

# Contents

1	Introduction . . . . .	1
2	Overview of Supervised Learning . . . . .	9
3	2.1 Introduction . . . . .	9
4	2.2 Variable Types and Terminology . . . . .	9
5	2.3 Two Simple Approaches to Prediction: Least Squares and Nearest Neighbors . . . . .	11
6	2.3.1 Linear Models and Least Squares . . . . .	11
7	2.3.2 Nearest-Neighbor Methods . . . . .	14
8	2.3.3 From Least Squares to Nearest Neighbors . . . . .	16
9	2.4 Statistical Decision Theory . . . . .	18
10	2.5 Local Methods in High Dimensions . . . . .	22
11	2.6 Statistical Models, Supervised Learning and Function Approximation . . . . .	28
12	2.6.1 A Statistical Model for the Joint Distribution $\Pr(X, Y)$ . . . . .	28
13	2.6.2 Supervised Learning . . . . .	29
14	2.6.3 Function Approximation . . . . .	29
15	2.7 Structured Regression Models . . . . .	32
16	2.7.1 Difficulty of the Problem . . . . .	32
17	2.8 Classes of Restricted Estimators . . . . .	33
18	2.8.1 Roughness Penalty and Bayesian Methods . . . . .	34

## Preface

vii

1	Introduction . . . . .	1
2	Overview of Supervised Learning . . . . .	9
3	2.1 Introduction . . . . .	9
4	2.2 Variable Types and Terminology . . . . .	9
5	2.3 Two Simple Approaches to Prediction: Least Squares and Nearest Neighbors . . . . .	11
6	2.3.1 Linear Models and Least Squares . . . . .	11
7	2.3.2 Nearest-Neighbor Methods . . . . .	14
8	2.3.3 From Least Squares to Nearest Neighbors . . . . .	16
9	2.4 Statistical Decision Theory . . . . .	18
10	2.5 Local Methods in High Dimensions . . . . .	22
11	2.6 Statistical Models, Supervised Learning and Function Approximation . . . . .	28
12	2.6.1 A Statistical Model for the Joint Distribution $\Pr(X, Y)$ . . . . .	28
13	2.6.2 Supervised Learning . . . . .	29
14	2.6.3 Function Approximation . . . . .	29
15	2.7 Structured Regression Models . . . . .	32
16	2.7.1 Difficulty of the Problem . . . . .	32
17	2.8 Classes of Restricted Estimators . . . . .	33
18	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
<b>3 Linear Methods for Regression</b>	<b>41</b>
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
<b>4 Linear Methods for Classification</b>	<b>79</b>
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

<b>5 Basis Expansions and Regularization</b>	<b>115</b>
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: <i>B</i> -splines . . . . .	160
Appendix: Computations for Smoothing Splines . . . . .	163
<b>6 Kernel Methods</b>	<b>165</b>
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

<b>7 Model Assessment and Selection</b>	<b>193</b>
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–Chervonenkis 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
<b>8 Model Inference and Averaging</b>	<b>225</b>
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
<b>9 Additive Models, Trees, and Related Methods</b>	<b>257</b>
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
<b>10</b>	<b>Boosting and Additive Trees</b>	<b>299</b>
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

<b>11 Neural Networks</b>	<b>347</b>
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
<b>12 Support Vector Machines and Flexible Discriminants</b>	<b>371</b>
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

<b>13 Prototype Methods and Nearest-Neighbors</b>	<b>411</b>
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
<b>14 Unsupervised Learning</b>	<b>437</b>
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
<b>References</b>	<b>509</b>

<b>Author Index</b>	<b>523</b>
---------------------	------------

<b>Index</b>	<b>527</b>
--------------	------------