

Chapman & Hall/CRC  
Data Mining and Knowledge Discovery Series

# Data Clustering in C++

## An Object-Oriented Approach

Guojun Gan



CRC Press  
Taylor & Francis Group  
Boca Raton London New York

---

CRC Press is an Imprint of the  
Taylor & Francis Group, an Informa business  
A CHAPMAN & HALL BOOK

---

# **Contents**

<b>List of Figures</b>	<b>xv</b>
<b>List of Tables</b>	<b>xix</b>
<b>Preface</b>	<b>xxi</b>
<b>I Data Clustering and C++ Preliminaries</b>	<b>1</b>
<b>1 Introduction to Data Clustering</b>	<b>3</b>
1.1 Data Clustering . . . . .	3
1.1.1 Clustering versus Classification . . . . .	4
1.1.2 Definition of Clusters . . . . .	5
1.2 Data Types . . . . .	7
1.3 Dissimilarity and Similarity Measures . . . . .	8
1.3.1 Measures for Continuous Data . . . . .	9
1.3.2 Measures for Discrete Data . . . . .	10
1.3.3 Measures for Mixed-Type Data . . . . .	10
1.4 Hierarchical Clustering Algorithms . . . . .	11
1.4.1 Agglomerative Hierarchical Algorithms . . . . .	12
1.4.2 Divisive Hierarchical Algorithms . . . . .	14
1.4.3 Other Hierarchical Algorithms . . . . .	14
1.4.4 Dendrograms . . . . .	15
1.5 Partitional Clustering Algorithms . . . . .	15
1.5.1 Center-Based Clustering Algorithms . . . . .	17
1.5.2 Search-Based Clustering Algorithms . . . . .	18
1.5.3 Graph-Based Clustering Algorithms . . . . .	19
1.5.4 Grid-Based Clustering Algorithms . . . . .	20
1.5.5 Density-Based Clustering Algorithms . . . . .	20
1.5.6 Model-Based Clustering Algorithms . . . . .	21
1.5.7 Subspace Clustering Algorithms . . . . .	22
1.5.8 Neural Network-Based Clustering Algorithms . . . . .	22
1.5.9 Fuzzy Clustering Algorithms . . . . .	23
1.6 Cluster Validity . . . . .	23
1.7 Clustering Applications . . . . .	24
1.8 Literature of Clustering Algorithms . . . . .	25
1.8.1 Books on Data Clustering . . . . .	25

1.8.2	Surveys on Data Clustering . . . . .	26
1.9	Summary . . . . .	28
<b>2</b>	<b>The Unified Modeling Language</b>	<b>29</b>
2.1	Package Diagrams . . . . .	29
2.2	Class Diagrams . . . . .	32
2.3	Use Case Diagrams . . . . .	36
2.4	Activity Diagrams . . . . .	38
2.5	Notes . . . . .	39
2.6	Summary . . . . .	40
<b>3</b>	<b>Object-Oriented Programming and C++</b>	<b>41</b>
3.1	Object-Oriented Programming . . . . .	41
3.2	The C++ Programming Language . . . . .	42
3.3	Encapsulation . . . . .	45
3.4	Inheritance . . . . .	48
3.5	Polymorphism . . . . .	50
3.5.1	Dynamic Polymorphism . . . . .	51
3.5.2	Static Polymorphism . . . . .	52
3.6	Exception Handling . . . . .	54
3.7	Summary . . . . .	56
<b>4</b>	<b>Design Patterns</b>	<b>57</b>
4.1	Singleton . . . . .	58
4.2	Composite . . . . .	61
4.3	Prototype . . . . .	64
4.4	Strategy . . . . .	67
4.5	Template Method . . . . .	69
4.6	Visitor . . . . .	72
4.7	Summary . . . . .	75
<b>5</b>	<b>C++ Libraries and Tools</b>	<b>77</b>
5.1	The Standard Template Library . . . . .	77
5.1.1	Containers . . . . .	77
5.1.2	Iterators . . . . .	82
5.1.3	Algorithms . . . . .	84
5.2	Boost C++ Libraries . . . . .	86
5.2.1	Smart Pointers . . . . .	87
5.2.2	Variant . . . . .	89
5.2.3	Variant versus Any . . . . .	90
5.2.4	Tokenizer . . . . .	92
5.2.5	Unit Test Framework . . . . .	93
5.3	GNU Build System . . . . .	95
5.3.1	Autoconf . . . . .	96
5.3.2	Automake . . . . .	97
5.3.3	Libtool . . . . .	97

5.3.4	Using GNU Autotools . . . . .	98
5.4	Cygwin . . . . .	98
5.5	Summary . . . . .	99
<b>II</b>	<b>A C++ Data Clustering Framework</b>	<b>101</b>
<b>6</b>	<b>The Clustering Library</b>	<b>103</b>
6.1	Directory Structure and Filenames . . . . .	103
6.2	Specification Files . . . . .	105
6.2.1	configure.ac . . . . .	105
6.2.2	Makefile.am . . . . .	106
6.3	Macros and <code>typedef</code> Declarations . . . . .	109
6.4	Error Handling . . . . .	111
6.5	Unit Testing . . . . .	112
6.6	Compilation and Installation . . . . .	113
6.7	Summary . . . . .	114
<b>7</b>	<b>Datasets</b>	<b>115</b>
7.1	Attributes . . . . .	115
7.1.1	The Attribute Value Class . . . . .	115
7.1.2	The Base Attribute Information Class . . . . .	117
7.1.3	The Continuous Attribute Information Class . . . . .	119
7.1.4	The Discrete Attribute Information Class . . . . .	120
7.2	Records . . . . .	122
7.2.1	The Record Class . . . . .	122
7.2.2	The Schema Class . . . . .	124
7.3	Datasets . . . . .	125
7.4	A Dataset Example . . . . .	127
7.5	Summary . . . . .	130
<b>8</b>	<b>Clusters</b>	<b>131</b>
8.1	Clusters . . . . .	131
8.2	Partitional Clustering . . . . .	133
8.3	Hierarchical Clustering . . . . .	135
8.4	Summary . . . . .	138
<b>9</b>	<b>Dissimilarity Measures</b>	<b>139</b>
9.1	The Distance Base Class . . . . .	139
9.2	Minkowski Distance . . . . .	140
9.3	Euclidean Distance . . . . .	141
9.4	Simple Matching Distance . . . . .	142
9.5	Mixed Distance . . . . .	143
9.6	Mahalanobis Distance . . . . .	144
9.7	Summary . . . . .	147

<b>10 Clustering Algorithms</b>	<b>149</b>
10.1 Arguments . . . . .	149
10.2 Results . . . . .	150
10.3 Algorithms . . . . .	151
10.4 A Dummy Clustering Algorithm . . . . .	154
10.5 Summary . . . . .	158
<b>11 Utility Classes</b>	<b>161</b>
11.1 The Container Class . . . . .	161
11.2 The Double-Key Map Class . . . . .	164
11.3 The Dataset Adapters . . . . .	167
11.3.1 A CSV Dataset Reader . . . . .	167
11.3.2 A Dataset Generator . . . . .	170
11.3.3 A Dataset Normalizer . . . . .	173
11.4 The Node Visitors . . . . .	175
11.4.1 The Join Value Visitor . . . . .	175
11.4.2 The Partition Creation Visitor . . . . .	176
11.5 The Dendrogram Class . . . . .	177
11.6 The Dendrogram Visitor . . . . .	179
11.7 Summary . . . . .	180
<b>III Data Clustering Algorithms</b>	<b>183</b>
<b>12 Agglomerative Hierarchical Algorithms</b>	<b>185</b>
12.1 Description of the Algorithm . . . . .	185
12.2 Implementation . . . . .	187
12.2.1 The Single Linkage Algorithm . . . . .	192
12.2.2 The Complete Linkage Algorithm . . . . .	192
12.2.3 The Group Average Algorithm . . . . .	193
12.2.4 The Weighted Group Average Algorithm . . . . .	194
12.2.5 The Centroid Algorithm . . . . .	194
12.2.6 The Median Algorithm . . . . .	195
12.2.7 Ward's Algorithm . . . . .	196
12.3 Examples . . . . .	197
12.3.1 The Single Linkage Algorithm . . . . .	198
12.3.2 The Complete Linkage Algorithm . . . . .	200
12.3.3 The Group Average Algorithm . . . . .	202
12.3.4 The Weighted Group Average Algorithm . . . . .	204
12.3.5 The Centroid Algorithm . . . . .	207
12.3.6 The Median Algorithm . . . . .	210
12.3.7 Ward's Algorithm . . . . .	212
12.4 Summary . . . . .	214

<b>13 DIANA</b>	<b>217</b>
13.1 Description of the Algorithm . . . . .	217
13.2 Implementation . . . . .	218
13.3 Examples . . . . .	223
13.4 Summary . . . . .	227
<b>14 The <math>k</math>-means Algorithm</b>	<b>229</b>
14.1 Description of the Algorithm . . . . .	229
14.2 Implementation . . . . .	230
14.3 Examples . . . . .	235
14.4 Summary . . . . .	240
<b>15 The c-means Algorithm</b>	<b>241</b>
15.1 Description of the Algorithm . . . . .	241
15.2 Implementaion . . . . .	242
15.3 Examples . . . . .	246
15.4 Summary . . . . .	253
<b>16 The <math>k</math>-prototypes Algorithm</b>	<b>255</b>
16.1 Description of the Algorithm . . . . .	255
16.2 Implementation . . . . .	256
16.3 Examples . . . . .	258
16.4 Summary . . . . .	263
<b>17 The Genetic <math>k</math>-modes Algorithm</b>	<b>265</b>
17.1 Description of the Algorithm . . . . .	265
17.2 Implementation . . . . .	267
17.3 Examples . . . . .	274
17.4 Summary . . . . .	277
<b>18 The FSC Algorithm</b>	<b>279</b>
18.1 Description of the Algorithm . . . . .	279
18.2 Implementation . . . . .	281
18.3 Examples . . . . .	284
18.4 Summary . . . . .	290
<b>19 The Gaussian Mixture Algorithm</b>	<b>291</b>
19.1 Description of the Algorithm . . . . .	291
19.2 Implementation . . . . .	293
19.3 Examples . . . . .	300
19.4 Summary . . . . .	306

<b>20 A Parallel <i>k</i>-means Algorithm</b>	<b>307</b>
20.1 Message Passing Interface . . . . .	307
20.2 Description of the Algorithm . . . . .	310
20.3 Implementation . . . . .	311
20.4 Examples . . . . .	316
20.5 Summary . . . . .	320
<b>A Exercises and Projects</b>	<b>323</b>
<b>B Listings</b>	<b>325</b>
B.1 Files in Folder ClusLib . . . . .	325
B.1.1 Configuration File <code>configure.ac</code> . . . . .	325
B.1.2 m4 Macro File <code>acinclude.m4</code> . . . . .	326
B.1.3 Makefile . . . . .	327
B.2 Files in Folder c1 . . . . .	328
B.2.1 Makefile . . . . .	328
B.2.2 Macros and <code>typedef</code> Declarations . . . . .	328
B.2.3 Class Error . . . . .	329
B.3 Files in Folder c1/algorithms . . . . .	331
B.3.1 Makefile . . . . .	331
B.3.2 Class Algorithm . . . . .	332
B.3.3 Class Average . . . . .	334
B.3.4 Class Centroid . . . . .	334
B.3.5 Class Cmean . . . . .	335
B.3.6 Class Complete . . . . .	339
B.3.7 Class Diana . . . . .	339
B.3.8 Class FSC . . . . .	343
B.3.9 Class GKmode . . . . .	347
B.3.10 Class GMC . . . . .	353
B.3.11 Class Kmean . . . . .	358
B.3.12 Class Kprototype . . . . .	361
B.3.13 Class LW . . . . .	362
B.3.14 Class Median . . . . .	364
B.3.15 Class Single . . . . .	365
B.3.16 Class Ward . . . . .	366
B.3.17 Class Weighted . . . . .	367
B.4 Files in Folder c1/clusters . . . . .	368
B.4.1 Makefile . . . . .	368
B.4.2 Class CenterCluster . . . . .	368
B.4.3 Class Cluster . . . . .	369
B.4.4 Class HClustering . . . . .	370
B.4.5 Class PClustering . . . . .	372
B.4.6 Class SubspaceCluster . . . . .	375
B.5 Files in Folder c1/datasets . . . . .	376
B.5.1 Makefile . . . . .	376

B.5.2	Class AttrValue . . . . .	376
B.5.3	Class AttrInfo . . . . .	377
B.5.4	Class CAttrInfo . . . . .	379
B.5.5	Class DAttrInfo . . . . .	381
B.5.6	Class Record . . . . .	384
B.5.7	Class Schema . . . . .	386
B.5.8	Class Dataset . . . . .	388
B.6	Files in Folder cl/distances . . . . .	392
B.6.1	Makefile . . . . .	392
B.6.2	Class Distance . . . . .	392
B.6.3	Class EuclideanDistance . . . . .	393
B.6.4	Class MahalanobisDistance . . . . .	394
B.6.5	Class MinkowskiDistance . . . . .	395
B.6.6	Class MixedDistance . . . . .	396
B.6.7	Class SimpleMatchingDistance . . . . .	397
B.7	Files in Folder cl/patterns . . . . .	398
B.7.1	Makefile . . . . .	398
B.7.2	Class DendrogramVisitor . . . . .	399
B.7.3	Class InternalNode . . . . .	401
B.7.4	Class LeafNode . . . . .	403
B.7.5	Class Node . . . . .	404
B.7.6	Class NodeVisitor . . . . .	405
B.7.7	Class JoinValueVisitor . . . . .	405
B.7.8	Class PCVisitor . . . . .	407
B.8	Files in Folder cl/utilities . . . . .	408
B.8.1	Makefile . . . . .	408
B.8.2	Class Container . . . . .	409
B.8.3	Class DataAdapter . . . . .	411
B.8.4	Class DatasetGenerator . . . . .	411
B.8.5	Class DatasetNormalizer . . . . .	413
B.8.6	Class DatasetReader . . . . .	415
B.8.7	Class Dendrogram . . . . .	418
B.8.8	Class nnMap . . . . .	421
B.8.9	Matrix Functions . . . . .	423
B.8.10	Null Types . . . . .	425
B.9	Files in Folder examples . . . . .	426
B.9.1	Makefile . . . . .	426
B.9.2	Agglomerative Hierarchical Algorithms . . . . .	426
B.9.3	A Divisive Hierarchical Algorithm . . . . .	429
B.9.4	The $k$ -means Algorithm . . . . .	430
B.9.5	The $c$ -means Algorithm . . . . .	433
B.9.6	The $k$ -prototypes Algorithm . . . . .	435
B.9.7	The Genetic $k$ -modes Algorithm . . . . .	437
B.9.8	The FSC Algorithm . . . . .	439
B.9.9	The Gaussian Mixture Clustering Algorithm . . . . .	441

B.9.10 A Parallel $k$ -means Algorithm . . . . .	444
<b>B.10 Files in Folder <code>test-suite</code> . . . . .</b>	<b>450</b>
B.10.1 Makefile . . . . .	450
B.10.2 The Master Test Suite . . . . .	451
B.10.3 Test of AttrInfo . . . . .	451
B.10.4 Test of Dataset . . . . .	453
B.10.5 Test of Distance . . . . .	454
B.10.6 Test of nnMap . . . . .	456
B.10.7 Test of Matrices . . . . .	458
B.10.8 Test of Schema . . . . .	459
<b>C Software . . . . .</b>	<b>461</b>
C.1 An Introduction to Makefiles . . . . .	461
C.1.1 Rules . . . . .	461
C.1.2 Variables . . . . .	462
C.2 Installing Boost . . . . .	463
C.2.1 Boost for Windows . . . . .	463
C.2.2 Boost for Cygwin or Linux . . . . .	464
C.3 Installing Cygwin . . . . .	465
C.4 Installing GMP . . . . .	465
C.5 Installing MPICH2 and Boost MPI . . . . .	466
<b>Bibliography . . . . .</b>	<b>469</b>
<b>Author Index . . . . .</b>	<b>487</b>
<b>Subject Index . . . . .</b>	<b>493</b>