

# Contents

<b>Preface</b>	<b>vii</b>
<b>1 Introduction</b>	<b>1</b>
1.1 What Is Data Mining? . . . . .	2
1.2 Motivating Challenges . . . . .	4
1.3 The Origins of Data Mining . . . . .	6
1.4 Data Mining Tasks . . . . .	7
1.5 Scope and Organization of the Book . . . . .	11
1.6 Bibliographic Notes . . . . .	13
1.7 Exercises . . . . .	16
<b>2 Data</b>	<b>19</b>
2.1 Types of Data . . . . .	22
2.1.1 Attributes and Measurement . . . . .	23
2.1.2 Types of Data Sets . . . . .	29
2.2 Data Quality . . . . .	36
2.2.1 Measurement and Data Collection Issues . . . . .	37
2.2.2 Issues Related to Applications . . . . .	43
2.3 Data Preprocessing . . . . .	44
2.3.1 Aggregation . . . . .	45
2.3.2 Sampling . . . . .	47
2.3.3 Dimensionality Reduction . . . . .	50
2.3.4 Feature Subset Selection . . . . .	52
2.3.5 Feature Creation . . . . .	55
2.3.6 Discretization and Binarization . . . . .	57
2.3.7 Variable Transformation . . . . .	63
2.4 Measures of Similarity and Dissimilarity . . . . .	65
2.4.1 Basics . . . . .	66
2.4.2 Similarity and Dissimilarity between Simple Attributes . . . . .	67
2.4.3 Dissimilarities between Data Objects . . . . .	69
2.4.4 Similarities between Data Objects . . . . .	72

2.4.5	Examples of Proximity Measures . . . . .	73
2.4.6	Issues in Proximity Calculation . . . . .	80
2.4.7	Selecting the Right Proximity Measure . . . . .	83
2.5	Bibliographic Notes . . . . .	84
2.6	Exercises . . . . .	88
<b>3</b>	<b>Exploring Data</b>	<b>97</b>
3.1	The Iris Data Set . . . . .	98
3.2	Summary Statistics . . . . .	98
3.2.1	Frequencies and the Mode . . . . .	99
3.2.2	Percentiles . . . . .	100
3.2.3	Measures of Location: Mean and Median . . . . .	101
3.2.4	Measures of Spread: Range and Variance . . . . .	102
3.2.5	Multivariate Summary Statistics . . . . .	104
3.2.6	Other Ways to Summarize the Data . . . . .	105
3.3	Visualization . . . . .	105
3.3.1	Motivations for Visualization . . . . .	105
3.3.2	General Concepts . . . . .	106
3.3.3	Techniques . . . . .	110
3.3.4	Visualizing Higher-Dimensional Data . . . . .	124
3.3.5	Do's and Don'ts . . . . .	130
3.4	OLAP and Multidimensional Data Analysis . . . . .	131
3.4.1	Representing Iris Data as a Multidimensional Array . . . . .	131
3.4.2	Multidimensional Data: The General Case . . . . .	133
3.4.3	Analyzing Multidimensional Data . . . . .	135
3.4.4	Final Comments on Multidimensional Data Analysis . . . . .	139
3.5	Bibliographic Notes . . . . .	139
3.6	Exercises . . . . .	141
<b>4</b>	<b>Classification:</b>	
	<b>Basic Concepts, Decision Trees, and Model Evaluation</b>	<b>145</b>
4.1	Preliminaries . . . . .	146
4.2	General Approach to Solving a Classification Problem . . . . .	148
4.3	Decision Tree Induction . . . . .	150
4.3.1	How a Decision Tree Works . . . . .	150
4.3.2	How to Build a Decision Tree . . . . .	151
4.3.3	Methods for Expressing Attribute Test Conditions . . . . .	155
4.3.4	Measures for Selecting the Best Split . . . . .	158
4.3.5	Algorithm for Decision Tree Induction . . . . .	164
4.3.6	An Example: Web Robot Detection . . . . .	166

4.3.7	Characteristics of Decision Tree Induction . . . . .	168
4.4	Model Overfitting . . . . .	172
4.4.1	Overfitting Due to Presence of Noise . . . . .	175
4.4.2	Overfitting Due to Lack of Representative Samples . . .	177
4.4.3	Overfitting and the Multiple Comparison Procedure . .	178
4.4.4	Estimation of Generalization Errors . . . . .	179
4.4.5	Handling Overfitting in Decision Tree Induction . . . .	184
4.5	Evaluating the Performance of a Classifier . . . . .	186
4.5.1	Holdout Method . . . . .	186
4.5.2	Random Subsampling . . . . .	187
4.5.3	Cross-Validation . . . . .	187
4.5.4	Bootstrap . . . . .	188
4.6	Methods for Comparing Classifiers . . . . .	188
4.6.1	Estimating a Confidence Interval for Accuracy . . . . .	189
4.6.2	Comparing the Performance of Two Models . . . . .	191
4.6.3	Comparing the Performance of Two Classifiers . . . . .	192
4.7	Bibliographic Notes . . . . .	193
4.8	Exercises . . . . .	198
<b>5</b>	<b>Classification: Alternative Techniques</b>	<b>207</b>
5.1	Rule-Based Classifier . . . . .	207
5.1.1	How a Rule-Based Classifier Works . . . . .	209
5.1.2	Rule-Ordering Schemes . . . . .	211
5.1.3	How to Build a Rule-Based Classifier . . . . .	212
5.1.4	Direct Methods for Rule Extraction . . . . .	213
5.1.5	Indirect Methods for Rule Extraction . . . . .	221
5.1.6	Characteristics of Rule-Based Classifiers . . . . .	223
5.2	Nearest-Neighbor classifiers . . . . .	223
5.2.1	Algorithm . . . . .	225
5.2.2	Characteristics of Nearest-Neighbor Classifiers . . . .	226
5.3	Bayesian Classifiers . . . . .	227
5.3.1	Bayes Theorem . . . . .	228
5.3.2	Using the Bayes Theorem for Classification . . . . .	229
5.3.3	Naïve Bayes Classifier . . . . .	231
5.3.4	Bayes Error Rate . . . . .	238
5.3.5	Bayesian Belief Networks . . . . .	240
5.4	Artificial Neural Network (ANN) . . . . .	246
5.4.1	Perceptron . . . . .	247
5.4.2	Multilayer Artificial Neural Network . . . . .	251
5.4.3	Characteristics of ANN . . . . .	255

5.5	Support Vector Machine (SVM) . . . . .	256
5.5.1	Maximum Margin Hyperplanes . . . . .	256
5.5.2	Linear SVM: Separable Case . . . . .	259
5.5.3	Linear SVM: Nonseparable Case . . . . .	266
5.5.4	Nonlinear SVM . . . . .	270
5.5.5	Characteristics of SVM . . . . .	276
5.6	Ensemble Methods . . . . .	276
5.6.1	Rationale for Ensemble Method . . . . .	277
5.6.2	Methods for Constructing an Ensemble Classifier . . . . .	278
5.6.3	Bias-Variance Decomposition . . . . .	281
5.6.4	Bagging . . . . .	283
5.6.5	Boosting . . . . .	285
5.6.6	Random Forests . . . . .	290
5.6.7	Empirical Comparison among Ensemble Methods . . . . .	294
5.7	Class Imbalance Problem . . . . .	294
5.7.1	Alternative Metrics . . . . .	295
5.7.2	The Receiver Operating Characteristic Curve . . . . .	298
5.7.3	Cost-Sensitive Learning . . . . .	302
5.7.4	Sampling-Based Approaches . . . . .	305
5.8	Multiclass Problem . . . . .	306
5.9	Bibliographic Notes . . . . .	309
5.10	Exercises . . . . .	315
<b>6</b>	<b>Association Analysis: Basic Concepts and Algorithms</b>	<b>327</b>
6.1	Problem Definition . . . . .	328
6.2	Frequent Itemset Generation . . . . .	332
6.2.1	The <i>Apriori</i> Principle . . . . .	333
6.2.2	Frequent Itemset Generation in the <i>Apriori</i> Algorithm . . . . .	335
6.2.3	Candidate Generation and Pruning . . . . .	338
6.2.4	Support Counting . . . . .	342
6.2.5	Computational Complexity . . . . .	345
6.3	Rule Generation . . . . .	349
6.3.1	Confidence-Based Pruning . . . . .	350
6.3.2	Rule Generation in <i>Apriori</i> Algorithm . . . . .	350
6.3.3	An Example: Congressional Voting Records . . . . .	352
6.4	Compact Representation of Frequent Itemsets . . . . .	353
6.4.1	Maximal Frequent Itemsets . . . . .	354
6.4.2	Closed Frequent Itemsets . . . . .	355
6.5	Alternative Methods for Generating Frequent Itemsets . . . . .	359
6.6	FP-Growth Algorithm . . . . .	363

6.6.1	FP-Tree Representation . . . . .	363
6.6.2	Frequent Itemset Generation in FP-Growth Algorithm . . . . .	366
6.7	Evaluation of Association Patterns . . . . .	370
6.7.1	Objective Measures of Interestingness . . . . .	371
6.7.2	Measures beyond Pairs of Binary Variables . . . . .	382
6.7.3	Simpson's Paradox . . . . .	384
6.8	Effect of Skewed Support Distribution . . . . .	386
6.9	Bibliographic Notes . . . . .	390
6.10	Exercises . . . . .	404
<b>7</b>	<b>Association Analysis: Advanced Concepts</b> . . . . .	<b>415</b>
7.1	Handling Categorical Attributes . . . . .	415
7.2	Handling Continuous Attributes . . . . .	418
7.2.1	Discretization-Based Methods . . . . .	418
7.2.2	Statistics-Based Methods . . . . .	422
7.2.3	Non-discretization Methods . . . . .	424
7.3	Handling a Concept Hierarchy . . . . .	426
7.4	Sequential Patterns . . . . .	429
7.4.1	Problem Formulation . . . . .	429
7.4.2	Sequential Pattern Discovery . . . . .	431
7.4.3	Timing Constraints . . . . .	436
7.4.4	Alternative Counting Schemes . . . . .	439
7.5	Subgraph Patterns . . . . .	442
7.5.1	Graphs and Subgraphs . . . . .	443
7.5.2	Frequent Subgraph Mining . . . . .	444
7.5.3	<i>Apriori</i> -like Method . . . . .	447
7.5.4	Candidate Generation . . . . .	448
7.5.5	Candidate Pruning . . . . .	453
7.5.6	Support Counting . . . . .	457
7.6	Infrequent Patterns . . . . .	457
7.6.1	Negative Patterns . . . . .	458
7.6.2	Negatively Correlated Patterns . . . . .	458
7.6.3	Comparisons among Infrequent Patterns, Negative Pat- terns, and Negatively Correlated Patterns . . . . .	460
7.6.4	Techniques for Mining Interesting Infrequent Patterns . . . . .	461
7.6.5	Techniques Based on Mining Negative Patterns . . . . .	463
7.6.6	Techniques Based on Support Expectation . . . . .	465
7.7	Bibliographic Notes . . . . .	469
7.8	Exercises . . . . .	473

<b>8</b>	<b>Cluster Analysis: Basic Concepts and Algorithms</b>	<b>487</b>
8.1	Overview . . . . .	490
8.1.1	What Is Cluster Analysis? . . . . .	490
8.1.2	Different Types of Clusterings . . . . .	491
8.1.3	Different Types of Clusters . . . . .	493
8.2	K-means . . . . .	496
8.2.1	The Basic K-means Algorithm . . . . .	497
8.2.2	K-means: Additional Issues . . . . .	506
8.2.3	Bisecting K-means . . . . .	508
8.2.4	K-means and Different Types of Clusters . . . . .	510
8.2.5	Strengths and Weaknesses . . . . .	510
8.2.6	K-means as an Optimization Problem . . . . .	513
8.3	Agglomerative Hierarchical Clustering . . . . .	515
8.3.1	Basic Agglomerative Hierarchical Clustering Algorithm . . . . .	516
8.3.2	Specific Techniques . . . . .	518
8.3.3	The Lance-Williams Formula for Cluster Proximity . . . . .	524
8.3.4	Key Issues in Hierarchical Clustering . . . . .	524
8.3.5	Strengths and Weaknesses . . . . .	526
8.4	DBSCAN . . . . .	526
8.4.1	Traditional Density: Center-Based Approach . . . . .	527
8.4.2	The DBSCAN Algorithm . . . . .	528
8.4.3	Strengths and Weaknesses . . . . .	530
8.5	Cluster Evaluation . . . . .	532
8.5.1	Overview . . . . .	533
8.5.2	Unsupervised Cluster Evaluation Using Cohesion and Separation . . . . .	536
8.5.3	Unsupervised Cluster Evaluation Using the Proximity Matrix . . . . .	542
8.5.4	Unsupervised Evaluation of Hierarchical Clustering . . . . .	544
8.5.5	Determining the Correct Number of Clusters . . . . .	546
8.5.6	Clustering Tendency . . . . .	547
8.5.7	Supervised Measures of Cluster Validity . . . . .	548
8.5.8	Assessing the Significance of Cluster Validity Measures . . . . .	553
8.6	Bibliographic Notes . . . . .	555
8.7	Exercises . . . . .	559
<b>9</b>	<b>Cluster Analysis: Additional Issues and Algorithms</b>	<b>569</b>
9.1	Characteristics of Data, Clusters, and Clustering Algorithms . . . . .	570
9.1.1	Example: Comparing K-means and DBSCAN . . . . .	570
9.1.2	Data Characteristics . . . . .	571

9.1.3	Cluster Characteristics . . . . .	573
9.1.4	General Characteristics of Clustering Algorithms . . . . .	575
9.2	Prototype-Based Clustering . . . . .	577
9.2.1	Fuzzy Clustering . . . . .	577
9.2.2	Clustering Using Mixture Models . . . . .	583
9.2.3	Self-Organizing Maps (SOM) . . . . .	594
9.3	Density-Based Clustering . . . . .	600
9.3.1	Grid-Based Clustering . . . . .	601
9.3.2	Subspace Clustering . . . . .	604
9.3.3	DENCLUE: A Kernel-Based Scheme for Density-Based Clustering . . . . .	608
9.4	Graph-Based Clustering . . . . .	612
9.4.1	Sparsification . . . . .	613
9.4.2	Minimum Spanning Tree (MST) Clustering . . . . .	614
9.4.3	OPOSSUM: Optimal Partitioning of Sparse Similarities Using METIS . . . . .	616
9.4.4	Chameleon: Hierarchical Clustering with Dynamic Modeling . . . . .	616
9.4.5	Shared Nearest Neighbor Similarity . . . . .	622
9.4.6	The Jarvis-Patrick Clustering Algorithm . . . . .	625
9.4.7	SNN Density . . . . .	627
9.4.8	SNN Density-Based Clustering . . . . .	629
9.5	Scalable Clustering Algorithms . . . . .	630
9.5.1	Scalability: General Issues and Approaches . . . . .	630
9.5.2	BIRCH . . . . .	633
9.5.3	CURE . . . . .	635
9.6	Which Clustering Algorithm? . . . . .	639
9.7	Bibliographic Notes . . . . .	643
9.8	Exercises . . . . .	647
<b>10</b>	<b>Anomaly Detection</b> . . . . .	<b>651</b>
10.1	Preliminaries . . . . .	653
10.1.1	Causes of Anomalies . . . . .	653
10.1.2	Approaches to Anomaly Detection . . . . .	654
10.1.3	The Use of Class Labels . . . . .	655
10.1.4	Issues . . . . .	656
10.2	Statistical Approaches . . . . .	658
10.2.1	Detecting Outliers in a Univariate Normal Distribution . . . . .	659
10.2.2	Outliers in a Multivariate Normal Distribution . . . . .	661
10.2.3	A Mixture Model Approach for Anomaly Detection . . . . .	662

10.2.4	Strengths and Weaknesses . . . . .	665
10.3	Proximity-Based Outlier Detection . . . . .	666
10.3.1	Strengths and Weaknesses . . . . .	666
10.4	Density-Based Outlier Detection . . . . .	668
10.4.1	Detection of Outliers Using Relative Density . . . . .	669
10.4.2	Strengths and Weaknesses . . . . .	670
10.5	Clustering-Based Techniques . . . . .	671
10.5.1	Assessing the Extent to Which an Object Belongs to a Cluster . . . . .	672
10.5.2	Impact of Outliers on the Initial Clustering . . . . .	674
10.5.3	The Number of Clusters to Use . . . . .	674
10.5.4	Strengths and Weaknesses . . . . .	674
10.6	Bibliographic Notes . . . . .	675
10.7	Exercises . . . . .	680
<b>Appendix A Linear Algebra</b>		<b>685</b>
A.1	Vectors . . . . .	685
A.1.1	Definition . . . . .	685
A.1.2	Vector Addition and Multiplication by a Scalar . . . . .	685
A.1.3	Vector Spaces . . . . .	687
A.1.4	The Dot Product, Orthogonality, and Orthogonal Projections . . . . .	688
A.1.5	Vectors and Data Analysis . . . . .	690
A.2	Matrices . . . . .	691
A.2.1	Matrices: Definitions . . . . .	691
A.2.2	Matrices: Addition and Multiplication by a Scalar . . . . .	692
A.2.3	Matrices: Multiplication . . . . .	693
A.2.4	Linear Transformations and Inverse Matrices . . . . .	695
A.2.5	Eigenvalue and Singular Value Decomposition . . . . .	697
A.2.6	Matrices and Data Analysis . . . . .	699
A.3	Bibliographic Notes . . . . .	700
<b>Appendix B Dimensionality Reduction</b>		<b>701</b>
B.1	PCA and SVD . . . . .	701
B.1.1	Principal Components Analysis (PCA) . . . . .	701
B.1.2	SVD . . . . .	706
B.2	Other Dimensionality Reduction Techniques . . . . .	708
B.2.1	Factor Analysis . . . . .	708
B.2.2	Locally Linear Embedding (LLE) . . . . .	710
B.2.3	Multidimensional Scaling, FastMap, and ISOMAP . . . . .	712



B.2.4 Common Issues . . . . .	715
B.3 Bibliographic Notes . . . . .	716
<b>Appendix C Probability and Statistics</b>	<b>719</b>
C.1 Probability . . . . .	719
C.1.1 Expected Values . . . . .	722
C.2 Statistics . . . . .	723
C.2.1 Point Estimation . . . . .	724
C.2.2 Central Limit Theorem . . . . .	724
C.2.3 Interval Estimation . . . . .	725
C.3 Hypothesis Testing . . . . .	726
<b>Appendix D Regression</b>	<b>729</b>
D.1 Preliminaries . . . . .	729
D.2 Simple Linear Regression . . . . .	730
D.2.1 Least Square Method . . . . .	731
D.2.2 Analyzing Regression Errors . . . . .	733
D.2.3 Analyzing Goodness of Fit . . . . .	735
D.3 Multivariate Linear Regression . . . . .	736
D.4 Alternative Least-Square Regression Methods . . . . .	737
<b>Appendix E Optimization</b>	<b>739</b>
E.1 Unconstrained Optimization . . . . .	739
E.1.1 Numerical Methods . . . . .	742
E.2 Constrained Optimization . . . . .	746
E.2.1 Equality Constraints . . . . .	746
E.2.2 Inequality Constraints . . . . .	747
<b>Author Index</b>	<b>750</b>
<b>Subject Index</b>	<b>758</b>
<b>Copyright Permissions</b>	<b>769</b>