

Cluster Analysis for Researchers

H. Charles Romesburg





E8565525





Lifetime Learning Publications Belmont, California

a division of Wadsworth, Inc. London, Singapore, Sydney, Tokyo, Toronto, Mexico City To Lafayette College, University of Pittsburgh, and Utah State University

Designer: Rick Chafian Copyeditor: Kirk Sargent Illustrator: John Foster

Composition: Science Typographers, Inc.

© 1984 by Wadsworth, Inc. All rights reserved. No part of this book may be reproduced, stored in a retrieval system, or transcribed, in any form or by any means, electronic, mechanical, photocopying, recording, or otherwise, without the prior written permission of the publisher, Lifetime Learning Publications, Belmont, California 94002, a division of Wadsworth, Inc.

Printed in the United States of America

1 2 3 4 5 6 7 8 9 10-88 87 86 85 84

Library of Congress Cataloging in Publication Data

Romesburg, H. Charles

Cluster analysis for researchers.

Bibliography: p. Includes index.

1. Cluster analysis. I. Title.

QA278.R66 1984 ISBN 0-534-03248-6 519.5'3

83-24835

Cluster Analysis for Researchers

Preface

PURPOSE OF THIS BOOK

This book explains and illustrates the most frequently used methods of hierarchical cluster analysis so that they can be understood and practiced by researchers with limited backgrounds in mathematics and statistics.

Widely applicable in research, these methods are used to determine clusters of similar objects. For example, ecologists use cluster analysis to determine which plots (i.e. objects) in a forest are similar with respect to the vegetation growing on them; medical researchers use cluster analysis to determine which diseases have similar patterns of incidence; and market researchers use cluster analysis to determine which brands of products the public perceives in a similar way. In all fields of research, there exists this basic and recurring need to determine clusters of objects.

This book will ground you in the basic methods of cluster analysis and guide you in all phases of their use. You will learn how to recognize when you have a research problem that requires cluster analysis, how to decide upon the most appropriate kind of data to collect, how to choose the best method of cluster analysis for your problem, how to obtain a computer program to perform the necessary calculations, and how to interpret the results.

INTENDED AUDIENCES

This is primarily a self-study text for researchers and graduate students in all fields of the physical sciences, the social sciences, the life sciences, as well as those in planning, management, and engineering. In addition, this is a reference book for applied statisticians and mathematicians, especially those who want to learn how researchers are using cluster analysis to solve a variety of research problems. Finally, this book will serve as a text, or a supplemental text, in applied statistics and mathematics programs for students enrolled in courses that aim to help them improve their abilities in using mathematical methods in *real* applications.

37/2

Preface

SPECIAL FEATURES

As well as examining the mathematics of cluster analysis, this book analyzes the *qualitative* aspects of cluster analysis, which help researchers to make the best choices of both data and methods for use in their research problems.

Nearly one hundred applications of cluster analysis are described in ways that nonspecialists will understand. Drawn from diverse research, these applications illustrate qualitative aspects of choosing and using methods in which researchers must be proficient if they are to make valid applications. By studying this wealth of examples, your ability to creatively use cluster analysis and other mathematical methods will improve dramatically.

ORGANIZATION OF MATERIAL

The material is divided into four parts and two appendices as follows:

Part I presents the basic calculations of cluster analysis and illustrates a variety of its uses. You will see how it can be used to a) develop interesting scientific questions; b) create research hypotheses; c) test research hypotheses; d) make general-purpose and specific-purpose classifications; and e) facilitate planning, management, and engineering.

Part II presents alternative methods for tailoring cluster analysis to specific applications. These include methods for standardizing the data, for estimating similarities among the objects to be clustered, and for clustering the objects. Also included is a chapter that shows how to report the results found using cluster analysis.

Part III shows how to use cluster analysis to make classifications. While Part I introduced this function of cluster analysis, Part III proceeds to supply considerable detail.

Part IV discusses and illustrates how to make the subjective decisions required to frame and validate applications. It shows how researchers are guided by norms within their research communities, both when they choose methods and when they validate applications.

Appendix 1 describes books and articles about cluster analysis and multivariate methods so that you can continue to learn beyond the basic methods presented in this book.

Appendix 2 describes computer programs for cluster analysis, including those in the widely available SAS and BMDP statistical packages, and including the CLUSTAR and CLUSTID programs available from Lifetime Learning Publications as a companion to this book.

There are exercises at the end of key chapters with answers given at the back of the book. For self-study, you should work the exercises and also independently rework the examples in the text.

xiii

ACKNOWLEDGMENTS

Development of the examples of applications was partly supported by a National Science Foundation grant (NSF/SER-8160606) for "Development of a Course in the Principles of Mathematical Applications, with Emphasis on Cluster Analysis." I thank the reviewers of earlier versions of the manuscript for their comments, and I also thank Lana Barr for typing it.

H. Charles Romesburg

Cluster Analysis for Researchers

To complement *Cluster Analysis for Researchers*, Lifetime Learning is pleased to offer this statistical software for applied researchers . . .

CLUSTAR/CLUSTID:

Computer Programs for Hierarchical Cluster Analysis

by Kim Marshall and H. Charles Romesburg, Ph.D., both of the College of Natural Resources at Utah State University

CLUSTAR and CLUSTID are separate Fortran IV programs developed for researchers in the physical, natural, and social sciences, as well as for those in planning, management, and engineering, who use cluster analysis in their work.

CLUSTAR performs hierarchical cluster analysis. It finds clusters of objects that are defined by quantitative, qualitative, or mixed-scale attributes. CLUSTAR's features include:

- fast computing—problems with 300 objects and 300 attributes typically run in less than two minutes
- ten similarity coefficients for quantitative attributes
- fourteen similarity coefficients for qualitative attributes
- the ability to handle mixtures of quantitative and qualitative attributes
- a variety of options for standardizing the data
- the four most-used clustering methods: average linkage, single linkage, complete linkage, and Ward's minimum variance methods
- format control to read SPSS, SAS and BMPD data files. Can be used to complement these statistical packages
- produces publication-quality dendograms on both line printer and CalComp plotter
- rearrangement of data and similarity matrices according to the order in which objects cluster in the dendogram
- · a variety of matrix correlation methods
- clearly labeled output
- clearly written User's Manual containing extensive examples
- designed for interactive as well as batch operating modes

CLUSTID is used to identify objects into a classification that has been created using CLUSTAR. In addition to the features of CLUSTAR, it provides:

- means, standard deviations, and ranges of data for each attribute by cluster
- identification of new objects into clusters (classes) and assesses how well they fit

System Requirements. The Fortran IV source code for CLUSTAR/CLUSTID is available on 9-track (EBCDIC) magnetic tape. It is designed to compile and run on a mainframe (or 32-bit scientific desktop) computer that supports a Fortran IV or Fortran 77 compiler, with no changes, or at most minimal changes, to the source code. The programs, which are well documented, have specifically been tested on the following systems: VAX 11 series, IBM 4300 series, UNIVAC 1100 series.

Pricing and Documentation. The price of CLUSTAR/CLUSTID on tape is \$175.00 and includes a User's Manual, documentation and listing of source code, and example test problems with output. The User's Manual is very detailed and contains specific instructions for implementation and use, including worked-out examples. Additional copies of the User's Manual can be purchased at \$8.95 per copy.

Note: These programs contain all the methods described in *Cluster Analysis for Researchers*. The tapes, while complementary to the book, are not essential for learning and understanding the methods described in the book.

OKDE	RFORM
Please	send me
	CLUSTAR/CLUSTID: Computer Programs for Hierarchical Cluster Analysis (0-534-03420-9). I enclose \$175.00, which includes the price of the User's Manual, and cost of shipping/handling.
	additional copy/ies of <i>User's Manual for Clustar/Clustid Computer Programs</i> (0-534-3251-6) @ \$8.95 each. Payment is enclosed (includes shipping/handling costs)
	copy/ies of Cluster Analysis for Researchers (0-534-03248-6) @ \$36.00 each.
	Bill me. I'll return any books I don't want within the 15-day trial period without further obligation and the invoice will be cancelled. For books I keep, I'll pay the amount above plus my local sales tax and a small amount for postage and handling.
	Check enclosed. Publisher pays postage and handling. 15-day return privilege still applies.
	☐ Charge my ☐ VISA ☐ MasterCard ☐ American Express
	Card # Exp. Date
	Prices subject to change without notice. Offer valid in U.S. and Canada only. Residents of CA, KY, MA, MI, NC, NJ, NY, and WA, please add sales tax.
	Please sign here:
	We cannot process your order without your signature.
Please p	print to ensure proper delivery.
Name _	
Compa	ny
Addres	S
	ate/Zip



Detach and mail to:

LIFETIME LEARNING PUBLICATIONS 10 DAVIS DRIVE BELMONT, CA 94002

Contents

Preface	x
1. A Road Map to This Book	1
 1.1 What Cluster Analysis Is About 2 1.2 The Methods of Cluster Analysis in This Book 1.3 Special Features of This Book 3 1.4 How to Use This Book 5 	2
PART I. OVERVIEW OF CLUSTER ANALYSIS	7
2. Basics—The Six Steps of Cluster Analysis	9
 2.1 Step 1—Obtain the Data Matrix 10 2.2 Step 2—Standardize the Data Matrix 11 2.3 Step 3—Compute the Resemblance Matrix 1 2.4 Step 4—Execute the Clustering Method 14 2.5 Step 5—Rearrange the Data and Resemblance Matrices 23 2.6 Step 6—Compute the Cophenetic Correlation Coefficient 24 Summary 27 Exercises 28 	1
3. General Features of Cluster Analysis	29
3.1 Relation of Cluster Analysis to Numerical Taxonomy 30 3.2 Using Cluster Analysis to Make Classifications 3.3 Scales of Measurement for Attributes 34 3.4 Cluster Analyzing Attributes 35 3.5 Computers and Cluster Analysis 36 Summary 37	31

vi

1200968

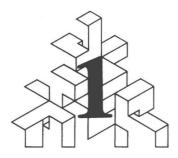
	4.	Applications of Cluster Analysis in Retroductive and Hypothetico-Deductive Science	38
		 4.1 Research Goal 1: Create a Question 40 4.2 Research Goal 2: Create a Hypothesis 44 4.3 Research Goal 3: Test a Hypothesis 46 4.4 The Importance of Background Knowledge 51 Summary 52 	
	5.	Applications of Cluster Analysis in Making Classifications 5.1 Using Cluster Analysis to Make General-Purpose Classifications 55 A Using Cluster Analysis to Make Specific Purpose	53
		5.2 Using Cluster Analysis to Make Specific-PurposeClassifications 59Summary 65	
	6.	Applications of Cluster Analysis in Planning and Engineering	66
		 6.1 Differences between Science, Planning, and Engineering Applications 67 6.2 Uses of Cluster Analysis in Planning 68 6.3 Uses of Cluster Analysis in Engineering 71 	
		Summary 72 Exercise 73	
PART II.	. Н	IOW TO DO CLUSTER ANALYSIS IN DEPTH	75
	7.	Standardizing the Data Matrix	77
		7.1 Reasons for Standardization 78 7.2 Standardizing Functions 78 7.3 Standardizing for <i>Q</i> -analysis and <i>R</i> -analysis 88 7.4 Data Transformations and Outliers 89 Summary 91 Exercises 92	
	8.	Resemblance Coefficients for Quantitative Attributes	93
		 8.1 Data Profiles 94 8.2 Resemblance Coefficients for Quantitative Attributes 96 8.3 How Resemblance Coefficients are Sensitive to Size Displacements Between Data Profiles 104 8.4 Examples of Applications Using Quantitative Resemblance Coefficients 108 	

	8.5 How Standardizing Can Compensate for Unwanted Size Displacements in Data Profiles 114	
	8.6 How to Handle Missing Data Matrix Values 115 Summary 117 Exercises 117	
9	. Clustering Methods	119
	 9.1 SLINK Clustering Method 120 9.2 CLINK Clustering Method 123 9.3 Clustering with Similarity and Dissimilarity Coefficients 128 9.4 Ward's Minimum Variance Clustering Method 129 9.5 Other Clustering Methods 135 9.6 Chaining 137 Summary 139 Exercise 139 	
10.	Resemblance Coefficients for Qualitative Attributes	141
	10.1 Qualitative Resemblance Coefficients 142 10.2 The Role of 0-0 Matches 154 10.3 Multistate Attributes 158 10.4 The Information in Qualitative Attributes 159 Summary 162 Exercises 162	
11.	Special Resemblance Coefficients for Ordinal-Scaled Attributes	164
	11.1 Kendall's Tau Coefficient, τ_{jk} 165 11.2 An Example of Kendall's Tau Coefficient 167 Summary 169 Exercise 169	
12.	Resemblance Coefficients for Mixtures of Quantitative and Qualitative Attributes	170
	 12.1 Strategies 171 12.2 An Example of the Combined Resemblance Matrix Approach 173 Summary 176 	
13.	Bypassing the Data Matrix	178
	13.1 Reasons for Bypassing the Data Matrix 17913.2 When Using the Data Matrix Is Inconvenient 180	

	13.3 When Using the Data Matrix Is Impossible 181 Summary 184	
14.	Matrix Correlation	185
	 14.1 Research Goals Involving the Correlation of Resemblance Matrices 188 14.2 Cluster-Analyzing Resemblance and Cophenetic Matrices 190 14.3 Alternatives to the Cophenetic Correlation Coefficient 190 	
	Summary 192	
15.	How to Present the Results of a Cluster Analysis	193
	15.1 Key Information 194 15.2 Optional Information 195 15.3 Ways of Presenting the Tree 198 Summary 199	
PART III. CLASSIFIO	HOW TO USE CLUSTER ANALYSIS TO MAKE CATIONS	201
16.	How to Make Classifications	203
	16.1 Steps in Making a Classification 204 16.2 Kinds of Classifications 206 16.3 Weighting Attributes 211 16.4 How to Determine Where to Cut the Tree 213 Summary 215	
17.	How to Identify Objects into a Classification	217
	17.1 How to Identify Objects 218 17.2 Strategies for Clustering "Too Many" Objects 220 Summary 221	
18.	Philosophy of Classification and Identification	223
	 18.1 Classifications as Islands in Attribute Spaces 224 18.2 The Uses of Classifications in Research 225 18.3 How Identification Helps Improve Classifications 227 18.4 How Attribute Spaces Affect Classifications 228 18.5 How to Choose and Sample an Attribute Space 229 Summary 233 	

PART IV.	CLUSTER ANALYSIS—PHILOSOPHY	235
19	19.1 A Model of Research 19.2 Objectivity and Subjectivity in Research Summary 242	237
20.	The Roles of Information, Tolerances, and Norms in Research 20.1 Information 245 20.2 Tolerances and Norms 246 Summary 252	244
21.	Framing and Validating in Cluster Analysis	253
	21.1 The Nature of Framing and Validating 21.2 Primary and Secondary Validity 256 Summary 259	
22.	Examples Illustrating How to Frame and Validate Applications of Cluster Analysis	261
	 22.1 Research Goal 1: Create a Question 262 22.2 Research Goal 2: Create a Hypothesis 263 22.3 Research Goal 3: Test a Hypothesis 266 22.4 Research Goal 4: Make a General-Purpose Classification 267 22.5 Research Goal 5: Make a Specific-Purpose Classification 269 	
	22.6 Research Goal 6: Facilitate Planning and Management Summary 276	274
23.	The Orders of Patterns of Similarity	277
	 23.1 What a Pattern of Data Is 278 23.2 Three Orders of Patterns of Similarities 278 23.3 How Patterns Become Information 282 23.4 Some Examples of the Orders of Patterns in Cluster Analysis 283 Summary 286 	

APPENDIX 1. BOOKS AND ARTICLES ON CLUSTER ANALYSIS AND OTHER MULTIVARIATE METHODS	288
A1.1 Books 288 A1.2 Articles 291	
APPENDIX 2. COMPUTER PROGRAMS FOR CLUSTER ANALYSIS	292
A2.1 SAS Programs 295 A2.2 BMDP Programs 296 A2.3 CLUSTAN Programs 298 A2.4 NTSYS Programs 299 A2.5 CLUSTAR and CLUSTID Programs 300 A2.6 Other Cluster Analysis Programs 304	
ANSWERS TO EXERCISES	305
GLOSSARY OF TERMS	314
REFERENCES	318
INDEX	330



A Road Map to This Book

OBJECTIVES

This book is an introduction to cluster analysis for researchers. It

- Presents the most often used methods of hierarchical cluster analysis so
 that they can be understood and applied by researchers with limited
 backgrounds in mathematics and statistics.
- Shows a variety of uses of cluster analysis that span the biological sciences, the social sciences, and the natural sciences, as well as planning and management.
- Explains how to use cluster analysis validly in research.

This chapter discusses

- What cluster analysis is about.
- What level of understanding you can expect to gain from this book.
- How you should use this book to meet your needs.