Contents

Preface		page xv	
1	Introd	uction	1
	1.1	What Is Learning?	1
	1.2	When Do We Need Machine Learning?	3
		Types of Learning	4
	1.4	Relations to Other Fields	6
	1.5	How to Read This Book	7
	1.6	Notation	8
Pai	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	Exercises	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	Evercises	35

5	The Bi	as-Complexity Trade-off	36
	5.1	The No-Free-Lunch Theorem	37
	5.2	Error Decomposition	40
	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	Discussing the Different Notions of Learnability	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
Paı	rt2 Fre	om Theory to Algorithms	
9		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	99

			Contents
10	Boostin	g	101
	10.1	Weak Learnability	102
		AdaBoost	105
	10.3	Linear Combinations of Base Hypotheses	108
		AdaBoost for Face Recognition	110
		Summary	111
		Bibliographic Remarks	111
		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
		Summary	135
		Bibliographic Remarks	136
	12.6	Exercises	136
13	Regular	ization 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
		Summary	146
	13.6	Bibliographic Remarks	146
	13.7	Exercises	147
14	Stochastic Gradient Descent		150
	14.1	Gradient Descent	151
		Subgradients	154
	14.3	Stochastic Gradient Descent (SGD)	156
		Variants	159
	14.5	Learning with SGD	162
		Summary	165
		Bibliographic Remarks	166
	14.8	Exercises	166
15	Support	t 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

ix

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
	16.4	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
		Structured Output Prediction	198
		Ranking	201
		Bipartite Ranking and Multivariate Performance Measures	206
		Summary	209
		Bibliographic Remarks	210
	17.8	Exercises	210
18	Decisio	on Trees	212
	18.1	Sample Complexity	213
		Decision Tree Algorithms	214
		Random Forests	217
		Summary	217
		Bibliographic Remarks	218
	18.6	Exercises	218
19	Neares	st Neighbor	219
	19.1	k Nearest Neighbors	219
		Analysis	220
	19.3	Efficient Implementation*	225
		Summary	225
		Bibliographic Remarks	225
	19.6	Exercises	225
20	Neural	Networks	228
		Feedforward Neural Networks	229
	20.2	Learning Neural Networks	230
		The Expressive Power of Neural Networks	231
		The Sample Complexity of Neural Networks	234
		The Runtime of Learning Neural Networks	235
	20.6	SGD and Backpropagation	236

		Contents
20.7	Summary	240
		240
		240
3 Add	ditional Learning Models	
	_	245
	•	246
		251
		257
	-	258
	, ,	261
	· · · · · · · · · · · · · · · · · · ·	261
	· .	262
011	du a	264
		264
		266
	9	268
		271
		273
		274
	•	276
		276
22.8	Exercises	276
Dimen	sionality Reduction	278
23.1	Principal Component Analysis (PCA)	279
23.2	Random Projections	283
23.3	Compressed Sensing	285
23.4	PCA or Compressed Sensing?	292
23.5	Summary	292
		292
23.7	Exercises	293
Genera	ative Models	295
24.1	Maximum Likelihood Estimator	295
24.2	Naive Bayes	299
24.3	Linear Discriminant Analysis	300
24.4	Latent Variables and the EM Algorithm	301
24.5	Bayesian Reasoning	305
24.6	Summary	307
24.7	Bibliographic Remarks	307
24.8	Exercises	308
Featur	e Selection and Generation	309
25.1	Feature Selection	310
		316
	-	319
	20.8 20.9 3 Add Online 21.1 21.2 21.3 21.4 21.5 21.6 21.7 Cluster 22.1 22.2 22.3 22.4 22.5 22.6 22.7 22.8 Dimens 23.1 23.2 23.3 23.4 23.5 23.6 23.7 Genera 24.1 24.2 24.3 24.4 24.5 24.6 24.7 24.8 Featur 25.1 25.2	21.1 Online Classification in the Realizable Case 21.2 Online Classification in the Unrealizable Case 21.3 Online Convex Optimization 21.4 The Online Perceptron Algorithm 21.5 Summary 21.6 Bibliographic Remarks 21.7 Exercises Clustering 22.1 Linkage-Based Clustering Algorithms 22.2 k-Means and Other Cost Minimization Clusterings 22.3 Spectral Clustering 22.4 Information Bottleneck* 22.5 A High-Level View of Clustering 22.6 Summary 22.7 Bibliographic Remarks 22.8 Exercises Dimensionality Reduction 23.1 Principal Component Analysis (PCA) 23.2 Random Projections 23.3 Compressed Sensing 23.4 PCA or Compressed Sensing? 23.5 Summary 23.6 Bibliographic Remarks 23.7 Exercises

χi

	25.4	Summary	321
	25.5	Bibliographic Remarks	321
	25.6	Exercises	322
Parl	t 4 Adv	vanced Theory	
26	Radem	nacher Complexities	325
	26.1	The Rademacher Complexity	325
		Rademacher Complexity of Linear Classes	332
		Generalization Bounds for SVM	333
	26.4	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
	29.3	Calculating the Natarajan Dimension	353
		On Good and Bad ERMs	355
	29.5	Bibliographic Remarks	357
	29.6	Exercises	357
30	Compr	ession Bounds	359
	30.1	Compression Bounds	359
	30.2	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
Арр	endix A	Technical Lemmas	369
Арр	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	