

CONTENTS

"THIS BOOK IS FOR SALE ONLY IN THE COUNTRY TO WHICH IT IS FIRST CONSIGNED
BY JOHN WILEY & SONS (ASIA) PTE LTD AND MAY NOT BE RE-EXPORTED"

	PREFACE	xvii
1	INTRODUCTION	1
	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	

- *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: $\Sigma_i = \text{arbitrary}$, 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
 - Summary, 63
 - Bibliographical and Historical Remarks, 64
 - Problems, 65
 - Computer exercises, 80
 - Bibliography, 82

3

MAXIMUM-LIKELIHOOD AND BAYESIAN PARAMETER ESTIMATION

84

- 3.1 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
- Summary, 139
- Bibliographical and Historical Remarks, 139
- Problems, 140
- Computer exercises, 155
- Bibliography, 159

4

NONPARAMETRIC TECHNIQUES**161**

- 4.1 Introduction, 161
- 4.2 Density Estimation, 161
- 4.3 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
- 4.4 k_n -Nearest-Neighbor Estimation, 174
 - 4.4.1 k_n -Nearest-Neighbor and Parzen-Window Estimation, 176
 - 4.4.2 Estimation of *A Posteriori* Probabilities, 177
- 4.5 The Nearest-Neighbor Rule, 177
 - 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

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

5

LINEAR DISCRIMINANT FUNCTIONS

215

5.1	Introduction,	215
5.2	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 1 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 Multicategory Generalizations, 265
 - 5.12.1 Kesler's Construction, 266
 - 5.12.2 Convergence of the Fixed-Increment Rule, 266
 - 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**282**

- 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

- 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

7

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

8

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
8.6.1	Grammars, 422
8.6.2	Types of String Grammars, 424
	Example 3 A Grammar for Pronouncing Numbers, 425
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
	Summary, 434
	Bibliographical and Historical Remarks, 435
	Problems, 437
	Computer exercises, 446
	Bibliography, 450

9**ALGORITHM-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
9.3	Bias and Variance, 465
9.3.1	Bias and Variance for Regression, 466
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
9.5	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, 485
 - 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

10**UNSUPERVISED LEARNING AND CLUSTERING****517**

- 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 1 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 On-line clustering, 559
 - 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

A**MATHEMATICAL FOUNDATIONS****601**

- 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
 - A.6.1 Chi-Squared Test, 629
- A.7 Information Theory, 630
 - A.7.1 Entropy and Information, 630

A.7.2 Relative Entropy, 632

A.7.3 Mutual Information, 632

A.8 Computational Complexity, 633

Bibliography, 635

INDEX