

Understanding Machine Learning

Machine learning is one of the fastest growing areas of computer science, with far-reaching applications. The aim of this textbook is to introduce machine learning, and the algorithmic paradigms it offers, in a principled way. The book provides an extensive theoretical account of the fundamental ideas underlying machine learning and the mathematical derivations that transform these principles into practical algorithms. Following a presentation of the basics of the field, the book covers a wide array of central topics that have not been addressed by previous textbooks. These include a discussion of the computational complexity of learning and the concepts of convexity and stability; important algorithmic paradigms including stochastic gradient descent, neural networks, and structured output learning; and emerging theoretical concepts such as the PAC-Bayes approach and compression-based bounds. Designed for an advanced undergraduate or beginning graduate course, the text makes the fundamentals and algorithms of machine learning accessible to students and nonexpert readers in statistics, computer science, mathematics, and engineering.

Shai Shalev-Shwartz is an Associate Professor in the School of Computer Science and Engineering at The Hebrew University, Israel.

Shai Ben-David is a Professor in the School of Computer Science at the University of Waterloo, Canada.





UNDERSTANDING MACHINE LEARNING

From Theory to Algorithms

Shai Shalev-Shwartz

The Hebrew University, Jerusalem

Shai Ben-David

University of Waterloo, Canada





CAMBRIDGE UNIVERSITY PRESS

32 Avenue of the Americas, New York, NY 10013-2473, USA

Cambridge University Press is part of the University of Cambridge.

It furthers the University's mission by disseminating knowledge in the pursuit of education, learning, and research at the highest international levels of excellence.

www.cambridge.org
Information on this title: www.cambridge.org/9781107057135

© Shai Shalev-Shwartz and Shai Ben-David 2014

This publication is in copyright. Subject to statutory exception and to the provisions of relevant collective licensing agreements, no reproduction of any part may take place without the written permission of Cambridge University Press.

First published 2014

Printed in the United States of America

 $A\ catalog\ record\ for\ this\ publication\ is\ available\ from\ the\ British\ Library.$

Library of Congress Cataloging in Publication data
Shalev-Shwartz, Shai.
Understanding machine learning: from theory to algorithms /
Shai Shalev-Shwartz, The Hebrew University, Jerusalem,
Shai Ben-David, University of Waterloo, Canada.
pages cm
Includes bibliographical references and index.
ISBN 978-1-107-05713-5 (hardback)
1. Machine learning. 2. Algorithms. I. Ben-David, Shai. II. Title.
Q325.5.S475 2014
006.3'1-dc23 2014001779

ISBN 978-1-107-05713-5 Hardback

Cambridge University Press has no responsibility for the persistence or accuracy of URLs for external or third-party Internet Web sites referred to in this publication and does not guarantee that any content on such Web sites is, or will remain, accurate or appropriate.



Triple-S dedicates the book to triple-M





Contents

Preface		page xv	
1	Introd	uction	1
	1.1	What Is Learning?	1
	1.2	When Do We Need Machine Learning?	3
	1.3		4
	1.4	Relations to Other Fields	6
	1.5	How to Read This Book	7
	1.6	Notation	8
Pa	rt 1 Fo	undations	
2	A Gen	tle Start	13
	2.1	A Formal Model – The Statistical Learning Framework	13
	2.2	Empirical Risk Minimization	15
	2.3	Empirical Risk Minimization with Inductive Bias	16
	2.4	Exercises	20
3	A Forn	nal Learning Model	22
	3.1	PAC Learning	22
	3.2	A More General Learning Model	23
	3.3	Summary	28
	3.4	Bibliographic Remarks	28
	3.5	e .	28
4	Learni	ng via Uniform Convergence	31
	4.1	Uniform Convergence Is Sufficient for Learnability	31
	4.2	Finite Classes Are Agnostic PAC Learnable	32
	4.3	Summary	34
	4.4	Bibliographic Remarks	35
	4.5	Exercises	35

vii



viii Contents

5	The Bi	as-Complexity Trade-off	36
	5.1	The No-Free-Lunch Theorem	37
	5.2	Error Decomposition	4(
	5.3	Summary	41
	5.4	Bibliographic Remarks	41
	5.5	Exercises	41
6	The V	C-Dimension	43
	6.1	Infinite-Size Classes Can Be Learnable	43
	6.2	The VC-Dimension	44
	6.3	Examples	46
	6.4	The Fundamental Theorem of PAC Learning	48
	6.5	Proof of Theorem 6.7	49
	6.6	Summary	53
	6.7	Bibliographic Remarks	53
	6.8	Exercises	54
7	Nonur	niform Learnability	58
	7.1	Nonuniform Learnability	58
	7.2	Structural Risk Minimization	60
	7.3	Minimum Description Length and Occam's Razor	63
	7.4	Other Notions of Learnability – Consistency	66
	7.5		67
	7.6	Summary	70
	7.7	Bibliographic Remarks	70
	7.8	Exercises	71
8	The R	untime of Learning	73
	8.1	Computational Complexity of Learning	74
	8.2	Implementing the ERM Rule	76
	8.3	Efficiently Learnable, but Not by a Proper ERM	80
	8.4	Hardness of Learning*	81
	8.5	Summary	82
	8.6	Bibliographic Remarks	82
	8.7		83
Par	t 2 Fro	om Theory to Algorithms	
9	Linear	Predictors	89
	9.1	Halfspaces	90
	9.2	Linear Regression	94
	9.3	Logistic Regression	97
	9.4	Summary	99
	9.5	Bibliographic Remarks	99
	9.6	Exercises Exercises	99
	,	· · · · · · · · · · · · · · · · · · ·	



		Contents	ix
10	Boosting	101	
	10.1 Weak Learnability	102	
	10.2 AdaBoost	105	
	10.3 Linear Combinations of Base Hypotheses	108	
	10.4 AdaBoost for Face Recognition	110	
	10.5 Summary	111	
	10.6 Bibliographic Remarks	111	
	10.7 Exercises	112	
11	Model Selection and Validation	114	
	11.1 Model Selection Using SRM	115	
	11.2 Validation	116	
	11.3 What to Do If Learning Fails	120	
	11.4 Summary	123	
	11.5 Exercises	123	
12	Convex Learning Problems	124	
	12.1 Convexity, Lipschitzness, and Smoothness	124	
	12.2 Convex Learning Problems	130	
	12.3 Surrogate Loss Functions	134	
	12.4 Summary	135	
	12.5 Bibliographic Remarks	136	
	12.6 Exercises	136	
13	Regularization and Stability	137	
	13.1 Regularized Loss Minimization	137	
	13.2 Stable Rules Do Not Overfit	139	
	13.3 Tikhonov Regularization as a Stabilizer	140	
	13.4 Controlling the Fitting-Stability Trade-off	144	
	13.5 Summary	146	
	13.6 Bibliographic Remarks	146	
	13.7 Exercises	147	
14	Stochastic Gradient Descent	150	
	14.1 Gradient Descent	151	
	14.2 Subgradients	154	
	14.3 Stochastic Gradient Descent (SGD)	156	
	14.4 Variants	159	
	14.5 Learning with SGD	162	
	14.6 Summary	165	
	14.7 Bibliographic Remarks	166	
	14.8 Exercises	166	
15	Support Vector Machines	167	
	15.1 Margin and Hard-SVM	167	
	15.2 Soft-SVM and Norm Regularization	171	
	15.3 Optimality Conditions and "Support Vectors"	* 175	



x Contents

	15.4	Duality*	175
	15.5	Implementing Soft-SVM Using SGD	176
	15.6	Summary	177
	15.7	Bibliographic Remarks	177
	15.8	Exercises	178
16	Kernel	Methods	179
	16.1	Embeddings into Feature Spaces	179
	16.2	The Kernel Trick	181
	16.3	Implementing Soft-SVM with Kernels	186
		Summary	187
		Bibliographic Remarks	188
	16.6	Exercises	188
17	Multicl	ass, Ranking, and Complex Prediction Problems	190
	17.1	One-versus-All and All-Pairs	190
	17.2	Linear Multiclass Predictors	193
	17.3	Structured Output Prediction	198
		Ranking	201
		Bipartite Ranking and Multivariate Performance Measures	206
		Summary	209
		Bibliographic Remarks	210
	17.8	Exercises	210
18	Decision	on Trees	212
		Sample Complexity	213
		Decision Tree Algorithms	214
		Random Forests	217
		Summary	217
		Bibliographic Remarks	218
	18.6	Exercises	218
19	Neares	st Neighbor	219
		k Nearest Neighbors	219
		Analysis	220
		Efficient Implementation*	225
		Summary	225
		Bibliographic Remarks	225
	19.6	Exercises	225
20		Notworks	228
20	Neural		220
20	20.1	Feedforward Neural Networks	229
20	20.1 20.2	Feedforward Neural Networks Learning Neural Networks	229 230
20	20.1 20.2 20.3	Feedforward Neural Networks Learning Neural Networks The Expressive Power of Neural Networks	229 230 231
20	20.1 20.2 20.3 20.4	Feedforward Neural Networks Learning Neural Networks The Expressive Power of Neural Networks The Sample Complexity of Neural Networks	229 230 231 234
20	20.1 20.2 20.3 20.4 20.5	Feedforward Neural Networks Learning Neural Networks The Expressive Power of Neural Networks	229 230 231



			Contents	хi
	20.7	Summary	240	
	20.8	Bibliographic Remarks	240	
	20.9	Exercises	240	
Part	t 3 Add	ditional Learning Models		
21	Online	Learning	245	
	21.1	Online Classification in the Realizable Case	246	
		Online Classification in the Unrealizable Case	251	
		Online Convex Optimization	257	
		The Online Perceptron Algorithm	258	
		Summary	261	
		Bibliographic Remarks	261	
		Exercises	262	
22	Cluste	ring	264	
	22.1	Linkage-Based Clustering Algorithms	266	
		k-Means and Other Cost Minimization Clusterings	268	
		Spectral Clustering	271	
		Information Bottleneck*	273	
		A High-Level View of Clustering	274	
		Summary	276	
		Bibliographic Remarks	276 276	
		Exercises	276	
23	Dimen	sionality Reduction	278	
		Principal Component Analysis (PCA)	279	
		Random Projections	283	
		Compressed Sensing	285	
		PCA or Compressed Sensing?	292	
		Summary	292	
		Bibliographic Remarks	292	
		Exercises	293	
24	Conor	ative Models	205	
24	0.0		295	
		Maximum Likelihood Estimator	295	
		Naive Bayes	299	
		Linear Discriminant Analysis	300	
		Latent Variables and the EM Algorithm	301	
		Bayesian Reasoning	305	
		Summary	307	
		Bibliographic Remarks	307	
	24.8	Exercises	308	
25	Featur	e Selection and Generation	309	
	25.1	Feature Selection	310	
	25.2	Feature Manipulation and Normalization	316	
	25.3	Feature Learning	319	



xii Contents

	25.4	Summary	321
		Bibliographic Remarks	321
	25.6	Exercises	322
Part	4 Adv	vanced Theory	
26	Radem	acher Complexities	325
	26.1	The Rademacher Complexity	325
		Rademacher Complexity of Linear Classes	332
		Generalization Bounds for SVM	333
		Generalization Bounds for Predictors with Low ℓ_1 Norm	335
	26.5	Bibliographic Remarks	336
27	Coveri	ng Numbers	337
	27.1	Covering	337
		From Covering to Rademacher Complexity via Chaining	338
	27.3	Bibliographic Remarks	340
28	Proof o	of the Fundamental Theorem of Learning Theory	341
	28.1	The Upper Bound for the Agnostic Case	341
	28.2	The Lower Bound for the Agnostic Case	342
	28.3	The Upper Bound for the Realizable Case	347
29	Multicl	ass Learnability	351
	29.1	The Natarajan Dimension	351
	29.2	The Multiclass Fundamental Theorem	352
		Calculating the Natarajan Dimension	353
		On Good and Bad ERMs	355
		Bibliographic Remarks Exercises	357
	29.0	Exercises	357
30	Compr	ession Bounds	359
		Compression Bounds	359
		Examples	361
	30.3	Bibliographic Remarks	363
31	PAC-Ba	ayes	364
	31.1	PAC-Bayes Bounds	364
		Bibliographic Remarks	366
	31.3	Exercises	366
Appe	endix A	Technical Lemmas	369
Appe	endix B	Measure Concentration	372
	B.1	Markov's Inequality	372
	B.2	Chebyshev's Inequality	373
	B.3	Chernoff's Bounds	373
	B.4	Hoeffding's Inequality	375



		Contents	xiii
B.5	Bennet's and Bernstein's Inequalities	376	
B.6	Slud's Inequality	378	
B.7	Concentration of χ^2 Variables	378	
Appendix C	Linear Algebra	380	
C.1	Basic Definitions	380	
C.2	Eigenvalues and Eigenvectors	381	
C.3	Positive Definite Matrices	381	
C.4	Singular Value Decomposition (SVD)	381	
References		385	
Index		395	





Preface

The term *machine learning* refers to the automated detection of meaningful patterns in data. In the past couple of decades it has become a common tool in almost any task that requires information extraction from large data sets. We are surrounded by a machine learning–based technology: Search engines learn how to bring us the best results (while placing profitable ads), antispam software learns to filter our email messages, and credit card transactions are secured by a software that learns how to detect frauds. Digital cameras learn to detect faces and intelligent personal assistance applications on smart-phones learn to recognize voice commands. Cars are equipped with accident-prevention systems that are built using machine learning algorithms. Machine learning is also widely used in scientific applications such as bioinformatics, medicine, and astronomy.

One common feature of all of these applications is that, in contrast to more traditional uses of computers, in these cases, due to the complexity of the patterns that need to be detected, a human programmer cannot provide an explicit, fine-detailed specification of how such tasks should be executed. Taking examples from intelligent beings, many of our skills are acquired or refined through *learning* from our experience (rather than following explicit instructions given to us). Machine learning tools are concerned with endowing programs with the ability to "learn" and adapt.

The first goal of this book is to provide a rigorous, yet easy-to-follow, introduction to the main concepts underlying machine learning: What is learning? How can a machine learn? How do we quantify the resources needed to learn a given concept? Is learning always possible? Can we know whether the learning process succeeded or failed?

The second goal of this book is to present several key machine learning algorithms. We chose to present algorithms that on one hand are successfully used in practice and on the other hand give a wide spectrum of different learning techniques. Additionally, we pay specific attention to algorithms appropriate for large-scale learning (a.k.a. "Big Data"), since in recent years, our world has become increasingly "digitized" and the amount of data available for learning is dramatically increasing. As a result, in many applications data is plentiful and computation



xvi Preface

time is the main bottleneck. We therefore explicitly quantify both the amount of data and the amount of computation time needed to learn a given concept.

The book is divided into four parts. The first part aims at giving an initial rigorous answer to the fundamental questions of learning. We describe a generalization of Valiant's Probably Approximately Correct (PAC) learning model, which is a first solid answer to the question "What is learning?" We describe the Empirical Risk Minimization (ERM), Structural Risk Minimization (SRM), and Minimum Description Length (MDL) learning rules, which show "how a machine can learn." We quantify the amount of data needed for learning using the ERM, SRM, and MDL rules and show how learning might fail by deriving a "no-free-lunch" theorem. We also discuss how much computation time is required for learning. In the second part of the book we describe various learning algorithms. For some of the algorithms, we first present a more general learning principle and then show how the algorithm follows the principle. While the first two parts of the book focus on the PAC model, the third part extends the scope by presenting a wider variety of learning models. Finally, the last part of the book is devoted to advanced theory.

We made an attempt to keep the book as self-contained as possible. However, the reader is assumed to be comfortable with basic notions of probability, linear algebra, analysis, and algorithms. The first three parts of the book are intended for first-year graduate students in computer science, engineering, mathematics, or statistics. It can also be accessible to undergraduate students with the adequate background. The more advanced chapters can be used by researchers intending to gather a deeper theoretical understanding.

ACKNOWLEDGMENTS

The book is based on Introduction to Machine Learning courses taught by Shai Shalev-Shwartz at Hebrew University and by Shai Ben-David at the University of Waterloo. The first draft of the book grew out of the lecture notes for the course that was taught at Hebrew University by Shai Shalev-Shwartz during 2010–2013. We greatly appreciate the help of Ohad Shamir, who served as a teaching assistant for the course in 2010, and of Alon Gonen, who served as TA for the course in 2011–2013. Ohad and Alon prepared a few lecture notes and many of the exercises. Alon, to whom we are indebted for his help throughout the entire making of the book, has also prepared a solution manual.

We are deeply grateful for the most valuable work of Dana Rubinstein. Dana has scientifically proofread and edited the manuscript, transforming it from lecture-based chapters into fluent and coherent text.

Special thanks to Amit Daniely, who helped us with a careful read of the advanced part of the book and wrote the advanced chapter on multiclass learnability. We are also grateful for the members of a book reading club in Jerusalem who have carefully read and constructively criticized every line of the manuscript. The members of the reading club are Maya Alroy, Yossi Arjevani, Aharon Birnbaum, Alon Cohen, Alon Gonen, Roi Livni, Ofer Meshi, Dan Rosenbaum, Dana Rubinstein, Shahar Somin, Alon Vinnikov, and Yoav Wald. We would also like to thank Gal Elidan, Amir Globerson, Nika Haghtalab, Shie Mannor, Amnon Shashua, Nati Srebro, and Ruth Urner for helpful discussions.