

Springer Series in Statistics

Trevor Hastie
Robert Tibshirani
Jerome Friedman

The Elements of Statistical Learning

Data Mining, Inference, and Prediction

Second Edition

 Springer

Contents

Preface to the Second Edition	vii
Preface to the First Edition	xi
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	43
3.1	Introduction	43
3.2	Linear Regression Models and Least Squares	44
3.2.1	Example: Prostate Cancer	49
3.2.2	The Gauss–Markov Theorem	51
3.2.3	Multiple Regression from Simple Univariate Regression	52
3.2.4	Multiple Outputs	56
3.3	Subset Selection	57
3.3.1	Best-Subset Selection	57
3.3.2	Forward- and Backward-Stepwise Selection	58
3.3.3	Forward-Stagewise Regression	60
3.3.4	Prostate Cancer Data Example (Continued)	61
3.4	Shrinkage Methods	61
3.4.1	Ridge Regression	61
3.4.2	The Lasso	68
3.4.3	Discussion: Subset Selection, Ridge Regression and the Lasso	69
3.4.4	Least Angle Regression	73
3.5	Methods Using Derived Input Directions	79
3.5.1	Principal Components Regression	79
3.5.2	Partial Least Squares	80
3.6	Discussion: A Comparison of the Selection and Shrinkage Methods	82
3.7	Multiple Outcome Shrinkage and Selection	84
3.8	More on the Lasso and Related Path Algorithms	86
3.8.1	Incremental Forward Stagewise Regression	86
3.8.2	Piecewise-Linear Path Algorithms	89
3.8.3	The Dantzig Selector	89
3.8.4	The Grouped Lasso	90
3.8.5	Further Properties of the Lasso	91
3.8.6	Pathwise Coordinate Optimization	92
3.9	Computational Considerations	93
	Bibliographic Notes	94
	Exercises	94

4	Linear Methods for Classification	101
4.1	Introduction	101
4.2	Linear Regression of an Indicator Matrix	103
4.3	Linear Discriminant Analysis	106
4.3.1	Regularized Discriminant Analysis	112
4.3.2	Computations for LDA	113
4.3.3	Reduced-Rank Linear Discriminant Analysis	113
4.4	Logistic Regression	119
4.4.1	Fitting Logistic Regression Models	120
4.4.2	Example: South African Heart Disease	122
4.4.3	Quadratic Approximations and Inference	124
4.4.4	L_1 Regularized Logistic Regression	125
4.4.5	Logistic Regression or LDA?	127
4.5	Separating Hyperplanes	129
4.5.1	Rosenblatt's Perceptron Learning Algorithm	130
4.5.2	Optimal Separating Hyperplanes	132
	Bibliographic Notes	135
	Exercises	135
5	Basis Expansions and Regularization	139
5.1	Introduction	139
5.2	Piecewise Polynomials and Splines	141
5.2.1	Natural Cubic Splines	144
5.2.2	Example: South African Heart Disease (Continued)	146
5.2.3	Example: Phoneme Recognition	148
5.3	Filtering and Feature Extraction	150
5.4	Smoothing Splines	151
5.4.1	Degrees of Freedom and Smoother Matrices	153
5.5	Automatic Selection of the Smoothing Parameters	156
5.5.1	Fixing the Degrees of Freedom	158
5.5.2	The Bias–Variance Tradeoff	158
5.6	Nonparametric Logistic Regression	161
5.7	Multidimensional Splines	162
5.8	Regularization and Reproducing Kernel Hilbert Spaces	167
5.8.1	Spaces of Functions Generated by Kernels	168
5.8.2	Examples of RKHS	170
5.9	Wavelet Smoothing	174
5.9.1	Wavelet Bases and the Wavelet Transform	176
5.9.2	Adaptive Wavelet Filtering	179
	Bibliographic Notes	181
	Exercises	181
	Appendix: Computational Considerations for Splines	186
	Appendix: B -splines	186
	Appendix: Computations for Smoothing Splines	189

6	Kernel Smoothing Methods	191
6.1	One-Dimensional Kernel Smoothers	192
6.1.1	Local Linear Regression	194
6.1.2	Local Polynomial Regression	197
6.2	Selecting the Width of the Kernel	198
6.3	Local Regression in \mathbb{R}^p	200
6.4	Structured Local Regression Models in \mathbb{R}^p	201
6.4.1	Structured Kernels	203
6.4.2	Structured Regression Functions	203
6.5	Local Likelihood and Other Models	205
6.6	Kernel Density Estimation and Classification	208
6.6.1	Kernel Density Estimation	208
6.6.2	Kernel Density Classification	210
6.6.3	The Naive Bayes Classifier	210
6.7	Radial Basis Functions and Kernels	212
6.8	Mixture Models for Density Estimation and Classification	214
6.9	Computational Considerations	216
	Bibliographic Notes	216
	Exercises	216
7	Model Assessment and Selection	219
7.1	Introduction	219
7.2	Bias, Variance and Model Complexity	219
7.3	The Bias–Variance Decomposition	223
7.3.1	Example: Bias–Variance Tradeoff	226
7.4	Optimism of the Training Error Rate	228
7.5	Estimates of In-Sample Prediction Error	230
7.6	The Effective Number of Parameters	232
7.7	The Bayesian Approach and BIC	233
7.8	Minimum Description Length	235
7.9	Vapnik–Chervonenkis Dimension	237
7.9.1	Example (Continued)	239
7.10	Cross-Validation	241
7.10.1	K -Fold Cross-Validation	241
7.10.2	The Wrong and Right Way to Do Cross-validation	245
7.10.3	Does Cross-Validation Really Work?	247
7.11	Bootstrap Methods	249
7.11.1	Example (Continued)	252
7.12	Conditional or Expected Test Error?	254
	Bibliographic Notes	257
	Exercises	257
8	Model Inference and Averaging	261
8.1	Introduction	261

8.2	The Bootstrap and Maximum Likelihood Methods	261
8.2.1	A Smoothing Example	261
8.2.2	Maximum Likelihood Inference	265
8.2.3	Bootstrap versus Maximum Likelihood	267
8.3	Bayesian Methods	267
8.4	Relationship Between the Bootstrap and Bayesian Inference	271
8.5	The EM Algorithm	272
8.5.1	Two-Component Mixture Model	272
8.5.2	The EM Algorithm in General	276
8.5.3	EM as a Maximization–Maximization Procedure	277
8.6	MCMC for Sampling from the Posterior	279
8.7	Bagging	282
8.7.1	Example: Trees with Simulated Data	283
8.8	Model Averaging and Stacking	288
8.9	Stochastic Search: Bumping	290
	Bibliographic Notes	292
	Exercises	293
9	Additive Models, Trees, and Related Methods	295
9.1	Generalized Additive Models	295
9.1.1	Fitting Additive Models	297
9.1.2	Example: Additive Logistic Regression	299
9.1.3	Summary	304
9.2	Tree-Based Methods	305
9.2.1	Background	305
9.2.2	Regression Trees	307
9.2.3	Classification Trees	308
9.2.4	Other Issues	310
9.2.5	Spam Example (Continued)	313
9.3	PRIM: Bump Hunting	317
9.3.1	Spam Example (Continued)	320
9.4	MARS: Multivariate Adaptive Regression Splines	321
9.4.1	Spam Example (Continued)	326
9.4.2	Example (Simulated Data)	327
9.4.3	Other Issues	328
9.5	Hierarchical Mixtures of Experts	329
9.6	Missing Data	332
9.7	Computational Considerations	334
	Bibliographic Notes	334
	Exercises	335
10	Boosting and Additive Trees	337
10.1	Boosting Methods	337
10.1.1	Outline of This Chapter	340

10.2	Boosting Fits an Additive Model	341
10.3	Forward Stagewise Additive Modeling	342
10.4	Exponential Loss and AdaBoost	343
10.5	Why Exponential Loss?	345
10.6	Loss Functions and Robustness	346
10.7	“Off-the-Shelf” Procedures for Data Mining	350
10.8	Example: Spam Data	352
10.9	Boosting Trees	353
10.10	Numerical Optimization via Gradient Boosting	358
10.10.1	Steepest Descent	358
10.10.2	Gradient Boosting	359
10.10.3	Implementations of Gradient Boosting	360
10.11	Right-Sized Trees for Boosting	361
10.12	Regularization	364
10.12.1	Shrinkage	364
10.12.2	Subsampling	365
10.13	Interpretation	367
10.13.1	Relative Importance of Predictor Variables	367
10.13.2	Partial Dependence Plots	369
10.14	Illustrations	371
10.14.1	California Housing	371
10.14.2	New Zealand Fish	375
10.14.3	Demographics Data	379
	Bibliographic Notes	380
	Exercises	384
11	Neural Networks	389
11.1	Introduction	389
11.2	Projection Pursuit Regression	389
11.3	Neural Networks	392
11.4	Fitting Neural Networks	395
11.5	Some Issues in Training Neural Networks	397
11.5.1	Starting Values	397
11.5.2	Overfitting	398
11.5.3	Scaling of the Inputs	398
11.5.4	Number of Hidden Units and Layers	400
11.5.5	Multiple Minima	400
11.6	Example: Simulated Data	401
11.7	Example: ZIP Code Data	404
11.8	Discussion	408
11.9	Bayesian Neural Nets and the NIPS 2003 Challenge	409
11.9.1	Bayes, Boosting and Bagging	410
11.9.2	Performance Comparisons	412
11.10	Computational Considerations	414
	Bibliographic Notes	415

Exercises	415
12 Support Vector Machines and Flexible Discriminants	417
12.1 Introduction	417
12.2 The Support Vector Classifier	417
12.2.1 Computing the Support Vector Classifier	420
12.2.2 Mixture Example (Continued)	421
12.3 Support Vector Machines and Kernels	423
12.3.1 Computing the SVM for Classification	423
12.3.2 The SVM as a Penalization Method	426
12.3.3 Function Estimation and Reproducing Kernels	428
12.3.4 SVMs and the Curse of Dimensionality	431
12.3.5 A Path Algorithm for the SVM Classifier	432
12.3.6 Support Vector Machines for Regression	434
12.3.7 Regression and Kernels	436
12.3.8 Discussion	438
12.4 Generalizing Linear Discriminant Analysis	438
12.5 Flexible Discriminant Analysis	440
12.5.1 Computing the FDA Estimates	444
12.6 Penalized Discriminant Analysis	446
12.7 Mixture Discriminant Analysis	449
12.7.1 Example: Waveform Data	451
Bibliographic Notes	455
Exercises	455
13 Prototype Methods and Nearest-Neighbors	459
13.1 Introduction	459
13.2 Prototype Methods	459
13.2.1 K -means Clustering	460
13.2.2 Learning Vector Quantization	462
13.2.3 Gaussian Mixtures	463
13.3 k -Nearest-Neighbor Classifiers	463
13.3.1 Example: A Comparative Study	468
13.3.2 Example: k -Nearest-Neighbors and Image Scene Classification	470
13.3.3 Invariant Metrics and Tangent Distance	471
13.4 Adaptive Nearest-Neighbor Methods	475
13.4.1 Example	478
13.4.2 Global Dimension Reduction for Nearest-Neighbors	479
13.5 Computational Considerations	480
Bibliographic Notes	481
Exercises	481

14 Unsupervised Learning	485
14.1 Introduction	485
14.2 Association Rules	487
14.2.1 Market Basket Analysis	488
14.2.2 The Apriori Algorithm	489
14.2.3 Example: Market Basket Analysis	492
14.2.4 Unsupervised as Supervised Learning	495
14.2.5 Generalized Association Rules	497
14.2.6 Choice of Supervised Learning Method	499
14.2.7 Example: Market Basket Analysis (Continued)	499
14.3 Cluster Analysis	501
14.3.1 Proximity Matrices	503
14.3.2 Dissimilarities Based on Attributes	503
14.3.3 Object Dissimilarity	505
14.3.4 Clustering Algorithms	507
14.3.5 Combinatorial Algorithms	507
14.3.6 K -means	509
14.3.7 Gaussian Mixtures as Soft K -means Clustering	510
14.3.8 Example: Human Tumor Microarray Data	512
14.3.9 Vector Quantization	514
14.3.10 K -medoids	515
14.3.11 Practical Issues	518
14.3.12 Hierarchical Clustering	520
14.4 Self-Organizing Maps	528
14.5 Principal Components, Curves and Surfaces	534
14.5.1 Principal Components	534
14.5.2 Principal Curves and Surfaces	541
14.5.3 Spectral Clustering	544
14.5.4 Kernel Principal Components	547
14.5.5 Sparse Principal Components	550
14.6 Non-negative Matrix Factorization	553
14.6.1 Archetypal Analysis	554
14.7 Independent Component Analysis and Exploratory Projection Pursuit	557
14.7.1 Latent Variables and Factor Analysis	558
14.7.2 Independent Component Analysis	560
14.7.3 Exploratory Projection Pursuit	565
14.7.4 A Direct Approach to ICA	565
14.8 Multidimensional Scaling	570
14.9 Nonlinear Dimension Reduction and Local Multidimensional Scaling	572
14.10 The Google PageRank Algorithm	576
Bibliographic Notes	578
Exercises	579

15 Random Forests	587
15.1 Introduction	587
15.2 Definition of Random Forests	587
15.3 Details of Random Forests	592
15.3.1 Out of Bag Samples	592
15.3.2 Variable Importance	593
15.3.3 Proximity Plots	595
15.3.4 Random Forests and Overfitting	596
15.4 Analysis of Random Forests	597
15.4.1 Variance and the De-Correlation Effect	597
15.4.2 Bias	600
15.4.3 Adaptive Nearest Neighbors	601
Bibliographic Notes	602
Exercises	603
16 Ensemble Learning	605
16.1 Introduction	605
16.2 Boosting and Regularization Paths	607
16.2.1 Penalized Regression	607
16.2.2 The “Bet on Sparsity” Principle	610
16.2.3 Regularization Paths, Over-fitting and Margins	613
16.3 Learning Ensembles	616
16.3.1 Learning a Good Ensemble	617
16.3.2 Rule Ensembles	622
Bibliographic Notes	623
Exercises	624
17 Undirected Graphical Models	625
17.1 Introduction	625
17.2 Markov Graphs and Their Properties	627
17.3 Undirected Graphical Models for Continuous Variables	630
17.3.1 Estimation of the Parameters when the Graph Structure is Known	631
17.3.2 Estimation of the Graph Structure	635
17.4 Undirected Graphical Models for Discrete Variables	638
17.4.1 Estimation of the Parameters when the Graph Structure is Known	639
17.4.2 Hidden Nodes	641
17.4.3 Estimation of the Graph Structure	642
17.4.4 Restricted Boltzmann Machines	643
Exercises	645
18 High-Dimensional Problems: $p \gg N$	649
18.1 When p is Much Bigger than N	649

18.2	Diagonal Linear Discriminant Analysis and Nearest Shrunken Centroids	651
18.3	Linear Classifiers with Quadratic Regularization	654
18.3.1	Regularized Discriminant Analysis	656
18.3.2	Logistic Regression with Quadratic Regularization	657
18.3.3	The Support Vector Classifier	657
18.3.4	Feature Selection	658
18.3.5	Computational Shortcuts When $p \gg N$	659
18.4	Linear Classifiers with L_1 Regularization	661
18.4.1	Application of Lasso to Protein Mass Spectroscopy	664
18.4.2	The Fused Lasso for Functional Data	666
18.5	Classification When Features are Unavailable	668
18.5.1	Example: String Kernels and Protein Classification	668
18.5.2	Classification and Other Models Using Inner-Product Kernels and Pairwise Distances	670
18.5.3	Example: Abstracts Classification	672
18.6	High-Dimensional Regression: Supervised Principal Components	674
18.6.1	Connection to Latent-Variable Modeling	678
18.6.2	Relationship with Partial Least Squares	680
18.6.3	Pre-Conditioning for Feature Selection	681
18.7	Feature Assessment and the Multiple-Testing Problem	683
18.7.1	The False Discovery Rate	687
18.7.2	Asymmetric Cutpoints and the SAM Procedure	690
18.7.3	A Bayesian Interpretation of the FDR	692
18.8	Bibliographic Notes	693
	Exercises	694
	References	699
	Author Index	729
	Index	737