

Contents

Preface	vii
1 Introduction	1
2 Overview of Supervised Learning	9
2.1 Introduction	9
2.2 Variable Types and Terminology	9
2.3 Two Simple Approaches to Prediction: Least Squares and Nearest Neighbors	11
2.3.1 Linear Models and Least Squares	11
2.3.2 Nearest-Neighbor Methods	14
2.3.3 From Least Squares to Nearest Neighbors	16
2.4 Statistical Decision Theory	18
2.5 Local Methods in High Dimensions	22
2.6 Statistical Models, Supervised Learning and Function Approximation	28
2.6.1 A Statistical Model for the Joint Distribution $\Pr(X, Y)$	28
2.6.2 Supervised Learning	29
2.6.3 Function Approximation	29
2.7 Structured Regression Models	32
2.7.1 Difficulty of the Problem	32
2.8 Classes of Restricted Estimators	33
2.8.1 Roughness Penalty and Bayesian Methods	34

2.8.2	Kernel Methods and Local Regression	34
2.8.3	Basis Functions and Dictionary Methods	35
2.9	Model Selection and the Bias–Variance Tradeoff	37
	Bibliographic Notes	39
	Exercises	39
3	Linear Methods for Regression	41
3.1	Introduction	41
3.2	Linear Regression Models and Least Squares	42
3.2.1	Example: Prostate Cancer	47
3.2.2	The Gauss–Markov Theorem	49
3.3	Multiple Regression from Simple Univariate Regression	50
3.3.1	Multiple Outputs	54
3.4	Subset Selection and Coefficient Shrinkage	55
3.4.1	Subset Selection	55
3.4.2	Prostate Cancer Data Example (Continued)	57
3.4.3	Shrinkage Methods	59
3.4.4	Methods Using Derived Input Directions	66
3.4.5	Discussion: A Comparison of the Selection and Shrinkage Methods	68
3.4.6	Multiple Outcome Shrinkage and Selection	73
3.5	Computational Considerations	75
	Bibliographic Notes	75
	Exercises	75
4	Linear Methods for Classification	79
4.1	Introduction	79
4.2	Linear Regression of an Indicator Matrix	81
4.3	Linear Discriminant Analysis	84
4.3.1	Regularized Discriminant Analysis	90
4.3.2	Computations for LDA	91
4.3.3	Reduced-Rank Linear Discriminant Analysis	91
4.4	Logistic Regression	95
4.4.1	Fitting Logistic Regression Models	98
4.4.2	Example: South African Heart Disease	100
4.4.3	Quadratic Approximations and Inference	102
4.4.4	Logistic Regression or LDA?	103
4.5	Separating Hyperplanes	105
4.5.1	Rosenblatt’s Perceptron Learning Algorithm	107
4.5.2	Optimal Separating Hyperplanes	108
	Bibliographic Notes	111
	Exercises	111

5	Basis Expansions and Regularization	115
5.1	Introduction	115
5.2	Piecewise Polynomials and Splines	117
5.2.1	Natural Cubic Splines	120
5.2.2	Example: South African Heart Disease (Continued)	122
5.2.3	Example: Phoneme Recognition	124
5.3	Filtering and Feature Extraction	126
5.4	Smoothing Splines	127
5.4.1	Degrees of Freedom and Smoother Matrices	129
5.5	Automatic Selection of the Smoothing Parameters	134
5.5.1	Fixing the Degrees of Freedom	134
5.5.2	The Bias–Variance Tradeoff	134
5.6	Nonparametric Logistic Regression	137
5.7	Multidimensional Splines	138
5.8	Regularization and Reproducing Kernel Hilbert Spaces	144
5.8.1	Spaces of Functions Generated by Kernels	144
5.8.2	Examples of RKHS	146
5.9	Wavelet Smoothing	148
5.9.1	Wavelet Bases and the Wavelet Transform	150
5.9.2	Adaptive Wavelet Filtering	153
	Bibliographic Notes	155
	Exercises	155
	Appendix: Computational Considerations for Splines	160
	Appendix: B -splines	160
	Appendix: Computations for Smoothing Splines	163
6	Kernel Methods	165
6.1	One-Dimensional Kernel Smoothers	165
6.1.1	Local Linear Regression	168
6.1.2	Local Polynomial Regression	171
6.2	Selecting the Width of the Kernel	172
6.3	Local Regression in $\mathbb{R}^p$	174
6.4	Structured Local Regression Models in $\mathbb{R}^p$	175
6.4.1	Structured Kernels	177
6.4.2	Structured Regression Functions	177
6.5	Local Likelihood and Other Models	179
6.6	Kernel Density Estimation and Classification	182
6.6.1	Kernel Density Estimation	182
6.6.2	Kernel Density Classification	184
6.6.3	The Naive Bayes Classifier	184
6.7	Radial Basis Functions and Kernels	186
6.8	Mixture Models for Density Estimation and Classification	188
6.9	Computational Considerations	190
	Bibliographic Notes	190
	Exercises	190

7	Model Assessment and Selection	193
7.1	Introduction	193
7.2	Bias, Variance and Model Complexity	193
7.3	The Bias–Variance Decomposition	196
7.3.1	Example: Bias–Variance Tradeoff	198
7.4	Optimism of the Training Error Rate	200
7.5	Estimates of In-Sample Prediction Error	203
7.6	The Effective Number of Parameters	205
7.7	The Bayesian Approach and BIC	206
7.8	Minimum Description Length	208
7.9	Vapnik–Chernovenkis Dimension	210
7.9.1	Example (Continued)	212
7.10	Cross-Validation	214
7.11	Bootstrap Methods	217
7.11.1	Example (Continued)	220
	Bibliographic Notes	222
	Exercises	222
8	Model Inference and Averaging	225
8.1	Introduction	225
8.2	The Bootstrap and Maximum Likelihood Methods	225
8.2.1	A Smoothing Example	225
8.2.2	Maximum Likelihood Inference	229
8.2.3	Bootstrap versus Maximum Likelihood	231
8.3	Bayesian Methods	231
8.4	Relationship Between the Bootstrap and Bayesian Inference	235
8.5	The EM Algorithm	236
8.5.1	Two-Component Mixture Model	236
8.5.2	The EM Algorithm in General	240
8.5.3	EM as a Maximization–Maximization Procedure	241
8.6	MCMC for Sampling from the Posterior	243
8.7	Bagging	246
8.7.1	Example: Trees with Simulated Data	247
8.8	Model Averaging and Stacking	250
8.9	Stochastic Search: Bumping	253
	Bibliographic Notes	254
	Exercises	255
9	Additive Models, Trees, and Related Methods	257
9.1	Generalized Additive Models	257
9.1.1	Fitting Additive Models	259
9.1.2	Example: Additive Logistic Regression	261
9.1.3	Summary	266
9.2	Tree-Based Methods	266

9.2.1	Background	266
9.2.2	Regression Trees	267
9.2.3	Classification Trees	270
9.2.4	Other Issues	272
9.2.5	Spam Example (Continued)	275
9.3	PRIM—Bump Hunting	279
9.3.1	Spam Example (Continued)	282
9.4	MARS: Multivariate Adaptive Regression Splines	283
9.4.1	Spam Example (Continued)	287
9.4.2	Example (Simulated Data)	288
9.4.3	Other Issues	289
9.5	Hierarchical Mixtures of Experts	290
9.6	Missing Data	293
9.7	Computational Considerations	295
	Bibliographic Notes	295
	Exercises	296

10 Boosting and Additive Trees **299**

10.1	Boosting Methods	299
10.1.1	Outline of this Chapter	302
10.2	Boosting Fits an Additive Model	303
10.3	Forward Stagewise Additive Modeling	304
10.4	Exponential Loss and AdaBoost	305
10.5	Why Exponential Loss?	306
10.6	Loss Functions and Robustness	308
10.7	“Off-the-Shelf” Procedures for Data Mining	312
10.8	Example—Spam Data	314
10.9	Boosting Trees	316
10.10	Numerical Optimization	319
10.10.1	Steepest Descent	320
10.10.2	Gradient Boosting	320
10.10.3	MART	322
10.11	Right-Sized Trees for Boosting	323
10.12	Regularization	324
10.12.1	Shrinkage	326
10.12.2	Penalized Regression	328
10.12.3	Virtues of the L_1 Penalty (Lasso) over L_2	330
10.13	Interpretation	331
10.13.1	Relative Importance of Predictor Variables	331
10.13.2	Partial Dependence Plots	333
10.14	Illustrations	335
10.14.1	California Housing	335
10.14.2	Demographics Data	339
	Bibliographic Notes	340
	Exercises	344

11 Neural Networks	347
11.1 Introduction	347
11.2 Projection Pursuit Regression	347
11.3 Neural Networks	350
11.4 Fitting Neural Networks	353
11.5 Some Issues in Training Neural Networks	355
11.5.1 Starting Values	355
11.5.2 Overfitting	356
11.5.3 Scaling of the Inputs	358
11.5.4 Number of Hidden Units and Layers	358
11.5.5 Multiple Minima	359
11.6 Example: Simulated Data	359
11.7 Example: ZIP Code Data	362
11.8 Discussion	366
11.9 Computational Considerations	367
Bibliographic Notes	367
Exercises	369
 12 Support Vector Machines and Flexible Discriminants	 371
12.1 Introduction	371
12.2 The Support Vector Classifier	371
12.2.1 Computing the Support Vector Classifier	373
12.2.2 Mixture Example (Continued)	375
12.3 Support Vector Machines	377
12.3.1 Computing the SVM for Classification	377
12.3.2 The SVM as a Penalization Method	380
12.3.3 Function Estimation and Reproducing Kernels	381
12.3.4 SVMs and the Curse of Dimensionality	384
12.3.5 Support Vector Machines for Regression	385
12.3.6 Regression and Kernels	387
12.3.7 Discussion	389
12.4 Generalizing Linear Discriminant Analysis	390
12.5 Flexible Discriminant Analysis	391
12.5.1 Computing the FDA Estimates	394
12.6 Penalized Discriminant Analysis	397
12.7 Mixture Discriminant Analysis	399
12.7.1 Example: Waveform Data	402
Bibliographic Notes	406
Exercises	406

13 Prototype Methods and Nearest-Neighbors	411
13.1 Introduction	411
13.2 Prototype Methods	411
13.2.1 K -means Clustering	412
13.2.2 Learning Vector Quantization	414
13.2.3 Gaussian Mixtures	415
13.3 k -Nearest-Neighbor Classifiers	415
13.3.1 Example: A Comparative Study	420
13.3.2 Example: k -Nearest-Neighbors and Image Scene Classification	422
13.3.3 Invariant Metrics and Tangent Distance	423
13.4 Adaptive Nearest-Neighbor Methods	427
13.4.1 Example	430
13.4.2 Global Dimension Reduction for Nearest-Neighbors .	431
13.5 Computational Considerations	432
Bibliographic Notes	433
Exercises	433
 14 Unsupervised Learning	 437
14.1 Introduction	437
14.2 Association Rules	439
14.2.1 Market Basket Analysis	440
14.2.2 The Apriori Algorithm	441
14.2.3 Example: Market Basket Analysis	444
14.2.4 Unsupervised as Supervised Learning	447
14.2.5 Generalized Association Rules	449
14.2.6 Choice of Supervised Learning Method	451
14.2.7 Example: Market Basket Analysis (Continued) . . .	451
14.3 Cluster Analysis	453
14.3.1 Proximity Matrices	455
14.3.2 Dissimilarities Based on Attributes	455
14.3.3 Object Dissimilarity	457
14.3.4 Clustering Algorithms	459
14.3.5 Combinatorial Algorithms	460
14.3.6 K -means	461
14.3.7 Gaussian Mixtures as Soft K -means Clustering . . .	463
14.3.8 Example: Human Tumor Microarray Data	463
14.3.9 Vector Quantization	466
14.3.10 K -medoids	468
14.3.11 Practical Issues	470
14.3.12 Hierarchical Clustering	472
14.4 Self-Organizing Maps	480
14.5 Principal Components, Curves and Surfaces	485
14.5.1 Principal Components	485
14.5.2 Principal Curves and Surfaces	491

14.6 Independent Component Analysis and Exploratory Projection Pursuit	494
14.6.1 Latent Variables and Factor Analysis	494
14.6.2 Independent Component Analysis	496
14.6.3 Exploratory Projection Pursuit	500
14.6.4 A Different Approach to ICA	500
14.7 Multidimensional Scaling	502
Bibliographic Notes	503
Exercises	504
 References	 509
 Author Index	 523
 Index	 527