CONTENTS

1

PREFACE

INTRODUCTION

	1.1 Machine Perception, 1	
	1.2 An Example, 1	
	1.2.1 Related Fields, 8	
	1.3 Pattern Recognition Systems, 9	
	1.3.1 Sensing, 9	
	1.3.2 Segmentation and Grouping, 9	
	1.3.3 Feature Extraction, 11	
	1.3.4 Classification, 12	
	1.3.5 Post Processing, 13	
	1.4 The Design Cycle, 14	
	1.4.1 Data Collection, 14	
	1.4.2 Feature Choice, 14	
	1.4.3 Model Choice, 15	
	1.4.4 Training, 15	
	1.4.5 Evaluation, 15	
	1.4.6 Computational Complexity, 16	
	1.5 Learning and Adaptation, 16	
	1.5.1 Supervised Learning, 16	
	1.5.2 Unsupervised Learning, 17	
	1.5.3 Reinforcement Learning, 17	
	1.6 Conclusion, 17	
	Summary by Chapters, 17	
	Bibliographical and Historical Remarks, 18	
	Bibliography, 19	
2	BAYESIAN DECISION THEORY	20
	2.1 Introduction, 20	

2.2 Bayesian Decision Theory—Continuous Features, 24
2.2.1 Two-Category Classification, 25
2.3 Minimum-Error-Rate Classification, 26
*2.3.1 Minimax Criterion, 27

vii

xvii

	*2.3.2 Neyman-Pearson Criterion, 28	
2.4	Classifiers, Discriminant Functions, and Decision Surfaces, 29	
	2.4.1 The Multicategory Case, 29	
	2.4.2 The Two-Category Case, 30	
2.5	The Normal Density, 31	
	2.5.1 Univariate Density, 32	
	2.5.2 Multivariate Density, 33	
2.6	Discriminant Functions for the Normal Density, 36	
	2.6.1 Case 1: $\Sigma_i = \sigma^2 \mathbf{I}$, 36	
	2.6.2 Case 2: $\Sigma_i = \Sigma$, 39	
	2.6.3 Case 3: Σ_i = arbitrary, 41	
	Example 1 Decision Regions for Two-Dimensional	
	Gaussian Data, 41	
*2.7	Error Probabilities and Integrals, 45	
*2.8	Error Bounds for Normal Densities, 46	
	2.8.1 Chernoff Bound, 46	
	2.8.2 Bhattacharyya Bound, 47	
	Example 2 Error Bounds for Gaussian Distributions, 48	
	2.8.3 Signal Detection Theory and Operating Characteristics, 48	
2.9	Bayes Decision Theory—Discrete Features, 51	
	2.9.1 Independent Binary Features, 52	
	Example 3 Bayesian Decisions for Three-Dimensional	
	Binary Data, 53	
2.10	Missing and Noisy Features, 54	
	2.10.1 Missing Features, 54	
	2.10.2 Noisy Features, 55	
2.11	Bayesian Belief Networks, 56	
	Example 4 Belief Network for Fish, 59	
2.12	Compound Bayesian Decision Theory and Context, 62	
Sum	mary, 63	
Bibli	ographical and Historical Remarks, 64	
Prob	lems, 65	
Com	puter exercises, 80	
Bibli	iography, 82	
MA	XIMUM-LIKELIHOOD AND BAYESIAN	
	AMETER ESTIMATION	84
		٠.
	Introduction, 84	
3.2	Maximum-Likelihood Estimation, 85	
	3.2.1 The General Principle, 85	
	3.2.2 The Gaussian Case: Unknown μ , 88	
	3.2.3 The Gaussian Case: Unknown μ and Σ , 88	
	3.2.4 Bias, 89	
3.3	Bayesian Estimation, 90	
	3.3.1 The Class-Conditional Densities, 91	

3.3.2 The Parameter Distribution, 91
3.4 Bayesian Parameter Estimation: Gaussian Case, 92
3.4.1 The Univariate Case: $p(\mu|\mathcal{D})$, 92
3.4.2 The Univariate Case: $p(x|\mathcal{D})$, 95
3.4.3 The Multivariate Case, 95

3.5	Bayesian Parameter Estimation: General Theory, 97	
	Example 1 Recursive Bayes Learning, 98	
	3.5.1 When Do Maximum-Likelihood and Bayes Methods Differ?, 100)
	3.5.2 Noninformative Priors and Invariance, 101	
	3.5.3 Gibbs Algorithm, 102	
*3.6	Sufficient Statistics, 102	
	3.6.1 Sufficient Statistics and the Exponential Family, 106	
3.7	Problems of Dimensionality, 107	
	3.7.1 Accuracy, Dimension, and Training Sample Size, 107	
	3.7.2 Computational Complexity, 111	
	3.7.3 Overfitting, 113	
*3.8	Component Analysis and Discriminants, 114	
	3.8.1 Principal Component Analysis (PCA), 115	
	3.8.2 Fisher Linear Discriminant, 117	
	3.8.3 Multiple Discriminant Analysis, 121	
*3.9	Expectation-Maximization (EM), 124	
	Example 2 Expectation-Maximization for a 2D Normal Model,	126
3.10	Hidden Markov Models, 128	
	3.10.1 First-Order Markov Models, 128	
	3.10.2 First-Order Hidden Markov Models, 129	
	3.10.3 Hidden Markov Model Computation, 129	
	3.10.4 Evaluation, 131	
	Example 3 Hidden Markov Model, 133	
	3.10.5 Decoding, 135	
	Example 4 HMM Decoding, 136	
	3.10.6 Learning, 137	
Sum	mary, 139	
Bibli	iographical and Historical Remarks, 139	
Prob	lems, 140	
Com	puter exercises, 155	
Bibli	iography, 159	
NO	NPARAMETRIC TECHNIQUES	16
4.1	Introduction, 161	
	Density Estimation, 161	
	Parzen Windows, 164	
	4.3.1 Convergence of the Mean, 167	
	4.3.2 Convergence of the Variance, 167	
	4.3.3 Illustrations, 168	
	4.3.4 Classification Example, 168	
	4.3.5 Probabilistic Neural Networks (PNNs), 172	
	4.3.6 Choosing the Window Function, 174	
44	k_n -Nearest-Neighbor Estimation, 174	
	4.4.1 k_n -Nearest-Neighbor and Parzen-Window Estimation, 176	
	4.4.2 Estimation of <i>A Posteriori</i> Probabilities, 177	
45	The Nearest-Neighbor Rule, 177	
7.5	4.5.1 Convergence of the Nearest Neighbor, 179	
	4.5.2 Error Rate for the Nearest-Neighbor Rule, 180	
	4.5.3 Error Bounds, 180	
	4.5.4 The k-Nearest-Neighbor Rule, 182	
	TISIT THE K-MORIOSI-MORRIDON MUIC, 102	

 4.5.5 Computational Complexity of the k-Nearest-Neighbor Rule, 184 4.6 Metrics and Nearest-Neighbor Classification, 187 4.6.1 Properties of Metrics, 187 4.6.2 Tangent Distance, 188 *4.7 Fuzzy Classification, 192 *4.8 Reduced Coulomb Energy Networks, 195 4.9 Approximations by Series Expansions, 197 Summary, 199 Bibliographical and Historical Remarks, 200 Problems, 201 Computer exercises, 209 Bibliography, 213 LINEAR DISCRIMINANT FUNCTIONS
or posteriors, as an electrical particular as a superior and the property of the superior and the superior a
5.1 Introduction, 2155.2 Linear Discriminant Functions and Decision Surfaces, 216
5.2.1 The Two-Category Case, 216
5.2.2 The Multicategory Case, 218
5.3 Generalized Linear Discriminant Functions, 219
5.4 The Two-Category Linearly Separable Case, 223
5.4.1 Geometry and Terminology, 224
5.4.2 Gradient Descent Procedures, 224
5.5 Minimizing the Perceptron Criterion Function, 227
5.5.1 The Perceptron Criterion Function, 227
5.5.2 Convergence Proof for Single-Sample Correction, 229
5.5.3 Some Direct Generalizations, 232
5.6 Relaxation Procedures, 235
5.6.1 The Descent Algorithm, 235
5.6.2 Convergence Proof, 237
5.7 Nonseparable Behavior, 238
5.8 Minimum Squared-Error Procedures, 239 5.8.1 Minimum Squared-Error and the Pseudoinverse, 240
Example Constructing a Linear Classifier by Matrix
Pseudoinverse, 241
5.8.2 Relation to Fisher's Linear Discriminant, 242
5.8.3 Asymptotic Approximation to an Optimal Discriminant, 243
5.8.4 The Widrow-Hoff or LMS Procedure, 245
5.8.5 Stochastic Approximation Methods, 246
5.9 The Ho-Kashyap Procedures, 249
5.9.1 The Descent Procedure, 250
5.9.2 Convergence Proof, 251
5.9.3 Nonseparable Behavior, 253
5.9.4 Some Related Procedures, 253
*5.10 Linear Programming Algorithms, 256
5.10.1 Linear Programming, 256
5.10.2 The Linearly Separable Case, 257
5.10.3 Minimizing the Perceptron Criterion Function, 258
*5.11 Support Vector Machines, 259 5.11.1 SVM Training, 263
Example 2 SVM for the XOR Problem, 264

	5.12.3 Generalizations for MSE Procedures, 268
	Summary, 269
	Bibliographical and Historical Remarks, 270
	Problems, 271
	Computer exercises, 278
	Bibliography, 281
6	MULTILAYER NEURAL NETWORKS
	6.1 Introduction, 282
	6.2 Feedforward Operation and Classification, 284
	6.2.1 General Feedforward Operation, 286
	6.2.2 Expressive Power of Multilayer Networks, 287
	6.3 Backpropagation Algorithm, 288
	6.3.1 Network Learning, 289
	6.3.2 Training Protocols, 293
	6.3.3 Learning Curves, 295
	6.4 Error Surfaces, 296
	6.4.1 Some Small Networks, 296
	6.4.2 The Exclusive-OR (XOR), 298
	6.4.3 Larger Networks, 298
	6.4.4 How Important Are Multiple Minima?, 299
	6.5 Backpropagation as Feature Mapping, 299
	6.5.1 Representations at the Hidden Layer—Weights, 302
	6.6 Backpropagation, Bayes Theory and Probability, 303
	6.6.1 Bayes Discriminants and Neural Networks, 303
	6.6.2 Outputs as Probabilities, 304
	*6.7 Related Statistical Techniques, 305
	6.8 Practical Techniques for Improving Backpropagation, 306
	6.8.1 Activation Function, 307
	6.8.2 Parameters for the Sigmoid, 308
	6.8.3 Scaling Input, 308
	6.8.4 Target Values, 309
	6.8.5 Training with Noise, 310
	6.8.6 Manufacturing Data, 310
	6.8.7 Number of Hidden Units, 310
	6.8.8 Initializing Weights, 311
	6.8.9 Learning Rates, 312
	6.8.10 Momentum, 313
	6.8.11 Weight Decay, 314
	6.8.12 Hints, 315
	6.8.13 On-Line, Stochastic or Batch Training?, 316
	6.8.14 Stopped Training, 316
	6.8.15 Number of Hidden Layers, 317 6.8.16 Criterion Function, 318
	*6.9 Second-Order Methods, 318
	6.9.1 Hessian Matrix, 318
	6.9.2 Newton's Method, 319
	0.7.2 Itemon struction, 517

5.12 Multicategory Generalizations, 265 5.12.1 Kesler's Construction, 266

5.12.2 Convergence of the Fixed-Increment Rule, 266

6.9.3 Quickprop, 320 6.9.4 Conjugate Gradient Descent, 321 Example 1 Conjugate Gradient Descent, 322 *6.10 Additional Networks and Training Methods, 324 6.10.1 Radial Basis Function Networks (RBFs), 324 6.10.2 Special Bases, 325 6.10.3 Matched Filters, 325 6.10.4 Convolutional Networks, 326 6.10.5 Recurrent Networks, 328 6.10.6 Cascade-Correlation, 329 6.11 Regularization, Complexity Adjustment and Pruning, 330 Summary, 333 Bibliographical and Historical Remarks, 333 Problems, 335 Computer exercises, 343 Bibliography, 347	
STOCHASTIC METHODS	350
 7.1 Introduction, 350 7.2 Stochastic Search, 351 7.2.1 Simulated Annealing, 351 7.2.2 The Boltzmann Factor, 352 7.2.3 Deterministic Simulated Annealing, 357 7.3 Boltzmann Learning, 360 7.3.1 Stochastic Boltzmann Learning of Visible States, 360 7.3.2 Missing Features and Category Constraints, 365 7.3.3 Deterministic Boltzmann Learning, 366 7.3.4 Initialization and Setting Parameters, 367 *7.4 Boltzmann Networks and Graphical Models, 370 7.4.1 Other Graphical Models, 372 *7.5 Evolutionary Methods, 373 7.5.1 Genetic Algorithms, 373 7.5.2 Further Heuristics, 377 7.5.3 Why Do They Work?, 378 *7.6 Genetic Programming, 378 Summary, 381 Bibliographical and Historical Remarks, 381 Problems, 383 Computer exercises, 388 Bibliography, 391 	
NONMETRIC METHODS	394
 8.1 Introduction, 394 8.2 Decision Trees, 395 8.3 CART, 396 8.3.1 Number of Splits, 397 8.3.2 Query Selection and Node Impurity, 398 8.3.3 When to Stop Splitting, 402 8.3.4 Pruning, 403 	

	8.3.5 Assignment of Leaf Node Labels, 404
	Example 1 A Simple Tree, 404
	8.3.6 Computational Complexity, 406
	8.3.7 Feature Choice, 407
	8.3.8 Multivariate Decision Trees, 408
	8.3.9 Priors and Costs, 409
	8.3.10 Missing Attributes, 409
	Example 2 Surrogate Splits and Missing Attributes, 410
8.4	Other Tree Methods, 411
	8.4.1 ID3, 411
	8.4.2 C4.5, 411
	8.4.3 Which Tree Classifier Is Best?, 412
*8.5	Recognition with Strings, 413
	8.5.1 String Matching, 415
	8.5.2 Edit Distance, 418
	8.5.3 Computational Complexity, 420
	8.5.4 String Matching with Errors, 420
	8.5.5 String Matching with the "Don't-Care" Symbol, 421
8.6	Grammatical Methods, 421
6.0	8.6.1 Grammars, 422
	•
	8.6.2 Types of String Grammars, 424
	Example 3 A Grammar for Pronouncing Numbers, 425
o =	8.6.3 Recognition Using Grammars, 426
8.7	Grammatical Inference, 429
	Example 4 Grammatical Inference, 431
*8.8	Rule-Based Methods, 431
	8.8.1 Learning Rules, 433
	mary, 434
	ographical and Historical Remarks, 435
Prob	lems, 437
Com	puter exercises, 446
Bibli	ography, 450
ALC	GORITHM-INDEPENDENT MACHINE LEARNING 453
9.1	Introduction, 453
9.2	Lack of Inherent Superiority of Any Classifier, 454
	9.2.1 No Free Lunch Theorem, 454
	Example 1 No Free Lunch for Binary Data, 457
	*9.2.2 Ugly Duckling Theorem, 458
	9.2.3 Minimum Description Length (MDL), 461
	9.2.4 Minimum Description Length Principle, 463
	9.2.5 Overfitting Avoidance and Occam's Razor, 464
0.2	Bias and Variance, 465
9.3	
	9.3.1 Bias and Variance for Regression, 466
0.4	9.3.2 Bias and Variance for Classification, 468
9.4	Resampling for Estimating Statistics, 471
	9.4.1 Jackknife, 472
	Example 2 Jackknife Estimate of Bias and Variance of the Mode, 473
	9.4.2 Bootstrap, 474
95	Resampling for Classifier Design, 475

9.5.1 Bagging, 475	
9.5.2 Boosting, 476	
9.5.3 Learning with Queries, 480	
9.5.4 Arcing, Learning with Queries, Bias and Variance, 482	
9.6 Estimating and Comparing Classifiers, 482	
9.6.1 Parametric Models, 483	
9.6.2 Cross-Validation, 483	
9.6.3 Jackknife and Bootstrap Estimation of Classification Accuracy, 4	85
9.6.4 Maximum-Likelihood Model Comparison, 486	•
9.6.5 Bayesian Model Comparison, 487	
9.6.6 The Problem-Average Error Rate, 489	
9.6.7 Predicting Final Performance from Learning Curves, 492	
9.6.8 The Capacity of a Separating Plane, 494	
9.7 Combining Classifiers, 495	
9.7.1 Component Classifiers with Discriminant Functions, 496	
9.7.2 Component Classifiers without Discriminant Functions, 498	
Summary, 499	
Bibliographical and Historical Remarks, 500	
Problems, 502	
Computer exercises, 508	
Bibliography, 513	
UNSUPERVISED LEARNING AND CLUSTERING	51
10.1 Introduction, 517	
10.2 Mixture Densities and Identifiability, 518	
10.3 Maximum-Likelihood Estimates, 519	
10.4 Application to Normal Mixtures, 521	
10.4.1 Case 1: Unknown Mean Vectors, 522	
10.4.2 Case 2: All Parameters Unknown, 524	
10.4.3 k-Means Clustering, 526	
*10.4.4 Fuzzy k-Means Clustering, 528	
10.5 Unsupervised Bayesian Learning, 530	
10.5.1 The Bayes Classifier, 530	
10.5.2 Learning the Parameter Vector, 531	
Example Unsupervised Learning of Gaussian Data, 534	
10.5.3 Decision-Directed Approximation, 536	
10.6 Data Description and Clustering, 537	
10.6.1 Similarity Measures, 538	
10.7 Criterion Functions for Clustering, 542	
10.7.1 The Sum-of-Squared-Error Criterion, 542	
10.7.2 Related Minimum Variance Criteria, 543	
10.7.3 Scatter Criteria, 544	
Example 2 Clustering Criteria, 546	
*10.8 Iterative Optimization, 548	
10.9 Hierarchical Clustering, 550	
10.9.1 Definitions, 551	
10.9.2 Agglomerative Hierarchical Clustering, 552	
10.9.3 Stepwise-Optimal Hierarchical Clustering, 555	
10.9.4 Hierarchical Clustering and Induced Metrics, 556	
*10.10 The Problem of Validity, 557	

10.11.1 Unknown Number of Clusters, 561 10.11.2 Adaptive Resonance, 563 10.11.3 Learning with a Critic, 565 *10.12 Graph-Theoretic Methods, 566 10.13 Component Analysis, 568 10.13.1 Principal Component Analysis (PCA), 568 10.13.2 Nonlinear Component Analysis (NLCA), 569 *10.13.3 Independent Component Analysis (ICA), 570 10.14 Low-Dimensional Representations and Multidimensional Scaling (MDS), 573 10.14.1 Self-Organizing Feature Maps, 576 10.14.2 Clustering and Dimensionality Reduction, 580 Summary, 581 Bibliographical and Historical Remarks, 582 Problems, 583 Computer exercises, 593 Bibliography, 598 MATHEMATICAL FOUNDATIONS A.1 Notation, 601 A.2 Linear Algebra, 604 A.2.1 Notation and Preliminaries, 604 A.2.2 Inner Product, 605 A.2.3 Outer Product, 606 A.2.4 Derivatives of Matrices, 606 A.2.5 Determinant and Trace, 608 A.2.6 Matrix Inversion, 609 A.2.7 Eigenvectors and Eigenvalues, 609 A.3 Lagrange Optimization, 610 A.4 Probability Theory, 611 A.4.1 Discrete Random Variables, 611 A.4.2 Expected Values, 611 A.4.3 Pairs of Discrete Random Variables, 612 A.4.4 Statistical Independence, 613 A.4.5 Expected Values of Functions of Two Variables, 613 A.4.6 Conditional Probability, 614 A.4.7 The Law of Total Probability and Bayes Rule, 615 A.4.8 Vector Random Variables, 616 A.4.9 Expectations, Mean Vectors and Covariance Matrices, 617 A.4.10 Continuous Random Variables, 618 A.4.11 Distributions of Sums of Independent Random Variables, 620 A.4.12 Normal Distributions, 621 A.5 Gaussian Derivatives and Integrals, 623 A.5.1 Multivariate Normal Densities, 624 A.5.2 Bivariate Normal Densities, 626 A.6 Hypothesis Testing, 628

*10.11 On-line clustering, 559

Α

A.6.1 Chi-Squared Test, 629

A.7.1 Entropy and Information, 630

A.7 Information Theory, 630

A.7.2 Relative Entropy, 632 A.7.3 Mutual Information, 632 A.8 Computational Complexity, 633 Bibliography, 635

INDEX 637