the complexity and diversity of scientific inquiry and question the feasibility of prescribing universal methodological principles.

The hypothetico-deductive method is a widely recognized approach in the philosophy of science, describing how scientific theories and knowledge are developed and tested. It begins with the formulation of a hypothesis, which serves as a tentative explanation for a phenomenon or a set of observations. From this hypothesis, scientists deduce specific, testable predictions or consequences, often in the form of "if-then" statements. These predictions are then subjected to empirical testing through experiments or observations. If the results align with the predictions, the hypothesis is supported but not conclusively proven; if the results contradict the predictions, the hypothesis may need to be revised or rejected. This iterative process underscores the provisional nature of scientific knowledge.

Falsificationism emphasizes that scientific theories can never be conclusively proven but can be rigorously tested through attempts to falsify them. An example of this is Einstein's theory of general relativity, which predicted that light would bend near massive objects like the sun. This prediction was empirically tested during the solar eclipse of 1919, when astronomers observed starlight bending as it passed near the sun, providing a crucial opportunity to potentially falsify the theory—but instead offering strong support for it. According to this perspective, a theory is scientific only if it is falsifiable—that is, if it makes predictions that could, in principle, be shown to be false by empirical evidence. In this view, the strength of a scientific theory lies in its ability to withstand attempts at falsification, and progress in science occurs when falsified theories are replaced by better, more robust ones. This perspective shifts the focus from verification to critical testing, highlighting the dynamic and self-correcting nature of scientific inquiry.

One challenge within the hypothetico-deductive method is addressing the origin of hypotheses themselves. While the method provides a systematic way to test and refine hypotheses, it does not dictate where these initial ideas come from. In the past, the generation of hypotheses was often the direct result of careful observations of natural phenomena. However, as science has progressed, hypotheses have increasingly become products of creativity, intuition, or inspiration drawn from prior knowledge, analogies, or even serendipitous observations. This aspect highlights the interplay between the logical structure of scientific testing and the imaginative processes that fuel scientific discovery. Philosophers of science have long debated whether hypothesis generation is a purely rational process or one influenced by subjective and contextual factors, underscoring the complexity of scientific creativity.

Statistical inference has become a significant approach within the scientific method, providing a framework for deriving conclusions from data in the face of uncertainty. By employing probabilistic models and statistical techniques, scientists can estimate the likelihood that observed phenomena are consistent with a given hypothesis. Techniques such as hypothesis testing, point estimation, and confidence intervals allow researchers to quantify uncertainty and make data-driven decisions. This approach is particularly powerful in fields where direct experimentation is difficult or impossible, such as cosmology or epidemiology. However, reliance on statistical methods also raises important questions about the interpretation of probabilities (see Section B.2) and the potential for misuse, such as overfitting models or neglecting prior assumptions. Despite these challenges, statistical inference remains an indispensable tool for connecting empirical data to theoretical models in modern science.

The Bayesian approach is an application of the statistical reasoning to the scientific method. Based on Bayes' theorem (see Theorem B.3.2), the Bayesian approach provides a formal framework for updating the probability of a hypothesis as new evidence emerges. By iteratively adjusting probabilities, the Bayesian approach dynamically reflects how beliefs evolve as evidence accumulates. Each time an experiment is succesfully performed the likelihood of the hypothesis to be true increases. This iterative process allows for a dynamic adjustment of beliefs, reflecting how evidence accumulates over time. Bayesian methods are particularly useful in contexts of uncertainty or incomplete data, such as medical diagnosis, or climate modeling.

Let $P(h \mid e)$ denote the probability of a hypotheis h in the light of evidence e. $P(e \mid h)$ denote the probability to be ascribed to the evidence e on the assumption that the hypothesis h is correct, $P(h)$ the probability ascribed to h in the absence of knowledge of e, and $P(e)$ the probability ascribed to e in the absence of any assumption about the truth of h. The Bayes' theorem (see

Theorem B.3.2) can be written:

$$P(h \mid e) = P(h)\frac{P(e \mid h}{P(e)}$$

$P(h)$ is referred to as the prior probability since it is the probability ascribed to the hypothesis prior to consideration of the evidence e, and $P(h \mid e)$ is referred to as the posterior probability, the probability after the evidence e is taken into account. So the formula tell us how to change the probability of a hypothesis to some new, revised probability in the light of some specified evidence.

The factor $P(e/h)$ is a measure of how likely e is given h. It will take a maximum value of 1 if e follows from h and a minimum value of zero if the negation of e follows from h.

With suffiencient amount of evidence, bayes converges? (weigth of isotopes), making less relevant the problem of subjective priors (conjugate priors?)

■ **Example G.1** Something established barely changes with new experiments, bold confirmed congetures do ■

When an experiment fails to confirm a theory, Bayesian inference allows for a probabilistic adjustment of the theory's credibility by updating its posterior probability in light of the evidence, unlike falsificationism, which considers a theory definitively refuted when evidence contradicts its predictions.

Bayesian inference, while powerful, has notable limitations:

Objective prior probabilities of hypothesis are difficult to obtain (how do we list all possible hypothesis?). Subjective priors represent degrees of bileif. its reliance on subjective priors can introduce bias, requiring careful justification;

it is sometimes applied in contexts lacking a well-defined probability space, undermining its validity; and it cannot accommodate scientific inferences that leap to entirely new theories, as conditionalization is incapable of handling hypotheses or concepts absent from the prior probability space. Despite these limitations, Bayesian inference continues to shape modern scientific practices, highlighting the interplay between evidence, prior knowledge, and probabilistic reasoning.

Causality refers to the relationship between events where one event (the cause) brings about or influences another event (the effect), and it asserts that explaining a natural phenomenon involves identifying its causes. In the philosophy of science, there is ongoing debate about whether causal explanations differ fundamentally from those based on general laws, as deducing an event from a general law often implicitly reveals its cause. A key feature of causality is its inherent asymmetry, if x is the cause of y, then y cannot be the cause of x; this asymmetry is a crucial distinction that sets causal explanations apart from mere statistical correlations. Many challenges arise when relying on empirical observations to justify causal relationships. One perspective emphasizes the development of rigorous methodologies, generally by statisticians and computer scientists, to infer causality from observational data, addressing issues such as *confounding factors* (variables that obscure the true causal relationship) and the principle that correlation does not imply causation. *Randomized controlled trials* stand as a gold standard in causal inference, where confounding variables are systematically controlled by design to isolate the effect of the factor under investigation. In contrast, empiricists argue that causal relations cannot be directly observed and suggest that causality is merely a conceptual framework humans impose on the world to make sense of observed regularities.

G.8 The Limits of Science

[...] philosophical enquiry has its own propietary methods, which can reveal truths of a sort that science cannot. [...] They include logical reasoning, the use of thought experiments, and what it is called 'conceptual analysis', which tries to delimit a particular concept by relying on our intuitions about whether a particular case fall under it. [...] It is often felt that natural sciences such as physics, chemistry, and biology are in a more advanced state than social sciences such as economics, sociology, and anthropology; the former can formulate precise laws with great predictive power, while the latter usually cannot. [...] It is never possible to prove that a scientific theory is true, in the strict sense of proof, for the inference from data to theory is invariably non-deductive.

Non-detectable entities

[...] sicence can in principle explain everything? Or are there some phenomena that must forever elude scientific explaination? [...] However much the science of the future can explain, the explanations it gives will have to make use of certain fundamental laws and principles. Since nothing can explain itself, it follows tat at least some of these laws and principles will themselves remain unexplained [...] some things will never be explained, but does not tell use what they are.

Science has long been a powerful tool for understanding and shaping the world. However, its scope is not unlimited. There are domains where science struggles to provide answers, such as consciousness or moral values. Metaphysical questions, such as the nature of existence or why there is something rather than nothing, often fall outside the realm of empirical investigation. Similarly, science can describe the consequences of actions but cannot determine moral values or prescribe what ought to be done. This section contains a brief description of the main topics related to the limits of science.

Reductionism vs. Holism

One key debate in understanding the limits of science is the tension between *reductionism* and *holism*. Reductionism asserts that complex phenomena can be fully understood by breaking them down into their most basic components and laws. For example, biology might be reduced to chemistry, and chemistry to physics. However, holism argues that some phenomena, especially in systems like ecosystems, societies, or even consciousness, cannot be fully understood without considering the interactions and emergent properties of the whole system. This debate underscores the challenge of addressing complexity within scientific frameworks.

The different scientific disciplines are designed for explaining different types of phenomena [...] there is a distinction of labour betwen the different sciences: each specializes in explaining its own particular set of phenomenon [...] it is widely held than the different branches of science are not all on a par: some are more fundamental than others [...] physics can subsume all the higher-level sciences? [...] The objects studied by the higher-level sicences are multiply realized at the phisical level.

Scientific inquiry excels in answering questions about the natural world, but it encounters boundaries when addressing issues that are metaphysical, moral, or inherently subjective. For example, while science can study the mechanics of evolution, it does not address whether life has an intrinsic purpose. Similarly, while it can analyze the factors influencing human behavior, it cannot resolve normative questions about justice or fairness. These limitations highlight the need for interdisciplinary approaches and alternative methods of inquiry.

Realism vs. Anti-realism: As it was already mentioned in Section G.2, another critical debate in philosophy of science concerns the nature of scientific knowledge: does science uncover true aspects of reality (*scientific realism*), or does it merely provide useful models and predictions without necessarily representing reality (*scientific anti-realism*)? Anti-realism suggests that scientific theories as instruments for helping us predict observable phenomena, rather than as attempts to describe the underlying nature of reality. The scientific realism vs scientific anti-realism debate underscores a debate in philosophy between two opposing schools of though called *realism* and *idealism*. Realism holds that the physical world exists independently of human though and perception. Idealism claims that the physical world is in some way dependent on the concious activity of humans.

The underdetermination argument: Anti-realist emphasize that the empirical data to which scientific theores are responsible consist of fact about observable entities and processes. [...] fact about observable phenomena provide the ultimate data fro theories that posit unobservable entities and processes. [...] Anti-realists that aregue that the emprirical data 'underdetermine' the theories scientist put forward on their basis [...] the data can in principle be explained by many different, mutually incompatible, theories. [...] Undetermination lead naturally to the anti-realist conclusion that agnosticism is the rational attitude to take towards theories about the unobservable region of reality. [...] But, say the realists, it does not follow that all of these possible explanations are equally good. [...] why simple theories should be though more likely to be true.

Objetivity

Science is often regarded as an objective endeavor, but this view is contested. Scientific practices are influenced by the cultural, social, and personal contexts of researchers. For example, funding priorities, societal values, and individual biases can shape research questions, methodologies, and interpretations. The ideal of objectivity remains central to scientific inquiry, but recognizing these influences is crucial for understanding the limitations and potential biases inherent in scientific work.

Address the self-correcting nature of science

The Demarcation Problem

The *demarcation problem* addresses the challenge of distinguishing science from non-science or pseudoscience. This philosophical issue has significant implications for the credibility and authority of scientific knowledge. Karl Popper's criterion of falsifiability, a theory is scientific if it can be tested and potentially falsified, has been influential but not universally accepted. Some disciplines, like evolutionary psychology or string theory, straddle the line, sparking debate about their scientific status. The demarcation problem highlights the complexity of defining the scope and boundaries of science.

Science thrives on uncertainty, yet there are questions that may remain permanently beyond its reach. For example, the origins of the universe, the nature of dark matter, or the ultimate fate of existence may elude definitive answers. Furthermore, the tools and methodologies of science may be inherently limited in addressing phenomena that require new paradigms or approaches. This recognition does not diminish science but rather emphasizes its role as one part of a broader human quest for knowledge.

While science provides the means to achieve certain ends, it does not dictate the ethical use of its discoveries. Ethical questions, such as the use of genetic engineering or artificial intelligence, require value-based judgments that go beyond empirical evidence. Integrating ethical considerations with scientific progress is essential to navigate the societal impact of science responsibly.

References

Add references to the following entries from the Stanford Encyclopedia of Philosophy:

- Scientific Representation
- Scientific Explanation
- Scientific Method
- Scientific Discovery

?? contains an interesting review of the concept of science, the scientific method, and the role that technology plays in our society. The author proposes that the goal of science should be quality, although the concept of quality is left undefined, and how to reconcile the rational and romantic points of view in science. The book also contains some advice about which is the right state of mind to pursue a scientific problem, and how to deal with the inevitable failures.

H. About Quotes and Photos

What we know is little,
combined with tenacious concentration on a subject
and what we are ignorant of is immense.
Pierre-Simon Laplace

TODO: Explain why are important quotes and photos

H.0.1 Quotes

Itroduce this section.

Perfection is achieved not when there is nothing more to add, but when there is nothing left to take away. Antoine de Saint-Exupéry.

This is a critical idea in the theory of nescience, although there are some differencies. I think Saint-Exupéry is talking more about what we have called redudancy, rather than the concept of surfeit. Moreover, Saint-Exupéry is true as long as the inaccuracy is zero.

Computers are useless, they can only give you answers. Pablo Picasso.

As I have said in the Preface of the book, this quote triggered everything.

If presented with a choice between indifferent alternatives, then one ought to select the simplest one. Occam's razor principle.

I am sure that many people will claim that the theory of nescience is just Occam on steroids. By I think there are big differences, as I have already described in the book.

Mathematics may be defined as the subject in which we never know what we are talking about, nor whether what we are saying is true. Bertrand Russell.

Maybe I can talk here about Hilbert-Frege controversy, and what Russell means with this quote.

Sometimes it's the people no one imagines anything of who do the things that no one can imagine. Alan Turing.

Hopefully Turing is talking about me :)

Information is the resolution of uncertainty. Claude Shannon.

TODO: Explain

Some mathematical statements are true for no reason, they're true by accident. Gregory Chaitin.

TODO: Explain

All great work is the fruit of patience and perseverance, combined with tenacious concentration on a subject over a period of months or years. Santiago Ramón y Cajal.

Mention the book of Cajal.

To go where you don't know, you have to go the way you don't know. San Juan de la Cruz

TODO: Explain

We are all agreed that your theory is crazy. The question which divides us is whether it is crazy enough. Niels Bohr.

TODO: Explain

Wanderer, there is no road, the road is made by walking. Antonio Machado.

TODO: Explain

A little inaccuracy sometimes saves tons of explanations. Saki.

TODO: Explain

Everything should be made as simple as possible, but not simpler. Albert Einstein

TODO: Explain

There are known knowns. These are things we know that we know. There are known unknowns. That is to say, there are things that we know we don't know. But there are also unknown unknowns. There are things we don't know we don't know. Donald Rumsfeld.

TODO: Explain

It is not the answer that enlightens, but the question. Eugène Ionesco.

TODO: Explain

Invert, always invert. Carl Gustav Jacob Jacobi.

TODO: Explain

Always look for tricks. Antonio García.

TODO: Explain

Anyone who regards games simply as games and takes work too seriously has grasped little of either. Heinrich Heine.

TODO: Explain

Science may be regarded as the art of data compression. Li & Vitányi.

TODO: Explain

To be surprised, to wonder, is to begin to understand. José Ortega y Gasset.

TODO: Explain

We are to admit no more causes of natural things than such as are both true and sufficient to explain their appearances. Isaac Newton

TODO: Explain

What we know is little, and what we are ignorant of is immense. Pierre-Simon Laplace

TODO: Explain

When academics encounter a new idea that doesn't conform to their preconceptions, there's often a sequence of three reactions: first dismiss, then reject, and finally declare it obvious. S. Sloman and P. Fernbach.

TODO: Explain

H.0.2 Photos

In this Appendix we explain the intended meaning of the photographs included at the beginning of each chapter. All the photographs are royalty-free (or at least this is what Google Images says). Photographs have been preprocessed with GIMP[1], the GNU image manipulation program: we have applied a dotify filter (Artistic filter, GIMPressionist), and then altered the color map (Colors, Colorize) with a Hue/Saturation/Lightness levels of 24/84/10.

The Torch Bearers

The Torch Bearers is an aluminum sculpture created by the American artist Anny Hyatt Huntington, and donated to the city of Madrid in 1955. The sculpture is currently located at Universidad Complutense campus. The sculpture represents and old dying man that before to die pass the torch (a symbol of knowledge) to a young riding man that will continue the quest of perfect knowledge. The artist created other copies in bronze of the same sculpture that are located in Valencia, La Habana, and several cultural organizations around the United States.

Ancient Greek Philosophers

The carved busts of Greek philosophers Socrates, Antisthenes, Chrysippus, and Epicurus, located at the British Museum in London. The ideas and achievements of the ancient Greeks philosophers changed their world and had a huge influence in Western culture. Philosophers like Socrates, Plato and Aristotle formulated the first scientific explanations about how the world worked, and they pioneer a new way of thinking, based on reason and rational thought. The scientific explanation of how the Universe works formulated by Aristotle was accepted as true during more than two thousands years.

Ars Magna

Ars Generalis Ultima or Ars Magna (The Ultimate General Art) was a book published by the Spanish philosopher Raimundo Lulio in 1305. The book contained the description of a mechanical device capable of answering any argument or question abut Christian beliefs by means of using logic and reason. The machine operated by rotating a collection of concentrically arranged circles to combine a fixed set of fundamental concepts. In this way,

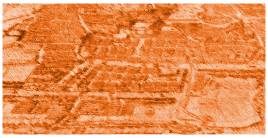
[1] www.gimp.org

the device could show all possible truths about the subject of inquiry. The method was an early attempt to use logical means to produce new knowledge, and it was the inspiration for the methodology of finding interesting questions described in this book.

Galileo's Telescope

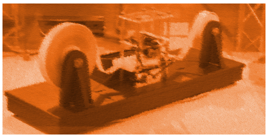
Galileo Galilei was an Italian astronomer, physicist, engineer, philosopher and mathematician. Galileo was the first scientist to clearly state the usefulness of mathematics to discover the laws of nature. Galileo also played a major role in the scientific revolution of the seventeenth century, introducing important innovations in the scientific method. In 1610, Galileo built a telescope and looked up at the heavens. His discoveries revolutionized the field of astronomy and changed our understanding of the Universe.

Königsberg Bridges



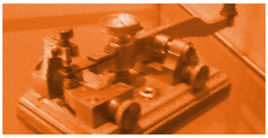
The old city of Königsberg in Prussia (now Kaliningrad, Russia) was laid on both sides of the Pregel river. The city had two large islands which were connected to each other and to mainland by seven bridges. The seven bridges problem is a classical problem in mathematics that asks to devise a walk that would cross each of the seven bridges once and only once, starting and ending at any point, not necessarily the same. The Swiss mathematician Leonhard Euler proved in 1736 that the problem has no solution. The work of Euler laid the foundations of a new mathematical discipline: Graph Theory.

The Turing Machine



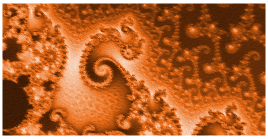
In 1936, the British mathematician Alan Turing proposed a formal model for a hypothetical machine and claimed that his machine could compute anything that humans could compute following an algorithm. The model was a highly convincing one, and simple enough to allow precise mathematical analysis. If fact, the model had many of the ideas that ten years later electrical engineers used to build real computers. The Turing machine was one of this few moments in the history of science in which theory preceded practice.

Morse key



A switching device used to send messages along a wire. The system sends pulses of electric current using the Morse code. Morse code is named after Samuel F. B. Morse, the inventor of the telegraph. The code is composed by a standardized sequence of short and long signals called *dots* and *dashes*, although it is not a binary code, since the code alphabet also includes symbols for the separation between letters and words. The average bit length per character for the English language is 2.53, a remarkable result, given the fact that the code was designed intuitively, without knowing any of the (later discovered) results of coding theory.

Mandelbrot Set



The Mandelbrot set is created by sampling the complex numbers, and determining for each sample whether the result of iterating a function goes to infinity. Treating the real and imaginary parts of each number as image coordinates, pixels are colored according to how rapidly the sequence diverges, with black used for points where the sequence does not diverge. Images of the Mandelbrot set exhibit an elaborate boundary that reveals progressively ever-finer, self-similar, recursive detail at increasing magnifications. However, according to Kolmogorov complexity, the set presents a very low complexity.

XXX: XXX

Xxx xxxx x xxx xx xxxxxx

Athena's Owl

A silver coin depicting the owl that traditionally accompanies Athena. Athena is the virgin goddess of wisdom in Greek mythology. The owl has been used as a symbol of knowledge, wisdom, perspicacity and erudition throughout the Western world, perhaps because their ability to see in the dark. The German philosopher Hegel famously noted that "the owl of [Athena] spreads its wings only with the falling of the dusk", meaning that philosophy comes to understand a historical condition just as it passes away. In this sense, Hegel asserts that Philosophy cannot be prescriptive because it understands only in hindsight.

The Thinker

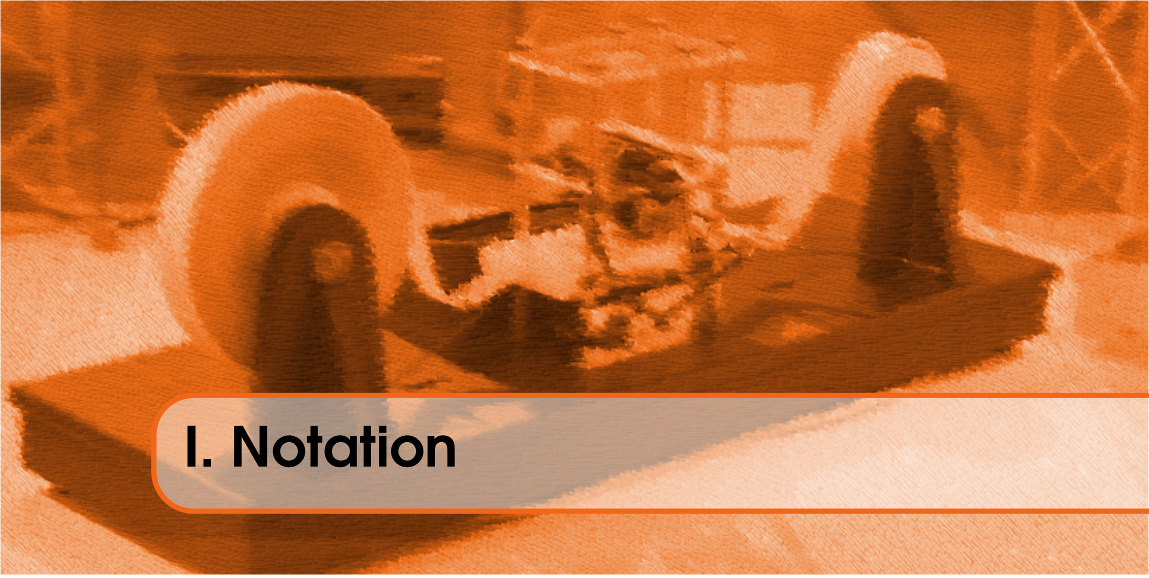
The Thinker is a bronze sculpture created by the French artist Auguste Rodin. The sculpture represents a nude male figure sitting on a rock with his chin resting on one hand. Originally created as part of a larger composition (The Gates of Hell), later the artist decided to treat the figure as an independent work, and at a larger size. There are about 28 full size castings located in museums and public places all around the world (Geneva, Brussels, San Francisco, New York, Buenos Aires, etc.), and many others at different scales. A common interpretation of the sculpture is as an image of the deep thoughts required to find the right questions in philosophy.

R.U.R.

R.U.R. (Rossum Universal Robots) was a highly successful science fiction play written by the Czech Karel Čapek in 1920. The play introduced for the first time the word 'robot' as an alternative to other words used at that time like 'automaton' or 'android'. The word 'robot' derives from the Czech 'robota' meaning "forced labor of the kind that serfs had to perform on their masters' lands". The drama occurs in R.U.R., a factory that makes intelligent robots from artificial flesh and bones, so perfect that they can be mistaken for humans (the name Rossum is derived from the Czech word 'rozum' that means 'reason'). At the beginning robots were happy to work for humans, but then a rebellion starts and all the humans are murdered. At the end of the plot, robots realize that they do not have the knowledge to make new robots, and that by exterminating humans they have triggered their own extinction. The play is considered as a tragic satire about a naive humankind, the dangers of technology, and the obsolescence of God.

Wikipedia Monument

The Wikipedia Monument is located in the city of Słubice, Poland. The statue was designed by Armenian sculptor Mihran Hakobyan, and it was unveiled on October 2014, becoming the world's first monument to the online encyclopedia. The inscription reads: "With this monument the citizens of Słubice would like to pay homage to thousands of anonymous editors all over the world, who have contributed voluntarily to the creation of Wikipedia, the greatest project co-created by people regardless of political, religious or cultural borders. In the year this monument is unveiled Wikipedia is available in more than 280 languages and contains about 30 million articles. The benefactors behind this monument feel certain that with Wikipedia as one of its pillars the knowledge society will be able to contribute to the sustainable development of our civilization, social justice and peace among nations."



I. Notation

When academics encounter a new idea that doesn't conform to their preconceptions,
there's often a sequence of three reactions:
first dismiss, then reject, and finally declare it obvious.
S. Sloman and P. Fernbach

$\mathbb{N}$	set of natural numbers (including 0)
$\mathbb{Z}$	set or integers
$\mathbb{Z}^+$	set or positive integers
$\mathbb{Q}$	set of rational numbers
$\mathbb{R}$	set of real numbers
$\mathbb{R}^+$	set of positive real numbers
$x \in A$	x is a member of A
$:$	set formation
$A \subset B$	A is a subset of B
$A \subseteq B$	A is a subset or equal to B
$\varnothing$	empty set
$d(A)$	cardinality of A
$A \cup B$	union of A and B
$A \cap B$	intersection of A and B

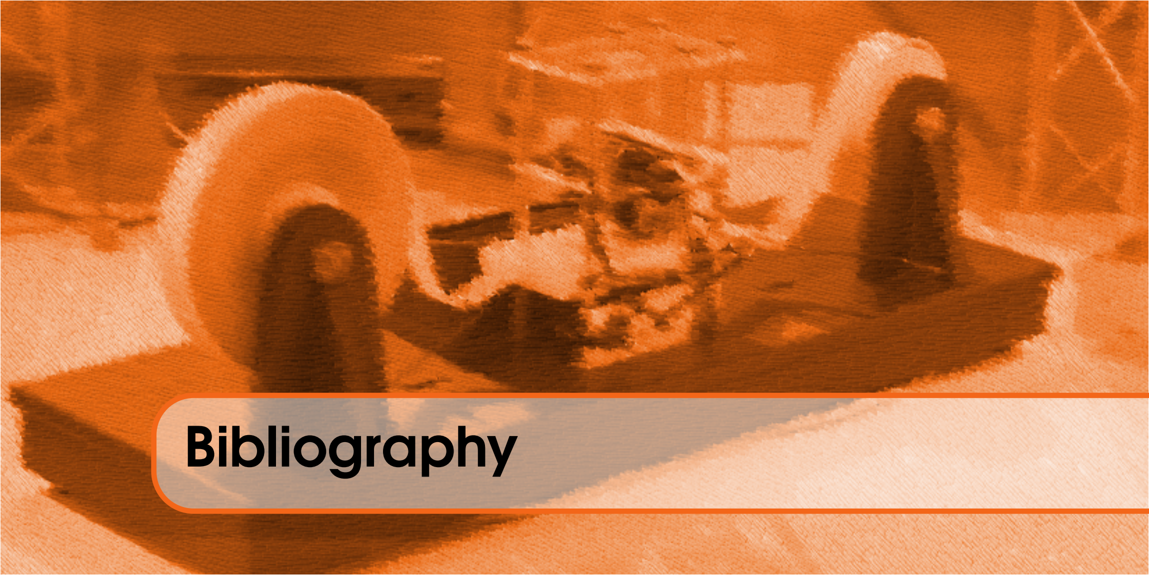
$A \backslash B$	set difference
$\bar{A}$	complement of A
$\mathcal{P}(A)$	power set
(x,y)	ordered pair
$A \times B$	cartesian product
A^n	n-fold cartesian product
R	binary relation
$\leq$	total order
$\max(A)$	maximun
$\min(A)$	minimum
$f(x) = y$	function
$f(x) = \infty$	undefined element
I_A	identity
f^{-1}	inverse function
$f \circ g$	composition
1_A	characteristic function
$abs(x)$	absolute value
$\lceil x \rceil$	ceil
$\lfloor x \rfloor$	floor
$l(s)$	length of string
λ	empty string
s^R	reverse string
$\mathcal{S}^n$	set of strings of length n
$\mathcal{S}^+$	set of all finite strings
$\mathcal{S}^*$	set of all finte string including the empty string
$<_p$	prefix
$\bar{s}$	Self delimited string
$\langle O \rangle$	Encoding as string of O
$G = (V,E)$	graph
$\deg(v)$	degree of a vertex
$N(v)$	neighborhood of a vertex
$indeg(v)$	in-degree of a vertex
$outdeg(v)$	out-degree of a vertex
Ω	sample space
$P(x)$	probability of x
$E(X)$	expectaion of X

T	Turing machine
Q	set of states
Γ	set of tape symbols
$\sqcup$	blank symbol

Σ	input symbols
q_o	initial state
q_f	final state
τ	transition function
C	configuration
C_o	initial configuration
C_f	final configuration
U	universal Turing machine
$\mathcal{E}$	Set of entities
$\mathcal{R}$	Set of representations
$\mathcal{R}_{\mathcal{E}}$	Set of representations of $\mathcal{E}$
$t \in \mathcal{T}$	Research topic
$d \in \mathcal{D}_t$	Description of a topic
$\mathcal{D}$	Set of descriptions
$\mathcal{D}_{\mathcal{T}}$	Set of valid descriptions of $\mathcal{T}$
$\mathcal{D}_t$	Set of descriptions of $t \in \mathcal{T}$
δ	Description function
$d_t^\star$	Perfect description of $t \in \mathcal{T}$
$d_{t,s}$	Joint description of $t, s \in \mathcal{T}$
$\mathcal{D}_{t,s}$	Set of joint descriptions of $t, s \in \mathcal{T}$
$d_{t,s}^\star$	Perfect joint description of $t, s \in \mathcal{T}$
$d_{t\|s^\star}$	Conditional description of t given s, $t, s \in \mathcal{T}$
$\mathcal{D}_{t\|s^\star}$	Set of conditional descriptions of t given s, $t, s \in \mathcal{T}$
$d_{t\|s^\star}^\star$	Perfect conditional description of t given s, $t, s \in \mathcal{T}$
$A \subset \mathcal{T}$	Research area
$\hat{A}$	Know subset of the area $A \subset \mathcal{T}$
$\mathcal{D}_{\hat{A}}$	Desription of the area A given the known subset $\hat{A}$
$\mathcal{D}_{\hat{A}}$	Set of descriptions of the area A given the known subset $\hat{A}$
$d_{\hat{A}}^\star$	Perfect description of the area A given the known subset $\hat{A}$
RG	relevance graph
R_t	relevance of topic t
IP_t	interestingness of topic t as a problem
M_t	maturity of topic t
AG	applicability graph
A_t	applicability of topic t
IT_t	interestingness of topic t as a tool
T'	set of known topics
$Q_{t_1 \to t_2}$	interesting question
$IQ_{t_1 \to t_2}$	interestingness of question $Q_{t_1 \to t_2}$
$\mathbb{F}$	unknown frontier

$\mathbb{S}$ new topics area
$S_{\{t_1,t_2\}}$ new topic
$IS_{\{t_1,t_2\}}$ interestingness of a new topic
IT_A interestingess of an area as tool
IP_A interestingess of an area as problem

$\hat{\imath}(\hat{\mathbf{y}},\mathbf{y})$ inaccuracy of predicted values



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