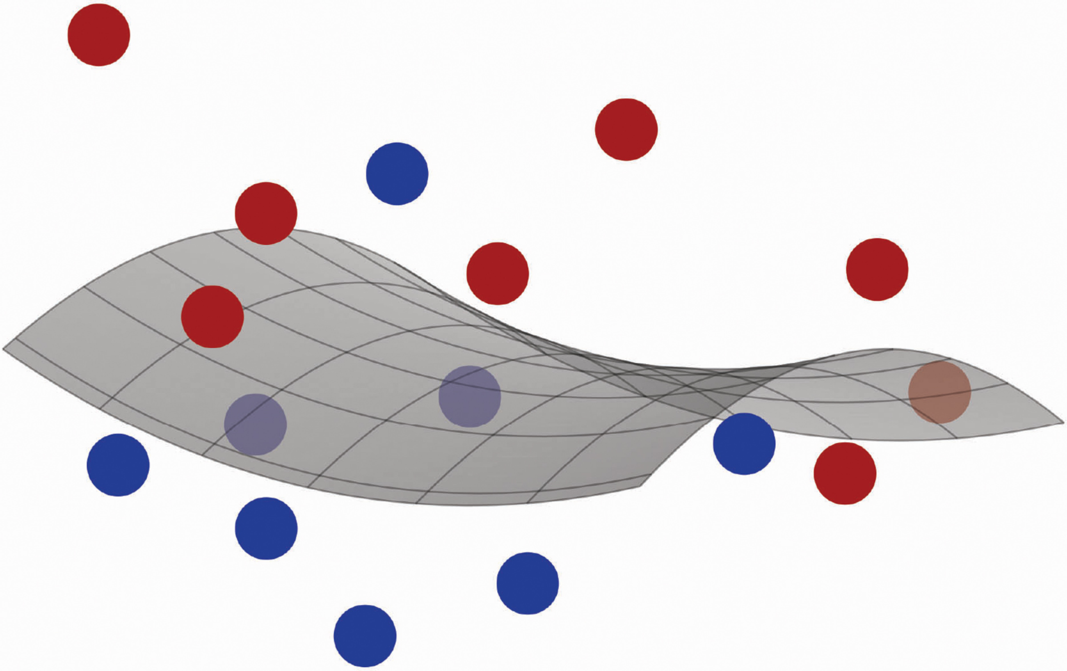
Foundations of Machine Learning

second edition



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Preface

This book is a general introduction to machine learning that can serve as a reference book for researchers and a textbook for students. It covers fundamental modern topics in machine learning while providing the theoretical basis and conceptual tools needed for the discussion and justification of algorithms. It also describes several key aspects of the application of these algorithms.

We have aimed to present the most novel theoretical tools and concepts while giving concise proofs, even for relatively advanced results. In general, whenever possible, we have chosen to favor succinctness. Nevertheless, we discuss some crucial complex topics arising in machine learning and highlight several open research questions. Certain topics often merged with others or treated with insufficient attention are discussed separately here and with more emphasis: for example, a different chapter is reserved for multi-class classification, ranking, and regression.

Although we cover a very wide variety of important topics in machine learning, we have chosen to omit a few important ones, including graphical models and neural networks, both for the sake of brevity and because of the current lack of solid theoretical guarantees for some methods.

The book is intended for students and researchers in machine learning, statistics and other related areas. It can be used as a textbook for both graduate and advanced undergraduate classes in machine learning or as a reference text for a research seminar. The first three or four chapters of the book lay the theoretical foundation for the subsequent material. Other chapters are mostly self-contained, with the exception of chapter 6 which introduces some concepts that are extensively used in later ones and chapter 13, which is closely related to chapter 12. Each chapter concludes with a series of exercises, with full solutions presented separately.

The reader is assumed to be familiar with basic concepts in linear algebra, probability, and analysis of algorithms. However, to further help, we have included an extensive appendix presenting a concise review of linear algebra, an introduction to convex optimization, a brief probability review, a collection of concentration inequalities useful to the analyses and discussions in this book, and a short introduction to information theory.

Our goal has been to give a unified presentation of multiple topics and areas, as opposed to a more specialized presentation adopted by some books which favor a particular viewpoint, such as for example a Bayesian view, or a particular topic, such as for example kernel methods. The theoretical foundation of this book and its deliberate emphasis on proofs and analysis make it also very distinct from many other presentations.

In this second edition, we have updated the entire book. The changes include a different writing style in most chapters, new figures and illustrations, many simplifications, some additions to existing chapters, in particular chapter 6 and chapter 17, and several new chapters. We have added a full chapter on model selection (chapter 4), which is an important topic that was only briefly discussed in the previous edition. We have also added a new chapter on Maximum Entropy models (chapter 12) and a new chapter on Conditional Maximum Entropy models (chapter 13) which are both essential topics in machine learning. We have also significantly changed the appendix. In particular, we have added a full section on Fenchel duality to appendix B on convex optimization, made a number of changes and additions to appendix D dealing with concentration inequalities, added appendix E on information theory, and updated most of the material. Additionally, we have included a number of new exercises and their solutions for existing and new chapters.

Most of the material presented here takes its origins in a machine learning graduate course (*Foundations of Machine Learning*) taught by the first author at the Courant Institute of Mathematical Sciences in New York University over the last fourteen years. This book has considerably benefited from the comments and suggestions from students in these classes, along with those of many friends, colleagues and researchers to whom we are deeply indebted.

We are particularly grateful to Corinna Cortes and Yishay Mansour who made a number of key suggestions for the design and organization of the material presented in the first edition, with detailed comments that we have fully taken into account and that have greatly improved the presentation. We are also grateful to Yishay Mansour for using a preliminary version of the first edition of the book for teaching, and for reporting his feedback to us.

We also thank for discussions, suggested improvement, and contributions of many kinds the following colleagues and friends from academic and corporate research laboratories: Jacob Abernethy, Cyril Allauzen, Kareem Amin, Stephen Boyd, Aldo Corbisiero, Giulia DeSalvo, Claudio Gentile, Spencer Greenberg, Lisa Hellerstein, Sanjiv Kumar, Vitaly Kuznetsov, Ryan McDonald, Andrès Muñoz Medina, Tyler Neylon, Peter Norvig, Fernando Pereira, Maria Pershina, Borja de Balle Pigem, Ashish Rastogi, Michael Riley, Dmitry Storcheus, Ananda Theertha Suresh, Umar Syed, Csaba Szepesvári, Toshiyuki Tanaka, Eugene Weinstein, Jason Weston, Scott Yang, and Ningshan Zhang.

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1 Introduction

This chapter presents a preliminary introduction to machine learning, including an overview of some key learning tasks and applications, basic definitions and terminology, and the discussion of some general scenarios.

1.1 What is machine learning?

Machine learning can be broadly defined as computational methods using experience to improve performance or to make accurate predictions. Here, *experience* refers to the past information available to the learner, which typically takes the form of electronic data collected and made available for analysis. This data could be in the form of digitized human-labeled training sets, or other types of information obtained via interaction with the environment. In all cases, its quality and size are crucial to the success of the predictions made by the learner.

An example of a learning problem is how to use a finite sample of randomly selected documents, each labeled with a topic, to accurately predict the topic of unseen documents. Clearly, the larger is the sample, the easier is the task. But the difficulty of the task also depends on the quality of the labels assigned to the documents in the sample, since the labels may not be all correct, and on the number of possible topics.

Machine learning consists of designing efficient and accurate prediction *algorithms*. As in other areas of computer science, some critical measures of the quality of these algorithms are their time and space complexity. But, in machine learning, we will need additionally a notion of *sample complexity* to evaluate the sample size required for the algorithm to learn a family of concepts. More generally, theoretical learning guarantees for an algorithm depend on the complexity of the concept classes considered and the size of the training sample.

Since the success of a learning algorithm depends on the data used, machine learning is inherently related to data analysis and statistics. More generally, learning