Pr	eface	xvii
No	otation	s xxi
1	Introd	duction 1
	1.1	What Is Machine Learning? 1
	1.2	Examples of Machine Learning Applications 4
		1.2.1 Learning Associations 4
		1.2.2 Classification 5
		1.2.3 Regression 9
		1.2.4 Unsupervised Learning 11
		1.2.5 Reinforcement Learning 13
	1.3	Notes 14
	1.4	Relevant Resources 17
	1.5	Exercises 18
	1.6	References 20
2	Super	vised Learning 21
	2.1	Learning a Class from Examples 21
	2.2	Vapnik-Chervonenkis Dimension 27
	2.3	Probably Approximately Correct Learning 29
	2.4	Noise 30
	2.5	Learning Multiple Classes 32
	2.6	Regression 34
	2.7	Model Selection and Generalization 37
	2.8	Dimensions of a Supervised Machine Learning Algorithm 41
	2.9	Notes 42

viii

	2.10	Exercises 43
	2.11	References 47
3	Baye.	sian Decision Theory 49
	3.1	Introduction 49
	3.2	Classification 51
	3.3	Losses and Risks 53
	3.4	Discriminant Functions 55
	3.5	Association Rules 56
	3.6	Notes 59
	3.7	Exercises 60
	3.8	References 64
4	Para	metric Methods 65
	4.1	Introduction 65
	4.2	Maximum Likelihood Estimation 66
		4.2.1 Bernoulli Density 67
		4.2.2 Multinomial Density 68
		4.2.3 Gaussian (Normal) Density 68
	4.3	Evaluating an Estimator: Bias and Variance 69
	4.4	The Bayes' Estimator 70
	4.5	Parametric Classification 73
	4.6	Regression 77
	4.7	Tuning Model Complexity: Bias/Variance Dilemma 80
	4.8	Model Selection Procedures 83
	4.9	Notes 87
	4.10	
	4.11	References 90
5		ivariate Methods 93
	5.1	Multivariate Data 93
	5.2	
	5.3	Estimation of Missing Values 95
	5.4	Multivariate Normal Distribution 96
	5.5	Multivariate Classification 100
	5.6	Tuning Complexity 106
	5.7	Discrete Features 108
	5.8	Multivariate Regression 109
	5.9	Notes 111
	5.10	Exercises 112

Contents iχ 5.11 References 113 6 Dimensionality Reduction 115 6.1 Introduction 6.2 **Subset Selection** 116 6.3 Principal Component Analysis 120 6.4 Feature Embedding 127 6.5 Factor Analysis 130 6.6 Singular Value Decomposition and Matrix Factorization 135 6.7 Multidimensional Scaling 136 6.8 Linear Discriminant Analysis 140 6.9 Canonical Correlation Analysis 145 6.10 Isomap 148 6.11 Locally Linear Embedding 150 6.12 Laplacian Eigenmaps 153 6.13 Notes 155 6.14 Exercises 157 6.15 References 158 7 Clustering 161 7.1 161 Introduction 7.2 Mixture Densities 162 7.3 *k*-Means Clustering 163 7.4 Expectation-Maximization Algorithm 167 7.5 Mixtures of Latent Variable Models 172 Supervised Learning after Clustering 7.6 173 7.7 Spectral Clustering 175 7.8 Hierarchical Clustering 176 7.9 Choosing the Number of Clusters 178 7.10 Notes 179 7.11 Exercises 180 7.12 References 182 8 Nonparametric Methods 185 8.1 185 Introduction 8.2 Nonparametric Density Estimation 186 8.2.1 Histogram Estimator 187 8.2.2 Kernel Estimator 188

k-Nearest Neighbor Estimator

Generalization to Multivariate Data

190

192

8.2.3

8.3

χ

_	
8.4	±
8.	e
8.0	
8.	
8.8	
	8.8.1 Running Mean Smoother 201
	8.8.2 Kernel Smoother 203
	8.8.3 Running Line Smoother 204
8.9	9 How to Choose the Smoothing Parameter 204
8.	10 Notes 205
_	11 Exercises 208
8.	12 References 210
9 D	ecision Trees 213
9.	1 Introduction 213
9.3	2 Univariate Trees 215
	9.2.1 Classification Trees 216
	9.2.2 Regression Trees 220
9.3	3 Pruning 222
9.4	4 Rule Extraction from Trees 225
9.	5 Learning Rules from Data 226
9.0	6 Multivariate Trees 230
9.	7 Notes 232
9.8	8 Exercises 235
9.9	9 References 237
10 <i>Li</i>	near Discrimination 239
10	0.1 Introduction 239
10	0.2 Generalizing the Linear Model 241
10	0.3 Geometry of the Linear Discriminant 242
	10.3.1 Two Classes 242
	10.3.2 Multiple Classes 244
10	0.4 Pairwise Separation 246
10	0.5 Parametric Discrimination Revisited 247
10	0.6 Gradient Descent 248
10	0.7 Logistic Discrimination 250
	10.7.1 Two Classes 250
	10.7.2 Multiple Classes 254
10	0.8 Discrimination by Regression 257

10.9 Learning to Rank 260 10.10 Notes 263 10.11 Exercises 263 10.12 References 266 11 Multilayer Perceptrons 267 267 11.1 Introduction 11.1.1 Understanding the Brain 268 11.1.2 Neural Networks as a Paradigm for Parallel **Processing** 269 11.2 The Perceptron 11.3 Training a Perceptron 274 11.4 Learning Boolean Functions 277 11.5 Multilayer Perceptrons 279 11.6 MLP as a Universal Approximator 281 11.7 Backpropagation Algorithm 283 11.7.1 Nonlinear Regression 284 11.7.2 Two-Class Discrimination 286 11.7.3 Multiclass Discrimination 288 11.7.4 Multiple Hidden Layers 290 11.8 Training Procedures 290 11.8.1 Improving Convergence 290 11.8.2 Overtraining 11.8.3 Structuring the Network 292 11.8.4 Hints 295 11.9 Tuning the Network Size 297 11.10 Bayesian View of Learning 300 11.11 Dimensionality Reduction 301 11.12 Learning Time 304 11.12.1 Time Delay Neural Networks 304 11.12.2 Recurrent Networks 305 11.13 Deep Learning 306 11.14 Notes 309 11.15 Exercises 311 11.16 References 313 12 Local Models 317 12.1 Introduction 317

χi

12.2 Competitive Learning

318

xii

12.2.1 Online <i>k</i> -Means 318	
12.2.2 Adaptive Resonance Theory 323	
12.2.3 Self-Organizing Maps 324	
12.3 Radial Basis Functions 326	
12.4 Incorporating Rule-Based Knowledge 332	
12.5 Normalized Basis Functions 333	
12.6 Competitive Basis Functions 335	
12.7 Learning Vector Quantization 338	
12.8 The Mixture of Experts 338	
12.8.1 Cooperative Experts 341	
12.8.2 Competitive Experts 342	
12.9 Hierarchical Mixture of Experts 342	
12.10 Notes 343	
12.11 Exercises 344	
12.12 References 347	
13 Kernel Machines 349	
13.1 Introduction 349	
13.2 Optimal Separating Hyperplane 351	
13.3 The Nonseparable Case: Soft Margin Hyperplane	355
13.4 v-SVM 358	
13.5 Kernel Trick 359	
13.6 Vectorial Kernels 361	
13.7 Defining Kernels 364	
13.8 Multiple Kernel Learning 365	
13.9 Multiclass Kernel Machines 367	
13.10 Kernel Machines for Regression 368	
13.11 Kernel Machines for Ranking 373	
13.12 One-Class Kernel Machines 374	
13.13 Large Margin Nearest Neighbor Classifier 377	
13.14 Kernel Dimensionality Reduction 379	
13.15 Notes 380	
13.16 Exercises 382	
13.17 References 383	
14 Graphical Models 387	
14.1 Introduction 387	
14.2 Canonical Cases for Conditional Independence	389
14.3 Generative Models 396	

xiii Contents

	14.4	d-Separation 399
	14.5	Belief Propagation 399
		14.5.1 Chains 400
		14.5.2 Trees 402
		14.5.3 Polytrees 404
		14.5.4 Junction Trees 406
	14.6	Undirected Graphs: Markov Random Fields 407
	14.7	Learning the Structure of a Graphical Model 410
	14.8	Influence Diagrams 411
	14.9	Notes 412
	14.10	Exercises 413
	14.11	References 415
1 -	11:33.	w Markov Madala 417
15		n Markov Models 417
	15.1	
		Discrete Markov Processes 418
		Hidden Markov Models 421
	15.4	
		Evaluation Problem 423
		Finding the State Sequence 427
		Learning Model Parameters 429
		Continuous Observations 432
		The HMM as a Graphical Model 433
	15.10	Model Selection in HMMs 436
	_	Notes 438
		Exercises 440
	15.13	References 443
16	Rayes	ian Estimation 445
10	-	
		Introduction 445
	16.2	
		Distribution 449
		16.2.1 $K > 2$ States: Dirichlet Distribution 449
	100	16.2.2 $K = 2$ States: Beta Distribution 450
	16.3	Bayesian Estimation of the Parameters of a Gaussian
		Distribution 451
		16.3.1 Univariate Case: Unknown Mean, Known
		Variance 451

χiν

		16.3.2 Univariate Case: Unknown Mean, Unknown
		Variance 453
		16.3.3 Multivariate Case: Unknown Mean, Unknown
		Covariance 455
	16.4	Bayesian Estimation of the Parameters of a Function 456
		16.4.1 Regression 456
		16.4.2 Regression with Prior on Noise Precision 460
		16.4.3 The Use of Basis/Kernel Functions 461
		16.4.4 Bayesian Classification 463
	16.5	Choosing a Prior 466
	16.6	Bayesian Model Comparison 467
	16.7	Bayesian Estimation of a Mixture Model 470
	16.8	Nonparametric Bayesian Modeling 473
	16.9	Gaussian Processes 474
	16.10	Dirichlet Processes and Chinese Restaurants 478
	16.11	Latent Dirichlet Allocation 480
	16.12	Beta Processes and Indian Buffets 482
	16.13	Notes 483
	16.14	Exercises 484
	16.15	References 485
17	Comb	ining Multiple Learners 487
17		•
	17.1	Rationale 487
	17.2	8
	17.3	Model Combination Schemes 491
		Voting 492
	17.5	Error-Correcting Output Codes 496
	17.6	Bagging 498
		Boosting 499
		The Mixture of Experts Revisited 502
	17.9	Stacked Generalization 504
	17.10	Fine-Tuning an Ensemble 505
		17.10.1 Choosing a Subset of the Ensemble 506
		17.10.2 Constructing Metalearners 506
		Cascading 507
		Notes 509
	17.13	Exercises 511

Contents

17.14 References

513

Contents XV

18 Reinf	orcement Learning 517
18.1	Introduction 517
18.2	Single State Case: <i>K</i> -Armed Bandit 519
18.3	Elements of Reinforcement Learning 520
18.4	Model-Based Learning 523
	18.4.1 Value Iteration 523
	18.4.2 Policy Iteration 524
18.5	Temporal Difference Learning 525
	18.5.1 Exploration Strategies 525
	18.5.2 Deterministic Rewards and Actions 526
	18.5.3 Nondeterministic Rewards and Actions 527
	18.5.4 Eligibility Traces 530
18.6	
18.7	
	18.7.1 The Setting 534
	18.7.2 Example: The Tiger Problem 536
18.8	Notes 541
18.9	
18.10	References 544
19 Desig	n and Analysis of Machine Learning Experiments 547
19.1	Introduction 547
19.2	Factors, Response, and Strategy of Experimentation 550
19.3	Response Surface Design 553
19.4	Randomization, Replication, and Blocking 554
19.5	Guidelines for Machine Learning Experiments 555
19.6	Cross-Validation and Resampling Methods 558
	19.6.1 K-Fold Cross-Validation 559
	19.6.2 5×2 Cross-Validation 560
	19.6.3 Bootstrapping 561
19.7	Measuring Classifier Performance 561
19.8	Interval Estimation 564
19.9	Hypothesis Testing 568
19.10	Assessing a Classification Algorithm's Performance 570
	19.10.1 Binomial Test 571
	19.10.2 Approximate Normal Test 572
	19.10.3 <i>t</i> Test 572
19.11	Comparing Two Classification Algorithms 573
	19.11.1 McNemar's Test 573

xvi

	19.13 19.14 19.15 19.16	19.11.2 K -Fold Cross-Validated Paired t Test 573 19.11.3 5×2 cv Paired t Test 574 19.11.4 5×2 cv Paired F Test 575 Comparing Multiple Algorithms: Analysis of Variance 576 Comparison over Multiple Datasets 580 19.13.1 Comparing Two Algorithms 581 19.13.2 Multiple Algorithms 583 Multivariate Tests 584 19.14.1 Comparing Two Algorithms 585 19.14.2 Comparing Multiple Algorithms 586 Notes 587 Exercises 588 References 590
A	Proba	
	A.1	Elements of Probability 593
		A.1.1 Axioms of Probability 594
	4.0	A.1.2 Conditional Probability 594
	A.2	Random Variables 595
		A.2.1 Probability Distribution and Density Functions 595
		A.2.2 Joint Distribution and Density Functions 596
		A.2.4 Parasa' Puls 507
		A.2.5 Formattation 597
		A.2.5 Expectation 597
		A.2.6 Variance 598 A.2.7 Weak Law of Large Numbers 599
	A.3	A.2.7 Weak Law of Large Numbers 599 Special Random Variables 599
	A.3	A.3.1 Bernoulli Distribution 599
		A.3.2 Binomial Distribution 600
		A.3.3 Multinomial Distribution 600
		A.3.4 Uniform Distribution 600
		A.3.5 Normal (Gaussian) Distribution 601
		A.3.6 Chi-Square Distribution 602
		A.3.7 t Distribution 603
		A.3.8 <i>F</i> Distribution 603
	A.4	References 603

Contents

605

Index