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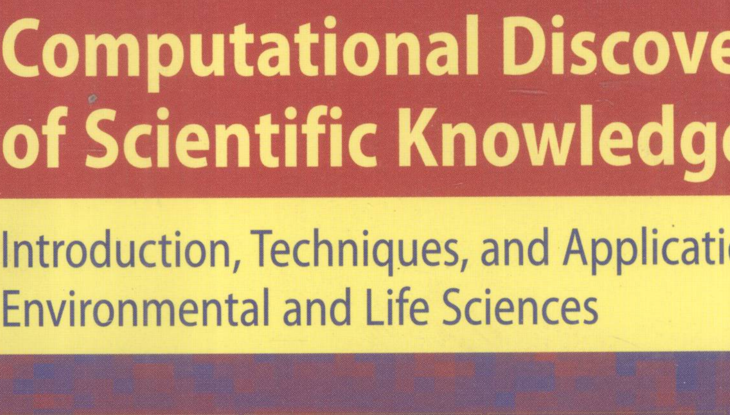
Ljupčo Todorovski (Eds.)

Computational Discovery of Scientific Knowledge

Introduction, Techniques, and Applications in Environmental and Life Sciences



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Preface

Advances in technology have enabled the collection of data from scientific observations, simulations, and experiments at an ever-increasing pace. For the scientist and engineer to benefit from these enhanced data-collecting capabilities, it is becoming clear that semi-automated data analysis techniques must be applied to find the useful information in the data. Techniques from both data mining and computational discovery can be used to that end.

Computational scientific discovery focuses on applying computational methods to automate scientific activities, such as finding laws from observational data. It has emerged from the view that science is a problem-solving activity and that problem solving can be cast as search through a space of possible solutions. Early research on computational discovery within the fields of artificial intelligence and cognitive science focused on reconstructing episodes from the history of science. This typically included identifying data and knowledge available at the time and implementing a computer program that models the scientific activities and processes that led to the scientist's insight.

Recent efforts in this area have focused on individual scientific activities (such as formulating quantitative laws) and have produced a number of new scientific discoveries, many of them leading to publications in the relevant scientific literatures. The discoveries made using computational tools include qualitative laws of metallic behavior, quantitative conjectures in graph theory, and temporal laws of ecological behavior. Work in this paradigm has emphasized formalisms used to communicate among scientists, including numeric equations, structural models, and reaction pathways.

However, in recent years, research on data mining and knowledge discovery has produced another paradigm. Data mining is concerned with finding patterns (regularities) in data. Even when applied to scientific domains, such as astronomy, biology, and chemistry, this framework employs formalisms developed by artificial intelligence researchers themselves, such as decision trees, rule sets, and Bayesian networks. Although such methods can produce predictive models that are highly accurate, their outputs are not cast in terms familiar to scientists, and thus typically are not very communicable.

Mining scientific data focuses on building highly predictive models, rather than producing knowledge in any standard scientific notation. In contrast, much of the work in computational scientific discovery has put a strong emphasis on formalisms used by scientists to communicate scientific knowledge, such as numeric equations, structural models, and reaction pathways. In this sense, computational scientific discovery is complementary to mining scientific data.

The book provides an introduction to computational approaches to the discovery of communicable scientific knowledge and gives an overview of recent advances in this area. The primary focus is on discovery in scientific and engineering disciplines, where communication of knowledge is often a central concern.

This volume has its origins in the symposium "Computational Discovery of Communicable Knowledge," organized by Pat Langley, held March 24-25, 2001 at Stanford University. A detailed report on the symposium can be found in the Proceedings of the DS-2001 Conference (S. Džeroski, and P. Langley. Computational discovery of communicable knowledge: Symposium report. In *Proceedings of the Fourth International Conference on Discovery Science*, pages 45-49. Springer, Berlin, 2001). Many of the presentations from that symposium have a corresponding chapter in the book. To achieve a more representative coverage of recent research in computational discovery, we have invited a number of additional contributions as well.

The book is organized as follows. The first chapter introduces the field of computational scientific discovery and provides a brief overview thereof. It also provides a more detailed overview of the contents of the book. The majority of the contributed chapters fall within two broad categories, which correspond to Parts I and II of the book, respectively. The first describes a number of computational discovery methods for system identification and automated modelling, while the second discusses a number of methods for computational discovery developed for biomedical and bioinformatics applications.

In the first part of the book, the focus is on establishing models of dynamic systems, i.e., systems that change their state over time. The models are mostly based on equations, in particular ordinary differential equations that represent a standard formalism for modelling dynamic systems in many engineering and scientific areas. This is in contrast to the bulk of previous research on equation discovery, which focuses on algebraic equations. Topics covered in this part include a reasoning tool for nonlinear system identification, the use of different forms of domain knowledge when inducing models of dynamic systems (including the use of existing models for theory revision, partial knowledge of the target model, knowledge on basic processes, and knowledge on measurement scales of the system variables), and applications to Earth sciences.

While the first part of the book focuses on a class of methods and covers a variety of scientific fields and areas, the second focuses on the field of biomedicine. The first three chapters are in line with the first part of the book and continue with the theme of model formation, but use representation formalisms specific to the biomedical field, such as chemical reaction networks and genetic pathways. The last two chapters present approaches to forming scientific hypotheses by connecting disconnected scientific literatures on the same topic. This part also includes a chapter on using learning in logic for predicting gene function.

We would like to conclude with some words of thanks. Pat Langley organized the symposium that motivated this volume and encouraged us to edit it. More importantly, he has pioneered research on computational scientific discovery and provided unrelenting support to our research in this area. We would also like to thank the participants of the symposium. Finally, we would like to thank all the contributors to this volume for their excellent contributions and their patience with the editors.

May 2007

Sašo Džeroski
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Lecture Notes in Artificial Intelligence (LNAI)

Vol. 4660: S. Džeroski, L. Todorovski (Eds.), Computational Discovery of Scientific Knowledge. X, 327 pages. 2007.

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Table of Contents

I Equation Discovery and Dynamic Systems Identification

II Computational Scientific Discovery in Biomedicine

Computational Discovery of Scientific Knowledge

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Abstract. This chapter introduces the field of computational scientific discovery and provides a brief overview thereof. We first try to be more specific about what scientific discovery is and also place it in the broader context of the scientific enterprise. We discuss the components of scientific behavior, that is, the knowledge structures that arise in science and the processes that manipulate them. We give a brief historical review of research in computational scientific discovery and discuss the lessons learned, especially in relation to work in data mining that has recently received substantial attention. Finally, we discuss the contents of the book and how it fits in the overall framework of computational scientific discovery.

1 Introduction

This book deals with computational approaches to scientific discovery. Research on computational scientific discovery aims to develop computer systems which produce results that, if a human scientist did the same, we would refer to as discoveries. Of course, if we hope to develop computational methods for scientific discovery, we must be more specific about the nature of such discoveries and how they relate to the broader context of the scientific enterprise.

The term science refers both to scientific knowledge and the process of acquiring such knowledge. It includes any systematic field of study that relates to observed phenomena (as opposed to mathematics) and that involves claims which can be tested empirically (as opposed to philosophy). We will attempt to characterize science more fully later in the chapter, but one thing is clear: Science is about knowledge.

Science is perhaps the most complex human intellectual activity, which makes it difficult to describe. Shrager and Langley (1990) analyze it in terms of the knowledge structures that scientists consider and the processes or activities they use to transform them. Basic knowledge structures that arise in science include observations, laws, and theories, and related activities include data collection, law formation, and theory construction.

S. Džeroski and L. Todorovski (Eds.): Computational Discovery, LNAI 4660, pp. 1–14, 2007.

There are two primary reasons why we might want to study scientific discovery from a computational perspective:

- to understand how humans perform this intriguing activity, which belongs to the realm of cognitive science; and
- to automate or assist in facets of the scientific process, which belongs to the realm of artificial intelligence.

Science is a highly complex intellectual endeavor, and discovery is arguably the most creative part of the scientific process. Thus, efforts to automate it completely would rightfully be judged as audacious, but, as Simon (1966) noted, one can view many kinds of scientific discovery as examples of problem solving through heuristic search. Most research in automating scientific discovery has focused on small, well-defined tasks that are amenable to such treatment and that allow measurable progress.

Traditional accounts of science (Klemke et al., 1998) focus on the individual, who supposedly observes nature, hypothesizes laws or theories, and tests them against new observations. Most computational models of scientific discovery share this concern with individual behavior. However, science is almost always a collective activity that is conducted by interacting members of a scientific community. The most fundamental demonstration of this fact is the emphasize placed on communicating one's findings to other researchers in journal articles and conference presentations.

This emphasis on exchanging results makes it essential that scientific knowledge be *communicable*. We will not attempt to define this term, but it seems clear that contributions are more communicable if they are cast in established formalisms and if they make contact with concepts that are familiar to most researchers in the respective field of study. The research reported in this book focuses on computational discovery of such communicable knowledge.

In the remainder of this chapter, we first examine more closely the scientific method and its relation to scientific discovery. After this, we discuss the components of scientific behavior, that is, the knowledge structures that arise in science and the processes that manipulate them. We then give a brief historical review of research in computational scientific discovery and discuss the lessons learned, especially in relation to work in data mining that has recently received substantial attention. Finally, we discuss the contents of the book and how it fits in the overall framework of computational scientific discovery.

2 The Scientific Method and Scientific Discovery

The Merriam-Webster Dictionary (2003) defines science as: "a) knowledge or a system of knowledge covering general truths or the operation of general laws, especially as obtained and tested through the scientific method, and b) such knowledge or such a system of knowledge concerned with the physical world and its phenomena". The scientific method, in turn, is defined as the "principles and procedures for the systematic pursuit of knowledge involving the recognition and formulation of a problem, the collection of data through observation and experiment, and the formulation and testing of hypotheses".

While there is consensus that science revolves around knowledge, there are different views in the philosophy of science (Klemke et al., 1998; Achinstein, 2004) about the nature of its content. The 'causal realism' position is that scientific knowledge is ontological, in that it identifies entities in the world, their causal powers, and the mechanisms through which they exert influence. In contrast, the 'constructive empiricism' tradition states that, scientific theories are objective, testable, and predictive. We believe that both frameworks are correct, in that they describe different facets of the truth.

The *scientific method* (Gower, 1996), dedicated to the systematic pursuit of reliable knowledge, incorporates a number of steps. First we must ask some meaningful question or identify a significant problem. We must next gather information relevant to the question, which might include existing scientific knowledge or new observations. We then formulate a hypothesis that could plausibly answer the question.

Next we must test this proposal by making observations and determining whether they are consistent with the hypothesis' predictions. When observations are consistent with the hypothesis, they lend it support and we may consider publishing it. If other scientists can reproduce our results, then the community comes to consider it as reliable knowledge. In contrast, if the observations are inconsistent, we should reject the hypothesis and either abandon it or, more typically, modify it, at which point the testing process continues. Hypotheses can take many different forms, including taxonomies, empirical laws, and explanatory theories, but all of them can be evaluated by comparing their implications to observed phenomena.

Most analyses of the scientific method come from philosophers of science, who have focused mainly on the evaluation of hypotheses and largely ignored their generation and revision. Unfortunately, what we refer to as discovery resides in just these activities. Thus, although there is a large literature on normative methods for making predictions from hypotheses, checking their consistency, and determining whether they are valid, there are remarkably few treatments of their production. Some (e.g., Popper (1959)) have even suggested that rational accounts of the discovery process are impossible. A few philosophers (e.g., Darden (2006); Hanson (1958); Lakatos (1976)) have gone against this trend and made important contributions to the topic, but most efforts have come from artificial intelligence and cognitive science.

Briefly, scientific discovery is the process by which a scientist creates or finds some hitherto unknown knowledge, such as a class of objects, an empirical law, or an explanatory theory. The knowledge in question may also be referred to as a scientific discovery. An important aspect of many knowledge structures, such as laws and theories, is their generality, in that they apply to many specific situations or many specific observations. We maintain that generality is an essential feature of a meaningful discovery, as will become apparent in the next section when we discuss types of scientific knowledge.

A defining aspect of discovery is that the knowledge should be new and previously unknown. Naturally, one might ask 'new to whom?'. We take the position that the knowledge should be unknown to the scientist in question with respect to the observations and background knowledge available to him when he made the discovery. This means that two or more scientists can make the same discovery independently, sometimes years apart, which has indeed happened in practice many times throughout the history of science. In this view, scientific discovery concerns a change in an individual's knowledge, which means that developing computer systems that reproduce events from the history of science can still provide important insights into the nature of discovery processes.

3 The Elements of Scientific Behavior

To describe scientific behavior, we follow Shrager and Langley (1990) and use as basic components knowledge structures and the activities that transform them. The former represent the raw materials and products of science, while the latter concern the process of producing scientific knowledge. The account below mostly follows the earlier treatise, but the definitions of several knowledge structures and activities have changed, reflecting improvements in our understanding over the past 15 years.

3.1 Scientific Knowledge Structures

Science is largely about understanding the world in which we live. To this end, we gather information about the world. Observation is the primary means of collecting this information, and observations are the primary input to the process of scientific discovery.

Observations (or data) represent recordings of the environment made by sensors or measuring instruments. Typically, the state of the environment varies over time or under different conditions, and one makes recordings for these different states, where what constitutes a state depends on the object of scientific study. We will refer to each of these recordings as an observation.

We can identify three important types of scientific knowledge – taxonomies, laws, and theories – that constitute the major products of the scientific enterprise. The creation of new taxonomies, laws, and theories, as well as revising and improving existing ones, make up the bulk of scientific discovery, making them some of the key activities in science.

- *Taxonomies* define or describe concepts for a domain, along with specialization relations among them. A prototypical example is the taxonomy for biological organisms, which are grouped into species, genera, families, and so forth, but similar structures play important roles in particle physics, chemistry, astronomy, and many other sciences. Taxonomies specify the concepts and terms used to state laws and theories.
- *Laws* summarize relations among observed variables, objects, or events. For example, Black's heat law states that mixing two substances produces a

temperature increases in one substance and a decrease in the other until they reach equilibrium. The law also describes a precise numeric relationship between the initial and final temperatures. The first statement is qualitative in form, whereas the latter is quantitative. Some laws may be quite general, whereas others may be very specific.

- *Theories* are statements about the structures or processes that arise in the environment. A theory is stated using terms from the domain's taxonomy and interconnects a set of laws into a unified theoretical account. For example, Boyle's law describes the inverse relation between the pressure and volume of a gas, whereas Charles' law states the direct relation between its temperature and pressure. The kinetic theory of gases provides a unifying account for both, explaining them in terms of Newtonian interactions among unobserved molecules.

Note that all three kinds of knowledge are important and present in the body of scientific knowledge. Different types of knowledge are generated at different stages in the development of a scientific discipline. Taxonomies are generated early in a field's history, providing the basic concepts for the discipline. After this, scientists formulate empirical laws based on their observations. Eventually, these laws give rise to theories that provide a deeper understanding of the structures and processes studied in the discipline.

A knowledge structure that a scientist has proposed, but that has not yet been tested with respect to observations, is termed an hypothesis. Note that taxonomies, laws, and theories can all have this status. As mentioned earlier, hypotheses must be evaluated to determine whether they are consistent with observations (and background knowledge). If it is consistent, we say that a hypothesis has been corroborated and it comes to be viewed as scientific knowledge. If an hypothesis is inconsistent with the evidence, then we either reject or modify it, giving rise to a new hypothesis that is further tested and evaluated.

Background knowledge is knowledge about the environment separate from that specifically under study. It typically includes previously generated scientific knowledge in the domain of study. Such knowledge differs from theories or laws at the hypothesis stage, in that the scientist regards it with relative certainty rather than as the subject of active evaluation. Scientific knowledge begins its life cycle as a hypothesis which (if corroborated) becomes background knowledge.

Besides the basic data and knowledge types considered above, several other types of structures play important roles in science. These include models, predictions, and explanations. These occupy an intermediate position, as they are derived from laws and theories and, as such, they are not primary products of the scientific process.

- *Models* are special cases of laws and theories that apply to particular situations in the environment and only hold under certain environmental conditions. These conditions specify the particular experimental or observational setting, with the model indicating how the law or theory applies in the setting. By applying laws and theories to a particular setting, models make it possible to use these for making predictions.

- *Predictions* represent expectations about the behavior of the environment under specific conditions. In science, a model is typically used to make a prediction, and then an actual observation is made of the behavior in the environment. Postdictions are analogous to predictions, except that the scientist generates them after making the observations he or she intends to explain. A prediction/postdiction that is consistent with the respective observation is successful and lends support to the model (and the respective law/theory) that produced it.
- *Explanations* are narratives that connect a theory to a law (or a model to a prediction) by a chain of inferences appropriate to the field. In such cases, we say that the theory explains the law. In some disciplines, inference chains must be deductive or mathematical. If a law cannot be explained by a theory (or a prediction by a model), we have an anomaly that brings either the theory or the observation into question.

3.2 Scientific Activities

Scientific processes and activities are concerned with generating and manipulating scientific data and knowledge structures. Here we consider the processes and activities in the same order as we discussed the structures that they generate in the previous subsection.

The process of observation involves inspecting the environmental setting by focusing an instrument, sometimes simply the agent's senses, on that setting. The result is a concrete description of the setting, expressed in terms from the agent's taxonomy and guided by the model of the setting. Since one can observe many things in any given situation, the observer must select some aspects to record and some to ignore.

As we have noted, scientific discovery is concerned with generating scientific knowledge in the form of taxonomies, laws and theories. These can be generated directly from observations (and possibly background knowledge), but, quite often, scientists modify an existing taxonomy, law, or theory to take into account anomalous observations that it cannot handle.

- *Taxonomy formation (and revision)* involves the organization of observations into classes and subclasses, along with the definition of those classes. This process may operate on, or take into account, an existing taxonomy or background knowledge. For instance, early chemists organized certain chemicals into the classes of acids, alkalis, and salts to summarize regularities in their taste and behavior. As time went on, they refined this taxonomy and modified the definitions of each class.
- *Inductive law formation (and revision)* involves the generation of empirical laws that cover observed data. The laws are stated using terms from the agent's taxonomy, and they are constrained by a model of the setting and possibly by the scientist's background knowledge. In some cases, the scientist may generate an entirely new law; in others, he may modify or extend an existing law.