

# Contents

<b>Preface to the Second Edition</b>	<b>vii</b>
<b>Preface to the First Edition</b>	<b>xi</b>
<b>1 Introduction</b>	<b>1</b>
<b>2 Overview of Supervised Learning</b>	<b>9</b>
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
<b>3</b>	<b>Linear Methods for Regression</b>	<b>43</b>
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

<b>4</b>	<b>Linear Methods for Classification</b>	<b>101</b>
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
<b>5</b>	<b>Basis Expansions and Regularization</b>	<b>139</b>
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

<b>6</b>	<b>Kernel Smoothing Methods</b>	<b>191</b>
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
<b>7</b>	<b>Model Assessment and Selection</b>	<b>219</b>
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
<b>8</b>	<b>Model Inference and Averaging</b>	<b>261</b>
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
<b>9</b>	<b>Additive Models, Trees, and Related Methods</b>	<b>295</b>
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
<b>10</b>	<b>Boosting and Additive Trees</b>	<b>337</b>
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
<b>11</b>	<b>Neural Networks</b>	<b>389</b>
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
<b>12 Support Vector Machines and Flexible Discriminants</b>	<b>417</b>
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
<b>13 Prototype Methods and Nearest-Neighbors</b>	<b>459</b>
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

<b>14 Unsupervised Learning</b>	<b>485</b>
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



<b>15 Random Forests</b>	<b>587</b>
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
 <b>16 Ensemble Learning</b>	 <b>605</b>
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
 <b>17 Undirected Graphical Models</b>	 <b>625</b>
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
 <b>18 High-Dimensional Problems: <math>p \gg N</math></b>	 <b>649</b>
18.1 When $p$ is Much Bigger than $N$ . . . . .	649

18.2	Diagonal Linear Discriminant Analysis and Nearest Shrunk 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
	<b>References</b>	<b>699</b>
	<b>Author Index</b>	<b>729</b>
	<b>Index</b>	<b>731</b>

# 1

## Introduction

*Statistical learning* plays a key role in many areas of science, finance and industry. Here are some examples of learning problems:

- Predict whether a patient, hospitalized due to a heart attack, will have a second heart attack. The prediction is to be based on demographic, diet and clinical measurements for that patient.
- Predict the price of a stock in 6 months from now, on the basis of company performance measures and economic data.
- Identify the numbers in a handwritten ZIP code, from a digitized image.
- Estimate the amount of glucose in the blood of a diabetic person, from the infrared absorption spectrum of that person's blood.
- Identify the risk factors for prostate cancer, based on clinical and demographic variables.

The science of learning plays a key role in the fields of statistics, data mining and artificial intelligence, intersecting with areas of engineering and other disciplines.

This book is about learning from data. In a typical scenario, we have an outcome measurement, usually quantitative (such as a stock price) or categorical (such as heart attack/no heart attack), that we wish to predict based on a set of *features* (such as diet and clinical measurements). We have a *training set* of data, in which we observe the outcome and feature