

# Contents

<b>List of Figures</b>	<b>xiii</b>
<b>List of Tables</b>	<b>xv</b>
<b>List of Algorithms</b>	<b>xvii</b>
<b>Preface</b>	<b>xix</b>
<b>I Clustering, Data, and Similarity Measures</b>	<b>1</b>
<b>1 Data Clustering</b>	<b>3</b>
1.1 Definition of Data Clustering . . . . .	3
1.2 The Vocabulary of Clustering . . . . .	5
1.2.1 Records and Attributes . . . . .	5
1.2.2 Distances and Similarities . . . . .	5
1.2.3 Clusters, Centers, and Modes . . . . .	6
1.2.4 Hard Clustering and Fuzzy Clustering . . . . .	7
1.2.5 Validity Indices . . . . .	8
1.3 Clustering Processes . . . . .	8
1.4 Dealing with Missing Values . . . . .	10
1.5 Resources for Clustering . . . . .	12
1.5.1 Surveys and Reviews on Clustering . . . . .	12
1.5.2 Books on Clustering . . . . .	12
1.5.3 Journals . . . . .	13
1.5.4 Conference Proceedings . . . . .	15
1.5.5 Data Sets . . . . .	17
1.6 Summary . . . . .	17
<b>2 Data Types</b>	<b>19</b>
2.1 Categorical Data . . . . .	19
2.2 Binary Data . . . . .	21
2.3 Transaction Data . . . . .	23
2.4 Symbolic Data . . . . .	23
2.5 Time Series . . . . .	24
2.6 Summary . . . . .	24

<b>3</b>	<b>Scale Conversion</b>	<b>25</b>
3.1	Introduction . . . . .	25
3.1.1	Interval to Ordinal . . . . .	25
3.1.2	Interval to Nominal . . . . .	27
3.1.3	Ordinal to Nominal . . . . .	28
3.1.4	Nominal to Ordinal . . . . .	28
3.1.5	Ordinal to Interval . . . . .	29
3.1.6	Other Conversions . . . . .	29
3.2	Categorization of Numerical Data . . . . .	30
3.2.1	Direct Categorization . . . . .	30
3.2.2	Cluster-based Categorization . . . . .	31
3.2.3	Automatic Categorization . . . . .	37
3.3	Summary . . . . .	41
<b>4</b>	<b>Data Standardization and Transformation</b>	<b>43</b>
4.1	Data Standardization . . . . .	43
4.2	Data Transformation . . . . .	46
4.2.1	Principal Component Analysis . . . . .	46
4.2.2	SVD . . . . .	48
4.2.3	The Karhunen-Loève Transformation . . . . .	49
4.3	Summary . . . . .	51
<b>5</b>	<b>Data Visualization</b>	<b>53</b>
5.1	Sammon's Mapping . . . . .	53
5.2	MDS . . . . .	54
5.3	SOM . . . . .	56
5.4	Class-preserving Projections . . . . .	59
5.5	Parallel Coordinates . . . . .	60
5.6	Tree Maps . . . . .	61
5.7	Categorical Data Visualization . . . . .	62
5.8	Other Visualization Techniques . . . . .	65
5.9	Summary . . . . .	65
<b>6</b>	<b>Similarity and Dissimilarity Measures</b>	<b>67</b>
6.1	Preliminaries . . . . .	67
6.1.1	Proximity Matrix . . . . .	68
6.1.2	Proximity Graph . . . . .	69
6.1.3	Scatter Matrix . . . . .	69
6.1.4	Covariance Matrix . . . . .	70
6.2	Measures for Numerical Data . . . . .	71
6.2.1	Euclidean Distance . . . . .	71
6.2.2	Manhattan Distance . . . . .	71
6.2.3	Maximum Distance . . . . .	72
6.2.4	Minkowski Distance . . . . .	72
6.2.5	Mahalanobis Distance . . . . .	72

6.2.6	Average Distance . . . . .	73
6.2.7	Other Distances . . . . .	74
6.3	Measures for Categorical Data . . . . .	74
6.3.1	The Simple Matching Distance . . . . .	76
6.3.2	Other Matching Coefficients . . . . .	76
6.4	Measures for Binary Data . . . . .	77
6.5	Measures for Mixed-type Data . . . . .	79
6.5.1	A General Similarity Coefficient . . . . .	79
6.5.2	A General Distance Coefficient . . . . .	80
6.5.3	A Generalized Minkowski Distance . . . . .	81
6.6	Measures for Time Series Data . . . . .	83
6.6.1	The Minkowski Distance . . . . .	84
6.6.2	Time Series Preprocessing . . . . .	85
6.6.3	Dynamic Time Warping . . . . .	87
6.6.4	Measures Based on Longest Common Subsequences . . . . .	88
6.6.5	Measures Based on Probabilistic Models . . . . .	90
6.6.6	Measures Based on Landmark Models . . . . .	91
6.6.7	Evaluation . . . . .	92
6.7	Other Measures . . . . .	92
6.7.1	The Cosine Similarity Measure . . . . .	93
6.7.2	A Link-based Similarity Measure . . . . .	93
6.7.3	Support . . . . .	94
6.8	Similarity and Dissimilarity Measures between Clusters . . . . .	94
6.8.1	The Mean-based Distance . . . . .	94
6.8.2	The Nearest Neighbor Distance . . . . .	95
6.8.3	The Farthest Neighbor Distance . . . . .	95
6.8.4	The Average Neighbor Distance . . . . .	96
6.8.5	Lance-Williams Formula . . . . .	96
6.9	Similarity and Dissimilarity between Variables . . . . .	98
6.9.1	Pearson's Correlation Coefficients . . . . .	98
6.9.2	Measures Based on the Chi-square Statistic . . . . .	101
6.9.3	Measures Based on Optimal Class Prediction . . . . .	103
6.9.4	Group-based Distance . . . . .	105
6.10	Summary . . . . .	106
<b>II</b>	<b>Clustering Algorithms</b>	<b>107</b>
<b>7</b>	<b>Hierarchical Clustering Techniques</b>	<b>109</b>
7.1	Representations of Hierarchical Clusterings . . . . .	109
7.1.1	$n$ -tree . . . . .	110
7.1.2	Dendrogram . . . . .	110
7.1.3	Banner . . . . .	112
7.1.4	Pointer Representation . . . . .	112
7.1.5	Packed Representation . . . . .	114
7.1.6	Icicle Plot . . . . .	115
7.1.7	Other Representations . . . . .	115

7.2	Agglomerative Hierarchical Methods . . . . .	116
7.2.1	The Single-link Method . . . . .	118
7.2.2	The Complete Link Method . . . . .	120
7.2.3	The Group Average Method . . . . .	122
7.2.4	The Weighted Group Average Method . . . . .	125
7.2.5	The Centroid Method . . . . .	126
7.2.6	The Median Method . . . . .	130
7.2.7	Ward's Method . . . . .	132
7.2.8	Other Agglomerative Methods . . . . .	137
7.3	Divisive Hierarchical Methods . . . . .	137
7.4	Several Hierarchical Algorithms . . . . .	138
7.4.1	SLINK . . . . .	138
7.4.2	Single-link Algorithms Based on Minimum Spanning Trees . . . . .	140
7.4.3	CLINK . . . . .	141
7.4.4	BIRCH . . . . .	144
7.4.5	CURE . . . . .	144
7.4.6	DIANA . . . . .	145
7.4.7	DISMEA . . . . .	147
7.4.8	Edwards and Cavalli-Sforza Method . . . . .	147
7.5	Summary . . . . .	149
<b>8</b>	<b>Fuzzy Clustering Algorithms</b>	<b>151</b>
8.1	Fuzzy Sets . . . . .	151
8.2	Fuzzy Relations . . . . .	153
8.3	Fuzzy $k$ -means . . . . .	154
8.4	Fuzzy $k$ -modes . . . . .	156
8.5	The $c$ -means Method . . . . .	158
8.6	Summary . . . . .	159
<b>9</b>	<b>Center-based Clustering Algorithms</b>	<b>161</b>
9.1	The $k$ -means Algorithm . . . . .	161
9.2	Variations of the $k$ -means Algorithm . . . . .	164
9.2.1	The Continuous $k$ -means Algorithm . . . . .	165
9.2.2	The Compare-means Algorithm . . . . .	165
9.2.3	The Sort-means Algorithm . . . . .	166
9.2.4	Acceleration of the $k$ -means Algorithm with the $kd$ -tree . . . . .	167
9.2.5	Other Acceleration Methods . . . . .	168
9.3	The Trimmed $k$ -means Algorithm . . . . .	169
9.4	The $x$ -means Algorithm . . . . .	170
9.5	The $k$ -harmonic Means Algorithm . . . . .	171
9.6	The Mean Shift Algorithm . . . . .	173
9.7	MEC . . . . .	175
9.8	The $k$ -modes Algorithm (Huang) . . . . .	176
9.8.1	Initial Modes Selection . . . . .	178
9.9	The $k$ -modes Algorithm (Chaturvedi et al.) . . . . .	178

9.10	The $k$ -probabilities Algorithm . . . . .	179
9.11	The $k$ -prototypes Algorithm . . . . .	181
9.12	Summary . . . . .	182
<b>10</b>	<b>Search-based Clustering Algorithms</b>	<b>183</b>
10.1	Genetic Algorithms . . . . .	184
10.2	The Tabu Search Method . . . . .	185
10.3	Variable Neighborhood Search for Clustering . . . . .	186
10.4	Al-Sultan's Method . . . . .	187
10.5	Tabu Search-based Categorical Clustering Algorithm . . . . .	189
10.6	$J$ -means . . . . .	190
10.7	GKA . . . . .	192
10.8	The Global $k$ -means Algorithm . . . . .	195
10.9	The Genetic $k$ -modes Algorithm . . . . .	195
10.9.1	The Selection Operator . . . . .	196
10.9.2	The Mutation Operator . . . . .	196
10.9.3	The $k$ -modes Operator . . . . .	197
10.10	The Genetic Fuzzy $k$ -modes Algorithm . . . . .	197
10.10.1	String Representation . . . . .	198
10.10.2	Initialization Process . . . . .	198
10.10.3	Selection Process . . . . .	199
10.10.4	Crossover Process . . . . .	199
10.10.5	Mutation Process . . . . .	200
10.10.6	Termination Criterion . . . . .	200
10.11	SARS . . . . .	200
10.12	Summary . . . . .	202
<b>11</b>	<b>Graph-based Clustering Algorithms</b>	<b>203</b>
11.1	Chameleon . . . . .	203
11.2	CACTUS . . . . .	204
11.3	A Dynamic System-based Approach . . . . .	205
11.4	ROCK . . . . .	207
11.5	Summary . . . . .	208
<b>12</b>	<b>Grid-based Clustering Algorithms</b>	<b>209</b>
12.1	STING . . . . .	209
12.2	OptiGrid . . . . .	210
12.3	GRIDCLUS . . . . .	212
12.4	GDILC . . . . .	214
12.5	WaveCluster . . . . .	216
12.6	Summary . . . . .	217
<b>13</b>	<b>Density-based Clustering Algorithms</b>	<b>219</b>
13.1	DBSCAN . . . . .	219
13.2	BRIDGE . . . . .	221
13.3	DBCLASD . . . . .	222

13.4	DENCLUE . . . . .	223
13.5	CUBN . . . . .	225
13.6	Summary . . . . .	226
<b>14</b>	<b>Model-based Clustering Algorithms</b>	<b>227</b>
14.1	Introduction . . . . .	227
14.2	Gaussian Clustering Models . . . . .	230
14.3	Model-based Agglomerative Hierarchical Clustering . . . . .	232
14.4	The EM Algorithm . . . . .	235
14.5	Model-based Clustering . . . . .	237
14.6	COOLCAT . . . . .	240
14.7	STUCCO . . . . .	241
14.8	Summary . . . . .	242
<b>15</b>	<b>Subspace Clustering</b>	<b>243</b>
15.1	CLIQUE . . . . .	244
15.2	PROCLUS . . . . .	246
15.3	ORCLUS . . . . .	249
15.4	ENCLUS . . . . .	253
15.5	FINDIT . . . . .	255
15.6	MAFIA . . . . .	258
15.7	DOC . . . . .	259
15.8	CLTree . . . . .	261
15.9	PART . . . . .	262
15.10	SUBCAD . . . . .	264
15.11	Fuzzy Subspace Clustering . . . . .	270
15.12	Mean Shift for Subspace Clustering . . . . .	275
15.13	Summary . . . . .	285
<b>16</b>	<b>Miscellaneous Algorithms</b>	<b>287</b>
16.1	Time Series Clustering Algorithms . . . . .	287
16.2	Streaming Algorithms . . . . .	289
	16.2.1 LSEARCH . . . . .	290
	16.2.2 Other Streaming Algorithms . . . . .	293
16.3	Transaction Data Clustering Algorithms . . . . .	293
	16.3.1 LargeItem . . . . .	294
	16.3.2 CLOPE . . . . .	295
	16.3.3 OAK . . . . .	296
16.4	Summary . . . . .	297
<b>17</b>	<b>Evaluation of Clustering Algorithms</b>	<b>299</b>
17.1	Introduction . . . . .	299
	17.1.1 Hypothesis Testing . . . . .	301
	17.1.2 External Criteria . . . . .	302
	17.1.3 Internal Criteria . . . . .	303
	17.1.4 Relative Criteria . . . . .	304

17.2	Evaluation of Partitional Clustering . . . . .	305
17.2.1	Modified Hubert's $\Gamma$ Statistic . . . . .	305
17.2.2	The Davies-Bouldin Index . . . . .	305
17.2.3	Dunn's Index . . . . .	307
17.2.4	The SD Validity Index . . . . .	307
17.2.5	The S_Dbw Validity Index . . . . .	308
17.2.6	The RMSSTD Index . . . . .	309
17.2.7	The RS Index . . . . .	310
17.2.8	The Calinski-Harabasz Index . . . . .	310
17.2.9	Rand's Index . . . . .	311
17.2.10	Average of Compactness . . . . .	312
17.2.11	Distances between Partitions . . . . .	312
17.3	Evaluation of Hierarchical Clustering . . . . .	314
17.3.1	Testing Absence of Structure . . . . .	314
17.3.2	Testing Hierarchical Structures . . . . .	315
17.4	Validity Indices for Fuzzy Clustering . . . . .	315
17.4.1	The Partition Coefficient Index . . . . .	315
17.4.2	The Partition Entropy Index . . . . .	316
17.4.3	The Fukuyama-Sugeno Index . . . . .	316
17.4.4	Validity Based on Fuzzy Similarity . . . . .	317
17.4.5	A Compact and Separate Fuzzy Validity Criterion . . . . .	318
17.4.6	A Partition Separation Index . . . . .	319
17.4.7	An Index Based on the Mini-max Filter Concept and Fuzzy Theory . . . . .	319
17.5	Summary . . . . .	320
<b>III Applications of Clustering</b>		<b>321</b>
<b>18</b>	<b>Clustering Gene Expression Data</b>	<b>323</b>
18.1	Background . . . . .	323
18.2	Applications of Gene Expression Data Clustering . . . . .	324
18.3	Types of Gene Expression Data Clustering . . . . .	325
18.4	Some Guidelines for Gene Expression Clustering . . . . .	325
18.5	Similarity Measures for Gene Expression Data . . . . .	326
18.5.1	Euclidean Distance . . . . .	326
18.5.2	Pearson's Correlation Coefficient . . . . .	326
18.6	A Case Study . . . . .	328
18.6.1	C++ Code . . . . .	328
18.6.2	Results . . . . .	334
18.7	Summary . . . . .	334
<b>IV MATLAB and C++ for Clustering</b>		<b>341</b>
<b>19</b>	<b>Data Clustering in MATLAB</b>	<b>343</b>
19.1	Read and Write Data Files . . . . .	343
19.2	Handle Categorical Data . . . . .	347

19.3	M-files, MEX-files, and MAT-files . . . . .	349
19.3.1	M-files . . . . .	349
19.3.2	MEX-files . . . . .	351
19.3.3	MAT-files . . . . .	354
19.4	Speed up MATLAB . . . . .	354
19.5	Some Clustering Functions . . . . .	355
19.5.1	Hierarchical Clustering . . . . .	355
19.5.2	$k$ -means Clustering . . . . .	359
19.6	Summary . . . . .	362
<b>20</b>	<b>Clustering in C/C++</b>	<b>363</b>
20.1	The STL . . . . .	363
20.1.1	The <i>vector</i> Class . . . . .	363
20.1.2	The <i>list</i> Class . . . . .	364
20.2	C/C++ Program Compilation . . . . .	366
20.3	Data Structure and Implementation . . . . .	367
20.3.1	Data Matrices and Centers . . . . .	367
20.3.2	Clustering Results . . . . .	368
20.3.3	The Quick Sort Algorithm . . . . .	369
20.4	Summary . . . . .	369
<b>A</b>	<b>Some Clustering Algorithms</b>	<b>371</b>
<b>B</b>	<b>The <math>kd</math>-tree Data Structure</b>	<b>375</b>
<b>C</b>	<b>MATLAB Codes</b>	<b>377</b>
C.1	The MATLAB Code for Generating Subspace Clusters . . . . .	377
C.2	The MATLAB Code for the $k$ -modes Algorithm . . . . .	379
C.3	The MATLAB Code for the MSSC Algorithm . . . . .	381
<b>D</b>	<b>C++ Codes</b>	<b>385</b>
D.1	The C++ Code for Converting Categorical Values to Integers . . . . .	385
D.2	The C++ Code for the FSC Algorithm . . . . .	388
	<b>Bibliography</b>	<b>397</b>
	<b>Subject Index</b>	<b>443</b>
	<b>Author Index</b>	<b>455</b>