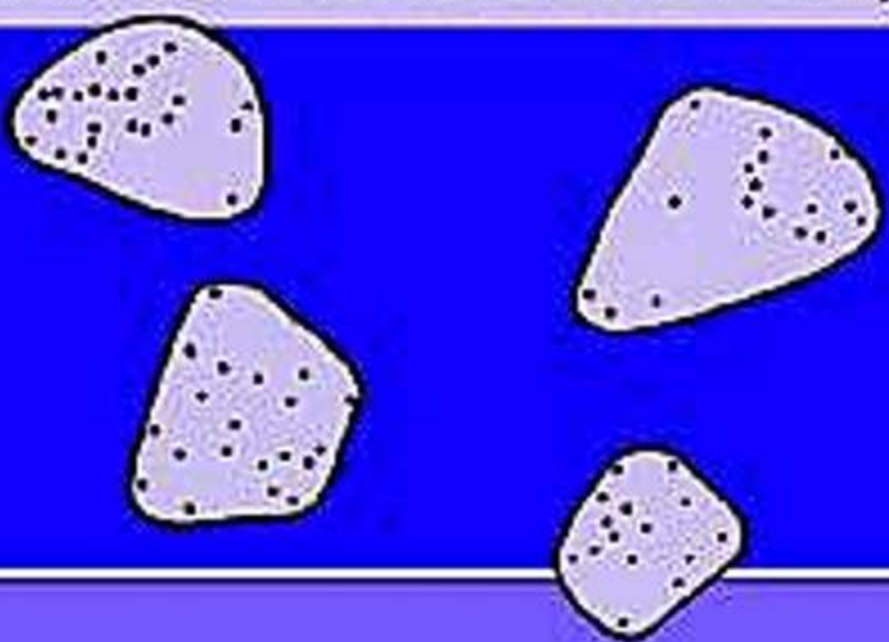
FINDING GROUPS IN DATA

An Introduction to Cluster Analysis



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An Introduction to Cluster Analysis

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To Our Parents And To Jean Haezendonck

Preface

Cluster analysis is a very practical subject. Some 30 years ago, biologists and social scientists began to look for systematic ways to find groups in their data. Because computers were becoming available, the resulting algorithms could actually be implemented. Nowadays clustering methods are applied in many domains, including artificial intelligence and pattern recognition, chemometrics, ecology, economics, the geosciences, marketing, medical research, political science, psychometrics, and many more. This has led to a lot of different methods, and articles on clustering have appeared not only in statistical journals but also in periodicals of all these domains. Clustering is known under a variety of names, such as numerical taxonomy and automatic data classification.

Our purpose was to write an applied book for the general user. We wanted to make cluster analysis available to people who do not necessarily have a strong mathematical or statistical background. Rather than giving an extensive survey of clustering methods, leaving the user with a bewildering multitude of methods to choose from, we preferred to select a few methods that together can deal with most applications. This selection was based on a combination of methodological aims (mainly robustness, consistency, and general applicability) and our own experience in applying clustering to a variety of disciplines.

The book grew out of several courses on cluster analysis that we taught in Brussels, Delft, and Fribourg. It was extensively tested as a textbook with students of mathematics, biology, economics, and political science. It is one of the few books on cluster analysis containing exercises. The first chapter introduces the main approaches to clustering and provides guidance to the choice between the available methods. It also discusses various types of data (including interval-scaled and binary variables, as well as similarity data) and explains how these can be transformed prior to the actual

clustering. The other six chapters each deal with a specific clustering method. These chapters all have the same structure. The first sections give a short description of the clustering method, explain how to use it, and discuss a set of examples. These are followed by two sections (marked with * because they may be skipped without loss of understanding) on the algorithm and its implementation, and on some related methods in the literature. The chapters are relatively independent (except for Chapter 3 which builds on Chapter 2), allowing instructors to cover only one chapter in a statistics course. Another advantage is that researchers can pick out the method they need for their current application, without having to read other chapters. (To achieve this structure, some things had to be repeated in the text.) Occasionally, we handed a single chapter to someone working on a particular problem.

Chapters 2, 3, and 4 are about partitioning methods, whereas Chapters 5, 6, and 7 cover hierarchical techniques. Whenever possible, we constructed methods that cannot only analyze data consisting of measurements (i.e., objects with variables) but also data consisting of dissimilarities between objects. (This excluded parametric approaches, such as those based on multivariate mixture distributions.) We also wanted the methods to be consistent for large data sets. All the selected methods are of the L_1 type, which means that they minimize sums of dissimilarities (rather than sums of *squared* dissimilarities, as in the classical nonrobust methods). Some of the methods are new, such as the approach for partitioning large data sets and the L_1 method for fuzzy clustering. Also, the clusterings are accompanied by graphical displays (called silhouettes and banners) and corresponding quality coefficients, which help the user to select the number of clusters and to see whether the method has found groups that were actually present in the data.

Current statistical software packages contain only a few clustering techniques and they are not the more modern methods. This forced us to write new programs, the use of which is described in the book. Their present version is for IBM-PC and compatible machines, but the source codes are very portable and have run on several types of mainframes without problems. The programs (together with their sources and the data sets used in the book) are available on floppy disks by writing to the authors. The programs are also being integrated in the workstation package S-PLUS of Statistical Sciences, Inc., P.O. Box 85625, Seattle, WA 98145-1625.

We are grateful to Frank Critchley, Jan de Leeuw, Gaetan Libert, Glenn Milligan, Frank Plastria, Marc Roubens, John Tukey, Bert van Zomeren, Howard Wainer, Michael Windham, and David Wishart for helpful suggestions and stimulating discussions on topics covered in this book and to

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Finding Groups in Data: An Introduction to Cluster Analysis
Leonard Kaufman and Peter J. Rousseeuw

CHAPTER 1

Introduction

1 MOTIVATION

Cluster analysis is the art of finding groups in data. To see what is meant by this, let us look at Figure 1. It is a plot of eight objects, on which two variables were measured. For instance, the weight of an object might be displayed on the horizontal axis and its height on the vertical one. Because this example contains only two variables, we can investigate it by merely looking at the plot.

In this small data set there are clearly two distinct groups of objects, namely {TIN, TAL, KIM, ILA} and {LIE, JAC, PET, LEO}. Such groups are called *clusters*, and to discover them is the aim of cluster analysis. Basically, one wants to form groups in such a way that objects in the same group are similar to each other, whereas objects in different groups are as dissimilar as possible.

The classification of similar objects into groups is an important human activity. In everyday life, this is part of the learning process: A child learns to distinguish between cats and dogs, between tables and chairs, between men and women, by means of continuously improving subconscious classification schemes. (This explains why cluster analysis is often considered as a branch of pattern recognition and artificial intelligence.) Classification has always played an essential role in science. In the eighteenth century, Linnaeus and Sauvages provided extensive classifications of animals, plants, minerals, and diseases (for a recent survey, see Holman, 1985). In astronomy, Hertzsprung and Russell classified stars in various categories on the basis of two variables: their light intensity and their surface temperature. In the social sciences, one frequently classifies people with regard to their behavior and preferences. In marketing, it is often attempted to identify market segments, that is, groups of customers with similar needs. Many more examples could be given in geography (clustering of regions), medicine

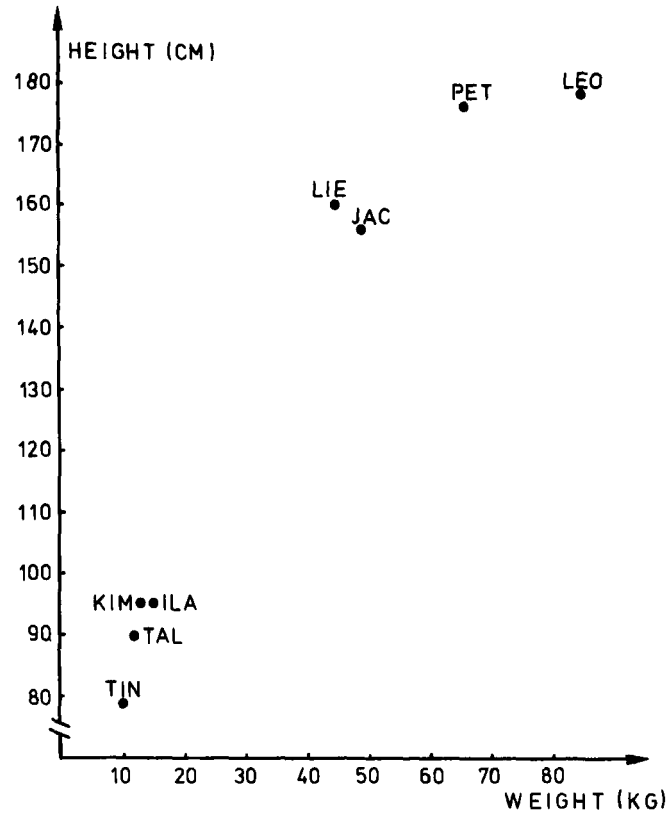


Figure 1 A plot of eight objects.

(incidence of specific types of cancer), chemistry (classification of compounds), history (grouping of archeological findings), and so on. Moreover, cluster analysis can be used not only to identify a structure already present in the data, but also to impose a structure on a more or less homogeneous data set that has to be split up in a "fair" way, for instance when dividing a country into telephone areas. Note that cluster analysis is quite different from discriminant analysis in that it actually establishes the groups, whereas discriminant analysis assigns objects to groups that were defined in advance.

In the past, clusterings were usually performed in a subjective way, by relying on the perception and judgment of the researcher. In the example of Figure 1, we used the human eye–brain system which is very well suited (through millenia of evolution) for classification in up to three dimensions.

However, the need to classify cases in more than three dimensions and the upcoming objectivity standards of modern science have given rise to so-called automatic classification procedures. Over the last 30 years, a wealth of algorithms and computer programs has been developed for cluster analysis. The reasons for this variety of methods are probably twofold. To begin with, automatic classification is a very young scientific discipline in vigorous development, as can be seen from the thousands of articles scattered over many periodicals (mostly journals of statistics, biology, psychometrics, computer science, and marketing). Nowadays, automatic classification is establishing itself as an independent scientific discipline, as witnessed by a full-fledged periodical (the *Journal of Classification*, first published in 1984) and the International Federation of Classification Societies (founded in 1985). The second main reason for the diversity of algorithms is that there exists no general definition of a cluster, and in fact there are several kinds of them: spherical clusters, drawn-out clusters, linear clusters, and so on. Moreover, different applications make use of different data types, such as continuous variables, discrete variables, similarities, and dissimilarities. Therefore, one needs different clustering methods in order to adapt to the kind of application and the type of clusters sought. Cluster analysis has become known under a variety of names, such as numerical taxonomy, automatic classification, botryology (Good, 1977), and typological analysis (Chandon and Pinson, 1981).

In this book, several algorithms are provided for transforming the data, for performing cluster analysis, and for displaying the results graphically. Section 2 of this introduction discusses the various types of data and what to do with them, and Section 3 gives a brief survey of the clustering methods contained in the book, with some guidelines as to which algorithm to choose. In particular the crucial distinction between partitioning and hierarchical methods is considered. In Section 4 a schematic overview is presented. In Section 5, it is explained how to use the program DAISY to transform your data.

2 TYPES OF DATA AND HOW TO HANDLE THEM

Our first objective is to study some types of data which typically occur and to investigate ways of processing the data to make them suitable for cluster analysis.

Suppose there are n objects to be clustered, which may be persons, flowers, words, countries, or whatever. Clustering algorithms typically operate on either of two input structures. The first represents the objects by means of p measurements or attributes, such as height, weight, sex, color,

and so on. These measurements can be arranged in an n-by-p matrix, where the rows correspond to the objects and the columns to the attributes. In Tucker's (1964) terminology such an objects-by-variables matrix is said to be *two-mode*, since the row and column entities are different. The second structure is a collection of proximities that must be available for all pairs of objects. These proximities make up an n-by-n table, which is called a *one-mode* matrix because the row and column entities are the same set of objects. We shall consider two types of proximities, namely dissimilarities (which measure how far away two objects are from each other) and similarities (which measure how much they resemble each other). Let us now have a closer look at the types of data used in this book by considering them one by one.

2.1 Interval-Scaled Variables

In this situation the n objects are characterized by p *continuous* measurements. These values are positive or negative real numbers, such as height, weight, temperature, age, cost, ..., which follow a linear scale. For instance, the time interval between 1905 and 1915 was equal in length to that between 1967 and 1977. Also, it takes the same amount of energy to heat an object of $-16.4°C$ to $-12.4°C$ as to bring it from $35.2°C$ to $39.2°C$. In general it is required that intervals keep the same importance throughout the scale.

These measurements can be organized in an n-by-p matrix, where the rows correspond to the objects (or cases) and the columns correspond to the variables. When the fth measurement of the ith object is denoted by x_{if} (where $i = 1, \ldots, n$ and $f = 1, \ldots, p$) this matrix looks like

$$\begin{array}{c} \\ n \text{ objects} \end{array} \begin{array}{c} \overset{p \text{ variables}}{\overbrace{\phantom{x_{11} \cdots x_{1f} \cdots x_{1p}}}} \\ \begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \vdots & & \vdots & & \vdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \vdots & & \vdots & & \vdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix} \end{array} \tag{1}$$

For instance, consider the following real data set. For eight people, the weight (in kilograms) and the height (in centimeters) is recorded in Table 1. In this situation, $n = 8$ and $p = 2$. One could have recorded many more variables, like age and blood pressure, but as there are only two variables in this example it is easy to make a scatterplot, which corresponds to Figure 1

Table 1 Weight and Height of Eight People, Expressed in Kilograms and Centimeters

Name	Weight (kg)	Height (cm)
Ilan	15	95
Jacqueline	49	156
Kim	13	95
Lieve	45	160
Leon	85	178
Peter	66	176
Talia	12	90
Tina	10	78

given earlier. Note that the units on the vertical axis are drawn to the same size as those on the horizontal axis, even though they represent different physical concepts. The plot contains two obvious clusters, which can in this case be interpreted easily: the one consists of small children and the other of adults.

Note that other variables might have led to completely different clusterings. For instance, measuring the concentration of certain natural hormones might have yielded a clear-cut partition into three male and five female persons. By choosing still other variables, one might have found blood types, skin types, or many other classifications.

Let us now consider the effect of changing measurement units. If weight and height of the subjects had been expressed in pounds and inches, the results would have looked quite different. A pound equals 0.4536 kg and an inch is 2.54 cm. Therefore, Table 2 contains larger numbers in the column of weights and smaller numbers in the column of heights. Figure 2, although plotting essentially the same data as Figure 1, looks much flatter. In this figure, the relative importance of the variable "weight" is much larger than in Figure 1. (Note that Kim is closer to Ilan than to Talia in Figure 1, but that she is closer to Talia than to Ilan in Figure 2.) As a consequence, the two clusters are not as nicely separated as in Figure 1 because in this particular example the height of a person gives a better indication of adulthood than his or her weight. If height had been expressed in feet (1 ft = 30.48 cm), the plot would become flatter still and the variable "weight" would be rather dominant.

In some applications, changing the measurement units may even lead one to see a very different clustering structure. For example, the age (in years) and height (in centimeters) of four imaginary people are given in

Table 2 Weight and Height of the Same Eight People, But Now Expressed in Pounds and Inches

Name	Weight (lb)	Height (in.)
Ilan	33.1	37.4
Jacqueline	108.0	61.4
Kim	28.7	37.4
Lieve	99.2	63.0
Leon	187.4	70.0
Peter	145.5	69.3
Talia	26.5	35.4
Tina	22.0	30.7

Table 3 and plotted in Figure 3. It appears that $\{A, B\}$ and $\{C, D\}$ are two well-separated clusters. On the other hand, when height is expressed in feet one obtains Table 4 and Figure 4, where the obvious clusters are now $\{A, C\}$ and $\{B, D\}$. This partition is completely different from the first because each subject has received another companion. (Figure 4 would have been flattened even more if age had been measured in days.)

To avoid this dependence on the choice of measurement units, one has the option of standardizing the data. This converts the original measurements to unitless variables. First one calculates the mean value of variable

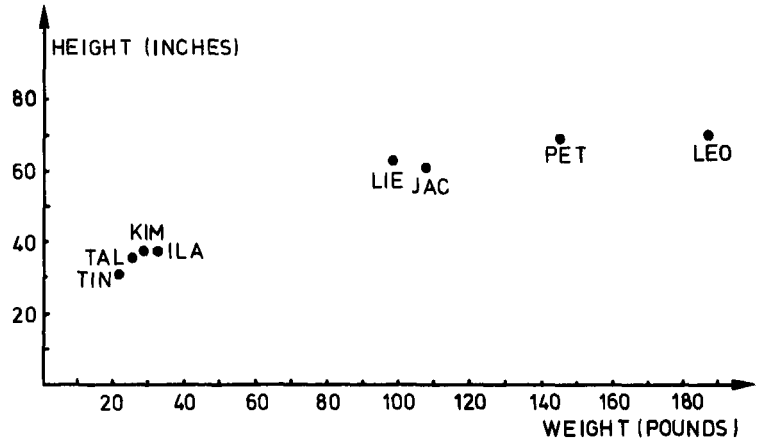


Figure 2 Plot corresponding to Table 2.

Table 3 Age (in years) and Height (in centimeters) of Four People

Person	Age (yr)	Height (cm)
A	35	190
B	40	190
C	35	160
D	40	160

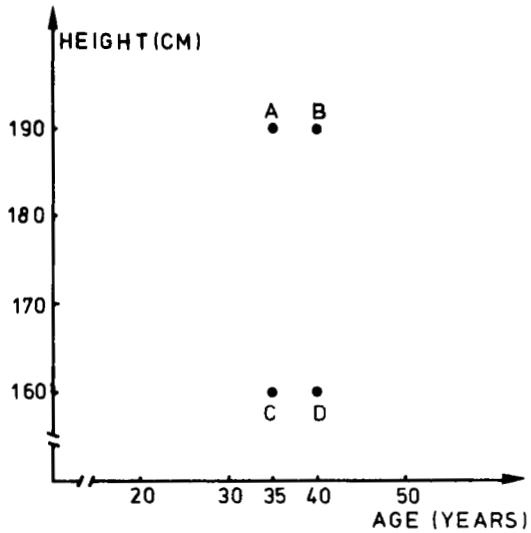


Figure 3 Plot of height (in centimeters) versus age for four people.

Table 4 Age (in years) and Height (in feet) of the Same Four People

Person	Age (yr)	Height (ft)
A	35	6.2
B	40	6.2
C	35	5.2
D	40	5.2

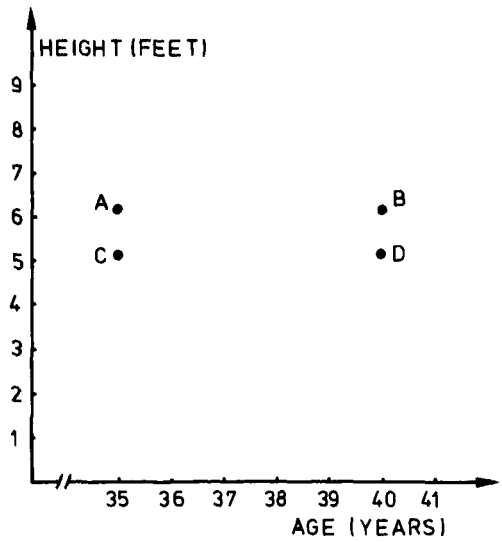


Figure 4 Plot of height (in feet) versus age for the same four people.

f, given by

$$m_f = \frac{1}{n}(x_{1f} + x_{2f} + \cdots + x_{nf}) \tag{2}$$

for each $f = 1, \ldots, p$. Then one computes a measure of the dispersion or "spread" of this fth variable. Traditionally, people use the standard deviation

$$\text{std}_f = \sqrt{\frac{1}{n-1}\left\{(x_{1f} - m_f)^2 + (x_{2f} - m_f)^2 + \cdots + (x_{nf} - m_f)^2\right\}}$$

for this purpose. However, this measure is affected very much by the presence of outlying values. For instance, suppose that one of the x_{if} has been wrongly recorded, so that it is much too large. In this case std_f will be unduly inflated, because $x_{if} - m_f$ is squared. Hartigan (1975, p. 299) notes that one needs a dispersion measure that is not too sensitive to outliers. Therefore, from now on we will use the *mean absolute deviation*

$$s_f = \frac{1}{n}\left\{|x_{1f} - m_f| + |x_{2f} - m_f| + \cdots + |x_{nf} - m_f|\right\} \tag{3}$$

where the contribution of each measurement x_{if} is proportional to the absolute value $|x_{if} - m_f|$. This measure is more robust (see, e.g., Hampel

et al., 1986) in the sense that one outlying observation will not have such a large influence on s_f. (Note that there exist estimates that are much more robust, but we would like to avoid a digression into the field of robust statistics.)

Let us assume that s_f is nonzero (otherwise variable f is constant over all objects and must be removed). Then the standardized measurements are defined by

$$z_{if} = \frac{x_{if} - m_f}{s_f} \tag{4}$$

and sometimes called *z-scores*. They are unitless because both the numerator and the denominator are expressed in the same units. By construction, the z_{if} have mean value zero and their mean absolute deviation is equal to 1. When applying standardization, one forgets about the original data (1) and uses the new data matrix

$$\begin{array}{c} \\ \text{objects} \end{array} \begin{array}{c} \text{variables} \\ \begin{bmatrix} z_{11} & \cdots & z_{1f} & \cdots & z_{1p} \\ \vdots & & \vdots & & \vdots \\ z_{i1} & \cdots & z_{if} & \cdots & z_{ip} \\ \vdots & & \vdots & & \vdots \\ z_{n1} & \cdots & z_{nf} & \cdots & z_{np} \end{bmatrix} \end{array} \tag{5}$$

in all subsequent computations. The advantage of using s_f rather than std_f in the denominator of (4) is that s_f will not be blown up so much in the case of an outlying x_{if}, and hence the corresponding z_{if} will still "stick out" so the ith object can be recognized as an outlier by the clustering algorithm, which will typically put it in a separate cluster. [This motivation differs from that of Milligan and Cooper (1988), who recommended the use of a nonrobust denominator.]

The preceding description might convey the impression that standardization would be beneficial in all situations. However, it is merely an option that may or may not be useful in a given application. Sometimes the variables have an absolute meaning, and should not be standardized (for instance, it may happen that several variables are expressed in the same units, so they should not be divided by different s_f). Often standardization dampens a clustering structure by reducing the large effects because the variables with a big contribution are divided by a large s_f.

For example, let us standardize the data of Table 3. The mean age equals $m_1 = 37.5$ and the mean absolute deviation of the first variable works out to be $s_1 = \{2.5 + 2.5 + 2.5 + 2.5\}/4 = 2.5$. Therefore, standardization converts age 40 to $+1$ and age 35 to -1. Analogously, $m_2 = 175$ cm and

Table 5 Standardized Age and Height of the Same Four People

Person	Variable 1	Variable 2
A	−1.0	1.0
B	1.0	1.0
C	−1.0	−1.0
D	1.0	−1.0

$s_2 = \{15 + 15 + 15 + 15\}/4 = 15$ cm, so 190 cm is standardized to +1 and 160 cm to −1. The resulting data matrix, which is unitless, is given in Table 5. Note that the new averages are zero and that the mean deviations equal 1. Of course, standardizing Table 4 would yield exactly the same result, so Table 5 is the standardized version of both Tables 3 and 4. Even when the data are converted to very strange units (such as the proverbial fortnights and furlongs), standardization will always yield the same numbers. However, plotting the values of Table 5 in Figure 5 does not give a very exciting result. Figure 5 looks like an intermediate between Figures 3 and 4 and shows no clustering structure because the four points lie at the vertices of a square. One could say that there are four clusters, each

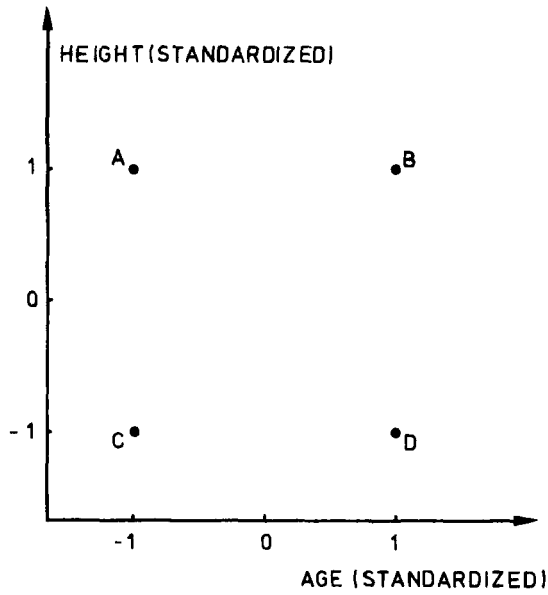


Figure 5 Standardized height versus standardized age.

consisting of a single point, or that there is only one big cluster containing four points.

From a philosophical point of view, standardization does not really solve the problem. Indeed, the choice of measurement units gives rise to relative *weights* of the variables. Expressing a variable in smaller units will lead to a larger range for that variable, which will then have a large effect on the resulting structure. On the other hand, by standardizing one attempts to give all variables an equal weight, in the hope of achieving objectivity. As such, it may be used by a practitioner who possesses no prior knowledge. However, it may well be that some variables are intrinsically more important than others in a particular application, and then the assignment of weights should be based on subject-matter knowledge (see, e.g., Abrahamowicz, 1985). On the other hand, there have been attempts to devise clustering techniques that are independent of the scale of the variables (Friedman and Rubin, 1967). The proposal of Hardy and Rasson (1982) is to search for a partition that minimizes the total volume of the convex hulls of the clusters. In principle such a method is invariant with respect to linear transformations of the data, but unfortunately no algorithm exists for its implementation (except for an approximation that is restricted to two dimensions). Therefore, the dilemma of standardization appears unavoidable at present and the programs described in this book leave the choice up to the user.

Of course, the data offered to the program may already be the result of some transformation: Often people find it useful to replace some variable by its inverse or its square, which may be more meaningful in that particular context. However, we shall assume from now on that such transformations have been performed prior to the cluster analysis.

The next step is to compute distances between the objects, in order to quantify their degree of dissimilarity. It is necessary to have a distance for each pair of objects i and j. The most popular choice is the *Euclidean distance*

$$d(i, j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \cdots + (x_{ip} - x_{jp})^2} \qquad (6)$$

(When the data are being standardized, one has to replace all x by z in this expression.) Formula (6) corresponds to the true geometrical distance between the points with coordinates $(x_{i1}, \ldots, x_{ip})$ and $(x_{j1}, \ldots, x_{jp})$. To illustrate this, let us consider the special case with $p = 2$. Figure 6 shows two points with coordinates (x_{i1}, x_{i2}) and (x_{j1}, x_{j2}). It is clear that the actual distance between objects i and j is given by the length of the hypothenuse of the triangle, yielding expression (6) by virtue of Pythagoras' theorem. For this reason, Gower (1971b) calls (6) the *Pythagorean distance*.

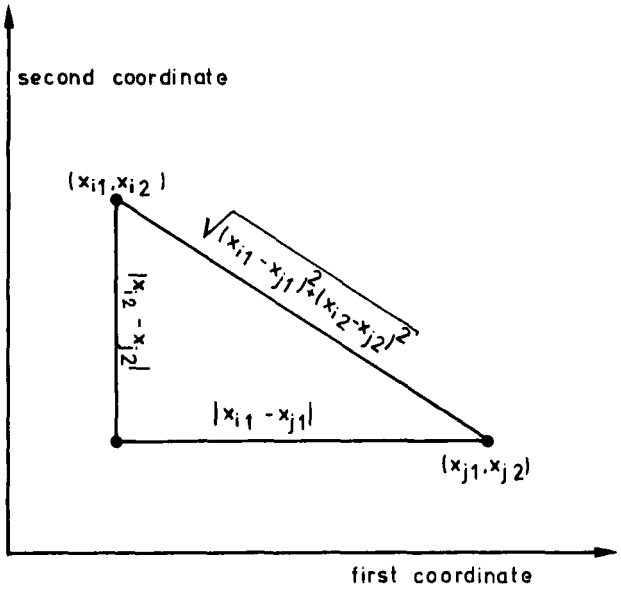


Figure 6 Illustration of the Euclidean distance formula.

Another well-known metric is the *city block* or *Manhattan distance*, defined by

$$d(i, j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \cdots + |x_{ip} - x_{jp}| \qquad (7)$$

In Figure 6, this corresponds to the sum of the lengths of the other two sides of the triangle. The Manhattan distance was used in a cluster analysis context by Carmichael and Sneath (1969) and owes its peculiar name to the following reasoning. Suppose you live in a city where the streets are all north–south or east–west, and hence perpendicular to each other. Let Figure 6 be part of a street map of such a city, where the streets are portrayed as vertical and horizontal lines. Then the actual distance you would have to travel by car to get from location i to location j would total $|x_{i1} - x_{j1}| + |x_{i2} - x_{j2}|$, corresponding to (7). This would be the shortest length among all possible paths from i to j. Only a bird could fly straight from point i to point j, thereby covering the Euclidean distance between these points. The use of the Manhattan distance is advised in those situations where for example a difference of 1 in the first variable and of 3 in the second variable is the same as a difference of 2 in the first variable and of 2 in the second.

Both the Euclidean metric (6) and the Manhattan metric (7) satisfy the following mathematical requirements of a distance function:

(D1) $d(i, j) \geq 0$
(D2) $d(i, i) = 0$
(D3) $d(i, j) = d(j, i)$
(D4) $d(i, j) \leq d(i, h) + d(h, j)$

for all objects i, j, and h. Condition (D1) merely states that distances are nonnegative numbers and (D2) says that the distance of an object to itself is zero. Axiom (D3) is the symmetry of the distance function. The *triangle inequality* (D4) looks a little bit more complicated, but is necessary to allow a geometrical interpretation. It says essentially that going directly from i to j is shorter than making a detour over object h.

Note that $d(i, j) = 0$ does not necessarily imply that $i = j$, because it can very well happen that two different objects have the same measurements for the variables under study. However, the triangle inequality implies that i and j will then have the same distance to any other object h, because $d(i, h) \leq d(i, j) + d(j, h) = d(j, h)$ and at the same time $d(j, h) \leq d(j, i) + d(i, h) = d(i, h)$, which together imply that $d(i, h) = d(j, h)$.

A generalization of both the Euclidean and the Manhattan metric is the *Minkowski distance* given by

$$d(i, j) = \left(|x_{i1} - x_{j1}|^q + |x_{i2} - x_{j2}|^q + \cdots + |x_{ip} - x_{jp}|^q\right)^{1/q}$$

where q is any real number larger than or equal to 1. This is also called the L_q metric, with the Euclidean ($q = 2$) and the Manhattan ($q = 1$) as special cases. Many other distance functions may be constructed (see, e.g., Bock, 1974, Section 3; Hartigan, 1975, Chapter 2; Romesburg, 1984, Chapter 8). The clustering programs accompanying this book provide a choice between Euclidean and Manhattan distances.

One sometimes computes weighted Euclidean distances like

$$d(i, j) = \sqrt{w_1(x_{i1} - x_{j1})^2 + w_2(x_{i2} - x_{j2})^2 + \cdots + w_p(x_{ip} - x_{jp})^2} \quad (8)$$

where each variable receives a weight according to its perceived importance. For instance, giving a variable weight 2 is the same thing as using it twice. However, applying such weighted distances on the raw data is equivalent to first choosing other measurement units, corresponding to rescaling the coordinates by the factors $\sqrt{w_1}, \ldots, \sqrt{w_p}$, and then computing ordinary distances. (Therefore, it was not necessary to provide weighted distances in

our programs.) This leads us back to the discussion on standardization. The essential question remains: Which weights should be assigned to the variables? If one thinks the measurement units were not particularly well chosen and one wants to assign equal weights to the variables, it is preferable to standardize the data first and then to compute ordinary Euclidean distances (6). But if one wants to keep the data intact, because the measurement scales are believed to be meaningful, it is best not to standardize (and hence to use the weights inherent in the raw data). Furthermore, if one wants to *impose* certain weights on the variables, due to prior beliefs or background information, one can either change the measurement units or apply weighted distances like (8), which boils down to the same thing.

In all this, it should be noted that a variable not containing any relevant information (say, the telephone number of each person) is worse than useless, because it will make the clustering less apparent. The occurrence of several such "trash variables" will kill the whole clustering because they yield a lot of random terms in the distances, thereby hiding the useful information provided by the other variables. Therefore, such noninformative variables must be given a zero weight in the analysis, which amounts to deleting them. A recent discussion of variable selection can be found in Fowlkes et al. (1988). In general, the selection of "good" variables is a nontrivial task and may involve quite some trial and error (in addition to subject-matter knowledge and common sense). In this respect, cluster analysis may be considered an exploratory technique.

It often happens that not all measurements are actually available, so there are some "holes" in the data matrix (1). Such an absent measurement is called a *missing value* and it may have several causes. The value of the measurement may have been lost or it may not have been recorded at all by oversight or lack of time. Sometimes the information is simply not available, as in the example of the birthdate of a foundling, or the patient may not remember whether he or she ever had the measles, or it may be impossible to measure the desired quantity due to the malfunctioning of some instrument. In certain instances the question does not apply (such as the color of hair of a bald person) or there may be more than one possible answer (when two experimenters obtain very different results). Because of all this, missing values are often encountered.

How can we handle a data set with missing values? In the matrix (1) we indicate the absent measurements by means of some code (like the number 999.99, if it did not already occur), that can then be recognized by the program. If there exists an object in the data set for which all measurements are missing, there is really no information on this object so it has to be deleted. Analogously, a variable consisting exclusively of missing values has to be removed too.

If the data are standardized, the mean value m_f of the fth variable is calculated by making use of the present values only. The same goes for s_f, so in the denominator of (2) and (3) we must replace n by the number of nonmissing values for that variable. The z-scores z_{if} can then be computed as in (4), but of course only when the corresponding x_{if} is not missing itself.

In the computation of distances (based on either the x_{if} or the z_{if}) similar precautions must be taken. When calculating the distances $d(i, j)$ given by (6) or (7), only those variables are considered in the sum for which the measurements for both objects are present; subsequently the sum is multiplied by p and divided by the actual number of terms (in the case of Euclidean distances this is done before taking the square root). Obviously, such a procedure only makes sense when the variables are thought of as having the same weight (for instance, this can be done after standardization). When computing these distances, one might come across a pair of objects that do not have any common measured variables, so their distance cannot be computed by means of the abovementioned approach. Several remedies are possible: One could remove either object or one could fill in some average distance value based on the rest of the data. A totally different approach consists of replacing all missing x_{if} by the mean m_f of that variable; then all distances can be computed. Applying any of these methods, one finally possesses a "full" set of distances. From this point on, many clustering algorithms can be applied, even though the original data set was not complete.

In any case, we now have a collection of distances (whether based on raw or standardized data that contained missing values or not) that we want to store in a systematic way. This can be achieved by arranging them in an n-by-n matrix. For example, when computing Euclidean distances between the objects of Table 1 we obtain

	ILA	JAC	KIM	LIE	LEO	PET	TAL	TIN
ILA	0	69.8	2.0	71.6	108.6	95.7	5.8	17.7
JAC	69.8	0	70.8	5.7	42.2	26.3	75.7	87.2
KIM	2.0	70.8	0	72.5	109.9	96.8	5.1	17.3
LIE	71.6	5.7	72.5	0	43.9	26.4	77.4	89.2
LEO	108.6	42.2	109.9	43.9	0	19.1	114.3	125.0
PET	95.7	26.3	96.8	26.4	19.1	0	101.6	112.9
TAL	5.8	75.7	5.1	77.4	114.3	101.6	0	12.2
TIN	17.7	87.2	17.3	89.2	125.0	112.9	12.2	0

(9)

The distance between object JAC and object LEO can be located at the intersection of the fifth row and the second column, yielding 42.2. The same

number can also be found at the intersection of the second row and the fifth column, because the distance between JAC and LEO is equal to the distance between LEO and JAC. This is the symmetry property (D3), which holds for any pair of objects [formula (6) gives the same result when i and j are interchanged]. Therefore, a distance matrix is always symmetric. Moreover, note that the entries on the main diagonal are always zero, because the distance of an object to itself has to be zero. (The same remarks apply to the Manhattan or any other distance.) Therefore, it would suffice to write down only the lower triangular half of the distance matrix, which looks like

	ILA	JAC	KIM	LIE	LEO	PET	TAL
JAC	69.8						
KIM	2.0	70.8					
LIE	71.6	5.7	72.5				
LEO	108.6	42.2	109.9	43.9			
PET	95.7	26.3	96.8	26.4	19.1		
TAL	5.8	75.7	5.1	77.4	114.3	101.6	
TIN	17.7	87.2	17.3	89.2	125.0	112.9	12.2

(10)

Note that in the latter form there are only seven rows and seven columns, because the upper row and the rightmost column of (9) were superfluous.

When the data are represented as in (9) or (10), the cluster structure we saw so easily in Figure 1 is rather hidden from visual inspection. Nevertheless, the clustering methods discussed in Chapters 2, 4, 5, and 6 only make use of this information, without having to return to the original data matrix.

2.2 Dissimilarities

This leads us to our second input data structure, namely an n-by-n matrix like (9), often presented as in (10). The entries of such a matrix may be Euclidean or Manhattan distances. However, there are many other possibilities, so we no longer speak of distances but of *dissimilarities* (or dissimilarity coefficients). Basically, dissimilarities are nonnegative numbers $d(i, j)$ that are small (close to zero) when i and j are "near" to each other and that become large when i and j are very different. We shall usually assume that dissimilarities are symmetric and that the dissimilarity of an object to itself is zero, but in general the triangle inequality does *not* hold. Indeed, it is often assumed that dissimilarities satisfy (D1), (D2), and (D3) (see, e.g., Bock, 1974, p. 25), although none of these properties is really essential and there are clustering methods that do not require any of them. But the main difference with distances is that (D4) can no longer be relied on.

Table 6 Subjective Dissimilarities between 11 Sciences

Astronomy	0.00										
Biology	7.86	0.00									
Chemistry	6.50	2.93	0.00								
Computer sci.	5.00	6.86	6.50	0.00							
Economics	8.00	8.14	8.21	4.79	0.00						
Geography	4.29	7.00	7.64	7.71	5.93	0.00					
History	8.07	8.14	8.71	8.57	5.86	3.86	0.00				
Mathematics	3.64	7.14	4.43	1.43	3.57	7.07	9.07	0.00			
Medicine	8.21	2.50	2.93	6.36	8.43	7.86	8.43	6.29	0.00		
Physics	2.71	5.21	4.57	4.21	8.36	7.29	8.64	2.21	5.07	0.00	
Psychology	9.36	5.57	7.29	7.21	6.86	8.29	7.64	8.71	3.79	8.64	0.00

Dissimilarities can be obtained in several ways. Often they can be computed from variables that are binary, nominal, ordinal, interval, or a combination of these (a description of such variables and possible formulas will be given later in this chapter). Also, dissimilarities can be simple subjective ratings of how much certain objects differ from each other, from the point of view of one or more observers. This kind of data is typical in the social sciences and in marketing.

Let us consider an example of this type. Fourteen postgraduate economics students (coming from different parts of the world) were asked to indicate the subjective dissimilarities between 11 scientific disciplines. All of them had to fill in a matrix like Table 6, where the dissimilarities had to be given as integer numbers on a scale from 0 (identical) to 10 (very different). The actual entries of Table 6 are the averages of the values given by the students. It appears that the smallest dissimilarity is perceived between mathematics and computer science, whereas the most remote fields were psychology and astronomy.

Another example of the construction of dissimilarities is to record how often consonants are misunderstood, because when two consonants are often confused (like "s" and "z") this indicates that their dissimilarity is small [see, e.g., Johnson's (1967) analysis of the Miller and Nicely (1955) data]. Such experiments lead to asymmetric matrices, because "z" may be more often inadvertently taken for "s" than vice versa. However, in such situations one can easily symmetrize the data [for instance by averaging $d(i, j)$ with $d(j, i)$ for each pair of consonants].

If one wants to perform a cluster analysis on a set of *variables* that have been observed in some population, there are other measures of dissimilarity. For instance, one can compute the (parametric) Pearson product-moment

correlation

$$R(f,g) = \frac{\sum_{i=1}^{n}(x_{if} - m_f)(x_{ig} - m_g)}{\sqrt{\sum_{i=1}^{n}(x_{if} - m_f)^2}\sqrt{\sum_{i=1}^{n}(x_{ig} - m_g)^2}}$$

between the variables f and g, or alternatively the (nonparametric) Spearman correlation. Both coefficients lie between -1 and $+1$ and do not depend on the choice of measurement units. The main difference between them is that the Pearson coefficient looks for a linear relation between the variables f and g, whereas the Spearman coefficient searches for a monotone relation. Both coefficients are provided by most statistical packages, like SPSS, BMDP, or SAS, so they can simply be taken from their routine output. Correlation coefficients are useful for clustering purposes because they measure the extent to which two variables are related.

For instance, the Pearson correlation between the variables weight and height in Table 1 is 0.957. It is very high because there appears to be a positive relationship between these two variables: The larger somebody's weight, the larger his or her height is likely to be, as can be seen from the upward trend in Figure 1. Table 7 also lists some other variables measured on the same eight people, namely their month and year of birth. We see no apparent relation between month of birth and weight: There is no obvious reason why someone born in November (of any year) would be likely to be heavier than someone born in February. Indeed, the correlation between month and weight is approximately zero (the actual value in this example is -0.036). A third situation occurs when we correlate weight with the year of birth: The people with a large birth year will typically possess a smaller weight and vice versa. In such a situation the correlation coefficient be-

Table 7 Data on Eight People. Weight is Expressed in Kilograms and Height in Centimeters. Also the Month and Year of Birth are Provided

Name	Weight	Height	Month	Year
Ilan	15	95	1	82
Jacqueline	49	156	5	55
Kim	13	95	11	81
Lieve	45	160	7	56
Leon	85	178	6	48
Peter	66	176	6	56
Talia	12	90	12	83
Tina	10	78	1	84

Table 8 (a) Pearson Correlation Coefficients between the Four Variables in Table 7, (b) Corresponding Dissimilarities Obtained Through Formula (11), and (c) Dissimilarities Computed by Means of (12)

Quantity		Weight	Height	Month	Year
(a) Correlations	Weight	1.000			
	Height	0.957	1.000		
	Month	−0.036	0.021	1.000	
	Year	−0.953	−0.985	0.013	1.000
(b) Dissimilarities	Weight	0.000			
According to (11)	Height	0.021	0.000		
	Month	0.518	0.489	0.000	
	Year	0.977	0.992	0.493	0.000
(c) Dissimilarities	Weight	0.000			
According to (12)	Height	0.043	0.000		
	Month	0.964	0.979	0.000	
	Year	0.047	0.015	0.987	0.000

comes strongly negative (in this example it is -0.953, which is close to -1, because the relation is nearly linear). Continuing like this, we can fill up Table 8(a).

Correlation coefficients, whether parametric or nonparametric, can be converted to dissimilarities $d(f, g)$, for instance by setting

$$d(f, g) = (1 - R(f, g))/2 \tag{11}$$

With this formula, variables with a high positive correlation receive a dissimilarity coefficient close to zero, whereas variables with a strongly negative correlation will be considered very dissimilar. In other applications one might prefer to use

$$d(f, g) = 1 - |R(f, g)| \tag{12}$$

in which case also variables with a strongly negative correlation will be assigned a small dissimilarity. Lance and Williams (1979) compared these formulas by means of real data, and concluded that (11) was unequivocally the best, whereas (12) still did relatively well. (A third possibility, given by $d(f, g) = 1 - R(f, g)^2$, turned out to be uniformly unsatisfactory.) Table 8(b) contains the dissimilarities computed according to (11), in which case weight and year are perceived to be very different. On the other hand, the

use of (12) yields Table 8(c) in which the variable year joins the cluster formed by weight and height.

Many other ad hoc dissimilarities between variables can be thought of. For example, in a psychological application (Lecompte et al., 1986) we once had to cluster nominal variables, some of which possessed two classes and some three. The resulting contingency tables of pairs of variables led to chi-squared statistics that could not be compared directly because they possessed different degrees of freedom. However, the computed significance level (also called P–value) of these statistics could be used to construct a dissimilarity measure. The stronger the relationship between two variables, the smaller their P–value becomes.

In many applications, the input data simply consist of a dissimilarity matrix, without any measurement values. Indeed, the dissimilarities may have been computed from attributes that were not published or even have been lost. It may also be that there never were any variables in the first place, because the dissimilarities were obtained in another way (from subjective assessments, confusion data, or whatever). For this reason it is useful to have clustering algorithms that can operate directly on a dissimilarity matrix, without having to resort to any measurements. This is the case for the programs PAM, FANNY, AGNES, and DIANA, which will be briefly introduced in Section 3.

2.3 Similarities

Instead of using a dissimilarity coefficient $d(i, j)$ to indicate how remote two objects i and j are, it is also possible to work with a *similarity coefficient* $s(i, j)$. The more objects i and j are alike (or close), the larger $s(i, j)$ becomes. Such a similarity $s(i, j)$ typically takes on values between 0 and 1, where 0 means that i and j are not similar at all and 1 reflects maximal similarity. Values in between 0 and 1 indicate various degrees of resemblance. Often it is assumed that the following conditions hold:

(S1) $0 \leq s(i, j) \leq 1$
(S2) $s(i, i) = 1$
(S3) $s(i, j) = s(j, i)$

for all objects i and j (see Bock, 1974). The numbers $s(i, j)$ can be arranged in an n-by-n matrix like (9) or (10), which is then called a *similarity matrix*. Both similarity and dissimilarity matrices are generally referred to as *proximity matrices*, or sometimes as *resemblance matrices*.

Similarities may arise in several ways. Like dissimilarities, they may be the results of subjective judgments. Also, there are formulas to compute similarities between objects characterized by attributes, even when these variables are of different types, as we shall see in Section 2.6 on mixed measurements.

In order to define similarities between *variables*, we can again resort to the Pearson or the Spearman correlation coefficient. However, neither correlation measure can be used directly as a similarity coefficient because they also take on negative values. Some transformation is in order to bring the coefficients into the zero-one range. There are essentially two ways to do this, depending on the meaning of the data and the purpose of the application. If variables with a strong negative correlation are considered to be very different because they are oriented in the opposite direction (like mileage and weight of a set of cars), then it is best to take something like

$$s(f, g) = (1 + R(f, g))/2 \tag{13}$$

which yields $s(f, g) = 0$ whenever $R(f, g) = -1$. On the other hand, there are situations in which variables with a strong negative correlation should be grouped, because they measure essentially the same thing. (For instance, this happens if one wants to reduce the number of variables in a regression data set by selecting one variable from each cluster.) In that case it is better to use a formula like

$$s(f, g) = |R(f, g)| \tag{14}$$

which yields $s(f, g) = 1$ when $R(f, g) = -1$.

It must be noted that people have sometimes used correlation coefficients for assessing similarity between *objects* by simply interchanging the roles of objects and variables in the expression of R. This does not make much sense because it involves such operations as averaging the measurements (in different units) of the same object. The use of the correlation coefficient between objects was criticized by Eades (1965), Fleiss and Zubin (1969), and others, on several grounds.

Suppose the data consist of a similarity matrix but one wants to apply a clustering algorithm designed for dissimilarities. Then it is necessary to transform the similarities into dissimilarities. The larger the similarity $s(i, j)$ between i and j, the smaller their dissimilarity $d(i, j)$ should be. Therefore, we need a decreasing transformation, such as

$$d(i, j) = 1 - s(i, j) \tag{15}$$

One could also take the square root of $1 - s(i, j)$, as advocated by Gower (1966) on the basis of a geometrical argument. This makes the differences between large similarities more important, but on the other hand makes it more difficult to obtain small dissimilarities. As a consequence, the resulting dissimilarity matrix might be rather homogeneous and less likely to yield clear-cut clusterings.

When applying (15) to correlation coefficients, expression (13) leads to formula (11), which means that negatively correlated variables are considered far apart. In the opposite case, (14) yields formula (12).

In order to be able to process similarities and correlation coefficients, the program DAISY executes (11), (12), and (15) as well as some other calculations. In Section 5 it will be explained how to use this program.

2.4 Binary Variables

Binary variables have only two possible outcomes (or states). For instance, when clustering people several binary variables may be used: male/female, smoker/nonsmoker, answered yes/no to a particular question, and so on. In the data matrix, such variables are often coded as zero or one. When variable f is binary, the objects i will have either $x_{if} = 0$ or $x_{if} = 1$. (It may be useful to allow a third code for missing values, e.g., to indicate that we do not know whether that particular person smokes or not.) Often 1 is taken to mean that a certain attribute is present (e.g., smoking), whereas 0 indicates its absence. Sometimes people treat binary variables just as if they were interval-scaled, that is, by applying the usual formulas for Euclidean or Manhattan distance. Although this may sometimes lead to decent results, it is good to know that there exist approaches designed specifically for binary data.

To begin with, there are special clustering algorithms for this situation, such as the *monothetic analysis* technique described in Chapter 7 and implemented in the program MONA. This algorithm operates directly on the binary data matrix, by dissecting the data according to a well-chosen variable. For instance, if the variable "smoking" were selected, the data would first be split into two clusters: the one consisting of smokers and the other of nonsmokers.

Another possibility is to compute a dissimilarity matrix (or a similarity matrix) from binary data and then simply to apply one of the clustering algorithms that operates on such a matrix (such as the methods described in Chapters 2, 4, 5, and 6). If all binary variables are thought of as having the same weight, one typically proceeds as follows. When computing a similarity $s(i, j)$ or a dissimilarity $d(i, j)$ between two objects i and j, one draws

a 2-by-2 contingency table (or association table) such as

		object j: 1	object j: 0	
object i	1	a	b	$a + b$
	0	c	d	$c + d$
		$a + c$	$b + d$	p

(16)

Here, a is the number of variables that equal 1 for both objects. Analogously, b is the number of variables f for which $x_{if} = 1$ and $x_{jf} = 0$, and so on. Obviously $a + b + c + d = p$, the total number of variables. (When missing values occur, one has to replace p by the number of variables that are available for both i and j. One could also compute weighted sums: If a variable is perceived to be very important, it may be given a higher weight than the other variables. In such a situation, p will be replaced by the sum of all the weights.) The values a, b, c, and d are then combined in a coefficient describing to what extent objects i and j agree with regard to the collection of binary variables.

Table 9 provides an example of binary data. For 8 people, a total of 10 binary variables were considered, such as male/female, blue eyes/brown eyes, round face/oval face, and so on. The attribute listed first is always the one coded as 1, for instance blue eyes = 1 and brown eyes = 0. When comparing Ilan with Talia, we make up a table like (16) which yields $a = 1$, $b = 3$, $c = 1$, and $d = 5$. Note that interchanging Ilan and Talia would permute b and c (while leaving a and d unchanged), so a good similarity or dissimilarity coefficient must treat b and c in the same way in order to satisfy (D3) or (S3).

At this point a crucial remark is in order. Following Gower (1971a, p. 858) and Bock (1974, Section 4) we can distinguish between *two* kinds of binary variables, depending on the particular application.

The binary variable "sex" possesses the possible states "male" and "female." Both are equally valuable and carry the same weight. There is no preference which outcome should be coded as 0 and which as 1. Such a variable is called *symmetric*. This is the first type of binary variable, which occurs very frequently. For symmetric variables, it is natural to work with *invariant* similarities, that is, the result must not change when some or all of the binary variables are coded differently. Therefore, a and d should play the same role. One looks for coefficients that only depend on the number of agreements ($a + d$) and the number of disagreements ($b + c$) between the objects i and j that are being compared. Table 10 gives the most common

Table 9 Binary Variables for Eight People

Person	Sex (Male = 1, Female = 0)	Married (Yes = 1, No = 0)	Fair Hair = 1, Dark Hair = 0	Blue Eyes = 1, Brown Eyes = 0	Wears Glasses (Yes = 1, No = 0)	Round Face = 1, Oval Face = 0	Pessimist = 1, Optimist = 0	Evening Type = 1, Morning Type = 0	Is an Only Child (Yes = 1, No = 0)	Left-Handed = 1, Right-Handed = 0
Ilan	1	0	1	1	0	0	1	0	0	0
Jacqueline	0	1	0	0	1	0	0	0	0	0
Kim	0	0	1	0	0	0	1	0	0	1
Lieve	0	1	0	0	0	0	0	1	1	0
Leon	1	1	0	0	1	1	0	1	1	0
Peter	1	1	0	0	1	0	1	1	0	0
Talia	0	0	0	1	0	1	0	0	0	0
Tina	0	0	0	1	0	1	0	0	0	0

Table 10 Some Invariant Coefficients for Binary Data

Name	$s(i, j)$	$d(i, j)$
Simple matching coefficient (Zubin, 1938; Dumas, 1955; Sokal and Michener, 1958; Sneath, 1962; Hill et al., 1965)	$\frac{a+d}{a+b+c+d}$	$\frac{b+c}{a+b+c+d}$
Rogers and Tanimoto (1960)	$\frac{a+d}{(a+d)+2(b+c)}$	$\frac{2(b+c)}{(a+d)+2(b+c)}$
Sokal and Sneath (1963) (Duran and Odell 1974)	$\frac{2(a+d)}{2(a+d)+(b+c)}$	$\frac{b+c}{2(a+d)+(b+c)}$

invariant similarities $s(i, j)$, together with the corresponding invariant dissimilarities $d(i, j) = 1 - s(i, j)$.

The most well known of these is the *simple matching* coefficient, which looks for the percentage of matches (i.e., agreements), or equivalently the percentage of mismatches (i.e., disagreements) between objects i and j. For the distance between Ilan and Talia it yields $d(i, j) = (3 + 1)/(1 + 3 + 1 + 5) = 0.4$. Sometimes it is also called *M-coefficient* or *affinity index*. If one treats binary variables as if they were interval-scaled and computes the Manhattan distance (without first standardizing the measurements), one obtains $d(i, j) = b + c$ which corresponds to the simple matching dissimilarity except for a constant factor p. In the same way, the Euclidean distance between objects i and j corresponds to the square root of the simple matching dissimilarity. Note that treating binary variables as if they were interval-scaled implies that they are assumed to be symmetric, because interchanging the codes 0 and 1 for some or all variables will still yield the same distance.

The other coefficients in Table 10 are less often used. In the Rogers and Tanimoto (1960) formulas, the disagreements $(b + c)$ carry twice the weight of the agreements $(a + d)$. On the other hand, Sokal and Sneath (1963) doubly weight the agreements. However, there is a simple monotone relation between all three coefficients, because the Rogers–Tanimoto dissimilarity can be written as a monotone function of the simple matching dissimilarity:

$$\frac{2(b + c)}{(a + d) + 2(b + c)} = \frac{2}{1/((b + c)/(a + b + c + d)) + 1} \tag{17}$$

and the same holds for the dissimilarity coefficient proposed by Sokal and Sneath:

$$\frac{b + c}{2(a + d) + (b + c)} = \frac{1}{2/((b + c)/(a + b + c + d)) - 1} \tag{18}$$

Therefore, it often makes little difference which of these three coefficients is used (especially if one applies a clustering algorithm that only depends on the ranks of the dissimilarities, such as the single linkage method discussed later). In this book, we prefer to work with the matching coefficient because it is simple and intuitive. In Section 5 we shall explain how to compute it by means of the program DAISY.

The situation changes drastically if one works with *asymmetric* binary variables, for which the outcomes are not equally important. An example of

such a variable is the presence or absence of a relatively rare attribute, such as bloodtype AB negative. While it can be said that two people with AB negative have something in common, it is not so clear if the same can be said of two people who do *not* have it. In medicine, one may want to study the incidence of diseases, the presence of which are indicated by 1 and their absence by 0. For a typical sample of people, the data matrix would contain many zeroes, and most of the counts of the contingency tables like (16) would be in d. Applying one of the invariant coefficients of Table 10 would lead to the conclusion that most people are very similar. Bock (1974, Section 4) gives an illuminating example concerning the color of flowers: The binary variable red = 1/not red = 0 is very asymmetric, as the statement "$x_{if} = 1$ and $x_{jf} = 1$" implies that flowers i and j have the same color, whereas "$x_{if} = 0$ and $x_{jf} = 0$" is much weaker and allows the flowers to have very different colors.

When working with asymmetric binary variables, we need other proximity coefficients. By convention, we shall always code the most important outcome (which is typically the rarest one) by 1, and the other by 0. Then the agreement of two 1s (called a *positive match* or a *1-1 match*) will be considered more significant than the agreement of two 0s (called a *negative match* or a *0-0 match*). Therefore, coefficients will be applied in which a, the number of positive matches, carries more weight than d, the number of negative matches. Such coefficients are no longer invariant and the most common of them, listed in Table 11, do not even count d at all.

The most famous noninvariant coefficient is due to Jaccard (1908) and looks like the simple matching coefficient except for leaving out d entirely. It has occasionally been called *S-coefficient*. The other formulas in Table 11 assign double weight to a or to $(b + c)$, and are monotonically related to the Jaccard coefficient in a manner analogous to (17) and (18). There are still other variants, some of which will be listed in Exercise 15. When

Table 11 Some Noninvariant Coefficients for Binary Data

Name	$s(i, j)$	$d(i, j)$
Jaccard coefficient (1908) (Sneath, 1957; Hill et al., 1965)	$\frac{a}{a + b + c}$	$\frac{b + c}{a + b + c}$
Dice (1945), Sorensen (1948)	$\frac{2a}{2a + b + c}$	$\frac{b + c}{2a + b + c}$
Sokal and Sneath (1963) (Duran and Odell, 1974)	$\frac{a}{a + 2(b + c)}$	$\frac{2(b + c)}{a + 2(b + c)}$

dealing with asymmetric binary variables, we prefer to use the Jaccard coefficient, which has also been implemented in the program DAISY.

There have been some philosophical debates as to whether or not negative matches should be counted at all. From a mathematical point of view, the invariant coefficients are more elegant, whereas in some applications it may be more appropriate to use a formula of Table 11. In our opinion there can be no single best coefficient because one should make the distinction between symmetric and asymmetric variables. Symmetric binary variables possess two equally important states, so for them the simple matching coefficient appears to be a logical choice. On the other hand, asymmetric binary variables are mostly concerned with the *presence* of a relatively rare attribute (coded 1), the absence of which (coded 0) is uneventful. By abuse of the word binary, one might call them monary variables. In this situation 0-0 matches do not contribute much to the similarity between two individuals, so the Jaccard coefficient appears to give a reasonable description. Therefore, DAISY lets the user decide whether the binary variables are symmetric, in which case simple matching will be performed, or asymmetric, in which situation the Jaccard coefficient will be computed.

To illustrate why it is important to make this distinction, let us return to the example of Table 9. Based on their interpretation, these binary variables appear to be symmetric. When the simple matching coefficient is used, we find

$$d(\text{JAC}, \text{LIE}) = 0.3 \qquad d(\text{ILA}, \text{PET}) = 0.5$$

On the other hand, applying the Jaccard coefficient (which would be rather inappropriate in this context) would yield

$$d(\text{JAC}, \text{LIE}) = 0.750 \qquad d(\text{ILA}, \text{PET}) = 0.714$$

The main point is not that the actual values are different (which was to be expected), but that the results are not monotone: In the first situation we find that $d(\text{JAC}, \text{LIE}) < d(\text{ILA}, \text{PET})$, whereas in the second situation it turns out that $d(\text{JAC}, \text{LIE}) > d(\text{ILA}, \text{PET})$, which could lead to quite different clusterings. [Applying either of the remaining coefficients of Table 10 would still yield $d(\text{JAC}, \text{LIE}) < d(\text{ILA}, \text{PET})$ because they have a monotone relation with the simple matching coefficient, while the measures of Table 11 all yield $d(\text{JAC}, \text{LIE}) > d(\text{ILA}, \text{PET})$ because they depend in a monotone way on the Jaccard coefficient.]

When both symmetric and asymmetric binary variables occur in the same data set, one can apply the "mixed variables" approach described in Section 2.6.

2.5 Nominal, Ordinal, and Ratio Variables

Apart from binary and interval-scaled variables, there exist at least three other types of data, which are less commonly used. We shall briefly describe these scales with some discussion as to how to treat them.

a. Nominal Variables

In the previous section we studied binary variables, which can only take on two states, typically coded as 1 and 0. This generalizes naturally to the concept of a nominal variable, which may take on more than two states. For instance, in Table 9 we had the binary variable blue eyes/brown eyes, which was appropriate for that collection of people. However, in larger populations one will need at least four states: blue eyes/brown eyes/green eyes/grey eyes. In general, we denote the number of states by M and code the outcomes as $1, 2, \ldots, M$ in the data matrix (sometimes the codes $0, 1, \ldots, M-1$ are also used). For instance, we could choose 1 = blue eyes, 2 = brown eyes, 3 = green eyes, and 4 = grey eyes. Note that these states are not ordered in any way: It is not because grey eyes are given a higher code number than brown eyes that they would in some sense be better. The code numbers are only used to facilitate data handling, but one could just as well code the different outcomes by letters or other symbols. Some examples of nominal variables are the nationality of people (for which M may be very large) or their marital status (bachelor/married/divorced/widowed).

Sometimes nominal variables are converted to binary ones. By collapsing some states until only two remain, a binary variable results. For instance, one can group green eyes with brown eyes and grey with blue. However, this clearly amounts to a loss of information. Another strategy would be to recode the data to a larger number of (asymmetric) binary variables, for instance by creating a new binary variable for each of the M nominal states, and then to put it equal to 1 if the corresponding state occurs and to 0 otherwise. After that, one could resort to one of the dissimilarity coefficients of the previous subsection.

By far the most common way of measuring the similarity or dissimilarity between some objects i and j that are characterized through nominal variables is to use the *simple matching* approach:

$$s(i, j) = \frac{u}{p} \quad \text{and} \quad d(i, j) = \frac{p - u}{p} \tag{19}$$

(Sokal and Michener, 1958). Here, u is the number of matches, that is, the number of variables for which objects i and j happen to be in the same

state. As before, p is the total number of variables (or, in a situation with missing values, the number of variables that are available for both i and j). Therefore, simple matching has exactly the same meaning as in the preceding section. For instance, it is invariant with respect to different codings of the variables because this does not affect the number of matches.

Again it is possible to give a higher weight to u, the number of agreements, or to $p - u$, the number of disagreements. Such variants were considered by Rogers and Tanimoto (1960) and Sokal and Sneath (1963), corresponding to the formulas in Table 10. It must also be noted that different variables may have different values of M. Therefore, Hyvarinen (1962) assigns more weight to matches in variables with a large number of states. Lingoes (1967) extends this by counting, for all variables, the frequency with which each state actually occurs and by giving a higher weight to matches corresponding to rare states. (This is reminiscent of the treatment of asymmetric binary variables.) Some other variants can be found in Bock (1974, Section 5).

We personally prefer the simple matching approach (19) because of its intuitive appeal and widespread acceptance. Simple matching dissimilarities can be computed by means of the program DAISY. It is not necessary to know the number of states for each variable because the program will itself produce an inventory with the number of states and the number of missing values. Also, the codes entered may be arbitrary real numbers, so the variables do not have to be coded in a discrete way. The main purpose of DAISY is to deliver a dissimilarity matrix which can be used by some of the clustering algorithms described in the following chapters.

b. Ordinal Variables

A *discrete* ordinal variable looks like a nominal variable, only now the M states are ordered in a meaningful sequence. The codes $1, \ldots, M$ are no longer arbitrary. The distance between two states becomes larger when their codes are further apart, so the states coded 1 and M differ most from each other.

Ordinal variables are very useful for registering subjective assessments of qualities that cannot be measured objectively. For example, you may ask someone to convey his or her appreciation of some paintings in terms of the following categories: detest = 1/dislike = 2/indifferent = 3/like = 4/admire = 5. This person's taste will then be modelled as an ordinal variable with $M = 5$ states. Another possibility is to rank 20 paintings in increasing order of appreciation, yielding an ordinal variable with states $1, 2, \ldots, 20$ and $M = 20$. (Note that in the latter example each state will occur exactly once, whereas in the first it may happen that some states occur very often and others not at all.) One may also obtain ordinal

variables from the discretization of interval-scaled quantities, by splitting up the continuous axis in a finite number of classes. Some examples are weight categories for boxers and tax brackets.

Sometimes there does exist an underlying interval-scaled variable, but it has not been measured. For instance, one can construct a ranking of the hardness of stones by making scratches on one stone with another, without necessarily being able to measure their hardness in absolute terms. Or one can organize a race without needing a stopwatch, by merely registering who came in first, second,..., and so on, as in the ancient olympics.

Continuous ordinal variables are very similar. They occur when the measurements are continuous, but one is not certain whether they are in anything like a linear scale, so the only trustworthy information is in the ordering of the observations. Indeed, if a scale is transformed by an exponential, a logarithmic or another nonlinear monotone transformation, it loses its interval property: A difference of 3.2 on one end of the new scale may be much more important than a difference of 3.2 on the other end. Therefore, one replaces the observations by their ranks $1,\ldots,M$ where M is the number of different values taken on by the continuous variable. (Of course, two equal measurements receive the same rank.) This is also very useful when the original data were roughly on an interval scale, but contained some gross errors. By switching to the ranks, such errors will have a much smaller influence on the result. It is as if we do have the running times of the race, but we are only interested in the ranking because we consider the exact time intervals irrelevant (imagine the last runner, seeing he is going to lose anyway and just walking the final part). Also, maybe we do not know whether the "right" variable should be the total running time or the average speed, which is on the inverse scale. In such situations, it is often useful to reduce the data to the essentials by converting them to ranks.

Whatever its origin, we are left with a variable with ordered states $1,2,\ldots,M$. It would be a waste of information to treat it as if it were nominal, because the further two states are apart, the larger the resulting dissimilarity should become. Therefore, most authors advise treating the ranks as interval-scaled and applying the usual formulas for obtaining dissimilarities (like the Euclidean or Manhattan distance). As it may happen that the ordinal variables under study possess different values of M, it is useful to convert all variables to the 0-1 range in order to achieve equal weighting of the variables. This can be done by replacing the rank r_{if} of the ith object in the fth variable by

$$z_{if} = \frac{r_{if} - 1}{M_f - 1} \tag{20}$$

where M_f is the highest rank for variable f. In this way, all z_{if} will lie between 0 and 1.

The program DAISY can be applied to a data set with ordinal variables, whether discrete or continuous. It will first convert each variable f to ranks $1, 2, \ldots, M_f$ in such a way that equal measurements lead to equal ranks and that each rank occurs at least once. Then it will replace all ranks by z_{if} as in (20). The final dissimilarity between objects i and j is then taken to be the Manhattan distance (7) divided by the number of variables that are non-missing for both objects.

Note that when the *variables* are to be clustered one can compute a full set of nonparametric correlations between them (say, Spearman coefficients) by means of any standard statistical package and then apply DAISY to transform these into a dissimilarity matrix by means of (11) or (12).

c. *Ratio Scale Variables*

We have seen that interval-scaled variables are positive or negative numbers on some kind of linear scale, for instance, the interval between 41°C and 51°C is equally important as the interval between −28°C and −18°C. By contrast, ratio-scaled variables are always positive measurements, for which the distinction between 2 and 20 has the same meaning as the distinction between 20 and 200. Typical examples are the concentration of a chemical substance in a certain solvent or the radiation intensity of some radioactive isotope. Often such ratio-scaled quantities follow exponential laws in time. For instance, the total amount of microorganisms that evolve in a time t (in a closed system with abundant nourishment) is approximately given by

$$Ae^{Bt} \tag{21}$$

where A and B are positive constants. Formula (21) is usually referred to as exponential growth and has been a reasonable model for the world population over certain time periods. Similarly, the concentration of some alien substances in human blood or the radiation intensity of an isotope can be modelled by an exponential decay formula

$$Ae^{-Bt} \tag{22}$$

In both (21) and (22), equal time intervals will lead to equal ratios of the quantities described, for instance, each year the radioactivity will decrease by the same percentage when compared to the level of the previous year.

When clustering objects that are characterized by ratio scale variables, one has at least three options. The first is to simply treat them *as if they were on an interval scale*. This is often done by people who only distinguish between qualitative and quantitative variables, without considering the fine

distinction between interval and ratio scales. In general, we would not recommend this because the scale might become distorted. A second approach, which is very common in chemistry, is to begin with a *logarithmic transformation* of the ratio scale variables x_{if}, at least when they are all nonzero, that is, one computes

$$y_{if} = \log(x_{if}) \tag{23}$$

and treats these y_{if} as interval-scaled. This is quite a sensible procedure, especially in situations where (21) or (22) apply. A third approach is to treat the x_{if} as *continuous ordinal data* and switch to their ranks. This could also be done after the logarithmic transformation (23) and would then yield exactly the same result. The ranks are then treated as interval-scaled data, in the way already described. This third approach is especially suitable when there are doubts whether the original data are interval or ratio scaled, or in case of uncertainty about the quality of the measurements. By only making use of the ordinal information, the distinction between interval and ratio disappears. Dissimilarities between objects (according to all three approaches) can be computed by means of the program DAISY, the use of which will be explained in Section 5.

2.6 Mixed Variables

In this section we have seen six types of variables:

symmetric binary
asymmetric binary
nominal
ordinal
interval
ratio

and we have discussed methods of dealing with data sets of one of these types. However, in practical applications it can easily happen that several kinds of variables occur in the same data set. For example, we could combine the interval variables of Table 7 with the binary variables of Table 9 because they pertain to the same individuals. A larger example is Table 12, listing certain characteristics of garden flowers. In the first column it is indicated whether the plant winters, that is, whether it may be left in the garden when it freezes. The second column shows whether the flower may stand in the shadow; those for which this is not so should be planted where

Table 12 Characteristics of Some Garden Flowers

Garden Flower	Winters (Yes = 1, No = 0)	Shadow (Yes = 1, No = 0)	Tubers (Yes = 1, No = 0)	Color of Flowers (White = 1, Yellow = 2, Pink = 3, Red = 4, Blue = 5)	Soil (Dry = 1, Normal = 2, Humid = 3)	Preference (Low = 1, High = 18)	Height (cm)	Planting distance (cm)
1. Begonia (*Bertinii boliviensis*)	0	1	1	4	3	15	25	15
2. Broom (*Cytisus praecox*)	1	0	0	2	1	3	150	50
3. Camellia (Japonica)	0	1	0	3	3	1	150	50
4. Dahlia (Tartini)	0	0	1	4	2	16	125	50
5. Forget-me-not (*Myosotis sylvatica*)	0	1	0	5	2	2	20	15
6. Fuchsia (Marinka)	0	1	0	4	3	12	50	40
7. Geranium (Rubin)	0	0	0	4	3	13	40	20
8. Gladiolus (Flowersong)	0	0	1	2	2	7	100	15
9. Heather (*Erica carnea*)	1	1	0	3	1	4	25	15
10. Hydrangea (Hortensis)	1	1	0	5	2	14	100	60
11. Iris (Versicolor)	1	1	1	5	3	8	45	10
12. Lily (*Lilium regale*)	1	1	1	1	2	9	90	25
13. Lily-of-the-valley (Convallaria)	1	1	0	1	2	6	20	10
14. Peony (*Paeonia lactiflora*)	1	1	1	4	2	11	80	30
15. Pink Carnation (Dianthus)	1	0	0	3	2	10	40	20
16. Red Rose (*Rosa rugosa*)	1	0	0	4	2	18	200	60
17. Scotch Rose (*Rosa pimpinella*)	1	0	0	2	2	17	150	60
18. Tulip (*Tulipa sylvestris*)	0	0	1	2	1	5	25	10

they are exposed to direct sunlight. These columns are symmetric binary variables, with equally important states. The third binary variable is coded 1 for tuberous plants and 0 for plants without tubers. This variable is asymmetric because two plants with tubers have at least something in common, whereas plants without tubers may grow in completely different ways. The next column describes the color of the flowers. This variable is nominal, with $m = 5$ states occurring in these data (white = 1, yellow = 2,

pink = 3, red = 4, and blue = 5). The fifth column says whether the plant thrives best in dry (1), normal (2), or humid (3) soil. This is an ordinal variable, the states being ranked according to increasing moisture. The sixth column is someone's preference ranking, going from 1 to 18. The code 18 next to the red rose indicates that this flower is best liked, whereas the code 1 is assigned to the plant least liked. This ordinal variable possesses many states, but each state occurs only once. The last columns list the height of the plants and the distances that should be left between them, both expressed in centimeters. Therefore, this data set contains only two interval-scaled variables out of a total of eight attributes.

Data with mixed variables can be treated in several ways. To begin with, it is possible not to mix these types at all but to perform a separate cluster analysis for each kind of variable. When the conclusions of these analyses more or less agree, all is well. However, when different results are obtained, it may be difficult to reconcile them.

Therefore, it is more practical to process the data together and then to perform a single cluster analysis. For instance, one can treat all variables as if they were interval-scaled. This is quite appropriate for symmetric binary variables, for the ranks originating from ordinal variables, and for the logarithms of ratio variables. However, for nominal variables with more than two states this does not make much sense because some codes may be further apart than others without reflecting an intrinsic "remoteness" of the corresponding states. Also, asymmetric binary variables would be treated symmetrically.

The opposite approach is to reduce everything to binary variables. How to do this for nominal variables was already discussed. It is also easy to obtain a binary variable from interval-scaled measurements y_{if} by cutting the measurement axis in two, that is, by applying a rule like

$$\text{if } y_{if} < a_f, \text{ then put } x_{if} = 0$$
$$\text{if } y_{if} \geq a_f, \text{ then put } x_{if} = 1$$

where the threshold a_f may be chosen by means of subject-matter information or simply by selecting a value in the center of the data. (It may even be that the y_{if} form two clear clusters in one dimension, in which case a_f may be chosen between them.) The same rule can be applied to ordinal and ratio variables. However, by converting the whole data set to binary attributes one may lose quite a bit of information, which is often considered a disadvantage.

In our opinion, the most convenient approach is to combine the different variables into a single proximity matrix, as was proposed by Ducker et al.

(1965), Rubin (1967), and Colless (1967). The definition of Gower (1971a) takes care of interval, nominal, and binary data. We shall describe a slight generalization of this method, also covering ordinal and ratio variables. Actually, Gower's original definition was a similarity coefficient between 0 and 1, but we shall transform it to a dissimilarity by means of (15). Conversely, one can always return to similarities by computing $s(i, j) = 1 - d(i, j)$ at the end.

Suppose the data set contains p variables of mixed nature. Then the dissimilarity $d(i, j)$ between objects i and j is defined as

$$d(i, j) = \frac{\sum_{f=1}^{p} \delta_{ij}^{(f)} d_{ij}^{(f)}}{\sum_{f=1}^{p} \delta_{ij}^{(f)}} \tag{24}$$

The indicator $\delta_{ij}^{(f)}$ is put equal to 1 when both measurements x_{if} and x_{jf} for the fth variable are nonmissing, and it is put equal to 0 otherwise. Moreover, $\delta_{ij}^{(f)}$ is also put equal to 0 when variable f is an asymmetric binary attribute and objects i and j constitute a 0-0 match. Expression (24) cannot be computed when all $\delta_{ij}^{(f)}$ are zero, in which case $d(i, j)$ must be assigned a conventional value or object i or j must be removed.

The number $d_{ij}^{(f)}$ is the contribution of the fth variable to the dissimilarity between i and j. We may assume that both x_{if} and x_{jf} are nonmissing: otherwise $d_{ij}^{(f)}$ does not have to be computed. If variable f is either *binary* or *nominal*, then $d_{ij}^{(f)}$ is defined as

$$\begin{aligned} d_{ij}^{(f)} &= 1 \quad \text{if } x_{if} \neq x_{jf} \\ &= 0 \quad \text{if } x_{if} = x_{jf} \end{aligned} \tag{25}$$

If all variables are nominal, expression (24) becomes the number of matches over the total number of available pairs, so it coincides with the simple matching coefficient (19). The same holds for symmetric binary variables, for which the simple matching coefficient of Table 10 is recovered. When the data consist of asymmetric binary variables, we obtain the Jaccard coefficient of Table 11 because the 0-0 matches are not counted (because their $\delta_{ij}^{(f)}$ equals zero).

If variable f is *interval-scaled*, then $d_{ij}^{(f)}$ is given by

$$d_{ij}^{(f)} = \frac{|x_{if} - x_{jf}|}{R_f} \tag{26}$$

where R_f is the range of variable f, defined as

$$R_f = \max_h x_{hf} - \min_h x_{hf} \tag{27}$$

where h runs over all nonmissing objects for variable f. Therefore, (26) is always a number between 0 and 1. *Ordinal* variables are first replaced by their ranks, after which (26) is applied. *Ratio* variables may be treated as interval variables: They can be converted to ranks or a logarithmic transformation may be carried out. In either case, (26) is applied to the result.

When all variables are interval-scaled, Gower's formula (24) becomes the Manhattan distance, assuming that the variables were first divided by their range [note that this standardization is quite different from (4)]. When all variables are ordinal, (24) yields the same result as the method described in Section 2.5. The same is true for ratio variables.

We conclude that the combined method (24) generalizes the dissimilarities of the homogeneous data discussed earlier. The computations can be performed with the program DAISY, as described in Section 5. For instance, it easily deals with Table 12. The same program is used for data with variables of a single type and for processing similarities and correlation coefficients. In all cases, it delivers a dissimilarity matrix that can be used to run four of the clustering programs of this book. Figure 15 of Section 4 contains a survey of the function of DAISY, among other information.

Note that we followed Gower in restricting $d_{ij}^{(f)}$ to the 0-1 range, so each variable yields a contribution between 0 and 1 to the average dissimilarity (24). [As a consequence, the resulting dissimilarity $d(i, j)$ also lies between 0 and 1, and can be turned back into Gower's original formula by computing $s(i, j) = 1 - d(i, j)$.] Why restrict ourselves to this range? Suppose we were to allow contributions with very different ranges, as done by Romesburg (1984) in his combined resemblance matrix approach. Then some interesting anomalies are possible. Take an example with a few asymmetric binary variables and many interval variables, the latter yielding contributions $d_{ij}^{(f)}$ around 3 or 4. Consider an asymmetric binary variable with $x_{if} = 0$ and $x_{jf} = 1$, which yields a contribution $d_{ij}^{(f)}$ of 1. Now change x_{jf} to 0, so we obtain a 0-0 match and the term $d_{ij}^{(f)}$ vanishes both in the numerator and the denominator. This yields a *larger* dissimilarity $d(i, j)$ than before. This effect is, of course, opposite to what was expected. It appears necessary to have equal ranges if one wants to be able to delete certain contributions, or else the effects of such deletions may be unwarranted.

As a final remark, it must be noted that it is even possible to cluster objects that are characterized by a combination of measurements and proximities. For instance, suppose we have a similarity matrix, a dissimilarity matrix, and a mixed collection of attributes, all pertaining to the same n objects. Then DAISY can convert the similarity matrix into a dissimilarity matrix as in (15), and compute another dissimilarity matrix from the attributes according to (24). The three resulting dissimilarity matrices can then be combined into a single one by means of

$$d(i, j) = \frac{w_1 d_1(i, j) + w_2 d_2(i, j) + w_3 d_3(i, j)}{w_1 + w_2 + w_3}$$

where w_1, w_2, and w_3 are some positive weights that may be chosen in a subjective way.

This section was devoted to clustering *objects* that are characterized by attributes of mixed types. In some situations, however, one might want to cluster the *variables* themselves. This was discussed by Lance and Williams (1979), who compute dissimilarities between variables of mixed types.

3 WHICH CLUSTERING ALGORITHM TO CHOOSE

Let us give an overview of the clustering methods implemented in this book, together with their most important characteristics and some hints toward typical applications. The choice of a clustering algorithm depends both on the type of data available and on the particular purpose. Sometimes several algorithms are applicable, and a priori arguments may not suffice to narrow down the choice to a single method. In such a situation it is probably a good idea to run more than one program and to carefully analyze and compare the resulting classifications, making use of their graphical displays. The interpretation of these results must then be based on insight into the meaning of the original data, together with some experience with the algorithms used. It is permissible to try several algorithms on the same data, because cluster analysis is mostly used as a descriptive or exploratory tool, in contrast with statistical tests which are carried out for inferential or confirmatory purposes. That is, we do not wish to prove (or disprove) a preconceived hypothesis; we just want to see what the data are trying to tell us.

Of course there exist very many clustering algorithms in the literature, and it would be infeasible to try to review all of them. Bock (1974)

undertook the monumental task of compiling an overall survey, which accurately reflects the state of the art in the early seventies, but the field has expanded very much since that time. Our own approach has been to select (and partly construct) six clustering methods, which together are believed to cover a majority of applications. This selection (which is subjective and necessarily debatable) has been based on a combination of some theoretical considerations (such as an attempt to achieve as much logical consistency and robustness as possible) and our own experience in applying clustering to a variety of disciplines. To each of these six algorithms we have dedicated one chapter which develops its background and describes how to run the corresponding computer program, illustrated with some examples.

3.1 Partitioning Methods

In this book we consider two kinds of clustering algorithms, namely partitioning and hierarchical methods. In the classification literature, the vast majority of algorithms is of either type. Therefore we have decided to provide three partitioning and three hierarchical programs.

A partitioning method constructs k clusters. That is, it classifies the data into k groups, which together satisfy the requirements of a partition:

Each group must contain at least one object.

Each object must belong to exactly one group.

These conditions imply that there are at most as many groups as there are objects:

$$k \leq n$$

The second condition says that two different clusters cannot have any objects in common and that the k groups together add up to the full data set. Figure 7 shows an example of a partition of 20 points into three clusters.

It is important to note that k is given by the user. Indeed, the algorithm will construct a partition with as many clusters as desired. Of course, not all values of k lead to "natural" clusterings, so it is advisable to run the algorithm several times with different values of k and to select that k for which certain characteristics or graphics look best, or to retain the clustering that appears to give rise to the most meaningful interpretation. It is also possible to have this decision made in an automatic way, that is, to let the computer try out all (or many) possible values of k and to choose the one which is best relative to some numerical criterion.

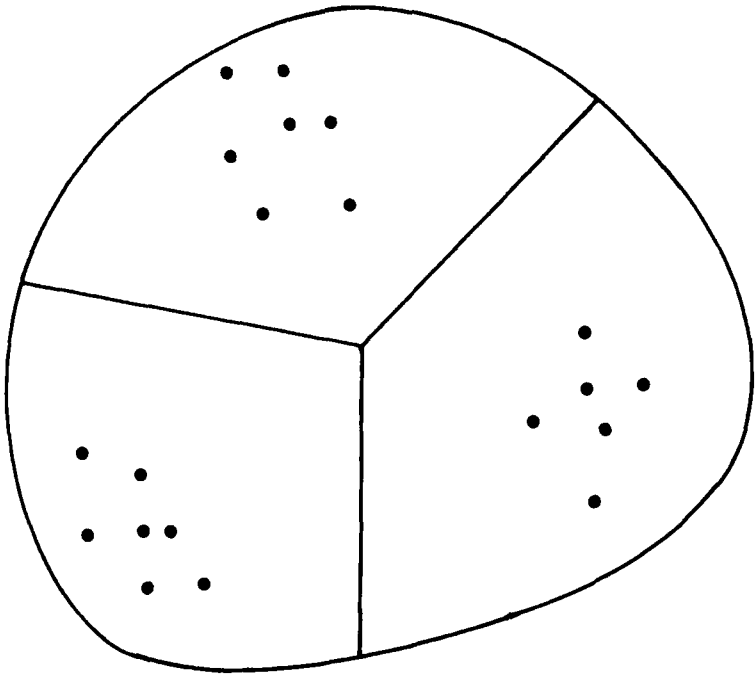


Figure 7 A partition with $n = 20$ and $k = 3$.

Partitioning methods are applied if one wants to classify the objects into k clusters, where k is fixed (although it may have been selected by the computer). Some examples are:

You have data on 100 bacteria. Do they form groups?

People give you subjective assessments on 12 countries. Does cluster analysis provide recognizable groups of states?

Performance criteria have been measured for 800 companies. Can groups of companies be found that perform in a similar way?

In general, the algorithm tries to find a "good" partition in the sense that objects of the same cluster should be close or related to each other, whereas objects of different clusters should be far apart or very different. The aim is usually to uncover a structure that is already present in the data, but sometimes the algorithm is used to impose a new structure, for example when partitioning a country into telephone areas.

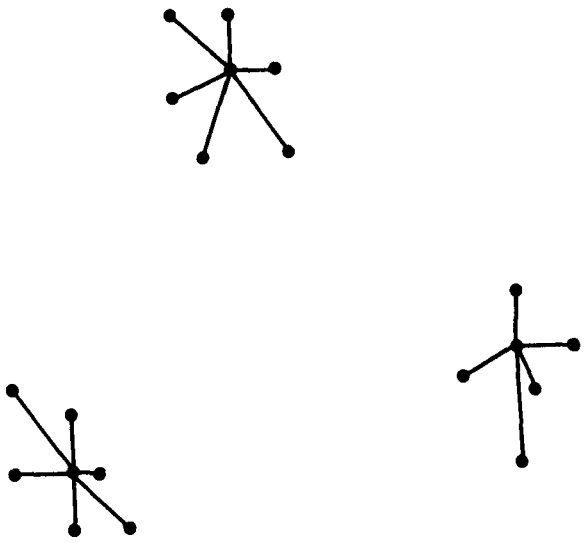


Figure 8 Illustration of partitioning around medoids for the example of Figure 7.

Partitioning Around Medoids (Chapter 2)

The program PAM clusters objects that are measured on p interval-scaled variables, and it can also be applied when the input data is a dissimilarity matrix (possibly set up by the program DAISY).

The idea of this partitioning algorithm is the following. In order to obtain k clusters, the method selects k objects (which are called *representative objects*) in the data set. The corresponding clusters are then found by assigning each remaining object to the nearest representative object. An example of such an allocation is shown in Figure 8 for objects characterized by two interval-scaled measurements (that is, $p = 2$). Of course, not every selection of k representative objects gives rise to a "good" clustering. The clue is that the representative objects must be chosen so that they are (in a certain sense) centrally located in the clusters they define. To be exact, the average distance (or average dissimilarity) of the representative object to all the other objects of the same cluster is being minimized. For this reason, such an optimal representative object we call the *medoid* of its cluster, and the method of partitioning around medoids we call the *k-medoid* technique.

Figure 8 also provides another way of looking at this method. Suppose the objects are really cities and it is desired to build three household appliance factories. To reduce transportation costs, the factories should be constructed in centrally located cities, so that the average distance to the

consumers is minimized. Stated in this form, we recognize a problem of industrial location that belongs to operations research.

On the other hand, people already familiar with cluster analysis will note a resemblance with the well-known k-means algorithm, which attempts to minimize the average *squared* distance, yielding so-called *centroids*. We have decided in favor of the k-medoid method because it is more robust with respect to outliers and because this method does not only deal with interval-scaled measurements but also with general dissimilarity coefficients.

By construction, the k-medoid method tries to find "spherical" clusters, that is, clusters that are roughly ball-shaped (as in Figure 8). It is therefore not suited to discover drawn-out clusters. The program PAM is especially recommended if one is also interested in the representative objects themselves, which may be very useful for data reduction or characterization purposes. The program also allows a more detailed analysis of the partition by providing clustering characteristics and a graphical display (a so-called *silhouette plot*), and an appropriate choice of k can be made on the basis of a validity index it computes.

Clustering Large Applications (Chapter 3)

The program CLARA was developed for the express purpose of analyzing large data sets. Its clustering objective is the same as in the program PAM: It also tries to find k representative objects that are centrally located in the cluster they define. But in PAM the collection of all pairwise distances between objects is stored in central memory, thereby consuming $O(n^2)$ memory space. This means that PAM cannot be used for large n (a typical upper bound is $n = 100$, but this depends on the central memory size). Therefore, CLARA no longer stores all dissimilarities, but only the actual measurements. This is paid for by the loss of some other features, the most important of which is that CLARA does not accept the input of a dissimilarity matrix (which would be too big anyway).

The program CLARA proceeds as follows. By means of a random number generator, a sample of objects is drawn from the data and clustered in the same way as in PAM. Then each object of the entire data set is assigned to the nearest medoid of the sample, as illustrated in Figure 9. This whole procedure is repeated several times and the solution with the best overall objective function is retained. In this way, the computation time also remains feasible.

As we are still in the k-medoid framework, CLARA shares the robustness of PAM, and it is also intended for spherical clusters. Also the majority of clustering characteristics and other tools are still available, albeit in approximate form.

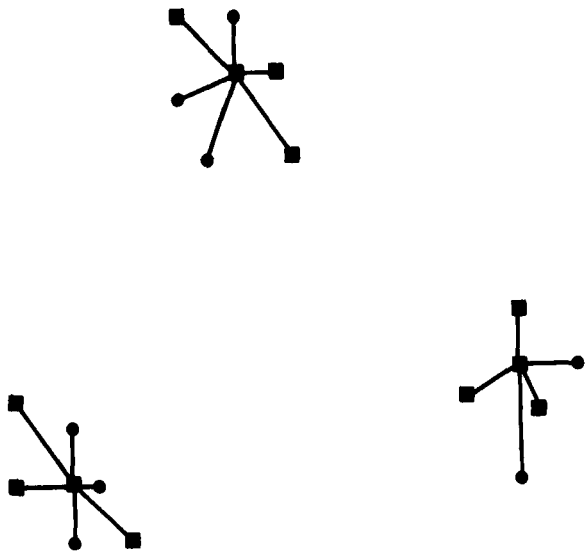


Figure 9 Illustration of the technique used in the program CLARA. The objects of the sample are indicated by small squares.

Fuzzy Analysis (Chapter 4)

The program FANNY can be applied to the same data sets as the program PAM, but its algorithm is of a different nature. Indeed, it employs the "fuzziness" principle, which means that FANNY is able to avoid "hard" decisions. Instead of saying "object *a* belongs to cluster 1," FANNY can say that "object *a* belongs for 90% to cluster 1, for 5% to cluster 2, and for 5% to cluster 3," meaning that *a* is probably to be assigned to cluster 1 but that there is still a glimpse of doubt in favor of clusters 2 and 3.

In Figure 10 we see some points that can be classified with a strong degree of certainty, as well as a few intermediate objects for which it is not clear to which cluster they should be assigned. In fuzzy analysis, these different situations can be described by means of so-called *membership coefficients* as found in Table 13. They reflect that *a* belongs mostly to cluster 1, that *b* belongs mostly to cluster 2, and that *c* belongs mostly to cluster 3. Note that the sum of the membership coefficients in each row equals 1. Object *d* is interesting because it is about halfway in between clusters 2 and 3, yielding a 45% membership in both. At the same time its membership coefficient in cluster 1 is only 10%, because it lies much further away from that cluster. The situation of object *e* is even more ambiguous, because it lies about equally far away from all three clusters, yielding

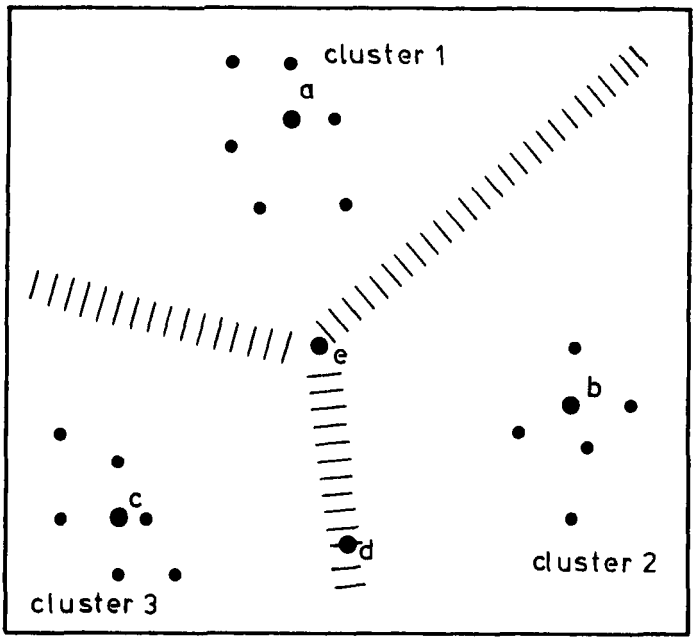


Figure 10 Example with intermediate points, to be classified in a fuzzy way.

membership coefficients of approximately 33%. The ability to describe such ambiguous situations is an important advantage of the fuzzy approach. Indeed, a "hard" clustering algorithm would have to assign object *e* to one of the clusters, leading to a distorted result.

The actual algorithm to calculate the membership coefficients is very different from other clustering methods and does not involve any represen-

Table 13 Membership Coefficients Corresponding to Figure 10

	Membership Coefficients		
Object	Cluster 1	Cluster 2	Cluster 3
a	0.90	0.05	0.05
b	0.05	0.90	0.05
c	0.10	0.10	0.80
d	0.10	0.45	0.45
e	0.33	0.33	0.34
⋮	⋮	⋮	⋮

tative objects. Unfortunately, the computations are rather complex and therefore neither transparent nor intuitive.

Another disadvantage is the massive output, because fuzzy analysis provides an entire n-by-k matrix of membership coefficients, that may be very hard to interpret because of its mere size. In the end one often resorts to the corresponding "hard" clustering, obtained by assigning each object to the cluster in which it has the largest membership coefficient. For this hard partition, FANNY yields the same kind of graphical display as does PAM, so it is possible to compare both outputs.

3.2 Hierarchical Methods

Hierarchical algorithms do not construct a single partition with k clusters, but they deal with all values of k in the same run. That is, the partition with $k = 1$ (all objects are together in the same cluster) is part of the output, and also the situation with $k = n$ (each object forms a separate cluster with only a single element). In between, all values of $k = 2, 3, \ldots, n - 1$ are covered in a kind of gradual transition: The only difference between $k = r$ and $k = r + 1$ is that one of the r clusters splits up in order to obtain $r + 1$ clusters (or, to put it differently, two of the $r + 1$ clusters combine to yield r clusters).

There are two kinds of hierarchical techniques: the agglomerative and the divisive. They construct their hierarchy in the opposite direction, possibly yielding quite different results. Figure 11 shows what happens with a data set with $n = 5$ objects. *Agglomerative* methods (indicated by the upper arrow, pointing to the right) start when all objects are apart (that is, at step 0 we have n clusters). Then in each step two clusters are merged, until only one is left. On the other hand, *divisive* methods start when all objects are together (that is, at step 0 there is one cluster) and in each following step a cluster is split up, until there are n of them. In this example the agglomerative and divisive hierarchies coincide, but usually they are different.

One might think that now partitioning methods are obsolete, as we obtain all values of k in a single run. However, this is not true because a clustering formed "along the way" is not necessarily very good. Indeed, a partitioning method tries to select the *best* clustering with k groups, which is not the goal of a hierarchical method. A hierarchical method suffers from the defect that it can never repair what was done in previous steps. Indeed, once an agglomerative algorithm has joined two objects, they cannot be separated any more. Also, whatever a divisive algorithm has split up cannot be reunited. This rigidity of hierarchical methods is both the key to their

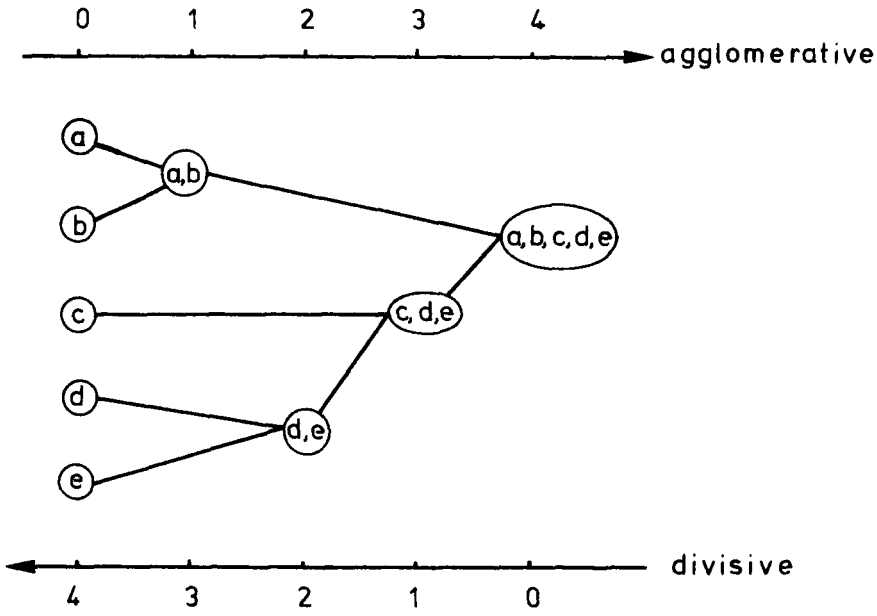


Figure 11 Distinction between agglomerative and divisive techniques.

success (because it leads to small computation times) and their main disadvantage (the inability to correct erroneous decisions).

On the other hand, hierarchical techniques do not really compete with partitioning methods because they do not pursue the same goal, as they try to describe the data in a totally different way. The structure in Figure 11 resembles an evolutionary tree, and indeed hierarchical methods have been found very useful in biological applications, for the classification of animals and plants (see Figure 12). Biologists have been most instrumental in the development of hierarchical methods, particularly in the framework of numerical taxonomy.

Agglomerative Nesting (Chapter 5)

The program AGNES accepts exactly the same data as PAM and FANNY. In fact, the interactive input dialogue is almost identical, except of course that k, the number of clusters, is no longer asked for. The program is agglomerative, so it executes a complete sequence of fusions as in Figure 11. In the first step, the two closest objects (that is, with smallest interobject

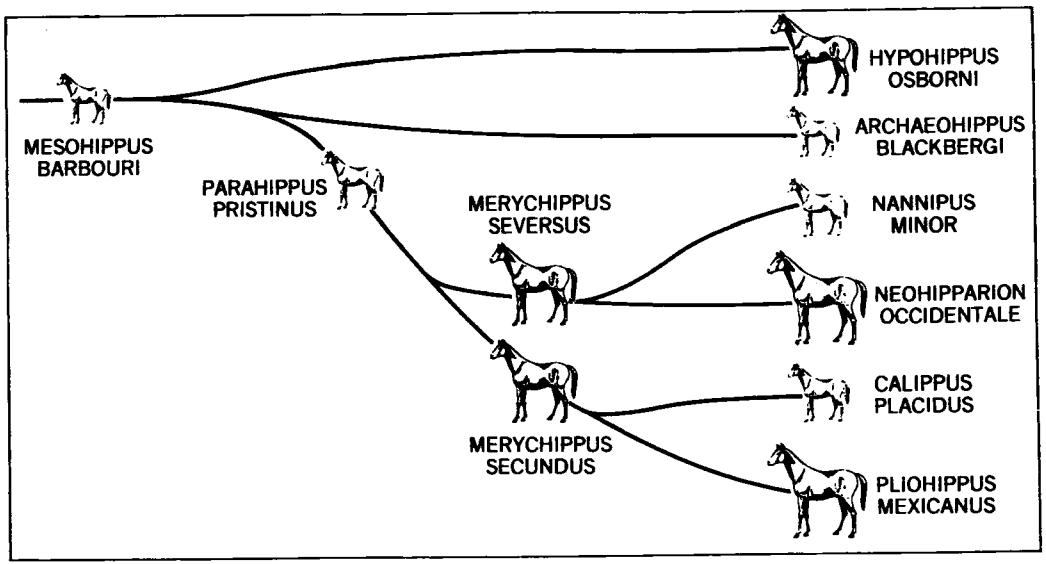


Figure 12 An example of a taxonomic tree (from Sokal, 1966).

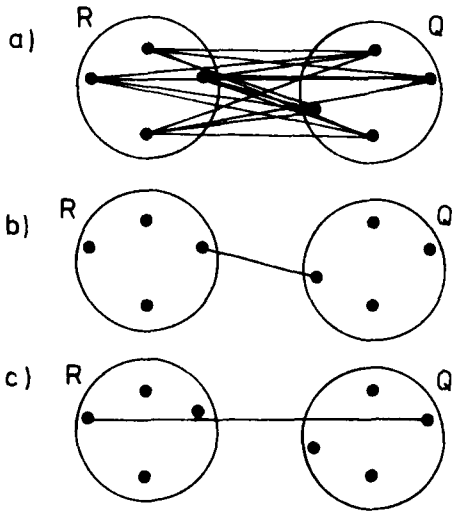


Figure 13 Representation of some definitions of intercluster dissimilarity: (a) Group average. (b) Nearest neighbor. (c) Furthest neighbor.

dissimilarity) are joined, leaving us with $n - 1$ clusters, one of which contains two objects whereas the others still have only a single member.

In all succeeding steps, the two closest clusters are merged. However, this calls for a definition of the dissimilarity between *clusters* (based on the dissimilarities between their objects). There exist many agglomerative algorithms, which only differ in their definition of between-cluster dissimilarity. We have selected the *unweighted pair-group average method* (UPGMA) to be incorporated in AGNES (this decision was made on several grounds, which will be explained in Chapter 5). In this method, the dissimilarity between clusters R and Q is taken to be the *average* of all dissimilarities $d(i, j)$, where i is any object of R and j is any object of Q. In Figure 13a, $d(R, Q)$ can be thought of as the average length of all lines between objects of R and objects of Q.

Figure 13 also displays two other well-known agglomerative methods. The *nearest neighbor* rule (also called *single linkage*) defines $d(R, Q)$ as the smallest dissimilarity between an object of R and an object of Q. On the other hand, the *furthest neighbor* rule (also called *complete linkage*) uses the largest dissimilarity between an object of R and an object of Q.

These three agglomerative methods are useful in different types of applications. The group average technique is aimed at finding roughly ball-shaped clusters as in Figure 14a. Being relatively robust, this method can even deal with rather potato-shaped clusters.

The nearest neighbor rule is not always appropriate in such situations: Whenever both clusters come too close to each other, even when this

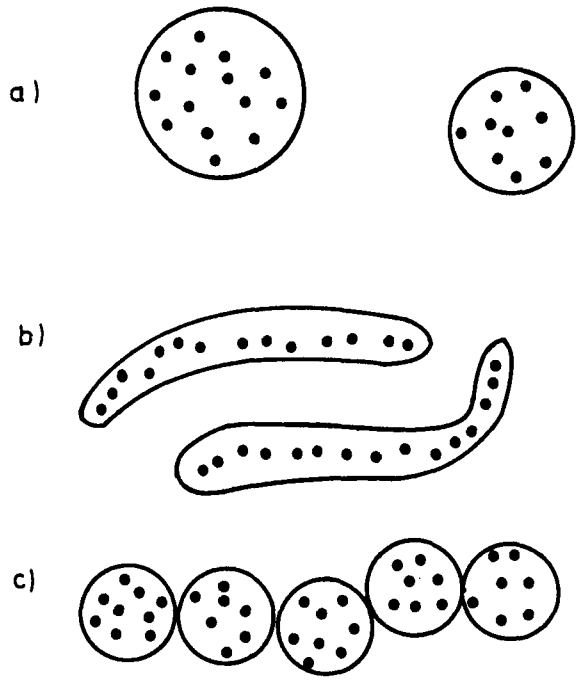


Figure 14 Some types of clusters: (a) Ball-shaped. (b) Elongated. (c) Compact but not well separated.

happens at just one point, the clusters immediately stick together (and remember, they cannot be separated in later steps). This is called the *chaining effect* because many objects may be chained together resulting in a drawn-out cluster, some members of which are very far from each other. On the other hand, this property can be turned to advantage in applications where one really *wants* to find such elongated clusters, as in Figure 14b.

The furthest neighbor rule possesses the opposite property: It tends to produce very compact clusters, which means that they have a small diameter. In other words, every member of such a cluster must be close to every other member of the same cluster and outlying points will not be incorporated. The resulting clusters are not necessarily well separated, because clusters will not be joined when they contain at least one pair of too distant points. (That is, they will only be merged in a much later stage of the amalgamation.) Therefore, furthest neighbor clustering is suitable for configurations like Figure 14c.

Divisive Analysis (Chapter 6)

The program DIANA analyzes the same data as AGNES and its interactive input is identical. To the user, the programs AGNES and DIANA appear to be twins because they can be run in the same way and they yield very similar output, except of course that they construct their hierarchies in the opposite direction.

The divisive approach offers a distinct advantage in that most users are interested in the main structure of their data, consisting of a few large clusters, rather than in a detailed description of the individual points. Agglomerative nesting starts with the details and then works its way up to large clusters, which may however be affected by unfortunate decisions in the first steps. On the other hand, divisive analysis starts with the main chunks. In the first step it splits the data into two parts and then goes on by dividing them further into smaller parts. Because the large clusters are determined first, they are less likely to suffer from earlier steps. (Moreover, one might even halt the algorithm at a stage where one is no longer interested in further splitting.)

On the other hand, divisive analysis poses some computational problems, at least in principle. Indeed, if the first step of the algorithm involved consideration of *all* possible divisions of the data into two subsets, it would be infeasible due to the large number of combinations. Because of this, the authors of most books and software packages have restricted their attention to the agglomerative hierarchical techniques. Therefore, divisive clustering algorithms are not generally available and rarely have been applied. However, there does exist a divisive method due to MacNaughton-Smith et al. (1964) that provides good results within very reasonable amounts of computation time. By implementing this technique in DIANA, we hope to make divisive clustering more accessible.

DIANA is suitable for approximately ball-shaped clusters, as is the group average method implemented in AGNES. Therefore, it is often useful to compare the output of AGNES with that of DIANA applied to the same data. Such comparison has been made easy because the results of both algorithms are displayed in a similar way (in a so-called *banner*).

Monothetic Analysis (Chapter 7)

The program MONA differs from the other algorithms in that it is intended for data consisting exclusively of binary variables. Each of these variables has only two states: 1 if a certain attribute is present and 0 if it is absent. (If variables of other types also occur, one should apply the program DAISY to compute dissimilarities as described in Section 5 and then run either PAM, FANNY, AGNES, or DIANA.)

The MONA algorithm is divisive and takes full advantage of the binary aspect. Indeed, at each step one of the variables is used to split the data, by separating the objects for which that variable takes on the value 1 from the objects for which it is 0. In order to decide which variable to use, one first computes a measure of the association between variables (for this reason, the algorithm is often called "association analysis") and then selects the variable that is most representative in the sense that it is most strongly associated with the other variables.

In Table 9 above, we have eight people on which 10 binary attributes are available. In the first step of the algorithm, the variable "married" is found to be the most representative, and hence the data are split up into the clusters {Ilan, Kim, Talia, Tina} and {Jacqueline, Leon, Lieve, Peter} because the people in the second group are married whereas those in the first are not. In the next step, each cluster is divided in the same way by means of one of the remaining variables. This illustrates a nice feature of the method: Not only do we obtain clusters, but we also know which variables were responsible for them.

Note that the clustering steps are based on one variable at a time. Therefore, this algorithm is said to be *monothetic*, whereas the other methods in this book use all variables simultaneously and hence are called *polythetic*. For instance, we can cluster the same data in a polythetic way, by first applying DAISY and then using the resulting dissimilarities as input for DIANA, yielding another divisive hierarchy. (Note that in DAISY we may even make a distinction between symmetric and asymmetric binary variables, whereas MONA does not distinguish between them.) Polythetic methods try to identify a multivariate structure in the p-dimensional space spanned by all variables, which may not show up in a monothetic analysis because it only treats the projections on the coordinate axes in a one-dimensional way. A monothetic analysis is therefore quite primitive, but on the other hand its simplicity also offers some advantages: The results are easily interpreted (because we know which variables caused the splits) and the algorithm is fast and able to deal with large data sets.

4 A SCHEMATIC OVERVIEW OF OUR PROGRAMS

To summarize what has been said in the previous sections, we look at a kind of flowchart. Figure 15 presents a schematic overview of the programs and the relations between them.

The second column lists the types of data discussed in Section 2. If you want to cluster objects that are characterized by some interval-scaled variables, you may apply PAM, FANNY, AGNES, and DIANA directly

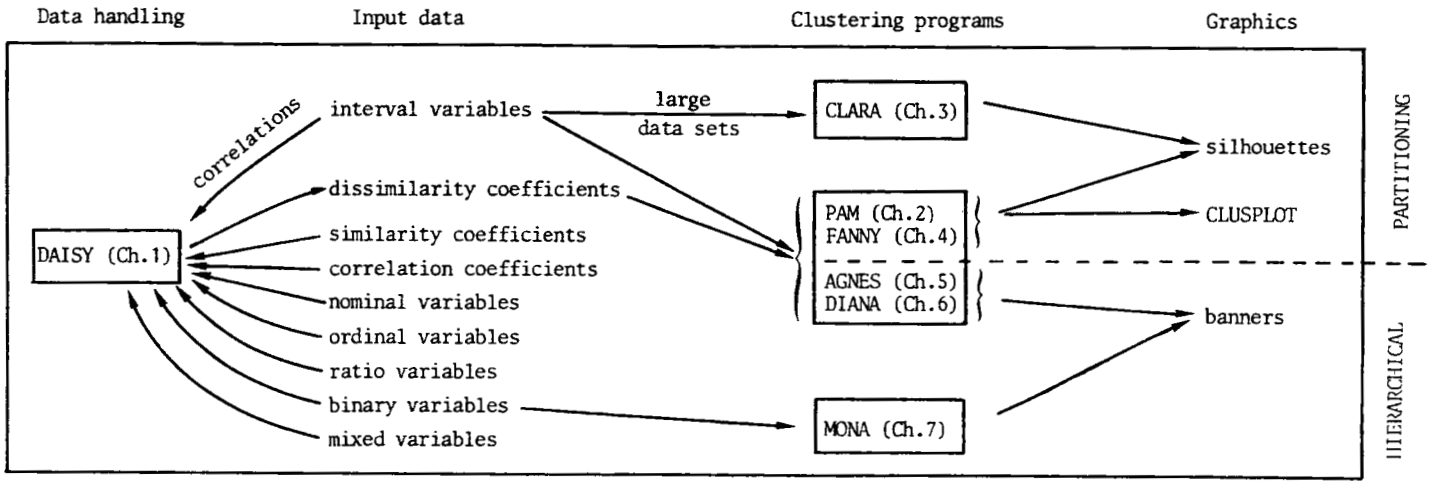


Figure 15 Function of the programs described in this book.

(or CLARA if your data set is very large). Moreover, you can also run PAM, FANNY, AGNES, and DIANA if you have a collection of pairwise dissimilarity coefficients between the objects. Should you have any of the other data types (that is, similarity coefficients, or correlations between variables, or objects characterized by attributes that are nominal, ordinal, ratio, binary, or even mixed) then DAISY will convert them to dissimilarities too. The purpose of this transformation is to enable you to apply the same four clustering programs.

When your data consists of interval-scaled measurements (the top entry in the second column), then you have the choice between two possibilities: If you want to cluster the *objects*, then you may directly apply one of the clustering algorithms (following the arrows to the right), but you may also cluster the *variables* by first computing correlation coefficients by means of DAISY (taking the arrow to the left) in order to convert them to dissimilarities, after which a clustering program can be run.

There is also a choice when you have objects with a collection of binary attributes. You may process them with DAISY (as indicated by the arrow to the left), but they may also be clustered directly by means of MONA, as described in Chapter 7. (Note that also variables of other types may be treated as binary attributes if one is willing to sacrifice a certain amount of information by grouping measurements.)

In the right half of Figure 15, the separation between hierarchical and partitioning methods is indicated. The programs AGNES, DIANA, and MONA are hierarchical and their results are displayed by means of banners. The programs CLARA, PAM, and FANNY are of the partitioning type and they use silhouettes for their graphical output. It is also possible to visualize a partition by constructing a faithful two-dimensional representation of the entities to be clustered (making use of multidimensional scaling) on which the clusters are portrayed as circles or ellipses. For this purpose, one may use the program CLUSPLOT described in Section 4 of the Appendix.

5 COMPUTING DISSIMILARITIES WITH THE PROGRAM DAISY

As already mentioned in the previous sections, it is useful to have a data handling program to prepare for the actual cluster analysis. This program has been called DAISY because its main function is to compute DISsimilAritY coefficients. Like the other programs used in this book, it is written in Fortran for the IBM PC (including XT and AT) and compatible microcomputers.

The program is entirely interactive. One only has to insert the floppy disk (which contains the file DAISY.EXE) in drive *A* and type

A:DAISY

(of course, the program may also be put in drive *B* or on a hard disk *C*). The user must then press the enter key (= carriage return), after which the computer loads the program and starts its execution. Next, questions appear on the screen, the answers to which have to be keyed in. This interactive dialogue is quite self-explanatory, so a manual is not really needed. Whenever the user types an "impossible" answer (like choosing option 5 when only four are available), DAISY will explain why this is unacceptable and simply ask the question again. (Some details on these messages can be found in the Appendix, because they are common to most of our programs.)

The data set itself can also be keyed in by the user or it may be read from a file that is already on a floppy or on a hard disk. If the data are entered with the keyboard, there is an option for storing them in a file, so that they may be reused in later runs. The output can be sent to the screen or to the printer or written in a file that is put on a floppy or on the hard disk.

DAISY starts by listing its four main options, as can be seen in the upper part of Figure 16. The first option is to compute dissimilarities between objects, according to formulas (24) to (27) in Section 2.6. The objects may be characterized by attributes that can be symmetric binary, asymmetric binary, nominal, ordinal, interval, ratio, or any combination of these. The flower data in Table 12 provide an example of such "mixed" measurements, because there are three binary, one nominal, two ordinal, and two interval variables. Figure 16 shows an entire interactive session, illustrating how DAISY may be applied to this example. For clarity, the answers typed by the user are underlined.

Note that DAISY allows to choose variables, so that one does not have to use all of them. This is often useful, because many applications include irrelevant variables or some variables may be related to others (in which case they may not provide any additional information). Sometimes the user has enough subject-matter knowledge to decide which variable to use or may only be interested in one particular aspect (say, the data contain both economic and demographic variables, but one wishes to obtain a clustering based on the economic quantities only). Therefore, choosing variables is possible in all our programs. To illustrate this facility, we only use six out of eight variables in Figure 16. That is, the whole data set is keyed in, but the

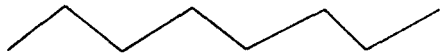
```
**********************************
*                                *
*   COMPUTING DISSIMILARITIES    *
*                                *
**********************************

This program has four options :
  1. Your data consists of a rectangular matrix of objects
     by variables, in which the variables may be of different
     types. You wish to cluster the objects.              (Please type 1)
  2. Your data consists of a rectangular matrix of
     objects by variables, but all variables are interval or ratio.
     You wish to calculate the Pearson correlation coefficients
     for clustering the variables.                        (Please type 2)
  3. Maybe you already have correlation
     coefficients between variables (either parametric
     or nonparametric). Your input data consist of a lower
     triangular matrix of pairwise correlations. You wish
     to calculate dissimilarities between the variables. (Please type 3)
  4. Your data consists of a lower triangular matrix of
     similarities between objects (with values between 0 and 1),
     which you would like to convert to dissimilarities. (Please type 4)
Please enter your choice : 1


THE PRESENT VERSION OF THE PROGRAM CAN HANDLE UP TO   100 OBJECTS.
(IF MORE ARE TO BE CONSIDERED, THE ARRAYS INSIDE THE PROGRAM MUST BE ADAPTED)

HOW MANY OBJECTS DOES YOUR DATA SET CONTAIN ?
---------------------------------------------
PLEASE GIVE A NUMBER BETWEEN 3 AND    100 : 18

THE PRESENT VERSION OF THE PROGRAM ALLOWS TO ENTER UP TO   80 VARIABLES,
OF WHICH AT MOST   50 CAN BE USED IN THE ACTUAL COMPUTATIONS.
(IF MORE ARE NEEDED, THE ARRAYS INSIDE THE PROGRAM MUST BE ADAPTED)

WHAT IS THE TOTAL NUMBER OF VARIABLES IN YOUR DATA SET ?
-------------------------------------------------------
PLEASE GIVE A NUMBER BETWEEN 1 AND     80 : 8

HOW MANY VARIABLES DO YOU WANT TO USE IN THE ANALYSIS ?
------------------------------------------------------
 (AT MOST    8 ) : 6

This option can handle variables of the following types  :
     SYMMETRIC BINARY (please type S)
     ASYMMETRIC BINARY (please type A)
     NOMINAL (please type N)
     ORDINAL (please type O)
     INTERVAL (please type I)
     RATIO to be treated as ORDINAL (please type O)
     RATIO to be treated as INTERVAL (please type I)
     RATIO to be logarithmically transformed (please type T)
         CAREFUL  :  A VARIABLE FOR WHICH A LOGARITHMIC
                     TRANSFORMATION IS REQUESTED MAY ONLY
                     CONTAIN POSITIVE NON-ZERO VALUES


VARIABLES TO BE USED     :   POSITION   LABEL (AT MOST 10 CHARACTERS)  TYPE
-------------------------:------------:-------------------------------:----
NUMBER      1            :   2          shadow                         S
NUMBER      2            :   3          tuberous                       A
NUMBER      3            :   4          color                          N
NUMBER      4            :   5          soil                           O
NUMBER      5            :   6          preference                     O
NUMBER      6            :   7          height                         I
```

Figure 16 Interactive session of DAISY with the data of Table 12.

```
PLEASE ENTER A TITLE FOR THE OUTPUT (AT MOST 60 CHARACTERS)
------------------------------------------------------------
Characteristics of garden flowers

DO YOU WANT TO READ THE DATA IN FREE FORMAT ?
---------------------------------------------
THIS MEANS THAT YOU ONLY HAVE TO INSERT BLANK(S) BETWEEN NUMBERS.
(NOTE: WE ADVISE USERS WITHOUT KNOWLEDGE OF FORTRAN FORMATS TO ANSWER YES.)
MAKE YOUR CHOICE (YES/NO) : yes

PLEASE GIVE THE NAME OF THE FILE CONTAINING THE DATA (e.g.TYPE A:EXAMPLE.DAT)
OR TYPE  KEY  IF YOU PREFER TO ENTER THE DATA BY KEYBOARD.
WHAT DO YOU CHOOSE ? key

DO YOU WANT TO SAVE YOUR DATA ON A FILE ?
PLEASE ANSWER YES OR NO : yes

ON WHICH FILE DO YOU WANT TO SAVE YOUR DATA ?
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME NAME
           THEN THE OLD FILE WILL BE OVERWRITTEN.)
TYPE e.g.  B:SAVE.DAT ..................... : a:flower.dat

OUTPUT SECTION
**************
A.  On which file do you want to output the dissimilarity matrix ?
    ----------------------------------------------------------
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME NAME
           THEN THE OLD FILE WILL BE OVERWRITTEN.)
TYPE e.g.  B:EXAMPLE.DIS .................. : a:flower.dis

B.  Where do you want the rest of the output ?
    ------------------------------------
   TYPE  CON  IF YOU WANT IT ON THE SCREEN
OR TYPE  PRN  IF YOU WANT IT ON THE PRINTER
OR TYPE THE NAME OF A FILE (e.g. B:EXAMPLE.OUT)
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME NAME
           THEN THE OLD FILE WILL BE OVERWRITTEN.)
WHAT DO YOU CHOOSE ? ..................... : a:flower.out

For the binary variables only the values 0 and 1 are allowed ;
all other values will be treated as missing measurements.
CAN MISSING DATA OCCUR FOR THE OTHER VARIABLES ?
PLEASE ANSWER YES OR NO : yes

IS THERE A UNIQUE VALUE WHICH IS TO BE INTERPRETED
AS A MISSING MEASUREMENT VALUE FOR ANY VARIABLE ?
PLEASE ANSWER YES OR NO : yes

PLEASE ENTER THIS VALUE NOW : 999.999


DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 TITLE  : Characteristics of garden flowers
 THERE ARE   18 OBJECTS
 INPUT OF A MATRIX OF MEASUREMENTS FOR THE CALCULATION
   OF DISSIMILARITIES BETWEEN OBJECTS

 THERE ARE    8 VARIABLES IN THE DATA SET,
  AND    6 OF THEM WILL BE USED IN THE ANALYSIS
 MISSING VALUES CAN OCCUR
 THE UNIQUE VALUE WHICH REPRESENTS MISSING MEASUREMENTS IS :
            999.9990000
 THE MEASUREMENTS WILL BE READ IN FREE FORMAT
 THE DATA WILL BE READ FROM THE KEYBOARD
 THE DATA WILL BE SAVED ON FILE : a:flower.dat
 THE DISSIMILARITIES WILL BE WRITTEN ON : a:flower.dis
 THE OTHER OUTPUT WILL BE WRITTEN ON : a:flower.out

 ARE ALL THESE PARAMETERS OK ?  YES OR NO : yes
```

Figure 16 (*Continued*)

```
PLEASE ENTER YOUR DATA FOR EACH OBJECT

 THE  8 MEASUREMENTS FOR OBJECT      1 :
0 1 1 4 3 15 25 15

 THE  8 MEASUREMENTS FOR OBJECT      2 :
1 0 0 2 1 3 150 50

 THE  8 MEASUREMENTS FOR OBJECT      3 :
0 1 0 3 3 1 150 50
```



```
 THE  8 MEASUREMENTS FOR OBJECT     17 :
1 0 0 2 2 17 150 60

 THE  8 MEASUREMENTS FOR OBJECT     18 :
0 0 1 2 1 5 25 10

 THE DATA WILL BE SAVED ON FILE :  a:flower.dat

This run has been successfully completed

The dissimilarity matrix is on file : a:flower.dis

The remaining output is on file : a:flower.out
```

Figure 16 (*Continued*)

distances are computed by means of formula (24) with only the six variables specified. However, note that all eight variables are being saved on the new file flower.dat to enable the user to run the analysis again with another combination of variables. (The user can then simply use flower.dat as input file for DAISY, without having to key in these numbers again.)

After stating that the program run has been successfully completed, DAISY also reminds us that we asked to put the dissimilarity matrix of the 18 objects on file flower.dis. To look at this dissimilarity matrix, we key in the command

TYPE A:FLOWER.DIS

and obtain Figure 17, which is of the same form as (10) in Section 2.1. The file flower.dis can be used as input for the programs PAM, FANNY, AGNES, and DIANA.

The other output file (named flower.out in this example) is given in Figure 18. It gathers the data specifications and chosen options, including a list of the variables used, with their position and type. When missing values have been announced, it provides the number of absent measurements for each variable. (In this example none actually occurred.) Sometimes there are so many missing values that certain computations can no longer be carried out, in which case the output file contains messages about this.

```
.900
.586  .624
.352  .567  .754
.549  .656  .456  .734
.219  .817  .441  .525  .451
.367  .640  .663  .358  .652  .223
.565  .336  .688  .278  .623  .679  .531
.608  .551  .374  .794  .329  .522  .723  .682
.496  .685  .508  .543  .230  .379  .578  .569
.501
.254  .813  .499  .569  .332  .377  .554  .477
.558  .360
.369  .698  .551  .434  .467  .483  .669  .362
.526  .392  .301
.510  .680  .503  .695  .247  .404  .605  .584
.329  .383  .459  .261
.173  .727  .580  .257  .477  .288  .473  .391
.536  .381  .312  .196  .438
.646  .505  .528  .471  .516  .535  .335  .418
.387  .514  .608  .556  .469  .547
.608  .532  .756  .256  .788  .537  .337  .534
.859  .558  .825  .690  .741  .513  .472
.719  .265  .688  .366  .721  .670  .469  .311
.792  .491  .769  .634  .674  .624  .405  .267
.598  .302  .822  .450  .617  .758  .592  .172
.510  .741  .548  .516  .598  .526  .480  .706
.483
```

Figure 17 Dissimilarity matrix produced by DAISY.

Therefore, the output file should always be looked at. Finally, an inventory is produced, in which for each nominal variable the number of (nonmissing) values is recorded. For each ordinal variable, the different values are ranked from smallest to largest, so the number of different values is also equal to the reported maximal rank.

Option 1, although primarily intended for mixed variables, can also be used if all variables are actually of the same type. For instance, one could process Table 9, which consists exclusively of symmetric binary variables, yielding the simple matching dissimilarity described in Section 2.4 (Exercise 20a). If we treat these data as nominal, we find the same result because symmetric binary attributes are also nominal variables with two states (Exercise 20b). If we were to consider the variables as asymmetric binary (1 = presence, 0 = absence), we would obtain the Jaccard dissimilarity (Exercise 20c). In the same vein we might apply DAISY to ordinal data sets, which are then processed as described in Section 2.5. We could also execute the program on the combination of Tables 7 and 9, because for each person we possess four interval-scaled measurements and 10 binary attributes (Exercise 21a).

DAISY's second option computes Pearson correlations between variables and then transforms these to dissimilarities according to formula (11) or (12) of Section 2.2. Figure 19 gives an example of the interactive input, starting from the line where option 2 is chosen (the earlier lines were, of course, as in Figure 16). In this example the correlations between the four variables of Table 7 are computed. It is assumed that these data already exist on a file named families.dat, which consists of eight lines, each

```
                    ********************************
                    *                              *
                    *   COMPUTING DISSIMILARITIES  *
                    *                              *
                    ********************************


 TITLE  : Characteristics of garden flowers


DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 THERE ARE   18 OBJECTS
 INPUT OF A MATRIX OF MEASUREMENTS FOR THE CALCULATION
   OF DISSIMILARITIES BETWEEN OBJECTS

 THERE ARE    8 VARIABLES IN THE DATA SET,
  AND    6 OF THEM WILL BE USED IN THE ANALYSIS
 THE LABELS OF THESE VARIABLES ARE :
         shadow       (POSITION :  2,  TYPE : S)
         tuberous     (POSITION :  3,  TYPE : A)
         color        (POSITION :  4,  TYPE : N)
         soil         (POSITION :  5,  TYPE : O)
         preference   (POSITION :  6,  TYPE : O)
         height       (POSITION :  7,  TYPE : I)
 MISSING VALUES CAN OCCUR
 THE UNIQUE VALUE WHICH REPRESENTS MISSING MEASUREMENTS IS :
           999.9990000
 THE MEASUREMENTS WILL BE READ IN FREE FORMAT

 THE DATA WILL BE SAVED ON FILE : a:flower.dat


 ANALYSIS OF MISSING DATA
 ------------------------
 VARIABLE shadow     HAS  NO MISSING VALUES
 VARIABLE tuberous   HAS  NO MISSING VALUES
 VARIABLE color      HAS  NO MISSING VALUES
 VARIABLE soil       HAS  NO MISSING VALUES
 VARIABLE preference HAS  NO MISSING VALUES
 VARIABLE height     HAS  NO MISSING VALUES


 THE TOTAL NUMBER OF MISSING VALUES IS      0

 SUMMARY OF THE VARIABLES
 ------------------------
 Variable shadow     is symmetric binary.
 Variable tuberous   is asymmetric binary.
 Variable color      is nominal. It takes   5 different values.
 Variable soil       is ordinal. Its maximal rank is     3.
 Variable preference is ordinal. Its maximal rank is    18.
 Variable height     is interval.

The dissimilarity matrix is on file : a:flower.dis

The remaining output is on file : a:flower.out
```

Figure 18 Output file produced by DAISY.

```
Please enter your choice : 2

The correlations can be converted to dissimilarities in two ways :

  1.  d = ( 1 - r ) / 2              (Please type 1)

     With this formula, variables with a high positive correlation receive
     a dissimilarity close to zero, whereas variables with a strongly negative
     correlation will be considered very dissimilar.
     In other applications one might prefer to use :

  2.  d = 1 - absolute value of r    (Please type 2)

     in which case also variables with a strongly negative correlation
     will be assigned a small dissimilarity.

Please enter your choice : 1

THE PRESENT VERSION OF THE PROGRAM CAN HANDLE UP TO   100 OBJECTS.
(IF MORE ARE TO BE CONSIDERED, THE ARRAYS INSIDE THE PROGRAM MUST BE ADAPTED)

HOW MANY OBJECTS DOES YOUR DATA SET CONTAIN ?
-------------------------------------------
PLEASE GIVE A NUMBER BETWEEN 3 AND    100 : 8

THE PRESENT VERSION OF THE PROGRAM ALLOWS TO ENTER UP TO   80 VARIABLES,
OF WHICH AT MOST   50 CAN BE USED IN THE ACTUAL COMPUTATIONS.
(IF MORE ARE NEEDED, THE ARRAYS INSIDE THE PROGRAM MUST BE ADAPTED)

WHAT IS THE TOTAL NUMBER OF VARIABLES IN YOUR DATA SET ?
-----------------------------------------------------
PLEASE GIVE A NUMBER BETWEEN 1 AND     80 : 4

HOW MANY VARIABLES DO YOU WANT TO USE IN THE ANALYSIS ?
-----------------------------------------------------
 (AT MOST    4 ) : 4

This option can handle variables of the following types   :
     INTERVAL (please type I)
     RATIO to be treated as INTERVAL (please type I)
     RATIO to be logarithmically transformed (please type T)
         CAREFUL  :  A VARIABLE FOR WHICH A LOGARITHMIC
                     TRANSFORMATION IS REQUESTED MAY ONLY
                     CONTAIN POSITIVE NON-ZERO VALUES

VARIABLES TO BE USED       LABEL (AT MOST 10 CHARACTERS)  TYPE
-------------------!!!!------!!!!!!!!!!-------------------!---
NUMBER     :         1      weight                         i
NUMBER     :         2      height                         i
NUMBER     :         3      month                          i
NUMBER     :         4      year                           i

PLEASE ENTER A TITLE FOR THE OUTPUT (AT MOST 60 CHARACTERS)
-----------------------------------------------------------
Eight_people_and_four_variables

DO YOU WANT TO READ THE DATA IN FREE FORMAT ?
--------------------------------------------
THIS MEANS THAT YOU ONLY HAVE TO INSERT BLANK(S) BETWEEN NUMBERS.
(NOTE: WE ADVISE USERS WITHOUT KNOWLEDGE OF FORTRAN FORMATS TO ANSWER YES.)
MAKE YOUR CHOICE (YES/NO) : yes

PLEASE GIVE THE NAME OF THE FILE CONTAINING THE DATA (e.g. TYPE A:EXAMPLE.DAT)
OR TYPE  KEY  IF YOU PREFER TO ENTER THE DATA BY KEYBOARD.
WHAT DO YOU CHOOSE ? a:families.dat
```

Figure 19 Interactive session for the computation of Pearson correlations and corresponding dissimilarities, for the variables of Table 7.

```
OUTPUT SECTION
**************
A.  On which file do you want to output the dissimilarity matrix ?
    ------------------------------------------------------------
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME NAME
           THEN THE OLD FILE WILL BE OVERWRITTEN.)
TYPE e.g.  B:EXAMPLE.DIS ..................... : a:families.dis

B.  Where do you want the rest of the output ?
    ----------------------------------------
   TYPE  CON  IF YOU WANT IT ON THE SCREEN
OR TYPE  PRN  IF YOU WANT IT ON THE PRINTER
OR TYPE THE NAME OF A FILE (e.g. B:EXAMPLE.OUT)
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME NAME
           THEN THE OLD FILE WILL BE OVERWRITTEN.)
WHAT DO YOU CHOOSE ? ..................... : CON

CAN MISSING DATA OCCUR IN THE MEASUREMENTS ?
PLEASE ANSWER YES OR NO : NO


DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 TITLE  : Eight people and four variables
 THERE ARE    8 OBJECTS
 INPUT OF A MATRIX OF INTERVAL OR RATIO MEASUREMENTS,
   FOR THE CALCULATION OF DISSIMILARITIES BETWEEN VARIABLES

 THE CORRELATIONS ARE CONVERTED TO DISSIMILARITIES BY THE FORMULA :
    d = ( 1 - r ) / 2

 THERE ARE    4 VARIABLES IN THE DATA SET,
  AND    4 OF THEM WILL BE USED IN THE ANALYSIS
 THERE ARE NO MISSING VALUES
 THE MEASUREMENTS WILL BE READ IN FREE FORMAT
 YOUR DATA RESIDE ON FILE        : a:families.dat

 THE DISSIMILARITIES WILL BE WRITTEN ON : a:families.dis
 THE OTHER OUTPUT WILL BE WRITTEN ON : CON

 ARE ALL THESE PARAMETERS OK ?  YES OR NO : yes

CORRELATION MATRIX
******************

      .957
     -.036      .021
     -.953     -.985      .013


 SUMMARY OF THE VARIABLES
 ------------------------
 Variable weight      is interval.
 Variable height      is interval.
 Variable month       is interval.
 Variable year        is interval.


This run has been successfully completed

The dissimilarity matrix is on file : a:families.dis
```

Figure 19 (*Continued*)

containing the four measurements of the corresponding person. This time the user decides to put the output on the screen, so it is just the bottom part of Figure 19.

The program prints the lower triangular half of the correlation matrix, corresponding to the values in Table 8(a) of Section 2.2. The final dissimilarity matrix (which is being stored on a file families.dis in this example) is identical to Table 8(b) because the user has chosen the transformation $d(f, g) = (1 - R(f, g))/2$. Based on this dissimilarity matrix, one can then perform a cluster analysis on the four variables.

Option 2 can also be used for another purpose. Indeed, suppose you have a data set consisting of interval-scaled measurements and you want to

```
Please enter your choice : 3

The correlations can be converted to dissimilarities in two ways :

  1.  d = ( 1 - r ) / 2              (Please type 1)

     With this formula, variables with a high positive correlation receive
     a dissimilarity close to zero, whereas variables with a strongly negative
     correlation will be considered very dissimilar.
     In other applications one might prefer to use :

  2.  d = 1 - absolute value of r    (Please type 2)

     in which case also variables with a strongly negative correlation
     will be assigned a small dissimilarity.

Please enter your choice : 2

THE PRESENT VERSION OF THE PROGRAM CAN HANDLE UP TO    50 VARIABLES.
(IF MORE ARE TO BE CONSIDERED, THE ARRAYS INSIDE THE PROGRAM MUST BE ADAPTED)

HOW MANY VARIABLES DOES YOUR DATA SET CONTAIN ?
-----------------------------------------------
PLEASE GIVE A NUMBER BETWEEN 3 AND     50 : 4

PLEASE ENTER A TITLE FOR THE OUTPUT (AT MOST 60 CHARACTERS)
-----------------------------------------------------------
Correlations_between_four_variables

DO YOU WANT TO READ THE DATA IN FREE FORMAT ?
--------------------------------------------
THIS MEANS THAT YOU ONLY HAVE TO INSERT BLANK(S) BETWEEN NUMBERS.
(NOTE: WE ADVISE USERS WITHOUT KNOWLEDGE OF FORTRAN FORMATS TO ANSWER YES.)
MAKE YOUR CHOICE (YES/NO) : yes

PLEASE GIVE THE NAME OF THE FILE CONTAINING THE DATA (e.g. TYPE A:EXAMPLE.DAT)
OR TYPE  KEY  IF YOU PREFER TO ENTER THE DATA BY KEYBOARD.
WHAT DO YOU CHOOSE ? key

DO YOU WANT TO SAVE YOUR DATA ON A FILE ?
PLEASE ANSWER YES OR NO : yes

ON WHICH FILE DO YOU WANT TO SAVE YOUR DATA ?
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME NAME
           THEN THE OLD FILE WILL BE OVERWRITTEN.)
TYPE e.g.  B:SAVE.DAT ..................... : a:variab.cor
```

Figure 20 Interactive session in which a correlation matrix is transformed into a dissimilarity matrix, as in Table 8(c).

cluster the *objects* by means of PAM, FANNY, AGNES, or DIANA, which allow you to specify a subset of variables for the actual computations. In such a situation it is quite useful to run DAISY's second option because it will give you the correlations between the variables, which may help you to decide which variables to delete: When two variables are strongly correlated, it makes sense to remove either of them.

```
OUTPUT SECTION
**************
A.  On which file do you want to output the dissimilarity matrix ?
    ------------------------------------------------------------
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME NAME
           THEN THE OLD FILE WILL BE OVERWRITTEN.)
TYPE e.g.  B:EXAMPLE.DIS ..................... : a:variab.dis

B.  Where do you want the rest of the output ?
    ------------------------------------------
   TYPE  CON  IF YOU WANT IT ON THE SCREEN
   TYPE  PRN  IF YOU WANT IT ON THE PRINTER
   TYPE THE NAME OF A FILE (e.g. B:EXAMPLE.OUT)
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME NAME
           THEN THE OLD FILE WILL BE OVERWRITTEN.)
WHAT DO YOU CHOOSE ? ..................... : a:variab.out


DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 TITLE  : Correlations between four variables
 THERE ARE    4 VARIABLES
 INPUT OF CORRELATION COEFFICIENTS BETWEEN VARIABLES

 THE CORRELATIONS ARE CONVERTED TO DISSIMILARITIES BY THE FORMULA :
    d = 1 - absolute value of r
 THE CORRELATIONS WILL BE READ IN FREE FORMAT
 THE DATA WILL BE READ FROM THE KEYBOARD
 THE DATA WILL BE SAVED ON FILE : a:variab.cor
 THE DISSIMILARITIES WILL BE WRITTEN ON : a:variab.dis
 THE OTHER OUTPUT WILL BE WRITTEN ON : a:variab.out

 ARE ALL THESE PARAMETERS OK ?  YES OR NO : yes

 FOR VARIABLE J, ENTER CORRELATIONS WITH VARIABLES 1,2,... ,(J-1)
  (CAREFUL : THE CORRELATIONS MUST BE BETWEEN -1 AND +1)

 CORRELATION BETWEEN VARIABLES     2 AND     1 :
0.957

 THE    2 CORRELATIONS WITH VARIABLE     3   :
-0.036 0.021

 THE    3 CORRELATIONS WITH VARIABLE     4   :
-0.953 -0.985 0.013

 THE DATA WILL BE SAVED ON FILE : a:variab.cor


This run has been successfully completed

The dissimilarity matrix is on file : a:variab.dis

The remaining output is on file : a:variab.out
```

Figure 20 *(Continued)*

The third option is based on the same formulas (11) and (12), but assumes that the user already has a full collection of correlation coefficients, possibly taken from the output of a standard statistical package. These correlations may be either parametric (Pearson's product-moment correlation) or nonparametric (Spearman's rank correlation). DAISY verifies whether these quantities lie between -1 and 1 and then converts them into dissimilarities, by means of which the variables may be clustered. Figure 20 shows a typical run, where the user enters the correlations between the four variables of Table 7 (which already appeared in Figure 19). The resulting dissimilarity matrix is identical to Table 8(c), because now formula (12) has been chosen.

Option 4 operates in an analogous way, except that now a (lower triangular) matrix of *similarities* between objects is converted into a matrix of dissimilarities. One may again choose between two formulas, namely $d(i, j) = 1 - s(i, j)$ as in (15), and $d(i, j) = (1 - s(i, j))^{1/2}$ as proposed by Gower (1966). During input, DAISY checks whether all entered similarities really lie between 0 and 1. The whole interactive session looks like that of option 3 in Figure 20.

EXERCISES AND PROBLEMS

Sections 1 and 2

1. Plot the data of Table 1 again with weight expressed in pounds (1 lb = 0.4536 kg) and height expressed in feet (1 ft = 30.48 cm). Compare the result with Figures 1 and 2.

2. For a data set with 10 objects and an interval-scaled variable f we have the following measurements x_{if}:

$$1, 2, 3, 4, 5, 6, 7, 8, 9, 55$$

containing one outlying value.

   (a) Compute the standard deviation std_f and the mean deviation s_f of this variable. Which is more affected by the outlier?

   (b) Compute the corresponding z-scores (4) with s_f and std_f, respectively. In which case does the outlier stick out most?

3. Suppose that we have a fixed set of $n - 1$ measurement values of variable f and an nth measurement that is an outlier equal to x. Prove

that

$$\lim_{x \to \infty} \frac{\text{std}_f}{s_f} = \frac{\sqrt{n}}{2} \frac{n}{n-1} \approx \frac{\sqrt{n}}{2}$$

showing that std_f is more affected by the outlier than s_f.

4. Show that the z-scores (4) always have mean zero and mean deviation equal to 1.

5. Standardize the variables of Table 4 and compare the result with Table 5.

6. Compute the Euclidean and Manhattan distances between the objects A, B, C, and D in Table 3.

7. Show that the Euclidean and Manhattan distances do not always result in the same ordering of the distances between pairs of objects. That is, there can be objects A, B, C, and D such that $d(A, B) < d(C, D)$ for the Euclidean distance whereas $d(A, B) > d(C, D)$ for the Manhattan distance.

8. Supposing that we have n objects, how many numbers are contained in a matrix of the type (9)? In (10)?

9. Construct a subjective dissimilarity matrix as in Table 6, but for another set of objects such as wines, colors, pets, ... Keep these data for clustering, using one of the methods described in Chapters 2, 4, 5, or 6.

10. Draw the graphs of the functions given by Eqs. (11) and (12) as well as of the function

$$d(f, g) = 1 - R(f, g)^2$$

Observe that for this last function a small change of $R(f, g)$ in the region near $R(f, g) = 0$ results in a much smaller change in $d(f, g)$ than for the function of (12).

11. Formula (17) writes the Rogers–Tanimoto dissimilarity r as a function of the simple matching coefficient m. Check that the function f given

by $r = f(m)$ is monotone and plot its graph. Do the same for $s = g(m)$ where s is the invariant dissimilarity of Sokal and Sneath [formula (18)]. Is there also a monotone relation between r and s?

12. Write the noninvariant dissimilarity coefficients of Dice and of Sokal and Sneath (both listed in Table 11) as monotone functions of the Jaccard dissimilarity.

13. Is it possible to write the Jaccard dissimilarity as a monotone function of the simple matching dissimilarity?

14. Check that the dissimilarities in Tables 10 and 11 satisfy (D1), (D2), and (D3), and that the similarities satisfy (S1), (S2), and (S3).

15. Bock (1974) and Romesburg (1984) consider several coefficients that were not given in Tables 10 and 11:

$$s(i, j) = [(a + d) - (b + c)]/[a + b + c + d] \quad \text{(Hamman)}$$

$$s(i, j) = [ad - bc]/[ad + bc] \quad \text{(Yule)}$$

$$s(i, j) = [a + d]/[(b + c) + 2(a + d)]$$

$$s(i, j) = d/[b + c] \quad \text{(Kulczynski)}$$

$$s(i, j) = a/[a + b + c + d] \quad \text{(Russell–Rao)}$$

(a) Check which of these five coefficients are invariant.

(b) None of these coefficients are similarities in the sense of conditions (S1) to (S3). Which of these conditions are violated?

16. The logarithmic transformation used for ratio-scaled variables cannot be carried out when a measurement equals zero. Suggest a solution to this problem based on the precision of the measurements (suppose that all measurements are nonnegative).

17. Consider the binary data set of Table 9. Calculate the dissimilarities $d(\text{JAC}, \text{LIE})$ and $d(\text{ILA}, \text{PET})$ using the mixed variables approach, assuming that the first six variables are symmetric and the last four variables are asymmetric.

Section 3

18. Consider Figure 11, which shows the result of applying a hierarchical clustering algorithm to a set of five objects. From this figure construct partitionings of the data set into 1, 2, 3, 4, and 5 clusters.

Section 4

19. Which clustering algorithms of this book are applicable to the data sets in Tables 6, 7, 9, and 12?

Section 5

20. Apply the program DAISY to the data of Table 9, by

(a) treating the variables as symmetric binary,

(b) treating the variables as nominal,

(c) treating the variables as asymmetric binary.

Which dissimilarity coefficients do we obtain? Why are the results of (a) identical to those of (b)? Explain how you would use this fact when faced with a data set consisting of symmetric binary variables, with states not coded as 0 and 1.

21. **(a)** Combine the data from Tables 7 and 9 and construct a dissimilarity matrix using the program DAISY. Consider all binary variables to be symmetric.

(b) Repeat this exercise after combining the two variables month and year into the variable birth using the formula

$$\text{birth} = \text{year} + \text{month}/12$$

22. Table 14 contains data concerning 12 countries. The variables (registered in 1983) are gross national product in dollars per inhabitant (x), average calorie intake per day (y), and average life expectancy at birth (z).

(a) Use the program DAISY to calculate the correlation coefficients and dissimilarities between the variables.

(b) Use DAISY to construct a dissimilarity matrix between the twelve countries.

Table 14 Three Variables on 12 Countries

Country	x	y	z
Belgium	12,180	3,800	71.0
Brazil	2,050	2,498	59.3
China	290	Missing	62.6
Cuba	Missing	2,672	64.3
France	11,730	3,412	73.8
Egypt	Missing	2,716	52.7
India	240	1,996	45.6
Israel	4,500	3,145	73.2
USA	11,360	3,537	76.5
USSR	Missing	3,443	69.0
Yugoslavia	Missing	3,510	67.8
Zaire	220	Missing	43.5

(c) Combine this dissimilarity matrix with that of Table 5 in Chapter 2, as described at the end of Section 2.6.

(d) Making use of subsequent chapters, the latter matrix can be used as input for the programs PAM, FANNY, AGNES, and DIANA, to cluster the countries.

Finding Groups in Data: An Introduction to Cluster Analysis
Leonard Kaufman and Peter J. Rousseeuw

CHAPTER 2

Partitioning Around Medoids (Program PAM)

1 SHORT DESCRIPTION OF THE METHOD

When partitioning a set of objects into k clusters the main objective is to find clusters, the objects of which show a high degree of similarity, while objects belonging to different clusters are as dissimilar as possible. Of course, many methods exist that try to achieve this aim. The algorithm used in the program PAM is based on the search for k *representative objects* among the objects of the data set. As evoked by their name, these objects should represent various aspects of the structure of the data. In the cluster analysis literature such representative objects are often called *centrotypes*. In the PAM algorithm the representative objects are the so-called *medoids* of the clusters (Kaufman and Rousseeuw, 1987). After finding a set of k representative objects, the k clusters are constructed by assigning each object of the data set to the nearest representative object.

To illustrate the algorithm used in PAM (a detailed description is given in Section 4) let us consider the data set represented in Figure 1. This data set contains 10 objects ($n = 10$) each characterized by two variables ($p = 2$), called x and y. The x and y values are given in Table 1.

Suppose the data set must be divided into two subsets or clusters ($k = 2$). In the algorithm one first considers possible choices of two representative objects and then constructs the clusters around these representative objects. As an example, suppose objects 1 and 5 are the selected representative objects. In Table 2 the dissimilarities from each of the objects to the two selected objects are given, as well as the smallest of these two dissimilarities and the corresponding representative object. (In this example we have simply used Euclidean distances between the points on

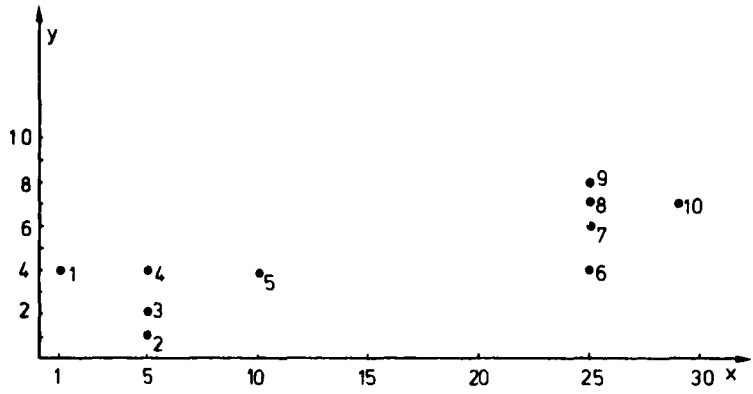


Figure 1 Two-dimensional example with 10 objects.

Table 1 Coordinates of the Objects of the Example of Figure 1

Number	x Coordinate	y Coordinate
1	1.0	4.0
2	5.0	1.0
3	5.0	2.0
4	5.0	4.0
5	10.0	4.0
6	25.0	4.0
7	25.0	6.0
8	25.0	7.0
9	25.0	8.0
10	29.0	7.0

the plot.) The average dissimilarity is 9.37. This value measures the tightness of the clusters and therefore the quality of the clustering.

In Table 3 the assignment is carried out for the case objects 4 and 8 are selected as representative objects. The clusterings associated with these two pairs of representative objects are shown in Figure 2.

The average dissimilarity for the case objects 4 and 8 are selected is 2.30, which is considerably less than the value of 9.37, found when 1 and 5 were the representative objects. In Section 4 an algorithm will be described, which for a given k makes it possible to select k representative objects which yield a very low average dissimilarity, and therefore a "good" partition. The clustering found with this algorithm is the same one as in

Table 2 Assignment of Objects to Two Representative Objects

Object Number	Dissimilarity from Object 1	Dissimilarity from Object 5	Minimal Dissimilarity	Closest Representative Object
1	0.00	9.00	0.00	1
2	5.00	5.83	5.00	1
3	4.47	5.39	4.47	1
4	4.00	5.00	4.00	1
5	9.00	0.00	0.00	5
6	24.00	15.00	15.00	5
7	24.08	15.13	15.13	5
8	24.19	15.30	15.30	5
9	24.33	15.52	15.52	5
10	28.16	19.24	19.24	5
			Average 9.37	

Table 3 Assignment of Objects to Two Other Representative Objects

Object Number	Dissimilarity from Object 4	Dissimilarity from Object 8	Minimal Dissimilarity	Closest Representative Object
1	4.00	24.19	4.00	4
2	3.00	20.88	3.00	4
3	2.00	20.62	2.00	4
4	0.00	20.22	0.00	4
5	5.00	15.30	5.00	4
6	20.00	3.00	3.00	8
7	20.10	1.00	1.00	8
8	20.22	0.00	0.00	8
9	20.40	1.00	1.00	8
10	24.19	4.00	4.00	8
			Average 2.30	

Table 3, but the two representative objects are 3 and 8 and in this way the average dissimilarity is 2.19.

There are basically two ways of entering the data in PAM. The most common way is by means of a matrix of measurement values. The rows of this matrix represent the objects and the columns correspond to variables, which must be on an interval scale. An example of such data is given in Table 1.

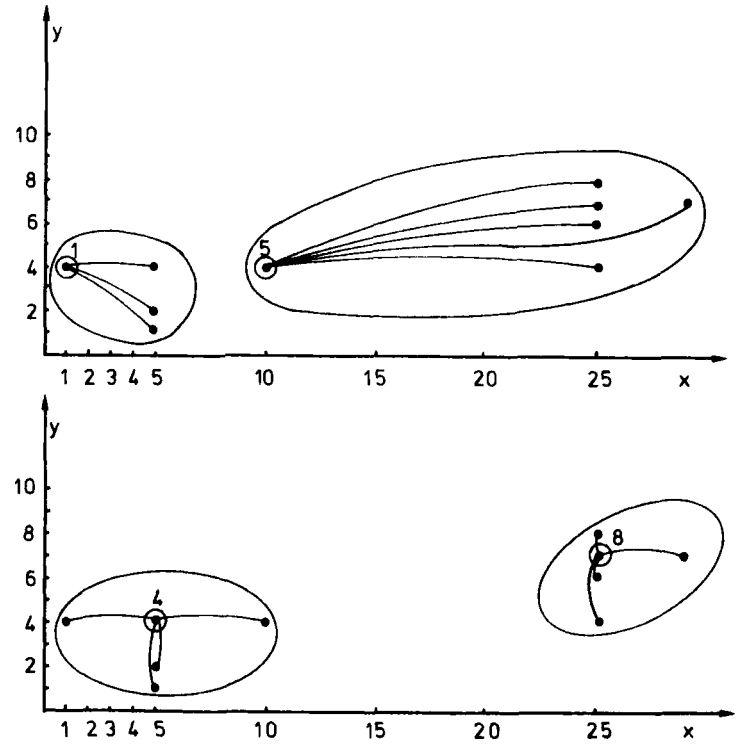


Figure 2 Clusterings corresponding to the selections described in Tables 2 and 3.

Alternatively the program can be used by entering a matrix of dissimilarities between objects. Such dissimilarities can be obtained in several ways. Often they are computed from variables that are not necessarily on an interval scale but which may also be binary, ordinal, or nominal. (This can be done by using the program DAISY of Chapter 1.) It also happens that dissimilarities are given directly, without resorting to any measurement values.

In many clustering problems one is particularly interested in a characterization of the clusters by means of typical or representative objects. These are objects that represent the various structural aspects of the set of objects being investigated. There can be many reasons for searching for representative objects. Not only can these objects provide a characterization of the clusters, but they can often be used for further work or research, especially when it is more economical or convenient to use a small set of k objects instead of the large set one started off with. In the method used in the

program PAM the representative object of a cluster is its medoid, which we define as that object of the cluster for which the average dissimilarity to all the objects of the cluster is minimal. (In fact, the name PAM comes from *P*artitioning *A*round *M*edoids.) As the objective is to find k such objects, we call this the *k-medoid method* (in the literature one also encounters the name k-median which to us seems less appropriate, as confusion can arise with the classical notion of median).

Another typical aspect of PAM is that it provides a large number of statistics by which a thorough investigation of the clustering results is made possible. Particularly worth mentioning are the medoids of the clusters (with their coordinates), the diameters and separations of the clusters, and also a graphical representation of the clusters by means of so-called silhouettes.

2 HOW TO USE THE PROGRAM PAM

The k-medoid method can be applied by using the program PAM. This program was written in Fortran and runs on an IBM PC, XT, AT, or compatible computer with at least 256K of internal storage. In Section 4 some details of the program are described and the Appendix discusses the implementation of the program.

The program PAM is operated entirely interactively. The data specifications and options must be entered by keyboard. The data set (consisting of the measurements or the dissimilarities) can be input by the keyboard or from a file located on a floppy or hard disk. If they are input from the keyboard, there is an option for saving them in a file. The output can be sent either to the screen, to the printer, or to a file which is then written on floppy or hard disk. In Section 2.1 we will describe how the program is operated. In Section 2.2 the output of the clustering results will be detailed. The case of missing measurement values, which is not of interest to all readers, is discussed in Section 2.3.

2.1 Interactive Use and Input

In order to run the program the first thing to do is to insert the diskette containing the file PAM.EXE. To load and run the program the user only has to type A:PAM in case the diskette is in drive A. The user must then press the key ENTER. (The carriage return or ENTER key, which instructs the computer to read the information, must follow each answer or input of

data. It will not be mentioned hereafter.) The program then generates the following screen:

```
PARTITIONING AROUND MEDOIDS

DO YOU WANT TO ENTER MEASUREMENTS ? (PLEASE ANSWER M)
OR DO YOU PREFER TO GIVE DISSIMILARITIES ?
(THEN ANSWER D) : m
```

Note that the user-supplied information (answers or data) is underlined.

The user now must select one of the two types of data to be used for the clustering algorithm. If he chooses measurements, the program will itself compute the dissimilarities before performing the clustering. This results in several additional options concerning the treatment of the measurements. We will suppose measurements were chosen in order to illustrate these options.

After the choice of input data type has been made, the following message appears:

```
THE PRESENT VERSION OF THE PROGRAM CAN HANDLE UP TO 100
OBJECTS.
(IF MORE ARE TO BE CLUSTERED, THE ARRAYS INSIDE THE PRO-
GRAM MUST BE ADAPTED)
HOW MANY OBJECTS ARE TO BE CLUSTERED ?
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
PLEASE GIVE A NUMBER BETWEEN 3 AND 100 : 10
```

The user then enters the number of cases in his data set. Note that there are limits on the size of the data set that can be handled. (These are due to the central memory limitation of the computer.) Also note that if an answer of less than 3 or more than 100 is given, the program reiterates the question. The next message concerns the number of clusters:

```
CLUSTERINGS WILL BE CARRIED OUT IN K1 TO K2 CLUSTERS.
PLEASE ENTER K1 : 2
PLEASE ENTER K2 : 2
```

If the values $K1$ and $K2$ are not satisfactory, special messages are given and they have to be entered again.

Subsequently, if input of measurements was chosen (see the first question), specific information related to the measurements must be entered. The questions and prompts are now discussed. (Note that these do not appear if input of dissimilarities was chosen.) The user first specifies the

total number of variables in his data set:

```
THE PRESENT VERSION OF THE PROGRAM ALLOWS TO ENTER UP TO
80 VARIABLES, OF WHICH AT MOST 20 CAN BE USED IN THE ACTUAL
COMPUTATIONS.
(IF MORE ARE NEEDED, THE ARRAYS INSIDE THE PROGRAM MUST BE
ADAPTED.)
WHAT IS THE TOTAL NUMBER OF VARIABLES IN YOUR DATA SET ?
-------------------------------------------------------
PLEASE GIVE A NUMBER BETWEEN 1 AND 80 : 5
```

As with the number of objects there are also limits on the number of variables. If a number is entered outside the range, a message appears and the question is restated.

In order to make it possible to cluster the same set of objects using different sets of variables, the program allows the choice of a subset of variables to be used for the clustering. The choice of variables must be made by the user:

```
HOW MANY VARIABLES DO YOU WANT TO USE IN THE ANALYSIS ?
-------------------------------------------------------
(AT MOST 5) : 2
```

Note that in the text this quantity is denoted by p. When the number of selected variables equals the total number of variables in the data set, a table is given in which each variable is to be identified by a label of at most 10 characters. On the other hand, when not all variables are uesd, the *position* of the selected variables must also be given. For our example, the following appears on screen:

```
VARIABLE TO BE USED:          POSITION    LABEL (AT MOST 10
                                          CHARACTERS)
------------------------------ ↓↓↓↓ ---↓↓↓↓↓↓↓↓↓↓---------
NUMBER 1 :                      2          x-coordina
NUMBER 2 :                      3          y-coordina
```

For each variable the position in the measurement matrix (column number) and its label must be entered on the same line. Note that after the position has been entered, blanks must be used to reach the area reserved for the label.

Also in this table checks on the input are carried out. For example, it is not allowed to enter the same variable twice. Finally, the user has the option of standardizing the measurements and a choice is given between two dissimilarity measures.

DO YOU WANT THE MEASUREMENTS TO BE STANDARDIZED (PLEASE ANSWER YES) OR NOT? (THEN ANSWER NO) . . . . . no

If this option is selected, the data are standardized as follows. First the mean (m_f) and the mean absolute deviation (s_f) of the fth variable are calculated:

$$m_f = \frac{1}{n}(x_{1f} + x_{2f} + \cdots + x_{nf})$$

$$s_f = \frac{1}{n}(|x_{1f} - m_f| + |x_{2f} - m_f| + \cdots + |x_{nf} - m_f|)$$

Then, each measurement x_{if} is replaced by the standardized value z_{if} defined as

$$z_{if} = \frac{x_{if} - m_f}{s_f} \tag{1}$$

which is often called a z-score. The advantages and disadvantages of such standardization were discussed in Section 2 of Chapter 1.

DO YOU WANT TO USE EUCLIDEAN DISTANCE ? (PLEASE ANSWER E) OR DO YOU PREFER MANHATTAN DISTANCE ? (THEN ANSWER M) . . e

Let us recollect that the Euclidean distance between two objects i and j is given by

$$d(i, j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \cdots + (x_{ip} - x_{jp})^2} \tag{2}$$

while their Manhattan distance corresponds to

$$d(i, j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \cdots + |x_{ip} - x_{jp}| \tag{3}$$

(For the interpretation of these formulas see Section 2 of Chapter 1.) If a standardization is carried out, the x_{if} are replaced by z_{if} in the last two

expressions. The answers to the following questions control the output of the program.

```
PLEASE ENTER A TITLE FOR THE OUTPUT (AT MOST 60 CHARACTERS)
-----------------------------------------------------------
Data of Table 1

DO YOU WANT LARGE OUTPUT ? (PLEASE ANSWER YES)
OR IS SMALL OUTPUT SUFFICIENT ? (THEN ANSWER NO)
(IN THE LATTER CASE NO DISSIMILARITIES ARE GIVEN) ..... yes

DO YOU WANT GRAPHICAL OUTPUT (SILHOUETTES) ? PLEASE AN-
SWER YES OR NO ..... yes

DO YOU WANT TO ENTER LABELS OF OBJECTS ? PLEASE ANSWER YES
OR NO ..... no
```

If labels of objects are to be entered this is made possible by the following screen:

```
EACH LABEL MAY CONSIST OF AT MOST 3 CHARACTERS
OBJECT          LABEL
--------------  ↓↓↓
NUMBER 1 :      AAA
NUMBER 2 :      BBB
NUMBER 3 :      CCC
NUMBER 4 :      DDD
NUMBER 5 :      EEE
```

If the labels are not provided by the user, they are constructed by the program as three-digit integers such as 001, 002, ... in which the leading zeroes are maintained. The following questions concern the input of the data.

```
DO YOU WANT TO READ THE DATA IN FREE FORMAT ?
THIS MEANS THAT YOU ONLY HAVE TO INSERT BLANK(S) BETWEEN
NUMBERS.
(NOTE : WE ADVISE USERS WITHOUT KNOWLEDGE OF FORTRAN
FORMATS TO ANSWER YES.)
MAKE YOUR CHOICE (YES / NO) : no

YOUR DESIRED FORTRAN FORMAT IS :
(BETWEEN BRACKETS AND AT MOST 60 CHARACTERS, e.g. (2F3.0,F1.0))
(5F5.1)
```

This format is chosen by the user to input the measurements or dissimilarities. It must be entered between brackets. (For the actual data only Fortran *F* formats and *E* formats are allowed because the dissimilarities are processed as real numbers. For ease of use *X* and */* are also allowed. Details about formats are described in the Appendix.)

Subsequently, information must be provided concerning the status of input and output. Several options make it possible to use the keyboard, screen, printer, and files on disk.

```
PLEASE GIVE THE NAME OF THE FILE CONTAINING THE DATA (e.g.
TYPE A:EXAMPLE.DAT)
OR TYPE KEY IF YOU PREFER TO ENTER THE DATA BY KEYBOARD.
WHAT DO YOU CHOOSE ? key
```

If the data are to be entered by keyboard, there is an option for saving them on a file.

```
DO YOU WANT TO SAVE YOUR DATA ON A FILE ?
PLEASE ANSWER YES OR NO: yes
ON WHICH FILE DO YOU WANT TO SAVE YOUR DATA ?
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME
           NAME THEN THE OLD FILE WILL BE OVERWRITTEN.)
TYPE e.g. B:SAVE.DAT ..... c:test.dat
```

The output can be directed toward the screen, a printer, or a file:

```
WHERE DO YOU WANT YOUR OUTPUT ?
-------------------------------
   TYPE CON IF YOU WANT IT ON THE SCREEN
OR TYPE PRN IF YOU WANT IT ON THE PRINTER
OR TYPE THE NAME OF A FILE (e.g. B:EXAMPLE.OUT)
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME
           NAME THEN THE OLD FILE WILL BE OVERWRITTEN.)
WHAT DO YOU CHOOSE ? ..... c:test.res
```

When measurements are to be entered, PAM makes provision for the occurrence of missing values in the data.

```
CAN MISSING DATA OCCUR IN THE MEASUREMENTS ?
PLEASE ANSWER YES OR NO : no
```

An affirmative answer to this question results in several prompts which, as they are not of interest to all users, will be discussed in Section 2.3.

Finally, the data specifications and chosen options are displayed:

```
DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------

TITLE : Data of Table 1
THERE ARE 10 OBJECTS
LABELS OF OBJECTS ARE NOT READ
INPUT OF MEASUREMENTS
LARGE OUTPUT IS WANTED
GRAPHICAL OUTPUT IS WANTED (SILHOUETTES)
CLUSTERINGS ARE CARRIED OUT IN 2 TO 2 CLUSTERS

THERE ARE 5 VARIABLES IN THE DATA SET,
   AND 2 OF THEM WILL BE USED IN THIS ANALYSIS
THE MEASUREMENTS WILL NOT BE STANDARDIZED
EUCLIDEAN DISTANCE WILL BE USED
THERE ARE NO MISSING VALUES
THE INPUT FORMAT FOR THE MEASUREMENTS IS
(5F5.1)
THE DATA WILL BE READ FROM THE KEYBOARD
THE DATA WILL BE SAVED ON FILE : C:TEST.DAT
YOUR OUTPUT WILL BE WRITTEN ON : C:TEST.RES

ARE ALL THESE SPECIFICATIONS OK ? YES OR NO : yes
```

If the user answers no to this question, the program returns to the first line (concerning the choice of measurements or dissimilarities). Otherwise it proceeds with the input of the actual data.

Let us first consider the situation of input of measurements. For the example of Table 1, if the data are entered in the preceding format, (5F5.1), the following screen will appear:

```
PLEASE ENTER YOUR DATA FOR EACH OBJECT

THE 5 MEASUREMENTS FOR OBJECT 001 :
  1.0  1.0  4.0  24.0  0.6
THE 5 MEASUREMENTS FOR OBJECT 002 :
  2.0  5.0  1.0  26.5  -0.3
THE 5 MEASUREMENTS FOR OBJECT 003 :
  3.0  5.0  2.0  27.0  0.4
THE 5 MEASUREMENTS FOR OBJECT 004 :
  4.0  5.0  4.0  23.5  0.2
THE 5 MEASUREMENTS FOR OBJECT 005 :
  5.0  10.0  4.0  24.5  -0.6
```

THE 5 MEASUREMENTS FOR OBJECT 006 :
6.0 25.0 4.0 25.5 0.1
THE 5 MEASUREMENTS FOR OBJECT 007 :
7.0 25.0 6.0 26.0 0.3
THE 5 MEASUREMENTS FOR OBJECT 008 :
8.0 25.0 7.0 23.5 −0.2
THE 5 MEASUREMENTS FOR OBJECT 009 :
9.0 25.0 8.0 22.0 0.0
THE 5 MEASUREMENTS FOR OBJECT 010 :
10.0 29.0 7.0 24.5 −0.3

Note that the first variable happens to be the number of the observation and that only the second and third variables are to be used in this particular analysis.

Let us now assume that the data consist of a set of dissimilarities. These are usually listed as in the matrix

$$\begin{array}{c} \\ a \\ b \\ c \\ d \\ e \end{array} \begin{array}{c} \begin{array}{ccccc} a & b & c & d & e \end{array} \\ \left[\begin{array}{ccccc} 0 & 2 & 6 & 10 & 9 \\ 2 & 0 & 5 & 9 & 8 \\ 6 & 5 & 0 & 4 & 5 \\ 10 & 9 & 4 & 0 & 3 \\ 9 & 8 & 5 & 3 & 0 \end{array}\right] \end{array} \tag{4}$$

For example, the dissimilarity between objects a and d equals 10. Observe that the matrix has nonnegative entries, zeroes on the diagonal, and is symmetric. Therefore, only the lower triangular part of the n-by-n matrix of dissimilarities is entered.

Be careful to delete the upper triangular part of the matrix, and also the diagonal, because otherwise wrong values might be read (especially if more than one line is used per object). We chose to read the lower triangular matrix instead of the upper one, because this makes it very easy to add objects to the data set by simply adding lines at the end of the data file.

When entering the dissimilarities by keyboard, the following screen appears:

FOR OBJECT J, ENTER THE DISSIMILARITIES TO OBJECTS
1,2,...,(J − 1)

DISSIMILARITY BETWEEN OBJECTS BBB AND AAA :
2.0
THE 2 DISSIMILARITIES FOR OBJECT CCC :
6.0 5.0

```
THE 3 DISSIMILARITIES FOR OBJECT DDD :
  10.0  9.0  4.0
THE 4 DISSIMILARITIES FOR OBJECT EEE :
  9.0  8.0  5.0  3.0
```

Conversely, the dissimilarities may also be read from a file which should then be organized as

```
 2.0
 6.0  5.0
10.0  9.0  4.0
 9.0  8.0  5.0  3.0
```

In some applications, similarities are given instead of dissimilarities. These cannot be used as input to the program but must first be converted to dissimilarities; this can, for example, be done by means of the program DAISY described in Chapter 1.

It is important to note that the input file requirements of PAM are completely identical to those of FANNY (Chapter 4), AGNES (Chapter 5), and DIANA (Chapter 6). This means that any input file constructed for either program will also run on the others. Also, the interactive dialogue is extremely similar for all four programs.

2.2 Output

In this section the output generated by PAM is described. Where necessary it is illustrated with the output of some test data. The output discussed in this section is obtained from a standard usage of the program, without missing values. (An example with missing values is given in Section 2.3. Outputs associated with special situations and error messages are discussed in the Appendix.)

The output of PAM is divided into five parts, two of which are not always obtained (parts c and e):

a. Identification of the Program and the Data Set

The phrase "PARTITIONING AROUND MEDOIDS" shows that the program PAM was used to obtain this output. The name of the data set is then printed as it was provided by the user.

b. Data Specifications and Chosen Options

Number of objects

Options concerning input and output:

- reading labels or not
- input of dissimilarities or measurements

- large or small output
- graphical output or not
- smallest and largest number of clusters

If measurement values are entered:

- number of variables in the data set
- which variables to be used in the analysis
- standardization or not
- the selected dissimilarity measure
- the absence or presence of missing values

The input format for measurements or dissimilarities.

Options for input and output (choice between keyboard and file for input and between screen, printer, and file for output).

c. Dissimilarities and Standardized Measurements

In case of dissimilarity input and if large output was asked for, the dissimilarities between objects are given before the clustering results.

In case of input of measurement values which are to be standardized, the average and mean absolute deviation of each variable are printed. In case of large output this is followed by the transformed measurements and the dissimilarities. If the measurements are not standardized and large output was requested, only the dissimilarities are listed.

In Figure 3, parts *a*, *b*, and *c* of the output are given for the data of Table 1.

d. Numerical Output Concerning Each Clustering

The number of clusters (number of representative objects).

The average dissimilarity for the solution found in the first part of the algorithm (called BUILD).

The average dissimilarity for the solution found in the second part of the algorithm (called SWAP).

(These two values are defined as the average dissimilarity between each object and its most similar representative object; details are discussed in Section 4.1.)

For each cluster the following information is printed:

- its medoid (with the label)
- its number of objects (size)

```
**********************************
*                                *
*  PARTITIONING AROUND MEDOIDS   *
*                                *
**********************************

TITLE  : Data of Table 1
DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 THERE ARE   10 OBJECTS
 LABELS OF OBJECTS ARE NOT READ
 INPUT OF MEASUREMENTS
 LARGE OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (SILHOUETTES)
 CLUSTERINGS ARE CARRIED OUT IN    2 TO    2 CLUSTERS

 THERE ARE    5 VARIABLES IN THE DATA SET,
  AND    2 OF THEM WILL BE USED IN THE ANALYSIS
 THE LABELS OF THESE VARIABLES ARE :
        x-coordina   (POSITION :  2)
        y-coordina   (POSITION :  3)
 THE MEASUREMENTS WILL NOT BE STANDARDIZED
 EUCLIDEAN DISTANCE WILL BE USED
 THERE ARE NO MISSING VALUES
 THE INPUT FORMAT FOR THE MEASUREMENTS IS
 (5F5.1)

 THE DATA WILL BE SAVED ON FILE : C:TEST.DAT

DISSIMILARITY MATRIX
--------------------

001
002      5.00
003      4.47     1.00
004      4.00     3.00     2.00
005      9.00     5.83     5.39     5.00
006     24.00    20.22    20.10    20.00    15.00
007     24.08    20.62    20.40    20.10    15.13     2.00
008     24.19    20.88    20.62    20.22    15.30     3.00     1.00
009     24.33    21.19    20.88    20.40    15.52     4.00     2.00     1.00
010     28.16    24.74    24.52    24.19    19.24     5.00     4.12     4.00
         4.12
```

Figure 3 PAM output, parts *a*, *b*, and *c*.

- the labels of its members (if no labels were read in the input, numbers are generated by the program)
- the coordinates of the medoid: This only occurs when there are measurements (when standardization is requested, only standardized coordinates are given)

The clustering vector: The jth element of this vector is the number of the cluster to which object j belongs (the clusters are numbered in such a way that when reading the clustering vector from left to right, cluster 1 is encountered before cluster 2, cluster 2 before cluster 3, and so on; therefore cluster 1 is defined as the cluster containing the first object).

The clustering characteristics:

- whether a cluster is a singleton
- whether a cluster is isolated: Two types of isolated clusters are considered in the program, L-clusters and L^*-clusters. They have

the following definitions (see Gordon, 1981):
C is an L-cluster if for each object i belonging to C:

$$\max_{j \in C} d(i, j) < \min_{h \notin C} d(i, h)$$

C is an L^*-cluster if:

$$\max_{i, j \in C} d(i, j) < \min_{l \in C, h \notin C} d(l, h) \tag{5}$$

It is clear that L^*-clusters are also L-clusters. It should be observed that the property of being isolated depends both on the internal structure of a cluster and its position relative to other clusters. When dividing the data into two clusters, it can happen that one is isolated and the other is not.

- the diameter and separation of each cluster: the left-hand side of Eq. (5) is called the diameter of cluster C and the right-hand side its separation.
- in each cluster, the average dissimilarity of the objects to the medoid and the maximum dissimilarity of any object to the medoid.

As an illustration, the numerical output of the example of Section 1 concerning the clustering into two clusters ($k = 2$) is given in Figure 4.

e. Graphical Output Concerning Each Clustering

If this was requested in the interactive part of the program, a graphical representation of each clustering is provided (except for the boundary cases $k = 1$ and $k = n$) displaying the silhouettes introduced by Rousseeuw (1987). Each cluster is represented by one silhouette, showing which objects lie well within the cluster and which objects merely hold an intermediate position. The entire clustering is displayed by plotting all silhouettes into a single diagram, allowing the user to compare the quality of the clusters. Such silhouettes are especially useful when the dissimilarities are on a ratio scale (as in the case of Euclidean distances) and when one is seeking compact and widely separated clusters.

Silhouettes are constructed in the following way: For each object i the value $s(i)$ is defined and then these numbers are combined into a plot. Take any object i of the data set. In order to define $s(i)$, first denote by A the cluster to which it has been assigned and then calculate

$$a(i) = \text{average dissimilarity of } i \text{ to all other objects of } A$$

```
*******************************************
*                                         *
*  NUMBER OF REPRESENTATIVE OBJECTS     2 *
*                                         *
*******************************************

RESULT OF BUILD
  AVERAGE DISSIMILARITY =         3.422

FINAL RESULTS
  AVERAGE DISSIMILARITY =         2.186

  CLUSTERS
  NUMBER   MEDOID    SIZE      OBJECTS
    1        003       5      001 002 003 004 005
    2        008       5      006 007 008 009 010

COORDINATES OF MEDOIDS
**********************

003        5.00      2.00
008       25.00      7.00

CLUSTERING VECTOR
*****************

             1  1  1  1  1  2  2  2  2  2

CLUSTERING CHARACTERISTICS
**************************

 CLUSTER     1 IS ISOLATED,
        WITH DIAMETER =       9.00 AND SEPARATION =       15.00
        THEREFORE IT IS AN L*-CLUSTER.

 CLUSTER     2 IS ISOLATED,
        WITH DIAMETER =       5.00 AND SEPARATION =       15.00
        THEREFORE IT IS AN L*-CLUSTER.

 THE NUMBER OF ISOLATED CLUSTERS =     2

 DIAMETER OF EACH CLUSTER
      9.00      5.00

 SEPARATION OF EACH CLUSTER
     15.00     15.00

 AVERAGE DISSIMILARITY TO EACH MEDOID
      2.57      1.80

 MAXIMUM DISSIMILARITY TO EACH MEDOID
      5.39      4.00
```

Figure 4 Numerical output for the clustering into two clusters of the example of Table 1.

This can only be done when A contains other objects apart from i, so at this point we assume that A is not a singleton.

Now consider any cluster C different from A and define

$$d(i, C) = \text{average dissimilarity of } i \text{ to all objects of } C$$

After computing $d(i, C)$ for all clusters $C \neq A$, we select the smallest of those:

$$b(i) = \min_{C \neq A} d(i, C)$$

The cluster B for which this minimum is attained [that is, $d(i, B) = b(i)$] is called the *neighbor* of object i. This is like the second-best choice for object

i: If cluster A is discarded, cluster B is closest to i. Therefore, it is very useful to know the neighbor of each object in the data set. Note that the construction of $b(i)$ depends on the availability of clusters differing from A, which explains why silhouettes are not defined for $k = 1$.

The number $s(i)$ is obtained by combining $a(i)$ and $b(i)$ as follows:

$$\begin{aligned} s(i) &= 1 - \frac{a(i)}{b(i)} && \text{if } a(i) < b(i) \\ &= 0 && \text{if } a(i) = b(i) \\ &= \frac{b(i)}{a(i)} - 1 && \text{if } a(i) > b(i) \end{aligned} \tag{6}$$

It is possible to write this in one formula:

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$

When cluster A contains only a single object, it is unclear how $a(i)$ should be defined and then we simply set $s(i) = 0$. This choice is of course arbitrary, but a value of zero appears to be most neutral. Indeed, from the preceding definition we easily see that

$$-1 \leq s(i) \leq 1$$

for each object i.

Note that $s(i)$ remains invariant when all the original dissimilarities are multiplied by a positive constant, but that an additive constant is not allowed. This explains why we explicitly assume that the dissimilarities are on a ratio scale, which means that a dissimilarity of 6 may be considered twice as large as a dissimilarity of 3. For instance, Euclidean distances are on a ratio scale.

To strengthen our intuition about the meaning of $s(i)$, let us look at a few extreme situations. When $s(i)$ is at its largest (that is, close to 1), this implies that the "within" dissimilarity $a(i)$ is much smaller than the smallest "between" dissimilarity $b(i)$. Therefore, we can say that i is "well classified", as there appears to be little doubt that i has been assigned to an appropriate cluster: The second-best choice (B) is not nearly as close as the actual choice (A).

A different situation occurs when $s(i)$ is about zero. Then $a(i)$ and $b(i)$ are approximately equal and hence it is not clear at all whether i should

have been assigned to A or to B. Object i lies equally far away from both, so it can be considered as an "intermediate" case.

The worst situation takes place when $s(i)$ is close to -1. Then $a(i)$ is much larger than $b(i)$, so i lies on the average much closer to B than to A. Therefore it would have seemed much more natural to assign object i to cluster B, so we can almost conclude that object i has been "misclassified".

To conclude, $s(i)$ measures how well object i matches the clustering at hand (that is, how well it has been classified). In the special case where there are only two clusters ($k = 2$), we note that moving object i from one cluster to the other will convert $s(i)$ to $-s(i)$.

Having computed the quantities $s(i)$ from the dissimilarities, we can now construct the graphical display. The silhouette of cluster A is a plot of the $s(i)$, ranked in decreasing order, for all objects i in A. On a line printer, we represent $s(i)$ by a row of asterisks, the length of which is proportional to $s(i)$. Therefore, the silhouette shows which objects lie well within their cluster and which ones are merely somewhere in between clusters. A wide silhouette indicates large $s(i)$ values and hence a pronounced cluster. The other dimension of a silhouette is its height, which simply equals the number of objects in A.

In order to obtain an overview, the silhouettes of the different clusters are printed below each other. In this way the entire clustering can be displayed by means of a single plot, which enables us to distinguish clear-cut clusters from weak ones. Above and below the plot there are scales going from 0.00 to 1.00 with steps of size 0.04 (to be read vertically). In the output of PAM, the following information is given for each object i:

The number of the cluster to which it belongs (under the header CLU).

The number of the neighboring cluster (under NEIG).

The value $s(i)$.

The three-character label of object i.

A line, the length of which is proportional to $s(i)$ (if this value is positive).

Also the following summary values are added:

The average of the $s(i)$ for all objects i in a cluster, which is called the *average silhouette width* of that cluster.

The average of the $s(i)$ for $i = 1, 2, \ldots, n$ which is called the *average silhouette width for the entire data set.*

This last number, which we will denote by $\bar{s}(k)$, can be used for the selection of a "best" value of k, by choosing that k for which $\bar{s}(k)$ is as

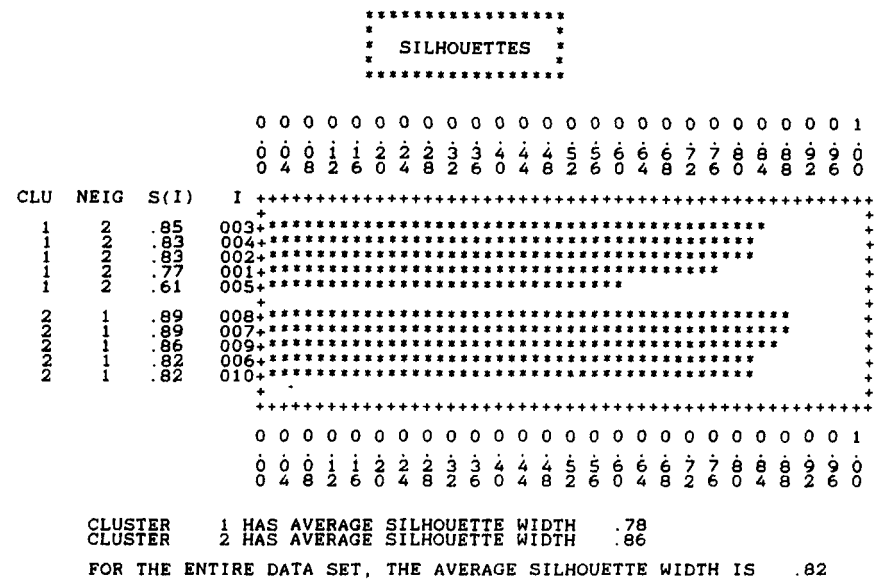


Figure 5 Graphical output for the clustering into two clusters of the data in Table 1.

high as possible. The choice of k is one of the most difficult problems of cluster analysis, for which no unique solution exists; for a recent survey of alternative criteria see Milligan and Cooper (1985).

The silhouettes for $k = 2$ of the example of Figure 1 are given in Figure 5. Both clusters appear to be quite pronounced because their silhouettes are relatively wide. We see that the average silhouette width for the entire data set is $\bar{s}(k) = 0.82$ when $k = 2$. After computing $\bar{s}(k)$ for all possible k we find that this value 0.82 is the highest, so we conclude that $k = 2$ is an appropriate number of clusters for this data set. It is possible to repeat this in all applications by computing what we call the *silhouette coefficient*:

$$\mathrm{SC} = \max_k \bar{s}(k) \tag{7}$$

where the maximum is taken over all k for which the silhouettes can be constructed, which means $k = 2, 3, \ldots, n - 1$. On the one hand, this gives us a selected value of k. On the other, the SC is a useful measure of the amount of clustering structure that has been discovered by the classification algorithm. The silhouette coefficient is a dimensionless quantity which is at most equal to 1 and which does not change when all the original dissimilarities are multiplied by a constant factor. Experience with the SC has led us

Table 4 Subjective Interpretation of the Silhouette Coefficient (SC), Defined as the Maximal Average Silhouette Width for the Entire Data Set

SC	Proposed Interpretation
0.71–1.00	A strong structure has been found
0.51–0.70	A reasonable structure has been found
0.26–0.50	The structure is weak and could be artificial; please try additional methods on this data set
≤ 0.25	No substantial structure has been found

to a rather subjective interpretation, which is summarized in Table 4. Indeed, an SC close to 1 points to a very clear structure and a low SC indicates that one might better apply an alternative method of data analysis.

Because the silhouettes and the SC are not restricted to a particular partitioning algorithm, Table 4 will also be used in Chapters 3 and 4. Readers wanting to gather some more experience with silhouettes in order to obtain a better feeling for their interpretation are referred to the examples in Section 3 of this chapter.

2.3 Missing Values

In PAM provision is made for the case that there are missing values in the input of measurements. As this situation does not interest all users and as it has a strong impact on both input and output, it is treated in a special subsection.

If the user answers yes to the question concerning the occurrence of missing data the following questions must be answered:

```
IS THERE A UNIQUE VALUE WHICH IS TO BE INTERPRETED
AS A MISSING MEASUREMENT VALUE FOR ANY VARIABLE ?
PLEASE ANSWER YES OR NO : no
```

If missing values can occur but there is no single code representing a missing measurement, the following questions are asked:

```
SHOULD MISSING VALUES BE FORESEEN FOR THE VARIABLE
TEMPERATUR ? PLEASE ANSWER YES OR NO : no
```

SHOULD MISSING VALUES BE FORESEEN FOR THE VARIABLE WEIGHT ? PLEASE ANSWER YES OR NO : yes
ENTER THE VALUE OF THE VARIABLE WHICH HAS TO BE INTERPRETED AS THE MISSING VALUE CODE : 9.999

SHOULD MISSING VALUES BE FORESEEN FOR THE VARIABLE HEIGHT ? PLEASE ANSWER YES OR NO : yes
ENTER THE VALUE OF THE VARIABLE WHICH HAS TO BE INTERPRETED AS THE MISSING VALUE CODE : 99.99

This means that missing values are only foreseen for the second and third variables. The actual measurements are introduced in the following dialogue:

THE 3 MEASUREMENTS FOR OBJECT 001 :
12.3 8.328 38.76
THE 3 MEASUREMENTS FOR OBJECT 002 :
-5.4 9.999 18.12
THE 3 MEASUREMENTS FOR OBJECT 003 :
10.7 9.999 41.71
THE 3 MEASUREMENTS FOR OBJECT 004 :
-4.6 2.981 20.83
THE 3 MEASUREMENTS FOR OBJECT 005 :
-4.8 3.156 99.99
THE 3 MEASUREMENTS FOR OBJECT 006 :
11.0 7.826 40.54

The following adaptations have been incorporated into the program to take missing data into account. If the data are standardized, the average m_f and mean absolute deviation s_f are calculated using only present values. When calculating the distances $d(i, j)$, only those variables are considered in the sum for which the measurements for both objects are present. Subsequently the sum of terms is multiplied by p and divided by the number of such variables (in the case of Euclidean distances this is done before taking the square root). If the measurements are standardized, the transformed values corresponding to missing data are given the value 99.99.

Another consequence of missing values is that in the output of the program, right after the data specifications, the number of missing values for each variable and their total number are listed. In Figure 6 the output is given corresponding to these data.

```
                    ********************************
                    *                              *
                    *  PARTITIONING AROUND MEDOIDS *
                    *                              *
                    ********************************

TITLE  : DATA WITH MISSING VALUES

DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 THERE ARE     6 OBJECTS
 LABELS OF OBJECTS ARE NOT READ
 INPUT OF MEASUREMENTS
 LARGE OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (SILHOUETTES)
 CLUSTERINGS ARE CARRIED OUT IN     2 TO     2 CLUSTERS

 THERE ARE     3 VARIABLES IN THE DATA SET,
  AND     3 OF THEM WILL BE USED IN THE ANALYSIS
 THE LABELS OF THESE VARIABLES ARE :
         TEMPERATUR    (POSITION :  1)
         WEIGHT        (POSITION :  2)
         HEIGHT        (POSITION :  3)
 THE MEASUREMENTS WILL BE STANDARDIZED
 MANHATTAN DISTANCE WILL BE USED
 MISSING VALUES CAN OCCUR
 THE MEASUREMENTS WILL BE READ IN FREE FORMAT

 THE DATA WILL BE SAVED ON FILE : b:miss.dat

 VARIABLE WEIGHT      CONTAINS     2 MISSING VALUES
 VARIABLE HEIGHT      CONTAINS     1 MISSING VALUES

 THE TOTAL NUMBER OF MISSING VALUES IS       3

VARIABLE TEMPERATUR HAS AVERAGE      3.200      MEAN DEVIATION      8.133
VARIABLE WEIGHT     HAS AVERAGE      5.573      MEAN DEVIATION      2.504
VARIABLE HEIGHT     HAS AVERAGE     31.992      MEAN DEVIATION     10.014

STANDARDIZED MEASUREMENTS
-------------------------
 ( 99.99 DENOTES A MISSING VALUE)

001        1.12      1.10       .68
002       -1.06     99.99     -1.39
003         .92     99.99       .97
004        -.96     -1.03     -1.11
005        -.98      -.97     99.99
006         .96       .90       .85

DISSIMILARITY MATRIX
--------------------

001
002        6.36
003         .74      6.50
004        6.00       .55      5.95
005        6.25       .22      5.72       .14
006         .54      6.38       .23      5.82      5.71

*********************************************
*                                           *
*  NUMBER OF REPRESENTATIVE OBJECTS     2   *
*                                           *
*********************************************

RESULT OF BUILD
  AVERAGE DISSIMILARITY =          .189

FINAL RESULTS
  AVERAGE DISSIMILARITY =          .189

  CLUSTERS
  NUMBER   MEDOID   SIZE      OBJECTS

    1       006       3      001 003 006

    2       005       3      002 004 005
```

Figure 6 Output from the missing data example.

```
COORDINATES OF MEDOIDS (USING STANDARDIZED MEASUREMENTS)
********************************************************

006          .96        .90        .85
005         -.98       -.97      99.99

CLUSTERING VECTOR
*****************

            1  2  1  2  2  1

CLUSTERING CHARACTERISTICS
**************************

 CLUSTER     1 IS ISOLATED,
        WITH DIAMETER  =          .74 AND SEPARATION =         5.71
        THEREFORE IT IS AN L*-CLUSTER.

 CLUSTER     2 IS ISOLATED,
        WITH DIAMETER  =          .55 AND SEPARATION =         5.71
        THEREFORE IT IS AN L*-CLUSTER.

 THE NUMBER OF ISOLATED CLUSTERS =     2

 DIAMETER OF EACH CLUSTER
       .74        .55

 SEPARATION OF EACH CLUSTER
      5.71       5.71

 AVERAGE DISSIMILARITY TO EACH MEDOID
       .26        .12

 MAXIMUM DISSIMILARITY TO EACH MEDOID
       .54        .22

                          ****************
                          *              *
                          *  SILHOUETTES *
                          *              *
                          ****************

                     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                     0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                     0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

 CLU  NEIG  S(I)   I +++++++++++++++++++++++++++++++++++++++++++++++++++++++++
                     +                                                       +
   1    2   .94   006+***************************************************    +
   1    2   .92   003+*************************************************      +
   1    2   .90   001+***********************************************        +
                     +                                                       +
   2    1   .97   005+*****************************************************  +
   2    1   .94   004+***************************************************    +
   2    1   .94   002+*****************************************************  +
                     +                                                       +
                     +++++++++++++++++++++++++++++++++++++++++++++++++++++++++

                     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                     0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                     0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

      CLUSTER    1 HAS AVERAGE SILHOUETTE WIDTH    .92
      CLUSTER    2 HAS AVERAGE SILHOUETTE WIDTH    .95

      FOR THE ENTIRE DATA SET, THE AVERAGE SILHOUETTE WIDTH IS    .93

The output is on file : b:miss.res
```

Figure 6 *(Continued)*

3 EXAMPLES

In the previous sections, the algorithm was illustrated with an example consisting of two-dimensional measurements. In this section we start with an example in which the basic data consist of a dissimilarity matrix. (The same example will be used in Chapters 4, 5, and 6.)

The data were obtained by distributing a questionnaire in a political science class, asking the students to provide subjective dissimilarity coefficients between 12 countries. This is similar to an experiment of Wish (1970), with the students' own country (Belgium) included. The countries selected were (in alphabetical order) Belgium, Brazil, China, Cuba, Egypt, France, India, Israel, USA, USSR, Yugoslavia, and Zaire. The final dissimilarity coefficients were obtained by taking the averages of the coefficients given by the students.

In Table 5 the data are listed and Figure 7 contains the first part of the output, including the dissimilarity matrix because the option of large output is selected.

Figure 7 also contains the clustering into a single cluster (selection of one representative object). An interesting feature is that Belgium is found as medoid for the entire data set. A possible explanation is that the Belgian students tend to perceive smaller differences between their own country and each of the others, than among foreign countries. Further results given are

Table 5 Dissimilarities between 12 Countries, Obtained by Averaging the Results of a Survey among Political Science Students

Country	Dissimilarities to Other Countries										
	BEL	BRA	CHI	CUB	EGY	FRA	IND	ISR	USA	USS	YUG
BRA	5.58										
CHI	7.00	6.50									
CUB	7.08	7.00	3.83								
EGY	4.83	5.08	8.17	5.83							
FRA	2.17	5.75	6.67	6.92	4.92						
IND	6.42	5.00	5.58	6.00	4.67	6.42					
ISR	3.42	5.50	6.42	6.42	5.00	3.92	6.17				
USA	2.50	4.92	6.25	7.33	4.50	2.25	6.33	2.75			
USS	6.08	6.67	4.25	2.67	6.00	6.17	6.17	6.92	6.17		
YUG	5.25	6.83	4.50	3.75	5.75	5.42	6.08	5.83	6.67	3.67	
ZAI	4.75	3.00	6.08	6.67	5.00	5.58	4.83	6.17	5.67	6.50	6.92

```
**********************************
*                                *
*  PARTITIONING AROUND MEDOIDS   *
*                                *
**********************************

TITLE  : Dissimilarities between 12 countries
DATA SPECIFICATIONS AND CHOSEN OPTIONS
---------------------------------------
 THERE ARE    12 OBJECTS
 LABELS OF OBJECTS ARE READ
 INPUT OF DISSIMILARITIES
 LARGE OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (SILHOUETTES)
 CLUSTERINGS ARE CARRIED OUT IN     1 TO     3 CLUSTERS
 THE DISSIMILARITIES WILL BE READ IN FREE FORMAT

 YOUR DATA RESIDE ON FILE        : COUNTRY.DAT


DISSIMILARITY MATRIX
--------------------

BEL
BRA      5.58
CHI      7.00     6.50
CUB      7.08     7.00     3.83
EGY      4.83     5.08     8.17     5.83
FRA      2.17     5.75     6.67     6.92     4.92
IND      6.42     5.00     5.58     6.00     4.67     6.42
ISR      3.42     5.50     6.42     6.42     5.00     3.92     6.17
USA      2.50     4.92     6.25     7.33     4.50     2.25     6.33     2.75
USS      6.08     6.67     4.25     2.67     6.00     6.17     6.17     6.92
         6.17
YUG      5.25     6.83     4.50     3.75     5.75     5.42     6.08     5.83
         6.67     3.67
ZAI      4.75     3.00     6.08     6.67     5.00     5.58     4.83     6.17
         5.67     6.50     6.92

*********************************************
*                                           *
*  NUMBER OF REPRESENTATIVE OBJECTS     1   *
*                                           *
*********************************************

FINAL RESULTS
  AVERAGE DISSIMILARITY =        4.590

  CLUSTERS
  NUMBER   MEDOID    SIZE      OBJECTS

    1        BEL       12      BEL BRA CHI CUB EGY FRA IND ISR USA USS
                               YUG ZAI

 DIAMETER OF EACH CLUSTER
      8.17

 AVERAGE DISSIMILARITY TO EACH MEDOID
      4.59

 MAXIMUM DISSIMILARITY TO EACH MEDOID
      7.08
```

Figure 7 First part of the output for the 12 countries example, including the clustering for $k = 1$.

the diameter of the cluster and the average and maximum dissimilarity to the medoid. The respective values of these cluster characteristics are 8.17, 4.59, and 7.08. Two of these values (diameter and maximum dissimilarity) can be found in Table 5 in which they have been circled. As mentioned in Section 2, silhouettes do not exist in the situation of a single cluster.

In Figure 8 the output is given for $k = 3$. The clustering obtained corresponds rather well to three groups of countries: Western, developing and Communist. It is remarkable that cluster 3, consisting of Cuba, China,

USSR, and Yugoslavia, is the only isolated cluster. These countries are perceived as being very similar (within the limited set of countries we considered). It is also interesting to note that the other values given (diameter and separation, average dissimilarity, and maximum dissimilarity) are very close to each other for the three clusters.

Figure 8 also contains the silhouettes of these clusters. The first silhouette is higher than the others because the first cluster contains more objects than the remaining two. Our first impression is that the silhouettes are not very wide, which indicates that the clustering structure is no better than reasonable. In the first cluster, USA possesses the largest $s(i)$, which means that it was classified with the least amount of doubt. On the other hand, Egypt only attains $s(i) = 0.02$, which means that it lies on the boundary of the first cluster. Because its neighbor is cluster 2, this means that it has approximately the same dissimilarity to clusters 1 and 2 [moving Egypt to cluster 2 would yield $s(i) = -0.02$]. The second cluster contains the remaining developing countries and possesses a rather narrow silhouette,

```
*******************************************
*                                         *
*  NUMBER OF REPRESENTATIVE OBJECTS     3 *
*                                         *
*******************************************

RESULT OF BUILD
  AVERAGE DISSIMILARITY =         2.583

FINAL RESULTS
  AVERAGE DISSIMILARITY =         2.507

  CLUSTERS
  NUMBER   MEDOID    SIZE      OBJECTS

     1       USA        5     BEL EGY FRA ISR USA

     2       ZAI        3     BRA IND ZAI

     3       CUB        4     CHI CUB USS YUG

CLUSTERING VECTOR
*****************

            1  2  3  3  1  1  2  1  1  3  3  2

CLUSTERING CHARACTERISTICS
**************************

 CLUSTER     3 IS ISOLATED,
        WITH DIAMETER =       4.50 AND SEPARATION =        5.25
        THEREFORE IT IS AN L*-CLUSTER.

 THE NUMBER OF ISOLATED CLUSTERS =     1

 DIAMETER OF EACH CLUSTER
      5.00      5.00      4.50

 SEPARATION OF EACH CLUSTER
      4.67      4.67      5.25

 AVERAGE DISSIMILARITY TO EACH MEDOID
      2.40      2.61      2.56

 MAXIMUM DISSIMILARITY TO EACH MEDOID
      4.50      4.83      3.83
```

Figure 8 Output of the 12 countries example for $k = 3$.

```
                    ****************
                    *              *
                    *  SILHOUETTES *
                    *              *
                    ****************

                    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                    0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                    0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

CLU  NEIG  S(I)   I +++++++++++++++++++++++++++++++++++++++++++++++++++++++++
                    +                                                       +
  1     2   .47   USA+************************                              +
  1     2   .44   FRA+**********************                                +
  1     2   .42   BEL+*********************                                 +
  1     2   .37   ISR+******************                                    +
  1     2   .02   EGY+*                                                     +
                    +                                                       +
  2     1   .28   ZAI+***************                                       +
  2     1   .25   BRA+************                                          +
  2     3   .17   IND+********                                              +
                    +                                                       +
  3     2   .48   CUB+************************                              +
  3     1   .44   USS+**********************                                +
  3     1   .31   YUG+***************                                       +
  3     2   .31   CHI+***************                                       +
                    +                                                       +
                    +++++++++++++++++++++++++++++++++++++++++++++++++++++++++

                    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                    0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                    0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

      CLUSTER    1 HAS AVERAGE SILHOUETTE WIDTH    .34
      CLUSTER    2 HAS AVERAGE SILHOUETTE WIDTH    .24
      CLUSTER    3 HAS AVERAGE SILHOUETTE WIDTH    .38

      FOR THE ENTIRE DATA SET, THE AVERAGE SILHOUETTE WIDTH IS    .33

The output is on file : COUNTRY.RES
```

Figure 8 (*Continued*)

which means that cluster 2 is not very clearly separated from the other clusters. It appears that Zaire and Brazil are more inclined toward the Western countries because their neighbor is cluster 1, whereas India [which has a smaller value of $s(i)$] seems to be closer to cluster 3. In the third cluster there is also a lack of unanimity: USSR and Yugoslavia seem to have more resemblance to the Western countries, whereas Cuba and China appear to be closer to the developing ones.

Note that silhouettes only depend on the actual partition of the objects and not on the clustering algorithm that was used to obtain it. As a consequence, silhouettes could be used to improve the results of cluster analysis [for instance, by moving an object with negative $s(i)$ to its neighbor] or to compare the output of different clustering algorithms applied to the same data.

However, we think that the main usefulness of silhouettes lies in the interpretation and validation of cluster analysis results. Often silhouettes can prevent us from drawing the wrong conclusions. For instance, suppose the data set consists of some dense clusters that are far away from each

other, but that we have set k too low. In this case, most clustering algorithms will combine some natural clusters in order to reduce the total number of groups to the specified value of k. Fortunately, the silhouette plot will often expose such artificial fusions. Indeed, joining different clusters will lead to large "within" dissimilarities and hence a large $a(i)$, resulting in small $s(i)$ values for the objects in such a conglomerate and yielding a narrow silhouette.

On the other hand, suppose that we have set k too high. Then some natural clusters have to be divided in an artificial way in order to conform to the specified number of groups. However, these artificial fragments will typically also show up through their narrow silhouettes. Indeed, the objects in such a fragment are on the average very close to the remaining part(s) of their natural cluster, and hence the "between" dissimilarities $b(i)$ will become very small, which also results in small $s(i)$ values.

This heuristic reasoning implies that the silhouettes should look best for a "natural" value of k. Therefore, we want the silhouettes to be as wide (or as dark) as possible. For each cluster, we have defined the *average silhouette width* as the average of the $s(i)$ for all objects i belonging to that cluster. This allows us to distinguish clear-cut from weak clusters in the same plot: Clusters with a larger average silhouette width are more pronounced. In Figure 8, we see that the average silhouette width of the second cluster is only 0.24, whereas the first and third clusters attain higher values.

We can also consider the *overall average silhouette width* for the entire plot, which is simply the average of the $s(i)$ for all objects i in the whole data set. In Figure 8 this yields 0.33. In general, each value of k will yield another overall average silhouette width $\bar{s}(k)$. One way to choose k appropriately is to select that value of k for which $\bar{s}(k)$ is as large as possible. For the 12 countries data, it turns out that the best choice in this respect is $k = 3$, hence the so-called silhouette coefficient (SC) equals 0.33. According to Table 4, this is interpreted as a weak structure, but indeed the features of this grouping will be confirmed when applying the clustering algorithms of Chapters 4, 5, and 6.

Let us now look at some rather extreme examples to obtain a better feeling for the meaning of silhouettes. First suppose we have eight objects that are divided over some very tight clusters, far away from each other. For instance, assume that five objects coincide with one geometrical point and the remaining three coincide with another geometrical point at a large distance from the first. This is an extremely sharp clustering structure, which should be recovered by any reasonable clustering algorithm when $k = 2$. The resulting silhouette plot in Figure 9 is as wide and as dark as possible. All $s(i)$ equal 1.00, so the overall average silhouette width attains its maximal value 1.00 (therefore, $k = 2$ is the best choice and the SC of

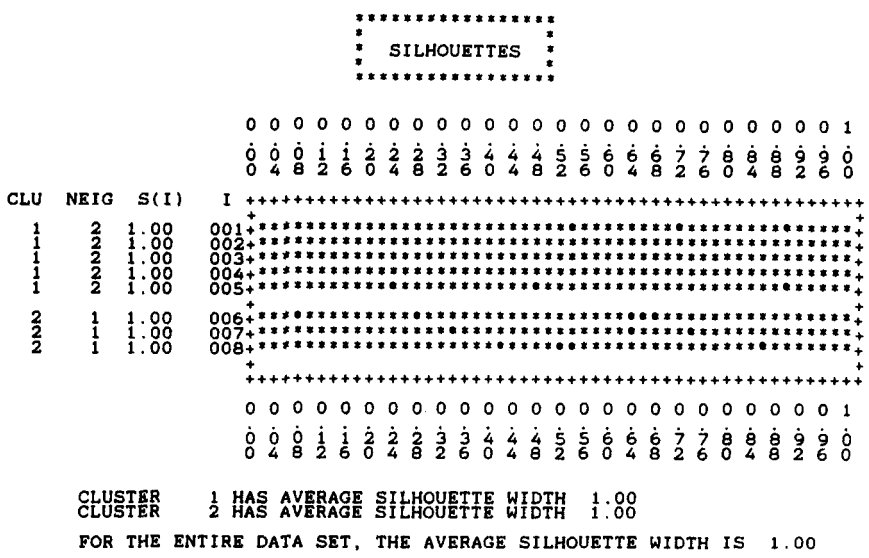


Figure 9 Silhouettes of an example in which eight objects are divided over two very tight clusters, for $k = 2$.

Table 4 equals 1.00). In general, a very large overall average silhouette width can be taken to mean that the algorithm has discovered a very strong clustering structure.

However, one must be careful with the interpretation of the last statement. For instance, a situation where the data set contains one far outlier is also an example of a strong clustering structure. Indeed, when the outlier is far enough, the other data look like a tight cluster by comparison. We may expect our clustering algorithm to provide the following picture for $k = 2$: one cluster containing just the outlier and the other cluster consisting of the bulk of the data. For instance, suppose seven objects have zero dissimilarities to each other and all have large dissimilarities to the eighth object, which is an outlier. The resulting silhouette plot is given in Figure 10, clearly separating object 8 from the rest. Because cluster 2 contains only a single object, its $s(i)$ was put equal to 0 by convention. In order to mark such singleton clusters in a more distinctive way, John Tukey (personal communication) suggested printing the number 1 in the rightmost column of the plot. The overall average silhouette width equals 0.88, which is very high (in general, one obtains $1 - 1/n$ where n is the total number of objects). Therefore, one should never merely accept a high overall average silhouette width at its face value, but also look at the graphical output itself

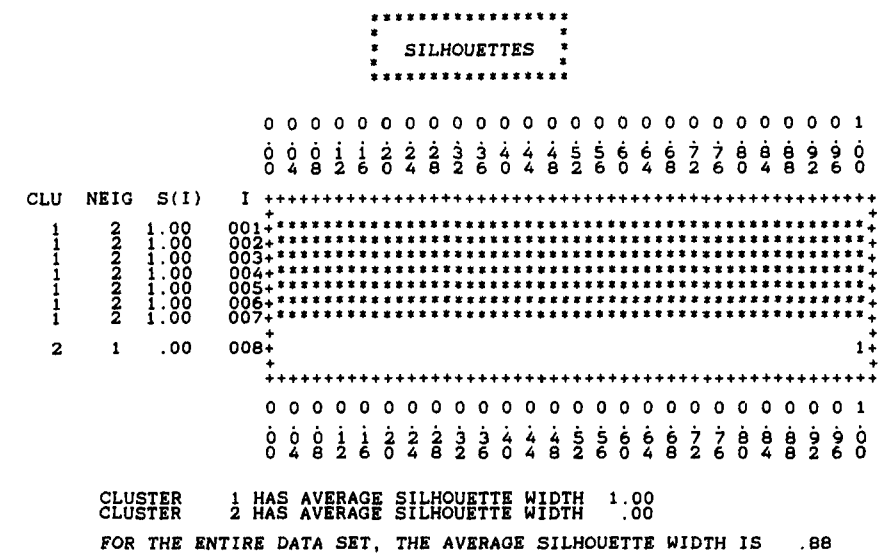


Figure 10 Silhouettes of a data set containing a distant outlier, for $k = 2$.

to find out what caused the large value. Depending on the subject matter and the task at hand, one might want to put the outlier aside for further investigation and run the clustering algorithm again on the remaining data.

When the clustering algorithm does not succeed in finding any "natural" clustering, the overall average silhouette width tends to become very low. An extreme case is when all dissimilarities between pairs of objects equal the same positive constant, so all off-diagonal entries of the dissimilarity matrix are identical. (In the case of Euclidean distances, this happens with the n vertices of a regular simplex in $n - 1$ dimensions.) In such a situation no clustering is more natural than any other, so there is a total absence of clustering structure. Whatever the value of k and whatever clustering algorithm is used, all $s(i)$ will be 0 [as well as the overall average silhouette width $\bar{s}(k)$ and the silhouette coefficient SC] and the silhouette plot (see Figure 11) stays completely empty. In actual applications one sometimes does encounter cases where even the largest value of $\bar{s}(k)$ is very small, pointing to a lack of clustering structure.

Figure 12 shows a plot of the well-known Ruspini data (1970). This data set consists of 75 points and was originally used by Ruspini in order to illustrate fuzzy clustering techniques. The actual coordinates, given in Table 6, were communicated to us by G. Libert. The points make up four groups, A, B, C, and D, as indicated in the plot. Because this example is two-

```
                    ****************
                    *               *
                    *  SILHOUETTES  *
                    *               *
                    ****************

                    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                    0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                    0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

CLU   NEIG   S(I)    I ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
                      +                                                          +
  1     2    .00    001+                                                         +
  1     2    .00    002+                                                         +
  1     2    .00    003+                                                         +
  1     2    .00    004+                                                         +
  1     2    .00    005+                                                         +
  1     2    .00    006+                                                         +
  1     2    .00    007+                                                         +
                      +                                                         1+
  2     1    .00    008+                                                         +
                      +                                                          +
                    ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

                    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                    0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                    0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

     CLUSTER    1 HAS AVERAGE SILHOUETTE WIDTH    .00
     CLUSTER    2 HAS AVERAGE SILHOUETTE WIDTH    .00

     FOR THE ENTIRE DATA SET, THE AVERAGE SILHOUETTE WIDTH IS    .00
```

Figure 11 Silhouettes of a data set without any clustering structure, for $k = 2$.

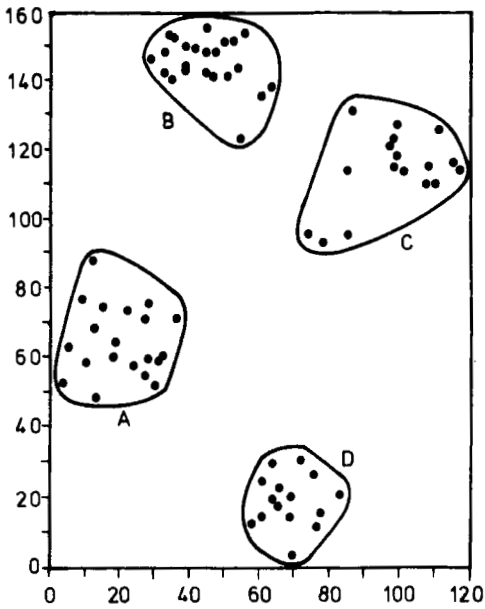


Figure 12 Plot of the two-dimensional data set of Ruspini. The loops are merely drawn to indicate four groups of points.

Table 6 Coordinates of the Ruspini Data

x	y	x	y	x	y
4	53	41	150	98	124
5	63	38	145	99	119
10	59	38	143	99	128
9	77	32	143	101	115
13	49	34	141	108	111
13	69	44	156	110	111
12	88	44	149	108	116
15	75	44	143	111	126
18	61	46	142	115	117
19	65	47	149	117	115
22	74	49	152	70	4
27	72	50	142	77	12
28	76	53	144	83	21
24	58	52	152	61	15
27	55	55	155	69	15
28	60	54	124	78	16
30	52	60	136	66	18
31	60	63	139	58	13
32	61	86	132	64	20
36	72	85	115	69	21
28	147	85	96	66	23
32	149	78	94	61	25
35	153	74	96	76	27
33	154	97	122	72	31
38	151	98	116	64	30

dimensional, we can now compare the silhouettes to the structure that we perceive by the naked eye. Figure 13 contains the silhouette plots of the k-medoid partitions with $k = 2, \ldots, 6$ (making use of Euclidean distance).

In the case of $k = 2$, one cluster is formed as the union of A with D, whereas the second combines B and C. As we saw before, artificial fusions are penalized by narrow silhouettes. For $k = 3$ we see that clusters B and C are found, but A and D still stick together. The corresponding silhouette plot shows clearly that both B and C are more pronounced than the union of A with D. For $k = 4$ the "right" solution is found, which leads to four silhouettes of about the same good quality. When $k = 5$ is imposed, the algorithm splits C into two parts. The second part contains the three lowest points of C (as viewed in Figure 12), that is, the three points of C with smallest y coordinates. This trio has a rather prominent silhouette and

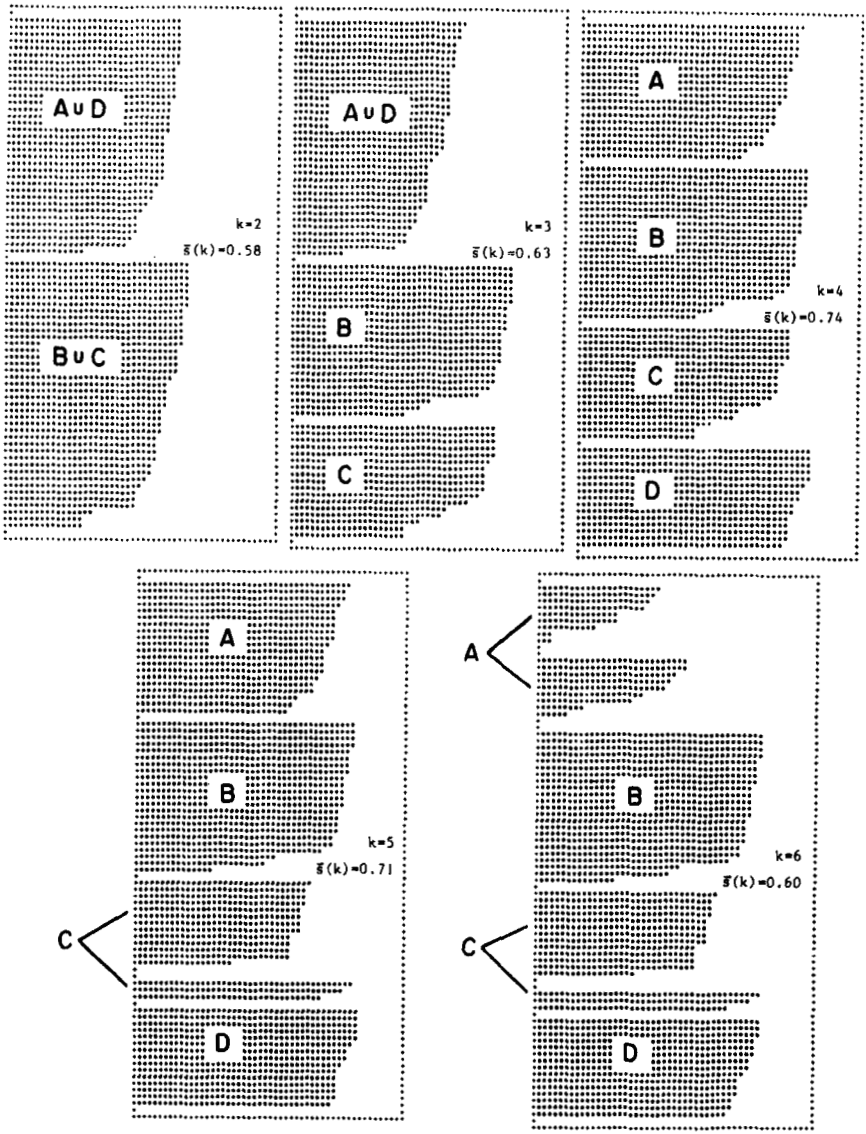


Figure 13 Silhouette plots of the Ruspini data, for k ranging from 2 to 6.

indeed some people consider it as a genuine cluster (see Delattre and Hansen, 1980). However, the silhouette of the major part of C becomes somewhat less wide because this cluster is not so well separated from the three-point one [indeed, one object has an $s(i)$ value of about zero because it lies rather close to the three-point cluster and therefore holds an intermediate position]. The last case ($k = 6$) leads to a more dramatic effect: Cluster A is being split up in an artificial way and consequently both parts obtain narrow silhouettes. For $k = 7, \ldots, 74$ the results are still worse.

In conclusion, the silhouette plots tell us that a partition into $k = 4$ clusters is probably most natural. Indeed, the overall average silhouette width $\bar{s}(k)$ is largest for this value (even if one tries all values of k ranging from 2 to 74). The second best $\bar{s}(k)$ is attained for $k = 5$ and the silhouette plot shows us the advantages and disadvantages of the corresponding clustering.

*4 MORE ON THE ALGORITHM AND THE PROGRAM

4.1 Description of the Algorithm

In the description of the k-medoid method given in Section 1, we minimize the *average* dissimilarity of objects to their closest representative object. However, in the program itself we prefer to minimize the *sum* of these dissimilarities, which is mathematically equivalent but gives rise to more accurate calculations. Therefore, from now on we shall only talk about the minimization of this sum.

The algorithm we are using in PAM consists of two phases. In a first phase, called BUILD, an initial clustering is obtained by the successive selection of representative objects until k objects have been found. The first object is the one for which the sum of the dissimilarities to all other objects is as small as possible. This object is the most centrally located in the set of objects. Subsequently, at each step another object is selected. This object is the one which decreases the objective function as much as possible. To find this object, the following steps are carried out:

1. Consider an object i which has not yet been selected.
2. Consider a nonselected object j and calculate the difference between its dissimilarity D_j with the most similar previously selected object, and its dissimilarity $d(j, i)$ with object i.
3. If this difference is positive, object j will contribute to the decision to select object i. Therefore we calculate

$$C_{ji} = \max\bigl(D_j - d(j, i), 0\bigr)$$

4. Calculate the total gain obtained by selecting object i:

$$\sum_j C_{ji}$$

5. Choose the not yet selected object i which

$$\underset{i}{\text{maximizes}} \sum_j C_{ji}$$

This process is continued until k objects have been found. In the second phase of the algorithm (called SWAP), it is attempted to improve the set of representative objects and therefore also to improve the clustering yielded by this set. This is done by considering all pairs of objects (i, h) for which *object i has been selected and object h has not.* It is determined what effect is obtained on the value of the clustering when a swap is carried out, i.e., when object i is no longer selected as a representative object but object h is. Here we should recall that in this subsection, the value of a clustering determined by k representative objects is defined as the sum of dissimilarities between each object and the most similar representative object.

To calculate the effect of a swap between i and h on the value of the clustering, the following calculations are carried out (steps 1 and 2):

1. Consider a nonselected object j and calculate its contribution C_{jih} to the swap:
   - **a.** If j is more distant from both i and h than from one of the other representative objects, C_{jih} is zero.
   - **b.** If j is not further from i than from any other selected representative object ($d(j, i) = D_j$), two situations must be considered:
     - **b1.** j is closer to h than to the second closest representative object

$$d(j, h) < E_j$$

       where E_j is the dissimilarity between j and the second most similar representative object. In this case the contribution of object j to the swap between objects i and h is

$$C_{jih} = d(j, h) - d(j, i)$$

     - **b2.** j is at least as distant from h than from the second closest representative object

$$d(j, h) \geq E_j$$

In this case the contribution of object j to the swap is

$$C_{jih} = E_j - D_j$$

It should be observed that in situation b1 the contribution C_{jih} can be either positive or negative depending on the relative position of objects j, h, and i. Only if object j is closer to i than to h is the contribution positive, which indicates that the swap is not favorable from the point of view of object j. On the other hand, in situation b2 the contribution is always positive because it cannot be advantageous to replace i by an object h further away from j than from the second closest representative object.

c. j is more distant from object i than from at least one of the other representative objects but closer to h than to any representative object. In this case the contribution of j to the swap is

$$C_{jih} = d(j, h) - D_j$$

2. Calculate the total result of a swap by adding the contributions C_{jih}:

$$T_{ih} = \sum_j C_{jih}$$

In the next steps it is decided whether to carry out a swap.

3. Select the pair (i, h) which

$$\underset{i,\,h}{\text{minimizes}}\, T_{ih}$$

4. If the minimum T_{ih} is negative, the swap is carried out and the algorithm returns to step 1. If the minimum T_{ih} is positive or 0, the value of the objective cannot be decreased by carrying out a swap and the algorithm stops.

Note that as all potential swaps are considered, the results of the algorithm do not depend on the order of the objects in the input file (except in case some of the distances between objects are tied).

4.2 Structure of the Program

The program PAM is written in Fortran and consists of approximately 1100 statement lines. Details about portability are given in the Appendix.

The program consists of a main unit, one function, and eight subroutines. In this section the purpose of each of these units is outlined.

The MAIN unit consists of the following parts:

- dimensions of the arrays
- setting the maximum values of the number of objects, the total number of variables, and the number of variables which can be used in a single analysis
- defining the unit for data input (called LUA) and the two units for output (LUB for the output of results and LUC for storing data entered by keyboard); in the present version they are given the values 1, 2, and 3
- call of the subroutine ENTR, which contains the interactive part of the program
- examination of objects and variables for missing values
- calls of the subroutines STAND (standardization) and DYSTA (computation of dissimilarities); these subroutines are associated with the input of measurements. After their input or calculation, the dissimilarities are stored in an array called DYS. In order to save memory space only the lower triangular part of the dissimilarity matrix is stored (an example is given in Figure 14). We chose the *lower* half matrix because this makes it possible to add new objects by simply adding some lines to the input file.
- parts *a*, *b*, and *c* of the output (see Section 2.2)
- a DO loop (DO 140 KK = KBEG,KEND) in which the subroutines BSWAP, CSTAT, and DARK are called; KK is the variable in which the number of clusters is stored (the subroutine DARK is called if graphical output was requested by the user, except if KK equals one or *n*)

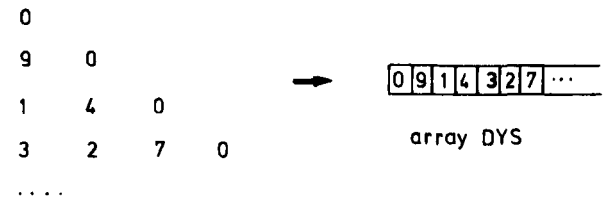


Figure 14 Illustration of the way dissimilarities are stored in a one-dimensional array. The first entry of the array is always 0 for convenience.

Subroutine ENTR: This subroutine controls the interactive use of the program and the input and output of data. It consists of the following parts:

- input of data specifications and chosen options
- if required by the user, input of labels of objects and information concerning missing values
- output of special messages
- output of a table with a recapitulation of data specifications and chosen options
- input of dissimilarities or measurement values

Subroutine QYN: Allows input of the answer to a yes–no question concerning options of the program (only the first letter of the answer is read and both upper and lowercase answers are allowed).

Function MEET: When a dissimilarity between objects L and J is needed, function MEET(L, J) gives the index of DYS where this dissimilarity is stored:

$$d(L, J) = \text{DYS}(\text{MEET}(L, J))$$

Subroutine NWLAB: This subroutine, which is accessed from the subroutine ENTR, is only called if no labels are provided. In it labels of objects are constructed:

$$001 \quad 002 \quad 003 \quad \cdots$$

They are stored in an integer matrix LAB(L, J) ($L = 1, 2, 3$ and $J = 1, 2, \ldots, n$) using the characters $0, 1, 2, \ldots, 9$ stored in a character type variable (NUM).

Subroutine STAND: In this subroutine, which is only called if standardization is requested, new standardized measurements are computed.

Subroutine DYSTA: Computes Euclidean or Manhattan distances (these are the dissimilarities that will be used in the clustering).

Subroutine BSWAP: Performs the clustering. It consists of two parts in which the BUILD and SWAP techniques are used.

Subroutine CSTAT: Gives the numerical output concerning each partition (except for the average dissimilarities, which are already computed in the subroutine BSWAP).

Subroutine DARK: Gives the graphical output for each partition.

Let us now investigate how the program can be adapted to special situations. Right after the dimension statements, four variables (MAXNN,

MAXTT, MAXPP, and MAXHH) are given values, which make it possible to use the program for clustering data sets of different sizes. MAXNN and MAXTT are the maximum numbers of objects and variables in the data set, whereas MAXPP is the maximum number of variables that are actually used in the computations. These values can be freely chosen by the user taking into account their effect on the storage requirements of the program. For example when clustering 50 objects measured on 10 variables (MAXNN = 50, MAXTT = 10, MAXPP = 10) the EXE file occupies 108,644 bytes, whereas for 100 objects and 20 variables (MAXNN = 100, MAXTT = 20, MAXPP = 20) 136,308 bytes are necessary. Often trial and error seems to be the easiest way of determining the maximum size of problems which can be solved on a particular computer.

The fourth variable defined after the dimensions is MAXHH, which gives the size of the array DYS and must be set equal to MAXNN(MAXNN − 1)/2 + 1.

The four variables MAXNN, MAXTT, MAXPP, and MAXHH are used as dimensions of arrays (vectors and matrices) in the subroutines. In the main program the dimensions of the arrays in the first five dimension statements must be set equal to the values of these four parameters. In Section 2 the following values were used:

$$\begin{aligned} \text{MAXNN} &= 100 \\ \text{MAXTT} &= 80 \\ \text{MAXPP} &= 20 \\ \text{MAXHH} &= 4951 \end{aligned}$$

If the program is used with input of dissimilarities, it is recommended to give a value of at least 1 to MAXTT and MAXPP.

Another important aspect of using the program on different computers is the time necessary to solve given problems. As an indication of the speed of the program, the times (in minutes) on an IBM/XT with an 8087 accelera-

Table 7 Computation Times (in minutes) on an IBM-XT with 8087 Accelerator for a Set of Randomly Generated Problems of Increasing Sizes

Objects	Variables	Clusters	Time
20	2	5	0.30
40	2	5	1.17
60	2	5	1.87
80	2	5	3.20
100	2	5	6.17

tor for a set of randomly generated problems of increasing sizes are given in Table 7.

Specific information concerning compilation of the program is given in the Appendix.

*5 RELATED METHODS AND REFERENCES

5.1 The *k*-Medoid Method and Optimal Plant Location

When constructing partitions with a fixed number k of clusters, it is often assumed that there exists a function which measures the quality of different clusterings of the same data set. This is also the case for the clustering method used in the program PAM. This method is based on a location model (the k-median model) with the following general formulation: Given a finite number of users, whose demands for a given service are known and must be satisfied, and given a finite set of possible locations among which k must be chosen for the location of service centers, select the locations in such a way as to minimize the total distance (or equivalently the average distance) travelled by the users. In the formulation used in clustering, the sets of users and of possible locations coincide and both correspond to the set of objects to be clustered. The location of a center is interpreted as the selection of an object as a representative object (or centrotype, median, or medoid) of a cluster. The distance travelled by a user corresponds to the dissimilarity between an object and the representative object of the cluster to which it belongs. The idea to use this model for cluster analysis was introduced by Vinod (1969) and later also discussed by Rao (1971), Church (1978), and Mulvey and Cowder (1979).

In the mathematical formulation of the k-medoid model the following notations are used:

The set of objects is denoted by X:

$$X = \{x_1, x_2, \ldots, x_n\}$$

The dissimilarity between objects x_i and x_j (also called objects i and j) is denoted by $d(i, j)$.

A solution of the model is determined by two types of decisions:

The selection of objects as representative objects in clusters: y_i is defined as a 0-1 variable, equal to 1 if and only if object i ($i = 1, 2, \ldots, n$) is selected as a representative object.

The assignment of each object j to one of the selected representative objects: z_{ij} is a 0-1 variable, equal to 1 if and only if object j is assigned to the cluster of which i is the representative object (and also the medoid).

The corresponding optimization model, which was first proposed by Vinod (1969), can then be written as:

$$\text{minimize} \sum_{i=1}^{n} \sum_{j=1}^{n} d(i, j) z_{ij} \tag{8}$$

subject to

$$\sum_{i=1}^{n} z_{ij} = 1, \qquad j = 1, 2, \ldots, n \tag{9}$$

$$z_{ij} \leq y_i, \qquad i, j = 1, 2, \ldots, n \tag{10}$$

$$\sum_{i=1}^{n} y_i = k, \qquad k = \text{number of clusters} \tag{11}$$

$$y_i, z_{ij} \in \{0, 1\}, \qquad i, j = 1, 2, \ldots, n \tag{12}$$

Constraints (9) express that each object j must be assigned to a single representative object. They imply [together with constraints (12)] that for a given j, one of the z_{ij} is equal to 1 and all others are 0. Constraints (10) ensure that an object j can only be assigned to an object i if this last object has been selected as a representative object. Indeed, if this is not the case, then y_i is 0 and the constraint [together with constraints (12)] implies that all z_{ij} are 0. If i is a representative object, then all the z_{ij} (for this i) can be either 0 or 1. Equation (11) expresses that exactly k objects are to be chosen as representative objects. As the clusters are formed by assigning each object to the most similar representative object, there will be exactly k nonempty clusters. (In case of ties the object is assigned to the representative object which was entered first.) Equation (9) implies that the dissimilarity between an object j and its representative object is given by

$$\sum_{i=1}^{n} d(i, j) z_{ij}$$

As all objects must be assigned, the total dissimilarity is given by

$$\sum_{j=1}^{n} \sum_{i=1}^{n} d(i, j) z_{ij} \tag{13}$$

which is the function to be minimized in the model.

The algorithm discussed in Section 4 yields a good but not necessarily optimal solution to model (8) to (12). A branch and bound method which always yields an optimal solution was discussed in Massart et al. (1983). Unfortunately this approach is only computationally feasible for relatively small problems with up to 50 or 60 objects. Another method was used by Klastorin (1985) in a comparison of several clustering algorithms. It is based on an algorithm proposed by Erlenkotter (1978) for the simple plant location problem.

Usually one does not know the number of clusters present in a data set. Because most partitioning methods provide a fixed number k of clusters, one must apply them for several values of k in order to find the most meaningful clustering. A possible way of selecting a value of k is by means of the silhouette coefficient (see Section 2). Another way is to search for sets of objects that persistently stay together in the clusterings obtained for several values of k. This approach has been investigated by Massart et al. (1983) and Plastria (1986). Another method, based on the bootstrap technique, was proposed by Moreau and Jain (1987). For one-dimensional observations, Müller and Sawitzki (1987) chose k by estimating the number of modes.

5.2 Other Methods Based on the Selection of Representative Objects

The objective of the k-medoid method is to minimize the sum of dissimilarities between the objects and their representative objects. This objective is suitable if a total value is liable to give a correct description of the structure being investigated.

One of the possible alternative aims is to try to minimize the largest distance from any object to the representative object of its cluster. The maximum dissimilarity between an object and its representative object is given by

$$\max_{j=1,\ldots,n} \sum_{i=1}^{n} d(i, j) z_{ij}$$

and the model of minimizing the maximum dissimilarity can be written as

$$\text{minimize} \max_{j=1,\ldots,n} \sum_{i=1}^{n} d(i, j) z_{ij}$$

subject to constraints (9) to (12). This is called the *k-center model* and, like the k-medoid model, it finds its equivalent in location theory and also in graph theory. Algorithms for the k-center model have been proposed by

Hakimi (1965). A characteristic of the clusterings obtained with the k-center model is that they are on average looser, but on the other hand they will never contain very loose clusters.

Another model using representative objects is the *covering model*. In this model the number of clusters is not fixed, but each object must be within a given distance D of its representative object. The objective is to minimize the number of representative objects necessary to achieve this aim. As in the k-medoid method, once the representative objects have been selected the clustering is obtained by assigning each object to its most similar selected representative object. The model can be stated as

$$\text{minimize} \sum_{i=1}^{n} y_i \tag{14}$$

subject to

$$\sum_{i=1}^{n} z_{ij} = 1, \qquad j = 1, 2, \ldots, n \tag{15}$$

$$z_{ij} \leq y_i, \qquad i, j = 1, 2, \ldots, n \tag{16}$$

$$\sum_{i=1}^{n} d(i, j) z_{ij} \leq D, \qquad j = 1, 2, \ldots, n \tag{17}$$

$$y_i, z_{ij} \in \{0, 1\}, \qquad i, j = 1, 2, \ldots, n \tag{18}$$

Constraints (17) express that each object j must lie within a maximum dissimilarity D of its representative object.

There are two reasons why the k-medoid, k-center, and covering models have been formulated as 0-1 linear programs such as (8) to (12) and (14) to (18). The first is that such a formulation can lead to their optimal solution using methods such as branch and bound. Unfortunately, this approach is only feasible for small problems. Another reason is that such a formulation makes it possible to quite easily impose a particular structure on the clustering being sought. For example, adding a simple constraint can limit the number of objects in the clusters or can prevent some of the objects from being selected as representative objects. Integer programming techniques can then be used to find optimal or good solutions. For a survey of integer programming see, for example, Garfinkel and Nemhauser (1972).

5.3 Methods Based on the Construction of Central Points

In the methods considered in the previous section each cluster is characterized by a centrally located object called the representative object. In case the objects are defined by measurement values, there exists an alternative

way of characterizing a cluster, namely by its *centroid*. This approach has been used extensively in the literature as a basis for clustering algorithms.

The centroid of a cluster v is defined as a point in p-dimensional space found by averaging the measurement values along each dimension (variable). For instance, its fth coordinate is

$$\bar{x}_f(v) = \frac{1}{n_v} \sum_{i \in C_v} x_{if}$$

where C_v represents the set of indices of cluster v (which contains n_v objects). Therefore, the centroid of cluster v is given by

$$\bar{x}(v) = \left(\bar{x}_1(v), \bar{x}_2(v), \ldots, \bar{x}_p(v)\right)$$

We note two important facts: The centroid does not have to be one of the objects in the original data set, and it is not defined when the data are dissimilarities not based on interval-scaled measurement values.

A possible measure for the tightness of a cluster is the error sum of squares, defined as the sum of squares of (Euclidean) distances between the objects of a cluster and its centroid:

$$\mathrm{ESS}(C_v) = \sum_{i \in C_v} \sum_{f=1}^{p} \left(x_{if} - \bar{x}_f(v)\right)^2 \tag{19}$$

The error sum of squares of the whole clustering is

$$\mathrm{ESS} = \sum_{v=1}^{k} \mathrm{ESS}(C_v) \tag{20}$$

Therefore a possible approach to the clustering problem is to look for a partition into k nonempty subsets that minimize the error sum of squares. Methods that try to achieve this aim are called *variance minimization techniques*. (Observe that a similar objective could be attained in a variant of the k-medoid method, by entering the *squares* of the dissimilarities as input to PAM.)

Many variance minimization techniques have been proposed, but we will limit ourselves to two widely used ones. Let us start with a relatively simple method suggested by Forgy (1965). This method consists of the following steps:

1. An initial partition of the objects into k nonempty subsets is randomly generated. Then go to step 2. The method can also start with a

set of central points, called seed points, in which case one proceeds with step 3.

2. Compute seed points as the centroids of the clusters of the current partition.
3. Assign each object to the cluster with the nearest seed point. The seed points remain fixed for an entire pass through the set of objects. If this is the first pass through the objects, go to step 2. In subsequent passes the clustering is compared to the previous clustering and if no change in the assignment of objects has occurred, stop. If there has been a change, go to step 2.

An efficient program for the method can ensure that an object is only moved if it is strictly closer to a different seed point and therefore the error sum of squares must decrease. As the number of possible different clusterings is finite, this ensures that the method converges. However, it cannot be foreseen how many repetitions of steps 2 and 3 will be required to reach a (locally) optimal solution. According to Anderberg (1973), five to ten iterations (passes through steps 2 and 3) are sufficient in most practical situations. A shortcoming of this method, and of many other variance minimization techniques, is that during step 3 it is possible that all objects of a cluster are assigned to other clusters, and at the same time no other objects are assigned to the centroid of this cluster. In this way the algorithm sometimes ends up with less than k clusters. (Note that this problem cannot occur for the k-medoid method.)

In a variant of this method, proposed by Jancey (1966), the new seed points of the clusters are found (in step 2) by reflection of the old seed points with respect to the centroids. In this way the steps taken (by the seed points) are amplified and a locally optimal solution is usually found in fewer iterations.

The *k-means method* of MacQueen (1967) is probably the most widely applied nonhierarchical clustering technique. It is very similar to Forgy's method, the only difference being that each time an object changes clusters the centroids of both its old and new cluster are recalculated. This can be done quite easily using an update equation for the centroid coordinates. If object i is moved from cluster v to cluster w, the coordinates of the new centroids are given by

$$\bar{x}_f(v') = \frac{1}{n_v - 1}\left(n_v \bar{x}_f(v) - x_{if}\right)$$

and

$$\bar{x}_f(w') = \frac{1}{n_w + 1}\left(n_w \bar{x}_f(w) + x_{if}\right)$$

where v' and w' represent the new clusters.

As in Forgy's method, an object is only moved if it is nearer to the new centroid. Therefore the sum of squares of distances to the centroids must decrease. Furthermore, in general, the centroids of the newly formed clusters will not coincide with the old ones. As the centroid is the point which minimizes the sum of squares of distances, the total sum of squares will decrease by an even larger quantity. An interesting feature of MacQueen's method is that the number of clusters cannot change. The reason for this is that if only two objects are left in a cluster and one of these is removed, the centroid of the new cluster (which is now a singleton) coincides with its object. This object then cannot be assigned to a different cluster. Finally, a drawback of this method (as well as those of Forgy and Jancey) is that the results (sometimes strongly) depend on the order of the objects in the input file, unlike the algorithm in PAM.

Many more variance minimization algorithms have been published, such as the method of Friedman and Rubin (1967) which has frequently been applied. However, it is not our aim to give a complete enumeration of these algorithms.

One of the problems with variance minimization methods is the effect of *outliers* on the value of the function to be minimized (formula 20). This has been our principal motivation for selecting the k-medoid method for PAM. Another reason was the possibility of obtaining representative objects in the clusters, which is very appealing and useful in a wide range of applications. It should be added that a method was proposed by Cooper (1963) which makes use of the criterion of the k-medoid method [Eq. (8)], but in which the representative objects are replaced by general p-dimensional points. This method and related ones are discussed by Massart and Kaufman (1983) and by Späth (1980). In another variant, proposed by Diday (1971, 1974), more general central regions of clusters are considered, which can consist of one or more objects or p-dimensional points; they are the so-called kernels.

To conclude the discussion of variance minimization, we will consider a method that combines the search for a tight clustering (with small error sum of squares) with the determination of an "optimal" number of clusters. Almost none of the partitioning methods tackles the problem of finding an adequate (natural) number of clusters. Ball and Hall (1965) proposed a

method called ISODATA the main features of which are:

The method starts with a clustering into a given number k of clusters, according to the method of Forgy.

In a second step, outliers and very small clusters are eliminated; they are disregarded for the remainder of the method.

Then perform either a lumping (fusion) or splitting of one of the clusters. This is done according to the following rules:

- perform a lumping if the current number of clusters is more than $2k$
- perform a splitting if the current number of clusters is less than $k/2$
- otherwise alternate between lumping and splitting
- stop if the same clustering is obtained twice.

Return to the first step with the newly obtained number of clusters (which replaces k), unless the user-specified maximum number of iterations is reached.

During lumping, clusters are merged with centroids nearer to each other than the lumping threshold, while during splitting clusters are divided if the average sum of squares of dissimilarities is greater than the splitting threshold. If no clusters meet the desired criteria, the algorithm returns to the first step. ISODATA requires a considerable amount of input from the user, which implies that the user already has some knowledge of the structure of the data set. According to Anderberg (1973), who discusses several versions of ISODATA and gives many references, the method is too elaborate to be used without periodic human intervention.

The methods of Ball and Hall (1965), Forgy (1965), Jancey (1966), and MacQueen (1967) are among the numerous methods implemented in the CLUSTAN package (Wishart, 1978).

The literature also contains some interesting special cases of variance minimization. Several algorithms have been proposed for the one-dimensional case in which a much smaller number of partitions has to be considered. The number of partitions that must be considered when partitioning a set of objects is a type 2 Stirling number. For n objects and k clusters it is of the order of $k^n/k!$, for example, 50 objects can be clustered into five clusters in approximately 7.4×10^{32} different ways. A complete enumeration of all partitions is clearly impossible except for very small clustering problems. Fisher (1958) has shown that for one-dimensional data the optimal clusters for the error sum of squares criterion must be contiguous; this of course reduces drastically the number of partitions to be

considered. Fisher proposed an algorithm for this case. He also extended the method to multidimensional data for which there exists a known complete ordering of the objects. This method is especially useful for the analysis of time series. Work along the same lines can be found in the paper by Vinod (1969). Another interesting special case is the clustering into two subsets ($k = 2$), which can serve as a basis for a divisive hierarchical method (see Chapter 6). An extensive discussion of these situations as well as many other nonhierarchical methods can be found in Bock (1974).

5.4 Some Other Nonhierarchical Methods

In two or three dimensions, an observer can distinguish clusters mainly on the basis of an impression of the density of objects in different areas. In particular, a cluster is often defined as a region in which the density of objects is locally higher than in other regions. Many clustering algorithms have been proposed which use the density of objects to construct clusters. Two general approaches have been used for a definition of this concept. In a first type of method, the density near an object is defined as the number of objects within a sphere (around this object) with a fixed radius R. Sometimes the objects are weighted by their dissimilarity to the central object being considered. In another approach, the density is defined as the inverse of the dissimilarity to the Tth nearest object or the inverse of the average dissimilarity to the T nearest objects. In both approaches there is an arbitrary element. In the first it is the radius R of the sphere and in the second it is the number T of objects considered. A too large value of R or of T will lead to a too small number of clusters. The most frequently applied density seeking method is Wishart's mode analysis (Wishart, 1969a) which attempts to isolate and remove outliers and to detect dense regions of space in which clusters of objects can be found. Based on this approach Wishart proposes two algorithms, one hierarchical and the other nonhierarchical. Another approach, used by Wolfe (1970) and Coomans and Massart (1981), is based on the search for k multivariate distributions and the determination of the most probable population for each object. An extensive discussion of density seeking methods can be found in the book by Chandon and Pinson (1981).

The vast majority of clustering methods are designed to classify a set of objects characterized by measurements of one or more variables. The same methods can be used to cluster a set of *variables* using their values on a given set of objects. In this situation one uses other types of dissimilarity measures, such as those based on correlation coefficients, but once the dissimilarities have been calculated the same algorithms can be used. However, the separate classification of objects (or variables) is sometimes

inadequate for finding relationships that can exist between groups of objects and groups of variables. For example, it is quite probable that the clustering of the objects would be different for different subsets of variables; this picture might become blurred if all variables are considered together. In order to discover relationships between subsets of objects and subsets of variables, methods are required that cluster objects and variables simultaneously. These are called two-way or block clustering methods. Hartigan (1972, 1975) and Good (1965) have proposed hierarchical methods for block clustering, while Kaufman and Plastria (1981) have introduced a partitioning algorithm. The subject of block clustering is discussed in some detail by Chandon and Pinson (1981).

5.5 Why Did We Choose the *k*-Medoid Method?

As mentioned in Section 5.3, the objective chosen in the *k*-medoid method is appealing because it is more robust than the error sum of squares employed in most methods. (The maximal dissimilarity used in the *k*-center method is even less robust.) Furthermore it allows a good characterization of all clusters that are not too elongated and makes it possible to isolate outliers in most situations.

As will be seen in later chapters, one of the themes of this book is the preference given to methods based on *average dissimilarities* instead of sums of squares of dissimilarities. Indeed, the *k*-medoid method minimizes the average dissimilarity of the objects to the representative objects they are assigned to. Our preference for average distances is also apparent in the choice of standardization of the variables, in which the mean absolute deviation is used and not the more classical standard deviation (see Section 2 of Chapter 1). In many branches of univariate and multivariate statistics it has been known for a long time that methods based on the minimization of sums (or averages) of dissimilarities or absolute residuals (the so-called L_1 methods) are much more robust than methods based on sums of squares (which are called L_2 methods). The computational simplicity of many of the latter methods does not make up for the fact that they are extremely sensitive to the effect of one or more outliers. [The effect of error perturbation on clustering algorithms was already examined by Milligan (1980), but his study did not contain the *k*-medoid method.]

Also note that the clustering found by PAM does not depend on the order in which the objects are presented (except when equivalent solutions exist, which very rarely occurs in practice). This is not the case for many other algorithms described in this section. Also, if we ask for k clusters we do obtain exactly k clusters, and not less.

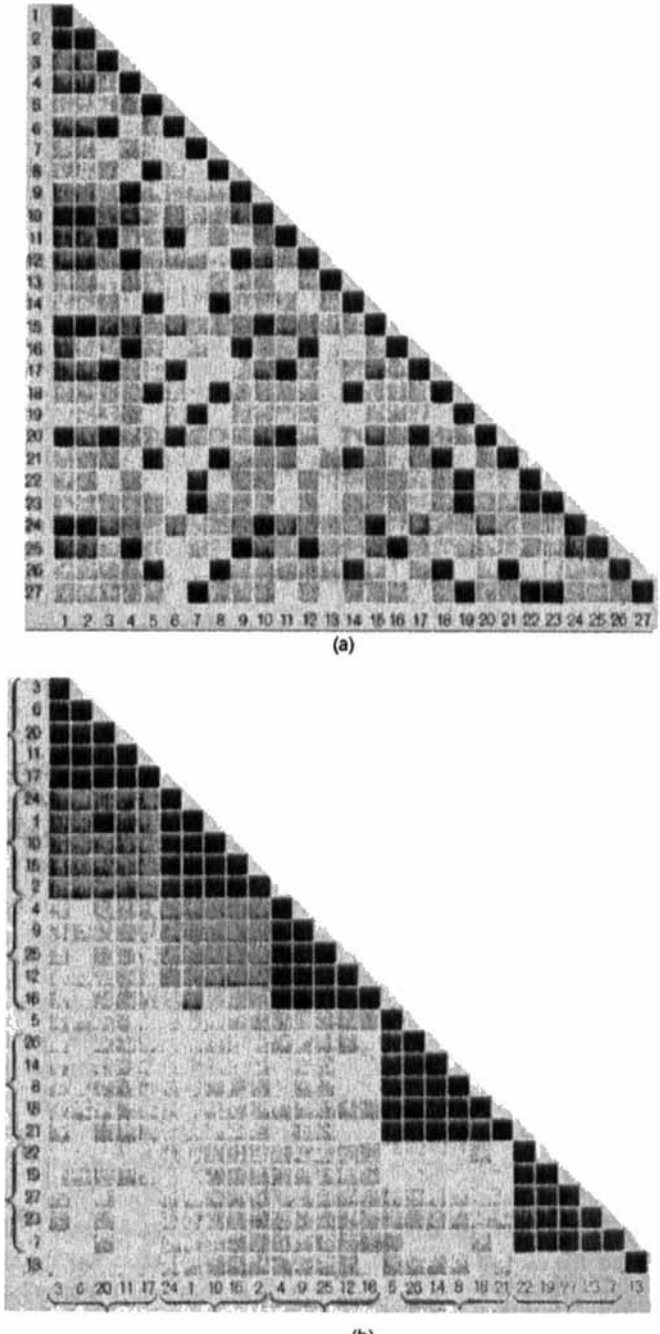


Figure 15 Shaded dissimilarity matrix of 27 objects: (a) In random order. (b) Ranked according to clusters (from Sokal, 1966).

The L_1 method described here is invariant with respect to translations and orthogonal transformations of the data points, but not with respect to affine transformations which change the interobject distances. However, we wanted to construct a method able to deal with general dissimilarity data, to which the notion of affine invariance does not apply. In fact, the affine invariant clustering methods in the literature make use of geometric notions (like centroids or tolerance ellipsoids) which do not exist for dissimilarity data. On the other hand, the medoids always exist, even when the data are only a collection of dissimilarities (see also Kaufman and Rousseeuw, 1987).

5.6 Graphical Displays

Whereas for hierarchical clustering (Chapters 5, 6, and 7) various versions of the dendrogram have been proposed and widely used to represent clustering results in a graphical way, for nonhierarchical methods relatively little has been done in the way of graphics. The main reason is that the tree-like structure yielded by hierarchical algorithms is suitable for an appealing graphical representation.

To display a partition, one of the approaches consists of a graphical representation of the matrix of dissimilarities between objects. The general idea consists of two phases. In the first phase the dissimilarities are replaced by symbols that give an impression of their magnitude. For example, black squares might represent small dissimilarities, white squares large dissimilarities, and shades of grey intermediate values. In a second phase, permutations of the objects are carried out (which change the rows and columns of the matrix) in such a way that the smallest dissimilarities are found close to the diagonal. Sokal (1966, p. 110) gave an interesting example, which is reproduced in Figure 15. A display like this can be generated automatically and drawn with a line printer. Recently, Gale, Halperin, and Costanzo (1984) proposed a more refined version based on so-called unclassed choropleth mapping.

Wainer (1983) gives a survey of methods for displaying multivariate data, in which each object is represented by an icon (such as a polygon), made up of parts that vary in size or shape with the measured attributes. Also some techniques are mentioned for allowing tables to communicate the data structure in a more efficient way, such as rounding, reordering, and blocking. Applying the latter to the dissimilarities between 12 countries (of Table 5) yields Figure 16, given to us by Howard Wainer (personal communication).

Another approach is to represent a partition using a diagram in which the groups are displayed as circles. Lines between the groups denote their

	B	*E*	*F*	*Is*	*US*	*Bzl*	*In*	*Z*	*Ch*	*Cu*	*U*
Belgium											
Egypt	5										
France	2	5									
Israel	3	5	4								
USA	3	5	2	3							
Brazil	6	5	6	6	5						
India	6	5	6	6	6	5					
Zaire	5	5	6	6	6	3	5				
China	7	8	7	6	6	7	6	6			
Cuba	7	6	7	6	7	7	6	7	4		
USSR	6	6	6	7	6	7	6	7	4	3	
Yugoslavia	5	6	5	6	7	7	6	7	5	4	4

Figure 16 Dissimilarities between 12 countries, with reordered objects and rounded entries, blocked according to clustering structure.

global dissimilarity. In one of these techniques, proposed by Carmichael and Sneath (1969) and called the method of *taxometric maps*, the diameter of a circle representing a cluster is proportional to the diameter of the cluster. Clusters with only one object are represented by points. It is attempted to place the clusters in the map in such a way that the distances between them are proportional to their actual distance (as defined by the clustering algorithm). For the pairs of clusters for which this is possible, a straight full line is drawn. When the distance on the map exceeds the actual distance, the straight line is divided into a full part of correct length and dashes for the remainder, and when it is too small a V-shaped line of correct length is drawn. An example is given in Figure 17. Taxometric maps are complementary to silhouettes because they depict the relationship between clusters but not the behavior of the individual objects within those clusters.

With the silhouettes defined by Rousseeuw (1987) it is possible to obtain more information on the objects themselves. The height of the silhouette of a cluster is proportional to the number of objects, while its width gives a picture of its tightness with respect to the other clusters. Furthermore,

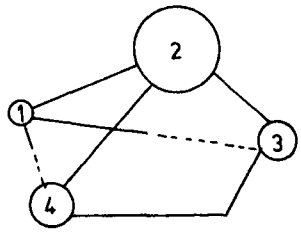


Figure 17 An example of a taxometric map.

information is immediately perceived concerning the individual objects. For example, a small (or even negative) value $s(i)$ denotes an object located at the outskirt of the cluster, whereas a value close to 1 shows the object to be centrally located. [In this way the $s(i)$ value can be compared with a correlation coefficient.] By looking at the neighbors one can find the objects located between two clusters. Additional information is given by the average silhouette width $\bar{s}(k)$ over the whole data set. This value can be used as a criterion to select the optimal number of clusters, but is by no means the only combination of $s(i)$ that could be computed for this purpose: One might also use transformations, medians, and so on. Like most validity coefficients, $\bar{s}$ could be used as an objective function for the clustering itself (that is, one might want to find a clustering that maximizes $\bar{s}$). Another idea would be to define $s(i)$ simply by $1 - a(i)/b(i)$, so $s(i)$ could become much smaller than -1, thereby penalizing misclassified points to a larger extent. Several other variants of the definition of $s(i)$ are possible. For instance, one could replace $a(i)$ and $b(i)$ of Eq. (6) by medians of dissimilarities (instead of average dissimilarities) in order to obtain more robustness. Also, when the clustering method is based on the selection of representative objects or the construction of central points, one could use the dissimilarities to these privileged entities in order to avoid the (lengthy) computation of average dissimilarities. However, we prefer the present definition because it only depends on the partition itself and not on the method used to construct it.

Silhouettes might be displayed in different ways, for instance, by using more sophisticated plotting devices instead of a line printer. One could also plot the negative $s(i)$ [we have not done so in PAM because very negative $s(i)$ rarely occur, and we wanted to use the width of the plot to its fullest advantage].

Recently, Edmonston (1986) proposed a graphical display that is very similar to the silhouette plot. It is called a clustergram and also contains a separate panel for each cluster. Each object is again represented by one printed line, in which two quantities are combined: the object's distance to the nearest object of another cluster (which is a kind of "neighbor") and the distance to the object's own cluster centroid.

The *distance graph* was proposed and used by Chen, Gnanadesikan, and Kettenring (1974) with further applications and developments by Cohen et al. (1977), Gnanadesikan, Kettenring, and Landwehr (1977, 1982), and Chambers and Kleiner (1982). For each cluster centroid, they plot the distances of every entity from that centroid (the symbol plotted is the cluster to which the entity was assigned). Figure 18 is an example of a distance graph. Although such a display gives an indication of the internal cohesiveness of a cluster, it does not allow the study of individual objects

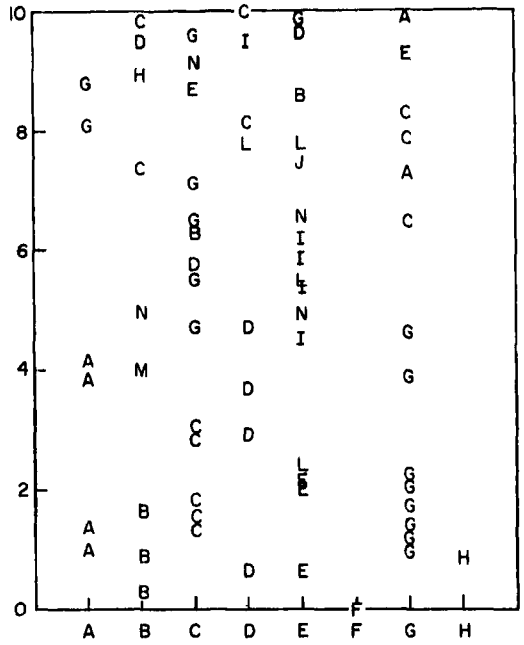


Figure 18 A distance graph of eight clusters (from Cohen et al., 1977). The centroids are listed on the horizontal axis. Distances of objects to these centroids are given on the vertical axis. The plotting symbol (*A* to *H*) identifies the cluster to which the object belongs.

because they remain anonymous in each list. Other variants display the (average) distances between the whole clusters, without further regard to the objects themselves. For a recent sociological application, see Andes (1985).

Another development is the introduction of *cluster validity profiles* (Bailey and Dubes, 1982). Although their name might suggest otherwise, the silhouettes proposed in this book are not related to these profiles. The latter displays are based exclusively on the ranks of the $n(n-1)/2$ entries of the triangular dissimilarity matrix. They originate from a method to investigate the validity of a certain clustering by means of formal testing against some null hypothesis. The adopted null hypothesis is due to random graph theory and states that the matrix of ranks of dissimilarities is chosen randomly from a uniform distribution on all $[n(n-1)/2]!$ possible rank matrices, supposing that there are no ties. A probability profile for a cluster shows, for each rank, the probability that an index of clustering is at least as good as the observed index (under the null hypothesis already specified). The resulting plots are drawn in function of dissimilarity ranks, whereas silhou-

ettes are drawn in function of the objects of the cluster. Profiles differ from silhouettes in an essential way because they are used with ordinal dissimilarities whereas silhouettes are constructed from dissimilarities on a ratio scale. Also their roots are different: Profiles are based on hypothesis testing in a mathematical framework, whereas silhouettes are developed as data analytical tools which are useful mainly because of their simplicity and intuitive appeal.

Finally Dunn and Landwehr (1976, 1980) proposed graphical representations for the changes in cluster characteristics when two clusterings are carried out on the same data set (for example, at two different time periods or with two sets of variables). Another problem discussed by these authors is the representation of relationships between clusters and one or several exogeneous variables (that is, variables not employed in the clustering).

The topic of graphical representation of clustering results has so far received too little attention in the literature. Some books on clustering do not even mention the subject. The most comprehensive discussion can be found in a book by Everitt (1978) on graphical techniques for multivariate data. Some general methods for the graphical representation of multivariate data, like Andrews' plots (1972), biplots (Gabriel, 1971), Chernoff's faces (1973), and Wegman's parallel coordinates (1985), frequently allow identification of clusters. Our own program CLUSPLOT, displaying the size, shape, and relative positions of the clusters, is briefly discussed in Section 4 of the Appendix.

EXERCISES AND PROBLEMS

1. Edwards and Cavalli-Sforza (1965) considered the following dissimilarity matrix between six families of bacteria:

	A	*B*	*C*	*D*	*E*	*F*
A	0					
B	5	0				
C	11	10	0			
D	11	6	6	0		
E	14	13	17	13	0	
F	14	15	21	15	6	0

Partition these data into two clusters with PAM and check that both are L^*-clusters. What is the "best" number of clusters according to the silhouettes? (Try all values of k.)

2. Show that for one-dimensional data the choice of a distance function (Euclidean or Manhattan) and of the standardization option has no effect on the clustering found by PAM.

3. Show that if a k-medoid clustering contains a doubleton (a cluster consisting of two objects), either object can be chosen as the medoid of that cluster.

4. The k-medoid method allocates objects to the nearest medoid. Give a geometrical interpretation of this fact when the data are two-dimensional and $k = 2$, by drawing the line which forms the boundary between the regions determined by both medoids. Do the same for two-dimensional data when $k = 3$.

5. Consider the countries data of Table 5. Multiply all dissimilarities by a constant factor (e.g., 5). Then use the program PAM to partition the countries into three clusters and compare the results with those described in Section 3. Repeat the exercise after adding a constant (e.g., 10) to each of the original dissimilarities.

6. Consider the following data set consisting of 28 two-dimensional points:

$$\begin{array}{lllllll} (0,1) & (0,2) & (0,3) & (1,0) & (1,1) & (1,2) & (1,3) \\ (1,4) & (1,8) & (1,9) & (2,1) & (2,2) & (2,4) & (2,7) \\ (2,9) & (3,3) & (3,5) & (3,7) & (3,8) & (4,4) & (4,6) \\ (4,7) & (5,4) & (5,5) & (5,6) & (6,3) & (6,4) & (6,5) \end{array}$$

   (a) Make a plot of these points.
   (b) Cluster this data set into two clusters by means of PAM, with the options "no standardization" and "Euclidean distance."
   (c) Repeat the clustering using only the first variable and then using only the second variable. Show that both variables are necessary to retrieve the cluster structure.

7. Cluster the squares of the integers between 0 and 50 (i.e., $0, 1, 4, 9, 16, 25, \ldots, 2500$) into 2 to 10 clusters by means of PAM.

8. Consider the dissimilarity matrix (4) in Section 2.
   (a) Cluster these data by means of PAM for $k = 2$.
   (b) If you have access to a program for multidimensional scaling (MDS), construct a two-dimensional representation of the five

objects characterized by (4). Indicate the clustering obtained by PAM on this plot and compare with the information obtained from the silhouettes.

9. Consider the artificial data set of Figure 1 of Chapter 4 (the actual data are listed in Section 2.1 of that chapter). Cluster these objects with PAM for $k = 3$, using the options "no standardization" and "Euclidean distance." What happens with the intermediate objects 6 and 13?

10. Atypical objects usually become singleton clusters. If too few clusters are requested, these objects are (wrongly) grouped with some other objects. A particular type of atypical object are the so-called bridges. These are objects located in between two or more clusters. Suppose too few clusters have been requested and a bridging object i has been assigned to one of the clusters. Can this be recognized from the values of $a(i)$ and $b(i)$ used to construct the silhouette for this object?

11. Show that for a one-dimensional data set the k-medoid clustering consists of contiguous clusters.

12. Show that when two clusters are required, the algorithm used in the program PAM always yields the exact minimum of the objective function.

13. (Research.) Construct a k-medoid algorithm for the special case of one-dimensional data, making use of the fact that all clusters must be contiguous. It is advisable to begin by sorting the observations in increasing order, because this allows one to exclude many possible clusters. Another simplification in one dimension is that there is no longer a need to store all distances between objects in central memory because the distances can easily be computed along the way. The program will therefore need little storage space.

Finding Groups in Data: An Introduction to Cluster Analysis
Leonard Kaufman and Peter J. Rousseeuw

CHAPTER 3

Clustering Large Applications (Program CLARA)

1 SHORT DESCRIPTION OF THE METHOD

The k-medoid partitioning method described in the previous chapter yields very satisfactory results in many situations. However, as can be gathered from the time and memory requirements discussed in Section 4 of that chapter, the program PAM is not practical for clustering large data sets. For this reason a method was constructed especially adapted to large applications (Kaufman and Rousseeuw, 1986). This method, which is also based on the k-medoid approach, has been implemented in the program CLARA (abbreviated from Clustering LARge Applications) that is the subject of this chapter.

The clustering of a set of objects with CLARA is carried out in two steps. First a sample is drawn from the set of objects and clustered into k subsets using the k-medoid method, which also gives k representative objects (this is done with the same algorithm as in PAM). Then, each object not belonging to the sample is assigned to the nearest of the k representative objects. This yields a clustering of the entire data set. A measure of the quality of this clustering is obtained by computing the average distance between each object of the data set and its representative object. After five samples have been drawn and clustered, the one is selected for which the lowest average distance was obtained.

The resulting clustering of the entire data set is then analyzed further. For each cluster, CLARA gives its size and its medoid and prints a complete list of its objects. Also a graphical representation of the clustering is provided, by means of the silhouettes that have been described in Section

2 of the previous chapter. (This is done for the selected sample, because a silhouette plot of the entire data set would become too large to be useful and also consume too much computational effort.)

It turns out that CLARA can deal with much larger data sets than can PAM: On an IBM/XT with 8087 coprocessor, we could easily cluster 2000 to 3000 objects.

2 HOW TO USE THE PROGRAM CLARA

The method briefly described in Section 1 can be applied by using the program CLARA, which is operated in much the same way as the program PAM of the previous chapter. The internal structure of CLARA can be found in Section 4 below. Details about the compilation and the implementation are given in the Appendix. The use of the program is quite simple: After evoking the file CLARA.EXE the selected options are entered interactively by the user. The data set is input by reading a file from a disk. The output of the program can be directed to the screen, to a printer, or to a disk. In the next subsection we will show a typical interactive session. Because the program is very similar to PAM, only those questions and options different from that program will be discussed in detail. In Section 2.2 we will look at the interpretation of the output. The treatment of missing values is explained in Section 2.3.

2.1 Interactive Use and Input

Starting up the program yields the following screen:

```
CLUSTERING LARGE APPLICATIONS

THE PRESENT VERSION OF CLARA CAN HANDLE DATA SETS WITH AT
LEAST 100 OBJECTS, AND AT MOST 3500 (IF FEWER THAN 100 OBJECTS
ARE TO BE CLUSTERED PLEASE USE THE PROGRAM PAM)

HOW MANY OBJECTS ARE TO BE CLUSTERED ?
-------------------------------------
PLEASE GIVE A NUMBER OF AT LEAST 100,  AND AT MOST 3500 : 1000
```

It should be noted here that CLARA stores the measurements in a single array of 3500 elements. This makes it possible to be flexible concerning the

size of the problems that the program can deal with. Only the total number of measurements must be taken into account. For example, one can solve problems with 100 objects and 35 variables and also problems with 3500 objects and a single variable.

```
CLARA CAN HANDLE UP TO 30 CLUSTERS.
HOW MANY CLUSTERS ARE WANTED ?
-------------------------------
PLEASE ENTER A NUMBER BETWEEN 1  AND 30 : 2
```

In CLARA only a fixed number of clusters may be requested. If several clusterings are wanted, repeated runs must be carried out.

```
IN THE PRESENT VERSION OF THE PROGRAM UP TO 150 VARIABLES
CAN BE ENTERED.
(IF  MORE  ARE  NEEDED,  THE  ARRAYS  INSIDE  THE  PROGRAM
 MUST BE ADAPTED)
WHAT IS THE TOTAL NUMBER OF VARIABLES IN YOUR DATA SET ?
-------------------------------------------------------
PLEASE GIVE A NUMBER BETWEEN 1 AND 150 : 8
```

CLARA only allows input of measurements and not of a dissimilarity matrix. Indeed, one of the problems of clustering large data sets is the size of the dissimilarity matrix. It was therefore decided not to reserve a large memory array for the dissimilarities. (The only dissimilarity matrix used in the program is the one between the elements of each sample, which is much smaller than the matrix for the entire data set.) Also note that the measurements are always read from a file, as the data sets are too large to enter them with the keyboard during an interactive session.

```
HOW MANY VARIABLES DO YOU WANT TO USE IN THE ANALYSIS ?
------------------------------------------------------
(NOTE THAT THE NUMBER OF VARIABLES MAY NOT EXCEED 3
 BECAUSE THE PROGRAM CAN STORE AT MOST 3500 MEASUREMENTS)
PLEASE ENTER A NUMBER BETWEEN 1 AND 3 : 3
VARIABLE TO BE USED:   POSITION   LABEL (AT MOST 10
                                  CHARACTERS)
-------------------------↓↓↓↓-----↓↓↓↓↓↓↓↓↓↓--------
NUMBER 1 :                1       var1
NUMBER 2 :                2       var2
NUMBER 3 :                3       var3
```

DO YOU WANT THE MEASUREMENTS TO BE STANDARDIZED ? (PLEASE ANSWER YES) OR NOT ? (THEN ANSWER NO) . . . . . yes

DO YOU WANT TO USE EUCLIDEAN DISTANCE ?
(PLEASE ANSWER E)
OR DO YOU PREFER MANHATTAN DISTANCE ?
(THEN ANSWER M) . . . . . e

PLEASE ENTER A TITLE FOR THE OUTPUT (AT MOST 60 CHARACTERS)

DATA SET WITH 1000 OBJECTS AND 8 VARIABLES

HOW MUCH OUTPUT DO YOU WANT ?
SMALL OUTPUT (PLEASE ANSWER 0)
MEDIUM SIZED OUTPUT (PLEASE ANSWER 1) :
INCLUDES DETAILS ON CLUSTERING
OR LARGE OUTPUT (PLEASE ANSWER 2) :
ALSO INCLUDES DETAILS ON THE DATA 0

DO YOU WANT GRAPHICAL OUTPUT (SILHOUETTES) ? PLEASE ANSWER YES OR NO : yes

DO YOU WANT TO READ THE DATA IN FREE FORMAT ?

THIS MEANS THAT YOU ONLY HAVE TO INSERT BLANK(S) BETWEEN NUMBERS.
(NOTE: WE ADVISE USERS WITHOUT KNOWLEDGE OF FORTRAN FORMATS TO ANSWER YES.)
MAKE YOUR CHOICE (YES/NO) . . . . . yes

PLEASE GIVE THE NAME OF THE FILE CONTAINING THE DATA (e.g. TYPE A:TEST.DAT) B:EX1000.DAT

WHERE DO YOU WANT YOUR OUTPUT ?

TYPE CON IF YOU WANT IT ON THE SCREEN
OR TYPE PRN IF YOU WANT IT ON THE PRINTER
OR TYPE THE NAME OF A FILE (e.g. B:EXAMPLE.OUT)
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME NAME THEN THE OLD FILE WILL BE OVERWRITTEN.)
WHAT DO YOU CHOOSE ? B:EX1000.RES

CAN MISSING DATA OCCUR IN THE MEASUREMENTS ?
PLEASE ANSWER YES OR NO . . . . . no

The situation of missing data is discussed in Section 2.3. It implies further input with detailed information concerning missing value codes and also adapted formulas for the computation of standardized measurements and distances.

```
DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
TITLE : DATA SET WITH 1000 OBJECTS AND 8 VARIABLES
THERE ARE 1000 OBJECTS
THE OBJECTS WILL BE CLUSTERED INTO 2 CLUSTERS
SMALL OUTPUT IS WANTED
GRAPHICAL OUTPUT IS WANTED (SILHOUETTES)

THERE ARE  8 VARIABLES IN THE DATA SET,
  AND  3 OF THEM WILL BE USED IN THE ANALYSIS
THE MEASUREMENTS WILL BE STANDARDIZED
EUCLIDEAN DISTANCE WILL BE USED
THERE ARE NO MISSING VALUES
THE MEASUREMENTS WILL BE READ IN FREE FORMAT
YOUR DATA RESIDE ON FILE : B:EX1000.DAT

YOUR OUTPUT WILL BE WRITTEN ON : B:EX1000.RES

ARE ALL THESE SPECIFICATIONS OK ? YES OR NO : yes
```

It should be noted here that the input for CLARA is almost identical to that of PAM (and also FANNY, AGNES, and DIANA). The differences are that in CLARA there are no labels of objects, only measurement input is allowed, and only a fixed number of clusters may be requested. Also note that if a data set of measurements is used for PAM and objects are added so that PAM cannot be used any more (because of either memory or computation time problems), the same input file is suitable for CLARA.

2.2 Output

The output generated by CLARA is divided into the following parts:

a. Identification of the Program and Selected Options
The output starts with the identification "CLUSTERING LARGE APPLICATIONS" and a list of options that were chosen by the user.

b. Standardized Measurements
If the measurements are standardized and large output is requested, the transformed measurement values are outputted. They are then accompanied

```
**********************************
*                                *
*  CLUSTERING LARGE APPLICATIONS *
*                                *
**********************************

DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 TITLE : DATA SET WITH 1000 OBJECTS AND 8 VARIABLES
 THERE ARE 1000 OBJECTS
 THE OBJECTS WILL BE CLUSTERED INTO    2 CLUSTERS
 SMALL OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (SILHOUETTES)

 THERE ARE     8 VARIABLES IN THE DATA SET,
  AND    3 OF THEM WILL BE USED IN THE ANALYSIS
 These variables are :
          var1          (POSITION :  1)
          var2          (POSITION :  2)
          var3          (POSITION :  3)
 THE MEASUREMENTS WILL BE STANDARDIZED
 EUCLIDEAN DISTANCE WILL BE USED
 THERE ARE NO MISSING VALUES
 THE MEASUREMENTS WILL BE READ IN FREE FORMAT

 YOUR DATA RESIDE ON FILE        : b:ex1000.dat

 VARIABLE var1       HAS AVERAGE       5.287    MEAN DEVIATION       4.977
 VARIABLE var2       HAS AVERAGE       5.326    MEAN DEVIATION       4.997
 VARIABLE var3       HAS AVERAGE       5.357    MEAN DEVIATION       4.978
```

Figure 1 CLARA output, parts a and b.

by the mean value and mean deviation of each variable, given by (2) and (3) of Chapter 1. Note that we chose to compute the mean value and mean deviation instead of more robust summary values (such as the median and the median deviation) because the former each need only a single pass through the objects and no additional arrays are required. This is particularly important for CLARA, in which the total computation time and storage are merely linear in the number of measurements. An example of parts a and b of the output is given in Figure 1.

c. Output Concerning Each Sample

This part of the output contains:

- A list of objects in the sample (the number of objects in each sample is $40 + 2k$, where k is the number of clusters).
- The average distance obtained from BUILD (this is merely an initial result of our k-medoid algorithm).
- The average distance obtained from SWAP (called the final result for this sample).

These values are the average distances between each object of the sample and its most similar representative object.

```
*********************************************
*                                           *
*  NUMBER OF REPRESENTATIVE OBJECTS     2   *
*                                           *
*********************************************


SAMPLE NUMBER     5
*****************

 RANDOM SAMPLE =
         5     25     93    161    189    191    208    225    242    308
       331    342    360    382    390    400    421    432    437    444
       463    506    528    547    613    641    747    760    777    785
       795    801    803    840    865    877    881    884    891    948
       954    955    976    992

 RESULT OF BUILD FOR THIS SAMPLE
   AVERAGE DISTANCE  =          .341

 FINAL RESULT FOR THIS SAMPLE
   AVERAGE DISTANCE  =          .317

 RESULTS FOR THE ENTIRE DATA SET
   TOTAL DISTANCE    =       328.923
   AVERAGE DISTANCE  =          .329

 CLUSTER SIZE MEDOID    COORDINATES OF MEDOID (STANDARDIZED MEASUREMENTS)

       1  530    840          .92        .89        .98

       2  470    161        -1.14      -1.14      -1.04

 AVERAGE DISTANCE TO EACH MEDOID
         .325       .333

 MAXIMUM DISTANCE TO EACH MEDOID
         .664       .785

 MAXIMUM DISTANCE TO A MEDOID DIVIDED BY MINIMUM
 DISTANCE OF THE MEDOID TO ANOTHER MEDOID
         .188       .223
```

Figure 2 CLARA output, part c (concerning one of the samples).

The total and average distance for the entire data set.

For each cluster the following information is given:

- its number of objects (size) in the entire data set
- its medoid
- the coordinates of the medoid (when standardization was requested, the standardized coordinates are given)

The following clustering characteristics of each cluster:

- the average distance to the medoid
- the maximum distance to the medoid
- the maximum distance to the medoid, divided by the minimum distance of the medoid to another medoid: This value gives an idea of the isolation of the cluster.

An example of the output concerning one sample is given in Figure 2.

d. Final Results

The list of objects in the selected sample, and the average distance for the entire data set are given.

The clustering vector (for the entire data set): The jth element of this array is the number of the cluster to which object j belongs (the clusters are numbered in such a way that when reading the vector from left to right, the clusters are encountered in ascending order).

If medium sized or large output is requested, a list of objects of each cluster is given (all objects of the data set are included).

The clustering characteristics of the final partition of the entire data set.

For an example of part d of the output, see Figure 3.

```
FINAL RESULTS
*************

SAMPLE NUMBER   5 WAS SELECTED, WITH OBJECTS =
        5      25      93     161     189     191     208     225     242     308
      331     342     360     382     390     400     421     432     437     444
      463     506     528     547     613     641     747     760     777     785
      795     801     803     840     865     877     881     884     891     948
      954     955     976     992

AVERAGE DISTANCE FOR THE ENTIRE DATA SET =          .329

CLUSTERING VECTOR
*****************

  1  2  2  1  1  2  2  1  2  1  1  1  1  1  2  2  1  2  1  1  1  2  1  1  1
  2  2  2  1  2  2  2  2  1  1  2  1  1  1  2  1  1  1  2  1  2  2  2  2  1
  2  2  2  1  1  2  1  2  2  2  1  1  2  1  2  1  1  1  1  1  2  1  1  2  1
  1  2  1  1  2  2  2  2  2  1  2  1  2  1  2  2  2  1  1  2  2  2  2  1  2
  1  1  2  1  2  1  1  2  1  2  2  1  1  1  1  1  2  1  2  1  1  2  2  1  1
  1  2  2  1  2  1  1  2  2  1  1  2  1  1  1  1  2  1  2  1  1  1  1  2  1
  1  2  1  1  2  1  1  1  1  2  2  1  2  1  1  2  2  1  2  1  1  1  2  2  1
  2  1  1  1  1  1  2  1  1  1  2  2  1  1  1  2  2  2  1  2  2  1  2  1  1
  1  2  1  1  1  1  1  1  1  2  1  1  2  2  1  2  1  1  2  1  1  2  2  2  1
  2  2  1  2  1  2  2  1  1  2  1  1  2  2  2  2  2  1  1  1  1  1  1  1  1
  1  1  2  1  1  1  2  2  2  1  2  1  1  1  2  1  1  1  2  1  2  1  1  1  2
  1  2  1  1  2  2  2  2  2  2  2  2  1  2  1  2  1  2  1  1  2  1  1  1  2
  2  1  1  1  2  1  1  1  1  1  1  2  1  1  2  2  1  2  1  1  1  2  2  1  1
  2  2  2  2  1  1  2  1  1  2  1  1  1  2  2  1  2  2  1  1  1  1  2  1  2
  1  1  2  1  2  2  1  1  2  2  2  1  2  1  (  1  2  2  1  1  1  2  1  2  1
  1  2  2  2  2  2  2  2  1  1  1  2  2  2  1  1  1  1  2  1  1  2  1  1  1
  2  2  2  1  2  1  2  2  2  1  1  2  2  2  2  2  1  1  2  2  1  2  1  1  2
  2  1  2  1  2  1  1  2  2  1  1  1  1  1  1  1  2  1  1  1  1  2  2  2  1
  2  2  2  2  1  2  1  2  2  2  2  1  2  1  2  1  1  1  1  2  2  2  2  1  1
  1  2  1  2  1  2  2  2  2  1  1  1  1  1  2  2  1  2  1  2  2  2  1  1  1
  1  1  2  2  2  1  2  1  1  2  2  1  1  1  1  1  2  1  2  2  1  1  2  1  1
  2  1  1  2  2  2  2  2  2  1  1  2  1  2  2  2  2  2  1  1  1  2  2  1  2
  2  2  2  1  2  1  1  2  1  2  1  2  2  1  1  2  2  1  2  1  1  2  2  1  1
  1  1  1  1  2  1  1  2  1  2  1  1  2  1  1  1  2  2  1  2  2  2  1  1  2
  2  1  1  1  2  2  1  1  1  2  2  1  1  1  2  1  1  1  2  1  1  2  2  2  2
  1  1  2  2  1  1  2  1  1  2  1  2  1  2  2  2  1  1  2  1  1  1  1  1  1
  2  1  2  2  2  1  2  1  1  1  2  1  1  1  2  1  1  2  2  2  2  1  2  1  1
  1  2  1  1  2  1  1  1  1  1  1  2  2  2  2  1  1  1  2  1  1  2  2  1  1
  1  1  1  2  2  1  1  1  1  2  2  2  1  2  2  2  1  1  2  2  2  2  2  1  1
  2  2  2  2  1  2  2  1  1  2  1  1  2  2  2  2  1  2  2  1  2  2  1  2  2
  1  2  1  1  2  2  1  2  2  1  1  2  2  2  1  2  2  1  1  1  1  1  2  1  2
  2  2  2  1  2  1  2  1  2  2  2  2  2  1  2  2  2  1  2  1  1  2  1  1  2
  1  2  1  1  2  1  2  2  1  2  2  1  2  1  1  2  2  2  2  1  2  1  2  2  1
  2  2  2  2  2  1  1  2  2  1  1  1  1  1  1  1  1  2  2  2  2  2  2  1  2
  1  2  1  1  2  1  2  2  1  2  1  2  1  1  1  2  2  2  2  1  2  1  1  1  1
  2  1  2  1  1  1  1  1  2  1  1  2  1  2  2  2  1  1  1  1  1  2  1  1  2
  1  2  2  2  1  2  1  2  2  1  1  2  2  1  1  2  2  2  1  1  2  2  2  2  1
  2  1  2  2  2  1  1  2  2  1  2  1  1  2  2  2  1  2  1  1  2  1  2  1  1
  1  2  1  1  1  1  2  1  2  1  2  2  1  1  2  2  1  2  2  1  1  1  2  2  2
  2  1  1  2  1  1  1  2  2  1  2  1  1  2  1  1  1  1  1  1  1  2  1  1  2

AVERAGE DISTANCE TO EACH MEDOID
          .325          .333

MAXIMUM DISTANCE TO EACH MEDOID
          .664          .785

MAXIMUM DISTANCE TO A MEDOID DIVIDED BY MINIMUM
DISTANCE OF THE MEDOID TO ANOTHER MEDOID
          .188          .223
```

Figure 3 CLARA output, part d (final results).

e. Graphical Output Concerning the Selected Sample

If the option of graphical output was chosen, a graphical representation of the selected sample is provided by means of the silhouettes that are also used in PAM (see Section 2.2 of Chapter 2). Only if $k = 1$ is no graphical representation given because in this case the silhouettes are not defined. An example of silhouettes for $k = 2$ is given in Figure 5 of Chapter 2. The silhouettes given by CLARA are similar to those of PAM. The only difference is that in CLARA only the objects of the selected sample are included, while in PAM all the objects of the data set were considered. An example for CLARA is shown in Figure 4 below.

2.3 Missing Values

In CLARA, provision is made for the case that there are missing measurement values. If the user says that there are missing data, the following additional question is asked:

```
IS THERE A UNIQUE VALUE WHICH IS TO BE INTERPRETED
AS A MISSING MEASUREMENT VALUE FOR ANY VARIABLE ?
PLEASE ANSWER YES OR NO : no
```

If this question is answered with a yes, the unique value must then be entered and the interactive dialogue is terminated. Otherwise, each of the variables is considered in turn, as in the lines:

```
SHOULD MISSING VALUES BE FORESEEN FOR THE VARIABLE AAA ?
PLEASE ANSWER YES OR NO : no

SHOULD MISSING VALUES BE FORESEEN FOR THE VARIABLE BBB ?
PLEASE ANSWER YES OR NO : yes
ENTER THE VALUE OF THIS VARIABLE WHICH HAS TO BE INTER-
PRETED AS THE MISSING VALUE CODE : -1
```

The provision of missing data has an effect on several computations carried out in CLARA. If the data are standardized, the averages m_f and mean deviations s_f are calculated using only present values. When calculating the distance between two objects, only those variables are considered in the sum for which the measurements for both objects are available; subsequently the sum of terms is multiplied by p and divided by the number of such variables (in the case of Euclidean distance, the multiplication and division are carried out before taking the square root).

In the output of CLARA, the provision for missing values yields the number of missing values for each variable and the total number of missing

```
                    ************************************
                    *                                  *
                    *  CLUSTERING LARGE APPLICATIONS   *
                    *                                  *
                    ************************************

TITLE : Randomly generated data set

DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------

 THERE ARE  200 OBJECTS
 THE OBJECTS WILL BE CLUSTERED INTO    3 CLUSTERS
 MEDIUM SIZED OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (SILHOUETTES)

 THERE ARE     2 VARIABLES IN THE DATA SET,
  AND    2 OF THEM WILL BE USED IN THE ANALYSIS
 These variables are :
         Var1          (POSITION :  1)
         Var2          (POSITION :  2)
 THE MEASUREMENTS WILL NOT BE STANDARDIZED
 EUCLIDEAN DISTANCE WILL BE USED
 THERE ARE NO MISSING VALUES
 THE MEASUREMENTS WILL BE READ IN FREE FORMAT

 YOUR DATA RESIDE ON FILE       : b:ex200.ran


*********************************************
*                                           *
*  NUMBER OF REPRESENTATIVE OBJECTS     3   *
*                                           *
*********************************************

  5 SAMPLES OF    46 OBJECTS WILL NOW BE DRAWN.


SAMPLE NUMBER    1
*****************

 RANDOM SAMPLE =
          3      4      8     12     14     19     23     27     33     41
         43     44     53     55     56     58     62     63     70     79
         87    107    115    120    121    129    130    135    138    139
        145    149    153    154    159    165    167    171    173    174
        176    179    181    183    185    199

 RESULT OF BUILD FOR THIS SAMPLE
   AVERAGE DISTANCE  =          2.347

 FINAL RESULT FOR THIS SAMPLE
   AVERAGE DISTANCE  =          2.252

 RESULTS FOR THE ENTIRE DATA SET
   TOTAL DISTANCE    =        367.925
   AVERAGE DISTANCE  =          1.840

 CLUSTER SIZE MEDOID    COORDINATES OF MEDOID

       1  120     23         -1.02       10.11

       2   60    135         20.13       12.42

       3   20    181         10.60       20.27

 AVERAGE DISTANCE TO EACH MEDOID
       2.363        .920        1.456

 MAXIMUM DISTANCE TO EACH MEDOID
       6.563       1.792        2.645

 MAXIMUM DISTANCE TO A MEDOID DIVIDED BY MINIMUM
 DISTANCE OF THE MEDOID TO ANOTHER MEDOID
         .425        .145         .214


SAMPLE NUMBER    2
*****************

 RANDOM SAMPLE =
          2      4      7     12     13     19     23     26     27     30
         37     42     44     58     62     63     65     67     87     95
         96     97    108    112    122    123    124    130    134    135
        136    140    145    151    154    161    170    173    175    178
        179    181    182    184    187    191

 RESULT OF BUILD FOR THIS SAMPLE
```

Figure 4 Example with 200 objects: Clustering into three clusters using the program CLARA.

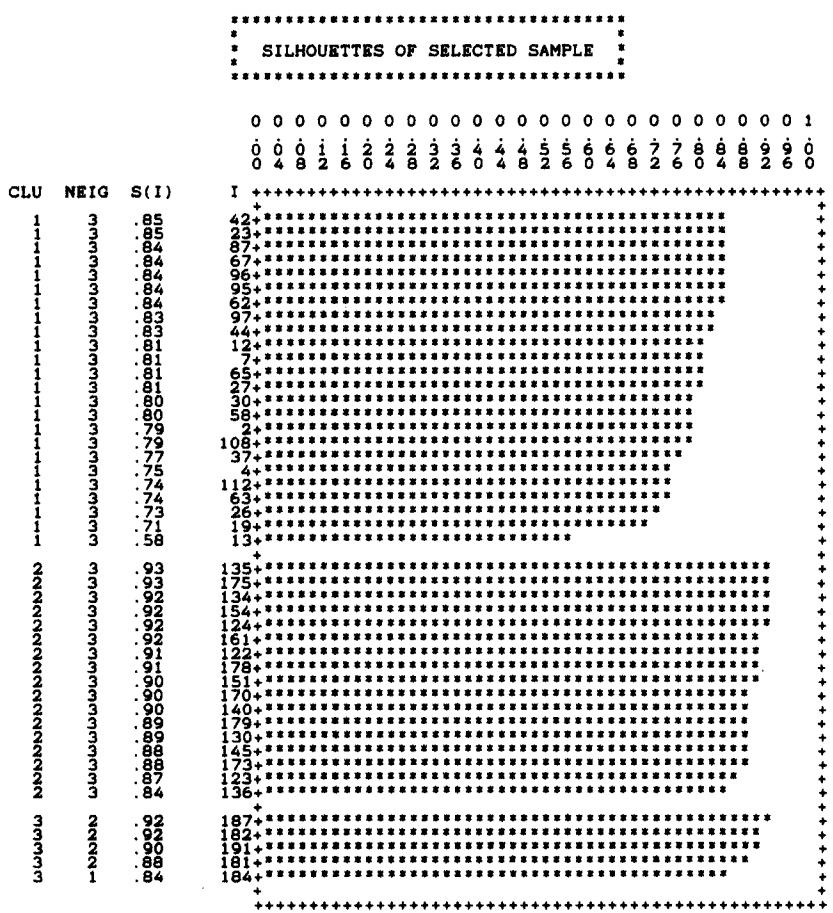
```
  AVERAGE DISTANCE  =          1.981

FINAL RESULT FOR THIS SAMPLE
  AVERAGE DISTANCE  =          1.441

RESULTS FOR THE ENTIRE DATA SET
  TOTAL DISTANCE    =        343.073
  AVERAGE DISTANCE  =          1.715

CLUSTER SIZE MEDOID    COORDINATES OF MEDOID

      1  120     42          .01        9.89

      2   60    135        20.13       12.42

      3   20    187         9.88       19.66

AVERAGE DISTANCE TO EACH MEDOID
      2.234         .920         .986

MAXIMUM DISTANCE TO EACH MEDOID
      5.518        1.792        2.863

MAXIMUM DISTANCE TO A MEDOID DIVIDED BY MINIMUM
DISTANCE OF THE MEDOID TO ANOTHER MEDOID
        .397         .143         .228


SAMPLE NUMBER    3
*****************

RANDOM SAMPLE =
      2     7     9    12    13    14    15    27    30    34
     35    42    68    69    71    73    81    86    88    91
    100   101   104   106   107   109   116   117   119   120
    128   135   138   140   145   148   150   152   167   169
    170   173   179   182   186   187

RESULT OF BUILD FOR THIS SAMPLE
  AVERAGE DISTANCE  =          2.067

FINAL RESULT FOR THIS SAMPLE
  AVERAGE DISTANCE  =          1.599

RESULTS FOR THE ENTIRE DATA SET
  TOTAL DISTANCE    =        354.655
  AVERAGE DISTANCE  =          1.773

CLUSTER SIZE MEDOID    COORDINATES OF MEDOID

      1  120     42          .01        9.89

      2   60    138        19.71       11.34

      3   20    182         9.25       19.87

AVERAGE DISTANCE TO EACH MEDOID
      2.234        1.112         .990

MAXIMUM DISTANCE TO EACH MEDOID
      5.518        2.284        2.557

MAXIMUM DISTANCE TO A MEDOID DIVIDED BY MINIMUM
DISTANCE OF THE MEDOID TO ANOTHER MEDOID
        .406         .169         .189


SAMPLE NUMBER    4
*****************

RANDOM SAMPLE =
      1     3     5    18    19    21    36    38    39    42
     44    45    49    64    67    72    78    88    89    93
    100   110   122   123   127   129   135   145   148   150
    152   156   159   161   165   168   170   173   175   177
    186   187   190   191   196   199

RESULT OF BUILD FOR THIS SAMPLE
  AVERAGE DISTANCE  =          2.373

FINAL RESULT FOR THIS SAMPLE
  AVERAGE DISTANCE  =          1.520

RESULTS FOR THE ENTIRE DATA SET
  TOTAL DISTANCE    =        346.295
  AVERAGE DISTANCE  =          1.731

CLUSTER SIZE MEDOID    COORDINATES OF MEDOID

      1  120    100         -.04        9.31

      2   60    127        20.07       12.16

      3   20    187         9.88       19.66
```

Figure 4 (*Continued*)

```
AVERAGE DISTANCE TO EACH MEDOID
      2.295          .852          .986

MAXIMUM DISTANCE TO EACH MEDOID
      5.565         1.705         2.863

MAXIMUM DISTANCE TO A MEDOID DIVIDED BY MINIMUM
DISTANCE OF THE MEDOID TO ANOTHER MEDOID
       .388          .135          .226


SAMPLE NUMBER     5
*****************

RANDOM SAMPLE =
        5     17     30     31     33     35     38     39     42     45
       46     51     53     62     68     69     74     77     80     82
       85     87     88     93    102    103    104    106    110    117
      122    128    135    147    151    157    161    172    176    177
      178    182    184    186    187    194

RESULT OF BUILD FOR THIS SAMPLE
  AVERAGE DISTANCE  =          2.151

FINAL RESULT FOR THIS SAMPLE
  AVERAGE DISTANCE  =          1.609

RESULTS FOR THE ENTIRE DATA SET
  TOTAL DISTANCE    =        343.156
  AVERAGE DISTANCE  =          1.716

CLUSTER SIZE MEDOID    COORDINATES OF MEDOID

      1  120     42          .01          9.89

      2   60    135        20.13         12.42

      3   20    182         9.25         19.87

AVERAGE DISTANCE TO EACH MEDOID
      2.234          .920          .990

MAXIMUM DISTANCE TO EACH MEDOID
      5.518         1.792         2.557

MAXIMUM DISTANCE TO A MEDOID DIVIDED BY MINIMUM
DISTANCE OF THE MEDOID TO ANOTHER MEDOID
       .406          .136          .194


FINAL RESULTS
*************

SAMPLE NUMBER    2 WAS SELECTED, WITH OBJECTS =
        2      4      7     12     13     19     23     26     27     30
       37     42     44     58     62     63     65     67     87     95
       96     97    108    112    122    123    124    130    134    135
      136    140    145    151    154    161    170    173    175    178
      179    181    182    184    187    191

AVERAGE DISTANCE FOR THE ENTIRE DATA SET =      1.715

CLUSTERING VECTOR
*****************

 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  2  2  2  2  2
 2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
 2  2  2  2  2  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3

 CLUSTER SIZE MEDOID OBJECTS

       1  120     42

                    1     2     3     4     5     6     7     8     9    10
                   11    12    13    14    15    16    17    18    19    20
                   21    22    23    24    25    26    27    28    29    30
                   31    32    33    34    35    36    37    38    39    40
                   41    42    43    44    45    46    47    48    49    50
                   51    52    53    54    55    56    57    58    59    60
                   61    62    63    64    65    66    67    68    69    70
                   71    72    73    74    75    76    77    78    79    80
                   81    82    83    84    85    86    87    88    89    90
```

Figure 4 (*Continued*)

```
                                  91   92   93   94   95   96   97   98   99  100
                                 101  102  103  104  105  106  107  108  109  110
                                 111  112  113  114  115  116  117  118  119  120

     2    60     135
                                 121  122  123  124  125  126  127  128  129  130
                                 131  132  133  134  135  136  137  138  139  140
                                 141  142  143  144  145  146  147  148  149  150
                                 151  152  153  154  155  156  157  158  159  160
                                 161  162  163  164  165  166  167  168  169  170
                                 171  172  173  174  175  176  177  178  179  180

     3    20     187
                                 181  182  183  184  185  186  187  188  189  190
                                 191  192  193  194  195  196  197  198  199  200


AVERAGE DISTANCE TO EACH MEDOID
      2.234          .920          .986

MAXIMUM DISTANCE TO EACH MEDOID
      5.518         1.792         2.863

MAXIMUM DISTANCE TO A MEDOID DIVIDED BY MINIMUM
DISTANCE OF THE MEDOID TO ANOTHER MEDOID
       .397          .143          .228
```




```
   1    3   .85      42+**********************************************
   1    3   .85      23+**********************************************
   1    3   .84      87+**********************************************
   1    3   .84      67+**********************************************
   1    3   .84      96+**********************************************
   1    3   .84      95+**********************************************
   1    3   .84      62+**********************************************
   1    3   .83      97+*********************************************
   1    3   .83      44+*********************************************
   1    3   .81      12+********************************************
   1    3   .81       7+********************************************
   1    3   .81      65+********************************************
   1    3   .81      27+********************************************
   1    3   .80      30+*******************************************
   1    3   .80      58+*******************************************
   1    3   .79       2+*******************************************
   1    3   .79     108+*******************************************
   1    3   .77      37+******************************************
   1    3   .75       4+*****************************************
   1    3   .74     112+******************************************
   1    3   .74      63+******************************************
   1    3   .73      26+*****************************************
   1    3   .71      19+***************************************
   1    3   .58      13+*****************************
                       +
   2    3   .93     135+************************************************
   2    3   .93     175+************************************************
   2    3   .92     134+***********************************************
   2    3   .92     154+***********************************************
   2    3   .92     124+***********************************************
   2    3   .92     161+**********************************************
   2    3   .91     122+**********************************************
   2    3   .91     178+**********************************************
   2    3   .90     151+*********************************************
   2    3   .90     170+*********************************************
   2    3   .90     140+*********************************************
   2    3   .89     179+*********************************************
   2    3   .89     130+*********************************************
   2    3   .88     145+*********************************************
   2    3   .88     173+*********************************************
   2    3   .87     123+********************************************
   2    3   .84     136+*******************************************
                       +
   3    2   .92     187+************************************************
   3    2   .92     182+***********************************************
   3    2   .90     191+**********************************************
   3    2   .88     181+*********************************************
   3    1   .84     184+*******************************************
                       +
                       ++++++++++++++++++++++++++++++++++++++++++++++++++
```

Figure 4 (*Continued*)

```
                    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                    0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                    0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

CLUSTER     1 HAS AVERAGE SILHOUETTE WIDTH    .79
CLUSTER     2 HAS AVERAGE SILHOUETTE WIDTH    .90
CLUSTER     3 HAS AVERAGE SILHOUETTE WIDTH    .89

FOR THE SELECTED SAMPLE, THE AVERAGE SILHOUETTE WIDTH IS    .84


Your output is written on file : a:ex200.res
```

Figure 4 (*Continued*)

values. If the measurements are standardized, the transformed values corresponding to missing data are given the value 99.99.

3 AN EXAMPLE

To illustrate CLARA, a set of 200 objects with two variables was randomly generated. Three groups of objects were constructed. In each group, the points were generated according to a spherical bivariate normal distribution with given mean vector $\mu = (\mu_x, \mu_y)$ and standard deviation σ for both x and y:

group 1:	120 objects	$\mu_x = 0$	$\mu_y = 10$	$\sigma = 1.7$
group 2:	60 objects	$\mu_x = 20$	$\mu_y = 12$	$\sigma = 0.7$
group 3:	20 objects	$\mu_x = 10$	$\mu_y = 20$	$\sigma = 1.0$

Table 1 contains the generated data used as input for the program (the actual input file consisted of 200 lines, one for each object).

In order to test CLARA, the 200 objects were clustered into $2, 3, 4, \ldots, 10$ clusters. Clearly, by the way the data were generated the best results should be obtained for $k = 3$. These results are presented in Figure 4.

A careful analysis of the output for $k = 3$ reveals many things about the structure of the data. The most important of these results, which can be used as guidelines for interpreting the output of CLARA, are the following:

All five samples yield the same (correct) clustering. This is of course expected for such a clear-cut situation. However, the medoids are not all the same and therefore the average distances for the entire data set are slightly different. The respective values for the five samples are 1.840, 1.715, 1.773, 1.731, and 1.716, which shows the usefulness of trying several samples.

Table 1 Example with 200 Generated Objects

x_i	y_i	x_i	y_i	x_i	y_i	x_i	y_i
−0.44	8.76	2.21	11.36	−1.74	11.95	20.87	12.96
1.52	8.76	−0.73	11.23	−1.80	9.55	19.96	12.68
−1.85	9.34	0.02	12.75	0.81	8.13	18.97	13.11
1.98	11.04	−1.70	9.29	−0.39	8.03	20.27	11.82
−1.43	12.13	0.50	4.67	1.67	12.55	19.80	11.92
2.67	6.25	0.65	9.20	−2.05	8.50	20.61	12.41
0.80	8.35	−0.18	10.80	−1.23	10.94	19.30	11.82
−0.81	11.05	−2.64	10.38	−1.46	11.76	18.38	12.38
1.62	8.52	−2.14	11.85	−0.37	8.88	20.91	11.58
2.68	11.47	0.18	10.14	−0.84	14.04	20.21	11.91
1.20	7.74	0.79	12.39	−0.92	9.02	20.82	12.60
0.90	8.48	−0.72	8.62	2.45	9.64	20.58	11.94
2.67	12.68	1.34	11.83	2.09	6.91	20.44	11.67
0.27	12.31	3.14	10.02	1.92	7.66	20.11	11.40
−1.10	9.39	0.44	11.17	3.12	13.81	19.65	13.62
0.87	10.16	−3.49	5.90	−0.22	12.29	20.55	11.93
2.34	10.69	−1.43	9.57	−1.34	10.62	19.56	13.01
−3.62	9.37	1.35	11.25	0.33	10.39	20.22	10.65
−2.49	12.75	−1.53	12.43	−2.09	8.62	19.56	10.93
0.37	8.03	1.36	8.97	−0.51	11.74	19.41	12.66
−0.48	8.48	−0.20	11.38	20.00	11.73	20.82	12.16
−1.39	9.28	2.56	9.33	19.84	12.99	19.76	12.56
−1.02	10.11	−0.16	12.39	21.49	11.25	19.11	12.48
0.60	8.31	0.40	9.58	19.96	11.98	19.59	13.35
−1.82	10.32	−0.60	5.28	19.99	11.99	20.58	12.21
2.34	10.70	3.19	11.96	21.12	11.83	20.83	11.77
−2.45	9.49	−1.94	9.52	20.07	12.16	19.47	11.88
−1.22	9.98	−0.04	9.85	19.41	11.44	20.30	13.16
−0.89	10.07	−0.41	8.95	20.24	10.96	20.40	13.36
−1.88	11.37	−0.42	8.04	19.67	13.21	20.74	12.10
0.79	11.35	−0.18	9.04	18.81	11.94	10.60	20.27
−2.18	10.58	2.28	9.89	19.84	11.76	9.25	19.87
2.71	10.91	−2.52	9.30	20.10	11.93	10.30	19.19
−1.37	8.66	1.78	8.68	20.70	12.17	7.96	20.19
−0.20	11.03	0.82	11.07	20.13	12.42	10.92	21.23
−3.60	12.97	−1.95	12.57	18.68	11.56	9.10	19.94
−1.39	6.79	−0.86	8.89	20.30	11.65	9.88	19.66
1.74	9.69	1.19	9.69	19.71	11.34	8.48	19.69
0.64	8.21	−2.88	9.86	20.50	11.88	8.73	20.33
0.88	12.39	1.04	11.21	21.04	11.51	9.12	22.42
−1.33	10.50	−2.90	12.02	20.00	11.66	10.22	19.42
0.01	9.89	5.52	9.59	19.38	12.68	9.19	18.98

Table 1 Example with 200 Generated Objects

x_i	y_i	x_i	y_i	x_i	y_i	x_i	y_i
−1.89	7.28	−0.84	6.64	19.81	11.74	11.04	18.50
−0.93	8.23	−0.07	11.84	19.25	12.81	9.53	18.82
1.97	9.78	0.58	9.74	20.45	10.95	10.26	19.57
−3.05	7.28	−0.03	10.62	19.24	11.77	10.03	19.52
−0.04	5.70	−0.52	11.10	19.36	12.42	9.51	20.19
2.53	8.88	1.98	9.76	18.55	11.65	8.92	19.75
−1.66	8.04	−1.27	9.17	19.21	12.86	9.64	19.27
−0.58	12.36	−0.04	9.31	19.89	11.29	9.33	19.86

Concerning the selected sample, one observes that:

- the final result for the sample is considerably better than the result of BUILD (1.441 instead of 1.981)
- the average and maximum distances are much larger for the first cluster than for the two others: This is to be expected because the first cluster has a larger standard deviation
- the maximum distance to the medoid divided by the minimum distance of the medoid to another medoid is also much larger in the first cluster, but still less than 0.5, which indicates a tight cluster (the values for the other two clusters are 0.143 and 0.228, indicating very tight clusters).

The silhouettes of the three clusters all have high average widths (0.79, 0.90, and 0.89): A glance at the three silhouettes shows a very good clustering. Looking at the individual values one observes that even in the most loose cluster (number 1), the lowest value is as high as 0.58 (for object 13), followed by 0.71 (for object 19). One also sees that clusters 1 and 2 are positioned more or less on both sides of cluster 3, because all of their objects have cluster 3 as neighbor, while the objects of cluster 3 have as neighbors clusters 1 and 2; however, as seen in the plot of Figure 5 this interpretation is only partially accurate.

From the silhouettes obtained for $k = 4$, shown in Figure 6, one can see that there are two quite weak clusters (1 and 2) and two very tight ones (3 and 4). This is also quite clear when looking at the average silhouette widths.

The clustering vector given in Figure 6 shows that the 120 objects from the first group (objects 1 to 120) have been artificially divided into the

clusters 1 and 2, while the other two generated groups have been left intact. Another way of obtaining this picture is from the ratio of the maximum distance to the medoid and the minimum distance of the medoid to another medoid. For clusters 1 and 2 the values 1.611 and 1.792 are obtained, while for clusters 3 and 4 the values are 0.137 and 0.245.

Finally, Table 2 contains the average silhouette width and optimal average distance for the entire data set, for clusterings with k ranging from 2 to 10. This table indicates the usefulness of the average silhouette width for selecting a "good" number of clusters (see also Section 2.2 of Chapter 2). This selection is based on the maximum average silhouette width, which is called the *silhouette coefficient* [see formula (7) of Chapter 2]. In the example, the value of the silhouette coefficient is 0.84. Looking at Table 4 of Chapter 2, this corresponds to a strong clustering structure. Additional information is obtained when comparing the silhouette coefficient with the second largest average silhouette width: The larger their difference, the more we are convinced that the selected value of k is distinctly better than competing values.

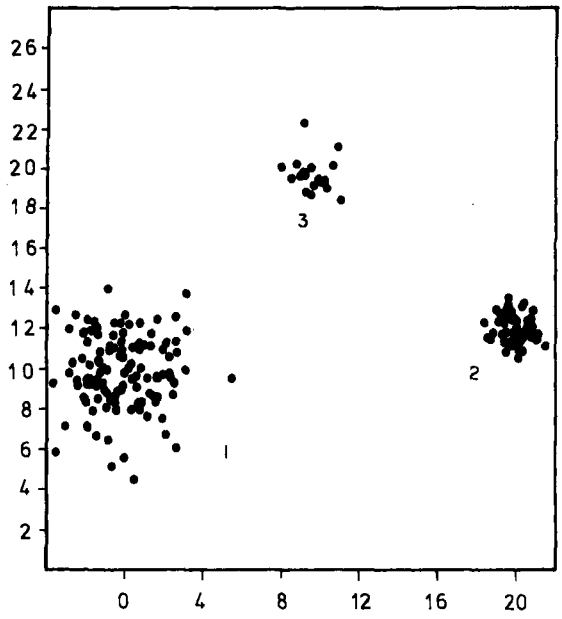


Figure 5 Example with 200 objects: Plot of the points of Table 1.

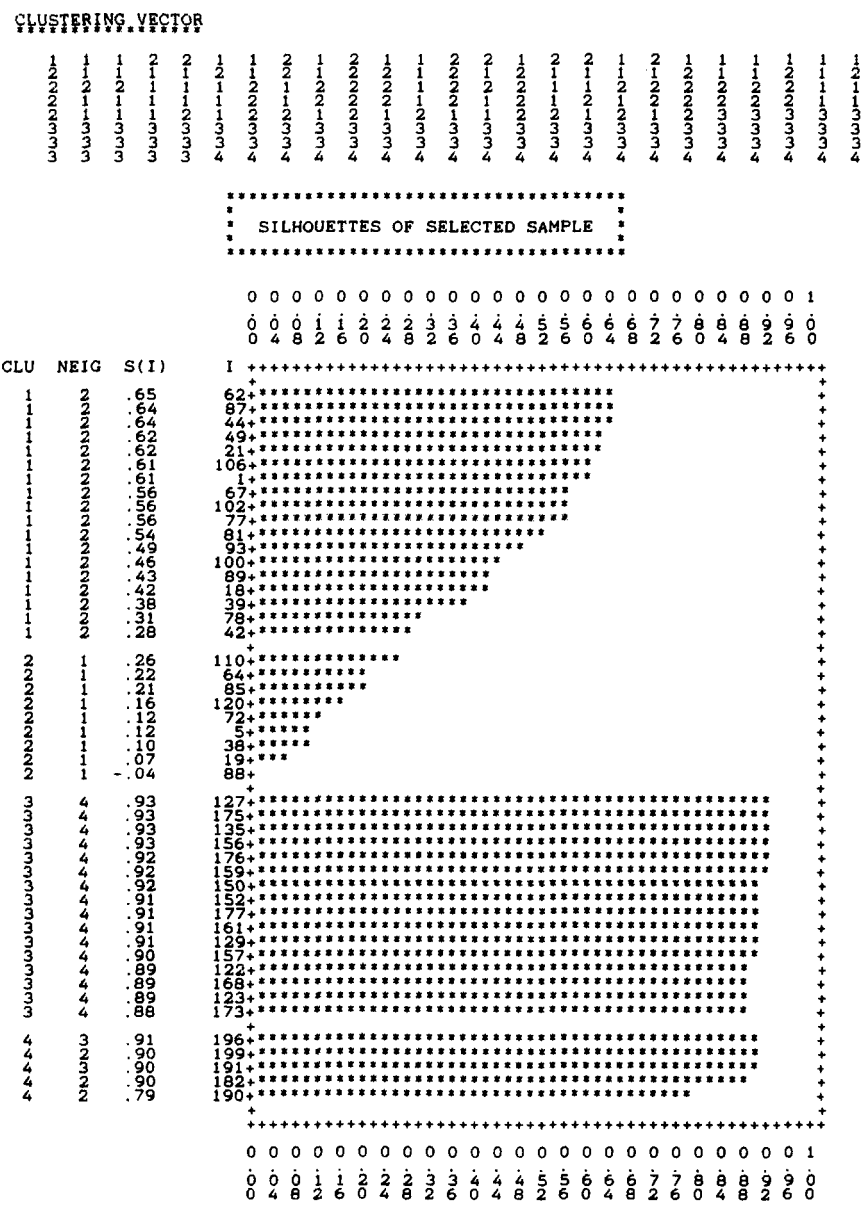


Figure 6 Example with 200 objects: Clustering vector and silhouettes for $k = 4$.

Table 2 Example with 200 Objects: Average Silhouette Width and Average Distance for the Entire Data Set, for Values of k between 2 and 10

k	Average Silhouette Width for the Selected Sample	Average Distance for the Entire Data Set
2	0.79	2.879
3	0.84	1.715
4	0.62	1.417
5	0.55	1.240
6	0.61	1.162
7	0.58	1.065
8	0.44	1.023
9	0.43	0.971
10	0.45	0.879

*4 MORE ON THE ALGORITHM AND THE PROGRAM

4.1 Description of the Algorithm

In the algorithm used in PAM, k objects (the medoids) are selected as being representative or centrally located, and the k clusters are constructed around these objects. The main computational effort made in the algorithm of PAM is a search among a large number of subsets of k objects, for a subset yielding a satisfactory, locally optimal clustering (there are C_n^k such subsets, but the algorithm only examines some of these). With increasing values of n the number of subsets increases dramatically: For fixed k the rate of increase is of the order of the kth power of n. As a consequence, it is clear that the exact k-medoid method is only feasible for relatively small (to medium-sized) numbers of objects because the computation time becomes enormous otherwise. Another factor with the same effect is the storage requirement. As discussed in Section 4 of Chapter 2, the number of memory locations used in PAM is mainly dependent on the number of objects, of which it is a quadratic function.

CLARA carries out the actual clustering in conjunction with the search for a set of representative objects or centrotypes, which should represent the different aspects of the structure of the data set. The method used in CLARA, which was first described by Kaufman and Rousseeuw (1986), is based on the selection of five (or more) random samples of objects. The random number generator used in the program was constructed by us in order to make it machine independent. (It should run on most computers because the largest integer used in it is less than 2^{30}.) The period of the generator is 2^{16}, which is good enough for our purposes.

The size of the samples depends on the number of clusters. For a clustering into k clusters, the size of the samples is given by $40 + 2k$. Because the number of clusters must lie between 1 and 30, the samples contain between 42 and 100 objects. Using a function of the number of clusters for the sample size is motivated by the objective of having a reasonable probability of finding objects from all the "existing" clusters in at least one of the generated samples.

For the construction of the first sample, objects are selected by the random number generator and ordered by increasing index. Each time an object is drawn, it is checked against already drawn objects. If it has not yet been selected, it is inserted at the correct position in the array.

If the sample size is only slightly smaller than the number of objects, it would often happen that the same object is drawn several times. For this reason, the random number generator is used to select the objects *not* belonging to the sample, whenever the number of objects is smaller than twice the sample size.

The construction of further samples is initiated by considering the medoids that have been found in previous samples. At each step of the algorithm, the current best set of medoids is stored in an array. (This best set is the one for which the average distance for the entire data set is the smallest found so far.) A new sample is constructed by adding objects to this best set, in the same way that objects were accumulated in the first sample.

After a sample of objects has been drawn, it is partitioned into k clusters using the same algorithm as in the program PAM. This algorithm consists of two parts, called BUILD and SWAP. In BUILD successive representative objects are selected, with the purpose of obtaining the smallest possible average distance between the objects (of the sample) and their most similar representative object. In SWAP it is attempted to decrease the average distance by replacing representative objects (more details on BUILD and SWAP are given in Section 4.1 of Chapter 2).

Once k representative objects have been selected, each object of the entire data set (and not only the sample) is assigned to the nearest representative object. The average distance obtained for the assignment is used as a measure of the quality of the clustering. After this calculation has been done for all five samples, the sample is withheld for which the average distance is as small as possible.

A further analysis is then carried out on the final partition. The list of objects of each cluster is given, together with the medoid and size of that cluster (in the entire data set). The program then lists, for each cluster, the average and maximum distance to its medoid. Also, the maximum distance is divided by the minimum distance of the medoid to another medoid. This

value gives information on the tightness of the cluster. A small value (for example 0.2) indicates a very tight cluster, while a value exceeding 1 suggests a weak cluster. Finally, a graphical representation of the clustering is given by means of the silhouette plot, as described in Section 2.2 of Chapter 2. This is only done for the selected sample because the silhouettes of the entire data set would become very large and consume a lot of computation time.

4.2 Structure of the Program

CLARA contains about 1425 statement lines. The program consists of a main unit, one function, and nine subroutines.

The Main Program Unit

This consists of the following parts:

Dimensions of the arrays.

Setting the maximum value of $n \times p$: This maximum value, called MAXXX in the program, is set equal to 3500. CLARA stores the measurement values in a one-dimensional array called X. The objects are stored as they are read and, as shown in Figure 7a, the p measurements for each object are stored contiguously. This approach uses the storage space much more efficiently than in the case of a two-dimensional array with bounds on both n and p.

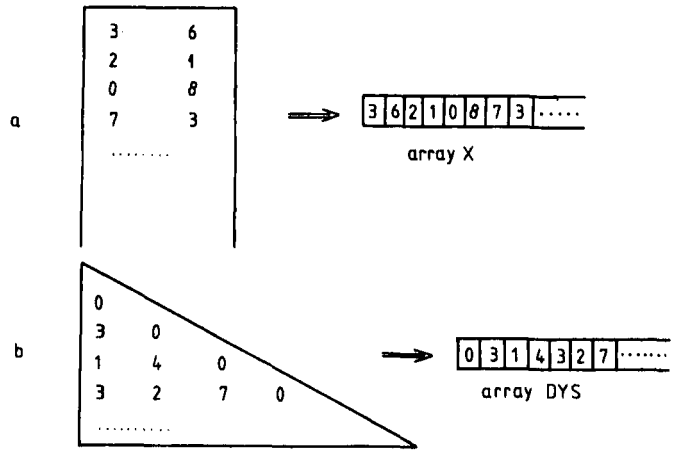


Figure 7 Storage of (a) measurement values and (b) distances in CLARA.

Setting the maximum number of variables in the data set to 150 (in the program this maximum number is denoted by MAXTT).

Defining the units for input of the data set (called LUA) and for output (LUB). These units are given the values 1 and 2, but these values may be changed according to the hardware configuration.

Setting NRAN, the number of samples to be drawn, equal to 5 (the user can change this line if more samples are wanted).

A call to the subroutine ENTR in which the options and parameters are entered and displayed and the data set is inputted.

Calculation of the number of objects of the samples.

Section in which missing measurements are examined.

If requested by the user, a call to the subroutine STAND (in which the data are standardized).

Output of the standardized measurements (providing large output was requested).

Output of the number of clusters and samples.

Do loop over the samples to be drawn (DO 400):

- drawing a sample or its complement: Calls to the subroutine RANDM. For all samples except the first, the currently best set of medoids is used to initiate the sample
- output of the objects of the sample
- calculation of the within-sample distances (subroutine DYSTA): If it was not possible to calculate all distances (due to missing values), a message is given and the next sample is drawn.
- calculation of the maximum distance S (this value is used for initialization purposes in the algorithm).
- carrying out the algorithm: subroutine BSWAP
- output of the average distance AZ
- assignment of the objects and calculation of ZB, the total distance for the entire data set (subroutine SELEC)
- if ZB is better (lower) than all previous values:
  - **a.** replace the best value found so far by ZB
  - **b.** store the sample number
  - **c.** store the objects of the sample
  - **d.** store the representative objects (medoids)
  - **e.** store the maximum distance

Test if for at least one sample it was possible to calculate all distances. If not, the program stops.

For the selected sample:

- print the sample number and the average distance
- recalculate the distances in the sample
- carry out the subroutine RESUL: construction of the clustering vector and (except for small output) a list of clusters
- graphical output showing the selected sample, in the subroutine BLACK (only if this option was chosen).

A summary of the main unit is shown in Figure 8.

Subroutine ENTR

This subroutine contains the interactive part of the program, in which the selected options are entered.

Subroutine QYN

Many of the questions asked in the subroutine ENTR have two possible answers: yes and no. In the subroutine QYN various equivalent answers to these questions are treated. For example the answers yes, Yes, y, and Y are considered equivalent.

Subroutine STAND

In this subroutine standardized measurements are computed. Before the actual standardization, the average and mean deviation of each variable are calculated and printed.

Subroutine DYSTA

Computes Euclidean or Manhattan distances between all objects of a sample (these distances will be used in the k-medoid algorithm). The distances are stored in an array called DYS. To save memory space, only the lower triangular part of the distance matrix is stored (an example is shown in Figure 7b). Also to save memory space, the same array is used again to store the distances for the next sample. Because the distances between objects of the optimal sample are needed for the silhouettes, these must be computed again when it has been determined which sample is the optimal one.

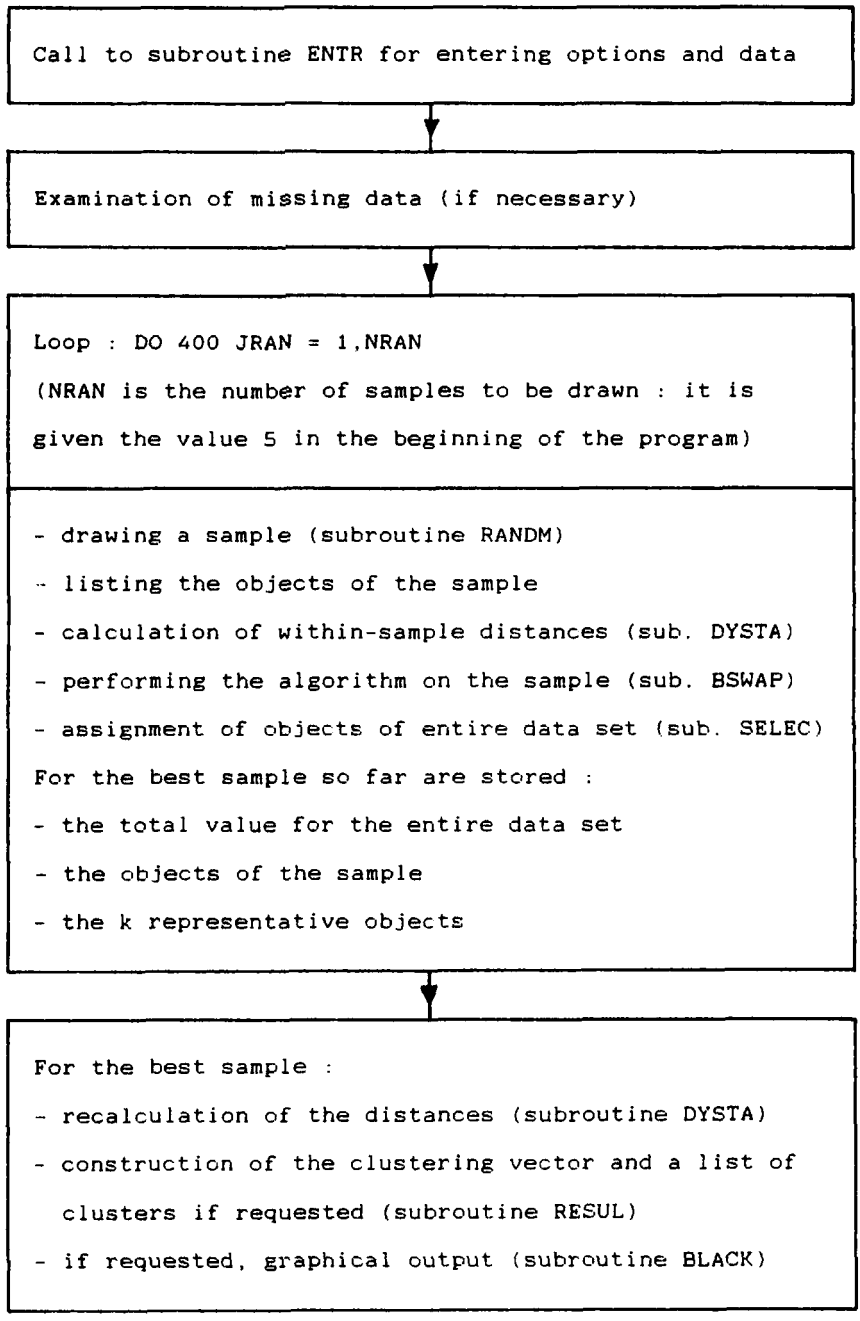


Figure 8 Description of the main unit of CLARA.

Function MEET

When the distance between two objects L and J is needed, the function MEET(L, J) gives the index of the array DYS where this distance is stored:

$$d(L, J) = \text{DYS}(\text{MEET}(L, J)).$$

Subroutine RANDM

Generates a pseudorandom number RAN in the interval]0, 1[each time it is called. The integer variable NRUN (equal to 2^{16}.RAN) is used as initial value. It is set equal to 0 in the main program, before the first call of the subroutine RANDM. Although NRUN is not changed in the main program, it is necessary as one of the arguments of the subroutine to ensure that a new pseudorandom number is generated at each call. If the program is run more than once on the same data set (with the same number of clusters), the same objects are selected in the samples.

Subroutine BSWAP

Performs the clustering. It consists of two parts in which the BUILD and SWAP techniques are used.

Subroutine SELEC

Consists of the following parts:

Assignment of the objects of the entire data set to their clusters. An object is assigned to a cluster if its distance to that representative object is smaller than to all other representative objects (in case of ties, the smallest numbered cluster is taken). In the situation of missing values, if an object is encountered for which it is not possible to calculate the distance to any representative object of the sample, the program stops (after giving a message).

During the process of assigning objects, the following statistics are calculated by updating mechanisms:

- average distance to each medoid
- maximum distance to each medoid
- number of objects in each cluster

Permutation of the vectors containing the clustering statistics: The numbering of the clusters in the output is the same as in the clustering vector. The permutation is carried out using an array called NEW in which the new numbering of clusters is stored.

Output of total and average distance for the entire data set.

Output for each cluster:

- size (number of objects)
- medoid
- coordinates of the medoid (if standardization was requested, only the standardized coordinates are given)
- average distance to the medoid
- maximum distance to the medoid

If there is more than one cluster: Computation of the maximum distance to a medoid divided by the minimum distance of the medoid to another medoid (if the minimum distance is zero, a message is printed).

Subroutine RESUL

The purpose of this subroutine is to provide a description of the clustering obtained from the optimal sample. It starts with the determination of the clustering vector. In order to save memory space, the number of the cluster to which an object belongs is stored in place of the first measurement value for this object, in the array X. This is done for all objects except the representative ones (the information lost in this way is not important, because once a nonrepresentative object has been assigned, its coordinates are no longer needed in the program). The clustering vector is then outputted, 30 elements per line (these 30 elements are stored in the array LYNE).

If at least medium-sized output was requested, another representation is given of the final clustering. In this case a list of clusters is provided, with, for each cluster:

The number of objects (size).

The medoid.

A list of its objects, in ascending order.

Subroutine BLACK

This subroutine constructs the graphical output for the selected sample. It produces the silhouettes of the clusters, in the same way as in PAM.

4.3 Limitations and Special Messages

CLARA was intended for clustering large sets of objects. For this reason it was necessary to build a number of limitations and restrictions into the program. The first such restriction is that the program only admits input of measurement values and not of dissimilarity coefficients. Indeed, a major problem of clustering large data sets is the required memory, because in

many situations it is impossible to store the $n(n-1)/2$ dissimilarities between n objects. Two restrictions that are consequences of the sampling method concern the minimum number of objects and the maximum number of clusters. Because it appeared that a reasonable maximum size of the sample is 100 objects (for reasons of both processing time and memory requirements), it was decided that the program should only be used with sets of at least 100 objects. In order to have a reasonable probability of drawing objects from the different groups, the number of clusters is limited to 30. The program only performs one clustering at a time because the data array is reused at the end, and therefore only a single value of k may be specified (as opposed to PAM and FANNY, in which all clusterings between minimum and maximum values of k are carried out in the same run). To save storage space, CLARA is the only clustering program in this book that does not allow the input of object labels. Another feature designed to limit the memory requirements is the method for storing the measurement values. Instead of a two-dimensional array (as in the other programs), a one-dimensional vector is used. This feature imposes a maximum total number of measurements instead of maxima on both the numbers of objects and variables. In the program, this maximum number is set equal to 3500. This makes it possible to consider either 3500 objects characterized by a single variable or, say, 100 objects defined on 35 variables.

As in the other clustering programs of this book, not all variables in the data set must be used in the clustering. The limitation on the total number of measurements, that was discussed in the previous paragraph, only concerns the measurements for the variables actually used. However, the total number of variables is also limited (to 150).

If missing values have been foreseen, the objects and the variables are examined for missing values. If an object or variable is encountered for which all values are missing it is printed, and after all objects and variables have been examined the program stops. (Actually, all objects are examined, but only those variables for which missing values have been foreseen.) If an object causes the program to stop, it should be removed by changing the input file. In order to delete a variable, a simple remedy is to no longer list it in the interactive input session.

During the standardization (subroutine STAND) the mean deviation of each variable is calculated. A special message is given for each variable with zero mean deviation. If there are any such variables, the program stops after all variables have been examined. Also here, the problem can be solved by removing such variables.

The subroutine DYSTA calculates the distances between all objects in the sample. During its execution all pairs of objects that do not have

common measurements (because there are too many missing data) are printed. If there are any such pairs, the sample is disregarded and the next sample is drawn. If such pairs of objects occur in all five samples, the program stops.

In the subroutine SELEC each object is assigned to one of the representative objects in the sample. If there is an object that does not have common measurements with any representative object (and therefore cannot be assigned), it is printed and the program stops.

4.4 Modifications and Extensions of CLARA

In order to cluster a data set on a particular computer system, one may have to adapt CLARA slightly. We shall consider some regularly encountered situations and discuss the possible solutions.

A first requirement for implementing the program concerns the availability of sufficient storage. The major part of the storage is taken by the vector X containing the measurement values. The default size of the vector is 3500. This value is stored in the variable MAXXX. If more than 3500 measurements are to be processed, the value of MAXXX must be increased (this can be done by adapting the corresponding statement located right after the dimension statements); also the dimension of the array X in the main program unit must be increased. (In the subroutines no changes have to be made because the variable MAXXX is passed on automatically.)

As an indication of the speed of the program, Table 3 gives the times (in minutes) on an IBM/XT with an 8087 coprocessor, for solving a set of randomly generated problems. The first data set (with 200 objects) is the one used in Section 3. All the runs were without standardization, using Euclidean distances and including large output and silhouettes.

A limitation of the program, which one sometimes wishes to avoid, is that at most 30 clusters can be determined. Indeed, in many large data sets there are outliers that should first be removed before looking for the actual clusters, and even if this is not the case there may be more than 30 groups.

Table 3 Computation Times (in minutes) on an IBM / XT with 8087 Coprocessor for a Set of Randomly Generated Problems of Increasing Sizes

	Number of Objects (Two-Dimensional)				
k	200	400	600	800	1000
2	2.30	2.92	3.52	4.12	4.70
5	5.67	7.47	6.92	8.20	9.77
10	13.75	17.52	17.88	21.65	21.98

A possible solution to this problem is to first cluster into 30 clusters and then to eliminate outliers or small clusters before running the program again on a reduced data set. Alternatively, the program could be adapted to accommodate more than 30 clusters. In this case the following changes must be made:

In the main program unit, the dimensions of the arrays NR and NRX must be increased.

In the subroutine ENTR, the test limiting the number of clusters (statement 170 and format 9040) must be adapted.

In the subroutine SELEC:

- the dimensions of the arrays NEW, NR, NRNEW, NS, NSNEW, NP, NPNEW, RADUS, RDNEW, TTD, TTNEW, and RATT must be increased
- the formats 9040, 9050, and 9060 should be adapted

In the subroutine RESUL, the dimension of the array NRX must be increased.

Here it should be noted that each sample contains $40 + 2k$ objects. The data set must contain at least as many objects. This should be taken into account when more than 30 clusters are wanted.

The probability of finding a large number of small samples is related to the sampling technique used in the program. For example, when clustering a set of 1000 objects, the probability of drawing at least one object from a cluster of 10 objects, in at least one of five samples of 50 objects, is 0.91. For a cluster of five objects this probability is reduced to 0.69 and for a singleton it is only 0.21. For larger data sets these probabilities are smaller. Therefore, it was made easy to increase the number of samples. This is done by changing the variable NRAN (the statement to be modified is located at the beginning of the program). No other changes must be made.

One might think of some other extensions to CLARA, such as:

Keeping track of the objective values encountered during execution, and maybe plotting them in a histogram to see if the selected value was much better than its competitors.

For each object, computing its minimal distance to any other object of the entire data set, as done by Kaufman et al. (1985) to identify outliers in a large data set.

Partitioning *extremely* large data sets by breaking them up into contiguous parts that are stored on an external device. Note that this

extension of CLARA is easy to make because the array X is not accessed very often during execution, and even then only sequentially. This modification was proposed by Bert van Zomeren (personal remark) and could be called CELIA (for Clustering Extremely Large Industrial Applications). Millions of objects can be clustered in this way.

*5 RELATED METHODS AND REFERENCES

Few authors of clustering algorithms have paid much attention to the specific problems encountered when clustering large data sets. The reason for this might be that these problems mainly concern the implementation of the methods, which depends on the computer hardware and software being used.

A first obstacle to solving problems with large sets of objects concerns the necessity to store and frequently retrieve the $n(n-1)/2$ dissimilarities between objects. Some authors have suggested either using an external storage device for this purpose or calculating the dissimilarities each time they are needed. Both methods usually result in considerable increases in computation time. This leads us to the second obstacle to solving large problems, namely, the substantial number of calculations necessary for the algorithms, particularly those of the partitioning type. In two subsections, devoted to partitioning and hierarchical methods, we will discuss the contributions of several authors to the challenge of clustering large data sets. In a final subsection, the implementation of CLARA on a parallel computer will be addressed.

5.1 Partitioning Methods for Large Data Sets

Steinhausen and Langer (1977) have made a suggestion for solving problems with large sets of objects, using any partitioning algorithm of the improvement type (such as most methods used for variance minimization; see Section 5.3 of Chapter 2). This suggestion consists of the following general steps:

1. Draw a sample from the set of objects and cluster the objects of the sample.
2. Assign the objects not belonging to the sample to the nearest of the clusters found during step 1.
3. Use the inflated clusters as the starting point of an iterative procedure.

The main difference between this suggestion and the method used in CLARA is that they only draw one sample whereas CLARA draws several of them. Also, most iterative procedures that can be used in step 3 are of order n^2, while the whole algorithm in CLARA is of order n. Finally, CLARA is more robust than most iterative procedures, as it is based on the minimization of a sum of distances instead of a sum of squares of distances.

Apart from this suggestion of Steinhausen and Langer, partitioning algorithms for clustering large sets of objects have been proposed by Hartigan (1975) and Diday (1971, 1975). The first proposal of Hartigan (1975) is a very simple *single pass sequential algorithm*, in which the objects are considered one by one and it is attempted to assign them to one of the previously generated clusters. If the distances of an object to all existing clusters exceed a known threshold value, a new cluster is initiated. [Deichsel (1980) gave a method of determining a threshold value for which the expected number of clusters is a given value k.] This single pass sequential algorithm involves very few calculations and is therefore well adapted to large sets of objects. However, it suffers from several shortcomings:

The results are strongly dependent on the order of the objects in the input file.

One is not sure of finding exactly k clusters.

The first clusters are usually much larger than the later ones since they get first chance at each object as it is allocated.

An inherent clustering philosophy (like optimization of a goal function) appears to be lacking, making it difficult to interpret the results.

Hartigan (1975) also proposed a more refined approach for solving large clustering problems. The set of objects is first clustered into about 100 clusters using a single pass sequential algorithm (here a guess must be made of the threshold value which will lead to 100 clusters). The centroids of the obtained clusters are determined and they themselves are clustered using the k-means algorithm (in this algorithm the centroids are given weights equal to the numbers of objects in the corresponding clusters produced by the sequential algorithm). The clusters of centroids are then used to obtain a partition of the entire data set into k clusters. This method suffers, however, from similar problems as the original single pass algorithm.

Diday (1975) proposed a family of so-called *sequential dynamic kernel algorithms*, which are closely related to his original dynamic kernel method (Diday, 1971). The latter is based on two functions:

A function g allowing the representation of a cluster of objects (using the kernel of the cluster, that can be either a set of points or a subset of objects): Usually the function g associates a value to the cluster.

A function f which makes it possible to use the representation given by g for the purpose of determining a new clustering.

The dynamic kernel method uses f and g alternatively until an equilibrium is reached (the method of Forgy discussed in Section 5.3 of Chapter 2 is a special case, because steps 2 and 3 of that method correspond to the use of some functions g and f). Starting with an initial set of kernels, each object of the data set is assigned to the "nearest" kernel, defining a first partition, that is used to yield a new set of kernels. This process is repeated until a stable clustering is obtained.

The sequential version of this method is based on the same principle but does not require storing all the data, while the computation times are not much longer. One starts with a first partition of the set of objects, together with a set of kernels. One then considers one cluster of the current partition and assigns each of its objects to the nearest kernel. When all objects of the cluster have been assigned, a new set of kernels is determined. This is done in the same way as in the original dynamic kernel method. The next cluster is then considered and again each of its objects is assigned to the nearest kernel. This process is continued until a complete pass through the clusters does not lead to a new assignment of any object. In a sense the method is intermediate between the method of Forgy (in which new seed points are determined when all objects are assigned) and the k-means method (in which each assignment of an object can lead to new seed points). The contribution of Diday is interesting because it generalizes a whole collection of clustering methods. Indeed, the kernels can be centroids, medoids, or even a whole set of points or objects.

5.2 Hierarchical Methods for Large Data Sets

(This subsection can be read most profitably after reading Chapter 5.) In the area of hierarchical cluster analysis, the techniques proposed for solving large problems can roughly be divided into two groups. The first group is concerned with the adaptation of existing algorithms in order to reduce either the storage or the number of calculations. A second group consists of new methods that have been specifically designed for clustering large data sets, although they are often based on concepts used in classical methods.

In the first group of techniques, most work has been done on variants of the single linkage algorithm that involve fewer calculations but yield the same results. We will not discuss these methods here because they are essentially identical with single linkage and suffer from the same problems. Methods of this type are given by Johnson (1967), Gower and Ross (1969), Sibson (1973), Jarvis and Patrick (1973), Hartigan (1975), Bentley and Friedman (1978), and Rohlf (1978). Another technique of the same group,

similar to single linkage but with a new approach and interesting novelties for computer implementation, was proposed by Hansen and Lehert (1980). Their method, called *clustering by connected components*, consists of linking all objects i and j for which $d(i, j) \leq \varepsilon$, where ε is some threshold and d is the Minkowski distance, of which the Euclidean and Manhattan distances are special cases (see Section 2.1 of Chapter 1). The basic idea is that there can be no direct link between i and j as soon as $|x_{if} - x_{jf}| > \varepsilon$ for any variable f, so that the actual distance $d(i, j)$ does not have to be computed for most pairs (i, j). This makes the algorithm very fast, but the disadvantages of single linkage remain, such as the chaining effect, the lack of robustness, and the asymptotic inconsistency (see Section 5.2 of Chapter 5).

Bruynooghe (1978) proposed several agglomerative hierarchical algorithms adapted to large data sets. These methods all make use of threshold values as well as the concept of *contracting aggregation strategy*. He denotes by $d(Q, R)$ the dissimilarity between two clusters Q and R belonging to a partition $\mathcal{P}$ (this dissimilarity of course depends on the clustering strategy being used). For a threshold ε the neighborhood of a class Q is then defined as

$$N(Q, \varepsilon) = \{R;\ R \in \mathcal{P}, d(Q, R) \leq \varepsilon, \quad R \neq Q\}$$

If $N(Q \cup R, \varepsilon) \subset (N(Q, \varepsilon) \cup N(R, \varepsilon))$ providing $d(Q, R) \leq \varepsilon$, the clustering method is called a contracting aggregation strategy. Bruynooghe showed that several agglomerative hierarchical methods, including single and complete linkage, are contracting aggregation strategies, and he uses this concept to increase the speed of such methods. He does not provide programs for his methods but states that for up to 1000 objects the computation time is approximately linear in the number of objects, while beyond that number it is quadratic.

In the second group of techniques, those specifically designed for clustering large data sets, Zupan (1982) proposed a method that proceeds by the construction of a binary tree using an update procedure. The most significant aspect of the procedure is that objects are inserted into the tree one at a time, and it can therefore be used effectively for classifying new objects once a first set of objects has been clustered. The way the hierarchical tree is built is neither agglomerative nor divisive. The method starts with the construction of a tree representing two objects (the first two objects in the data set). Such a tree is depicted in Figure 9.

Subsequently, objects are added to the tree one at a time until all objects have been incorporated. An object enters an existing tree by its root. The distance between the new object and each of the two descendants of the root is calculated and so is the distance between these two descendants. For

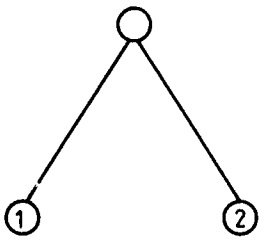


Figure 9 Initial tree for the method of Zupan (1982).

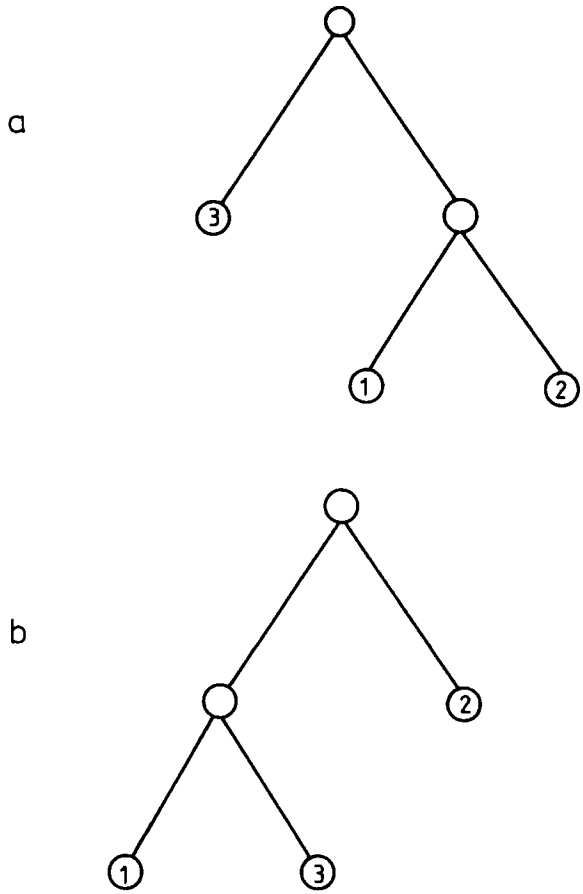


Figure 10 Adding an object to a tree in Zupan's method: (a) The object cannot be assigned to either descendant and forms a singleton. (b) The object is assigned to one of the two descendants.

these calculations, clusters are represented by their centroids and Euclidean distances are used. If the new object is further away from both descendants than the distance between these descendants, the new object forms a singleton in the tree. This situation is shown in Figure 10a. If this is not the case, the object is assigned to the closest of the two descendants, as in Figure 10b. The process is repeated with the descendants of the vertex (cluster) to which the new object has been assigned. This continues until the new object itself forms a vertex in the tree. For the example of Figure 10b the cluster $\{1, 3\}$ is separated into clusters $\{1\}$ and $\{3\}$.

In a book devoted to his method, Zupan (1982) gives a Fortran program and discusses a chemical application with 500 objects and 150 variables. The only computation times reported are on a relatively slow PDP 11/34 computer on which it took 40 hours to generate the entire tree. An analysis of the method shows that it suffers from several problems. The most important is that the method only yields a binary tree and gives no information on the strength or cohesion of the clusters (the level of the clusters). Another is that the results strongly depend on the order of the objects in the input file. Furthermore, the distance to the centroid of a cluster lacks robustness, although the method can easily be adapted to another measure. Finally, an advantage that the method shares with the algorithm used in CLARA is that it is easy to add objects to a previously obtained clustering without restarting the entire procedure.

Another hierarchical algorithm intended for large data sets was proposed by Openshaw (1980). Because this method is a monothetic divisive one, we postpone its discussion to Chapter 7.

5.3 Implementing CLARA on a Parallel Computer

The method used in CLARA was devised to tackle large clustering problems efficiently, even on quite small computer systems. However, when one is confronted with *very* large problems, with for example tens of thousands of objects, running CLARA on a small or medium-sized system can consume considerable computation time.

During the last few years there have been far-reaching innovations in the computing architecture available for solving scientific problems. The introduction of parallel systems has offered new software possibilities well adapted to the solution of many of these. The approach used in CLARA lends itself well to parallel processing. Each of the processors can be working independently on a sample, thereby taking maximum advantage of the parallelism. Communication between the processors, which is often a bottleneck in parallel systems, can be reduced to a minimum.

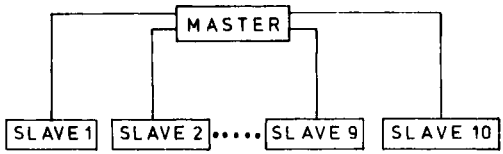


Figure 11 Structure of the ICAP 1 system.

In March 1987, an experiment was carried out (together with Phil Hopke of the University of Illinois at Champaign) to investigate the feasibility of using a parallel system for cluster analysis. The machine used was the ICAP 1 system at the IBM Research Center in Kingston, NY. This system consists of a central host processor connected by channels to 10 array processors, also called slaves. The host processor is an IBM 3081 and the slaves are Floating Point Systems FPS-164 array processors, connected as in Figure 11. Both the host and slave processors have bulk memory attached. There is also shared memory available, but it was not used in our experiment.

Software running on the ICAP usually consists of a master Fortran program running on the host processor, that calls Fortran subroutines to run on the slaves. In our experiment, all the subroutines were grouped into a slave program that could be made to run on some or all of the slaves.

The parallelism is controlled by a specific set of instructions that determine which routines must be executed on each slave and when this is done. A precompiler is used (on the host computer) to generate the source code for master and slave programs. More information on the ICAP system is given by Clementi and Logan (1985). The precompiler is discussed in detail by Chin et al. (1985).

When experimenting with the parallelization of CLARA, two strategies were implemented and compared. In a first approach, each slave processor is given a sample and the host processor waits until all samples have been analyzed. After clustering its sample, the slave also assigns each object in the entire data set to the nearest representative object found in the sample, and calculates the objective value. The representative objects and the objective value are then sent back to the host processor. When it has received this information from each slave, the host determines the best set of medoids and constructs a new set of samples around this best set. This strategy is easy to implement and allows a large number of samples to be analyzed. However, with this strategy there are often idle slave processors, waiting for samples to be completed on other slaves. The reason for this is

the substantial variation in time necessary to solve different samples, that is due to the SWAP algorithm used in CLARA (for a description of this algorithm see Section 4.1 of Chapter 2).

In a second approach, when the host processor receives a set of medoids and a total value from a slave, it immediately compares it with the best set found so far and updates this best set when necessary. A new sample is then constructed (around the currently best set) and sent back to the idle slave processor. In this way, there is a very short waiting time for the slave. It turns out that this second approach makes better use of the parallel system. Other aspects and strategies may be found in Kaufman et al. (1988). The same paper also discusses a parallel implementation of least median of squares regression (see Rousseeuw, 1984).

EXERCISES AND PROBLEMS

1. Consider the data set of Table 1. Cluster the objects into two, three, four, and five clusters with CLARA, but using the option of standardizing the data first. Compare the results with those of Section 3.

2. Cluster the data set of Table 1 by means of the program CLARA into two, three, and four clusters using only variable 1 and then using only variable 2. Choose the same options as in Section 3 (no standardization and Euclidean distance). Compare these two clusterings with each other and with the results in Section 3. Note in particular the relation between the quality of a clustering and the variability between the results for the five samples.

3. Consider a set of 500 objects from which random samples of 50 objects are drawn, with replacement.
   (a) Suppose five samples are drawn. Calculate the probability that at least one of these samples contains a given object.
   (b) Calculate the minimum number of samples necessary to have a 90% probability for at least one of these to include the given object.

4. A single atypical object, disconnected from the other data, can be considered an outlier. (If at least two such points lie close together, perhaps they should be called a cluster.) One way to identify an outlier is to have it show up as a singleton cluster. However, this is not so easy with CLARA because the probability that the object belongs to one of the selected samples is rather low, as seen in the preceding exercise. Also,

the number of clusters is limited in CLARA. Therefore, it would be useful to identify outliers first and then perhaps correct or delete them before running the CLARA algorithm. This could be done by computing

$$\min_{j \neq i} d(i, j)$$

for each object i in the data set and listing these values in decreasing order. Indeed, an outlier (in the sense described above) should have an unusually large value. Write a small program (or CLARA subroutine) to plot these values.

Finding Groups in Data: An Introduction to Cluster Analysis
Leonard Kaufman and Peter J. Rousseeuw

CHAPTER 4

Fuzzy Analysis (Program FANNY)

1 THE PURPOSE OF FUZZY CLUSTERING

Fuzzy clustering is a generalization of partitioning. In a partition, each object of the data set is assigned to one and only one cluster. Therefore, partitioning methods (such as those of Chapters 2 and 3) are sometimes said to produce a hard clustering, because they make a clear-cut decision for each object. On the other hand, a fuzzy clustering method allows for some ambiguity in the data, which often occurs.

Let us consider Figure 1, which contains 22 objects characterized by two interval-scaled variables. Our eye immediately sees three main clusters, as well as two intermediate points. Suppose that we run a partitioning method and ask for three clusters. In that case, the program would have to make a rather arbitrary choice whether to add object 6 to the cluster $\{1, 2, 3, 4, 5\}$ or to $\{7, 8, 9, 10, 11, 12\}$, because this object lies at approximately the same distance from both. Also, it would be very difficult to decide where to put object 13, which lies between the three main groups.

A fuzzy clustering technique is much better equipped to describe such situations because each object is "spread out" over the various clusters. For instance, a fuzzy clustering method is able to say that object 1 belongs for the most part to the first cluster, whereas object 13 should be divided almost equally between all three clusters. This degree of belonging is quantified by means of *membership coefficients* that range from 0 to 1. When we apply a fuzzy clustering method to the data of Figure 1, we obtain a list of membership coefficients as in Table 1.

Table 1 contains 66 membership coefficients. Looking at the first row, we see that object 1 belongs for 87% to cluster 1, for 6% to cluster 2, and for 7% to cluster 3. Note that the sum of the membership coefficients in each row equals 1 (or 100%). Also objects 2, 3, 4, and 5 belong mainly to the first

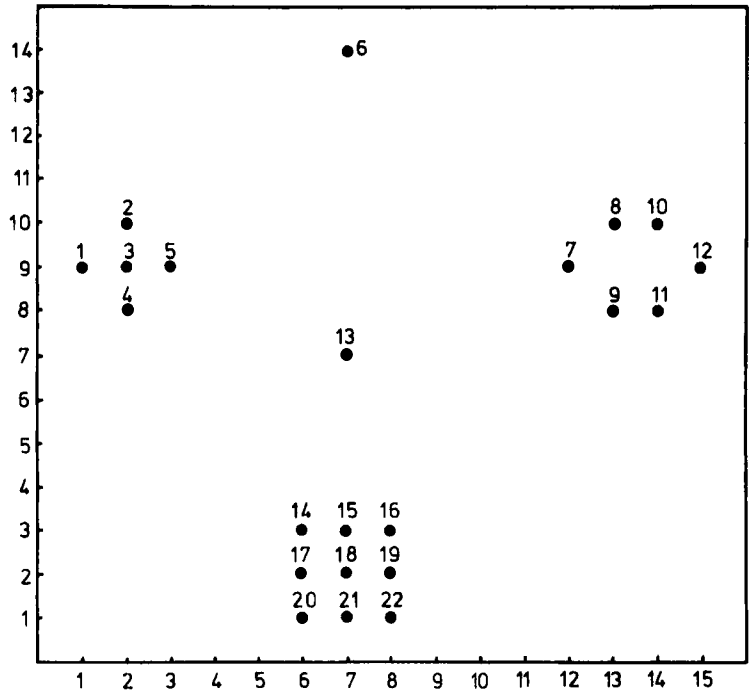


Figure 1 Data set with two intermediate objects.

cluster. Object 6 is an intermediate case, because it has substantial memberships (42% and 35%) in clusters 1 and 2, and a lower membership (23%) in cluster 3. This means that object 6 does not really belong to either cluster, but that it is still closer to clusters 1 and 2 than to cluster 3. One might say that object 6 forms a bridge between clusters 1 and 2.

The next objects (numbers 7 to 12) are quite strongly associated with cluster 2, whereas objects 14 to 22 have their largest memberships in cluster 3. Object 13 is hardest to classify, because it holds an intermediate position between clusters 1, 2, and 3. The fuzzy clustering does reflect this because the memberships of object 13 in the three clusters are nearly equal, showing no definite preference for any of them.

The main advantage of fuzzy clustering over hard clustering is that it yields much more detailed information on the structure of the data. On the other hand, this could also be considered a disadvantage, because the amount of output grows very fast with the number of objects and the number of clusters, so it may become too much to digest. Some other disadvantages are the absence of representative objects and the fact that

Table 1 A Fuzzy Clustering of the Data in Figure 1

	Membership		
Object	Cluster 1	Cluster 2	Cluster 3
1	0.87	0.06	0.07
2	0.88	0.05	0.07
3	0.93	0.03	0.04
4	0.86	0.06	0.08
5	0.87	0.06	0.07
6	0.42	0.35	0.23
7	0.08	0.82	0.10
8	0.06	0.87	0.07
9	0.06	0.86	0.08
10	0.06	0.87	0.07
11	0.06	0.86	0.08
12	0.07	0.84	0.09
13	0.36	0.27	0.37
14	0.12	0.08	0.80
15	0.08	0.07	0.85
16	0.10	0.10	0.80
17	0.08	0.06	0.86
18	0.04	0.04	0.92
19	0.07	0.07	0.86
20	0.10	0.08	0.82
21	0.07	0.06	0.87
22	0.09	0.09	0.82

fuzzy clustering algorithms are usually quite complicated and take considerable computation time. Nevertheless, we think that the fuzziness principle is very appealing because it allows a description of some of the uncertainties that often go with real data. Moreover, in Section 5.4 we will see that the list of memberships can itself be displayed graphically.

2 HOW TO USE THE PROGRAM FANNY

In order to perform fuzzy cluster analyses, we wrote the program FANNY which runs in an IBM-PC environment. The program handles data sets that either consist of interval-scaled measurements or of dissimilarities. As in the program PAM of Chapter 2, the actual algorithm only needs a collection of dissimilarities and does not depend on any measurements. When the data

do consist of measurements, FANNY starts by computing the interobject distances and then uses these to construct the fuzzy clustering from.

2.1 Interactive Use and Input

The program FANNY accepts the same data sets as does PAM and it is operated in a similar way. To run FANNY, it suffices to type

A:FANNY

which yields the following dialogue:

```
FUZZY ANALYSIS

DO YOU WANT TO ENTER MEASUREMENTS ?
(PLEASE ANSWER M)
OR DO YOU PREFER TO GIVE DISSIMILARITIES ?
(THEN ANSWER D) : m

THE PRESENT VERSION OF THE PROGRAM CAN HANDLE UP TO 100 OBJECTS.
(IF MORE ARE TO BE CLUSTERED, THE ARRAYS IN THE PROGRAM MUST BE ADAPTED)

HOW MANY OBJECTS ARE TO BE CLUSTERED ?
-------------------------------------
PLEASE GIVE A NUMBER BETWEEN 3 AND 100 : 22

CLUSTERINGS WILL BE CARRIED OUT IN K1 TO K2 CLUSTERS.
K1 SHOULD BE AT LEAST 2, AND K2 AT MOST 10.
  PLEASE ENTER K1 : 3
  PLEASE ENTER K2 : 3
```

FANNY yields fuzzy clusterings with k clusters, for all values of k between K1 and K2. Note that it is not allowed to ask for 1 cluster, which would be meaningless because all membership coefficients would equal 100%. Also, the maximal number of clusters has to be less than $n/2$, where n is the number of objects. There are numerical reasons for this restriction (having to do with the initialization of the algorithm) but it is also clear that large values of k would lead to a very extensive table of membership coefficients that would be hard to interpret.

The rest of the interactive input is identical to that of PAM:

```
THE PRESENT VERSION OF THE PROGRAM ALLOWS TO ENTER UP TO
80 VARIABLES, OF WHICH AT MOST 20 CAN BE USED IN THE ACTUAL
COMPUTATIONS.
(IF MORE ARE NEEDED, THE ARRAYS INSIDE THE PROGRAM MUST BE
ADAPTED)

WHAT IS THE TOTAL NUMBER OF VARIABLES IN YOUR DATA SET ?
--------------------------------------------------

PLEASE GIVE A NUMBER BETWEEN 1 AND 80 : 2

HOW MANY VARIABLES DO YOU WANT TO USE IN THE ANALYSIS ?
--------------------------------------------------

(AT MOST 2) : 2

VARIABLE TO BE USED          LABEL (AT MOST 10 CHARACTERS)
-----------------↓↓↓↓-----↓↓↓↓↓↓↓↓↓↓ ----------------
NUMBER :         1       x-coordina
NUMBER :         2       y-coordina

DO YOU WANT THE MEASUREMENTS TO BE STANDARDIZED ? (PLEASE
ANSWER YES)
OR NOT ? (THEN ANSWER NO) ..................................n

DO YOU WANT TO USE EUCLIDEAN DISTANCE ? (PLEASE ANSWER E)
OR DO YOU PREFER MANHATTAN DISTANCE ?
(THEN ANSWER M) ............................................e

PLEASE ENTER A TITLE FOR THE OUTPUT (AT MOST 60 CHARACTERS)
------------------------------------------------------------
Artificial data set with 22 points

DO YOU WANT LARGE OUTPUT ? (PLEASE ANSWER YES)
OR IS SMALL OUTPUT SUFFICIENT ? (THEN ANSWER NO)
(IN THE LATTER CASE NO DISSIMILARITIES ARE GIVEN) ..........n

DO YOU WANT GRAPHICAL OUTPUT (SILHOUETTES) ? PLEASE AN-
SWER YES OR NO .............................................y

DO YOU WANT TO ENTER LABELS OF OBJECTS ? PLEASE ANSWER YES
OR NO ......................................................n

DO YOU WANT TO READ THE DATA IN FREE FORMAT ?
--------------------------------------------

THIS MEANS THAT YOU ONLY HAVE TO INSERT BLANK(S) BETWEEN
NUMBERS.
```

(NOTE: WE ADVISE USERS WITHOUT KNOWLEDGE OF FORTRAN FORMATS TO ANSWER YES.)
MAKE YOUR CHOICE (YES/NO) : y

PLEASE TYPE THE NAME OF THE FILE CONTAINING THE DATA (e.g. A:EXAMPLE.DAT)
OR TYPE KEY IF YOU PREFER TO ENTER THE DATA BY KEYBOARD.
WHAT DO YOU CHOOSE ? a:22.dat

WHERE DO YOU WANT YOUR OUTPUT ?

TYPE CON IF YOU WANT IT ON THE SCREEN
OR TYPE PRN IF YOU WANT IT ON THE PRINTER
OR TYPE THE NAME OF A FILE (e.g. B:EXAMPLE.OUT)
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME NAME THEN THE OLD FILE WILL BE OVERWRITTEN.)
WHAT DO YOU CHOOSE ? a:22.fan

CAN MISSING DATA OCCUR IN THE MEASUREMENTS ?
PLEASE ANSWER YES OR NO : n

When there are missing measurements, these are treated in the same way as in PAM: The program tries to compute a complete dissimilarity matrix and then performs the actual clustering algorithm on the latter.

At the end of the interactive session, a summary of the data specifications and options appears on the screen:

DATA SPECIFICATIONS AND CHOSEN OPTIONS

TITLE : Artificial data set with 22 points
THERE ARE 22 OBJECTS
LABELS OF OBJECTS ARE NOT READ
INPUT OF MEASUREMENTS
SMALL OUTPUT
GRAPHICAL OUTPUT IS WANTED (SILHOUETTES)
CLUSTERINGS ARE CARRIED OUT IN 3 TO 3 CLUSTERS

THERE ARE 2 VARIABLES IN THE DATA SET,
AND 2 OF THEM WILL BE USED IN THE ANALYSIS
THE MEASUREMENTS WILL NOT BE STANDARDIZED
EUCLIDEAN DISTANCE WILL BE USED
THERE ARE NO MISSING VALUES
THE MEASUREMENTS WILL BE READ IN FREE FORMAT

```
YOUR DATA RESIDE ON FILE : a:22.dat
YOUR OUTPUT WILL BE WRITTEN ON : a:22.fan

ARE ALL THESE SPECIFICATIONS OK ? YES OR NO : y
```

In the present run, the data are read from a file called 22.dat, which looks like

```
 1   9
 2  10
 2   9
 2   8
 3   9
 7  14
12   9
13  10
13   8
14  10
14   8
15   9
 7   7
 6   3
 7   3
 8   3
 6   2
 7   2
 8   2
 6   1
 7   1
 8   1
```

These are the data of Figure 1. As soon as the program run is completed, a message appears on the screen and the output can be found in the file 22.fan.

2.2 Output

The output file of the preceding example is displayed in Figure 2. The first part gives some general information on the type of data and the chosen options, exactly as in PAM. Then the results for $k = 3$ are given, under the heading NUMBER OF CLUSTERS 3. Note that FANNY does not use any representative objects. Instead, the algorithm attempts to minimize the

objective function

$$\sum_{v=1}^{k} \frac{\sum_{i,j=1}^{n} u_{iv}^2 u_{jv}^2 d(i,j)}{2\sum_{j=1}^{n} u_{jv}^2}$$

where u_{iv} stands for the membership of object i in cluster v. At first sight this expression looks rather formidable, but we may note a few things. To begin with, it contains nothing but the dissimilarities $d(i, j)$ and the membership coefficients that we are trying to find. This explains why interval-scaled measurements are not required. Second, the sum in the numerator ranges over all *pairs* of objects $\{i, j\}$ (instead of making the sum of the distances of the objects to some cluster center, which does not exist here). Each pair $\{i, j\}$ is encountered twice because $\{j, i\}$ also occurs, which is why the sum is divided by 2. The outer sum is over all clusters v, so the objective function that we are trying to minimize is really a kind of total dispersion. More on this may be found in Sections 4 and 5, but for now it is enough to know that the algorithm is iterative and that it stops when the objective function converges. In Figure 2 we see that the algorithm needed five iteration steps and that the final value of the objective function is 16.0742.

Next, the actual memberships are printed. In this example there are three columns (because $k = 3$). Each object is identified by a three-character label (here the computer has generated the default labels 001, ..., 022, but the user may enter other labels when appropriate). The membership coefficients of this example were already listed in Table 1 and discussed in Section 1.

Some fuzzy clusterings are more fuzzy than others. When each object has equal memberships in all clusters (hence they are all $1/k$), we have complete fuzziness. On the other hand, when each object has a membership of 1 in some cluster (and hence a zero membership in all other clusters), the clustering is entirely hard (i.e., it is a partition). To measure how hard a fuzzy clustering is, we compute *Dunn's partition coefficient* (1976) given by

$$F_k = \sum_{i=1}^{n} \sum_{v=1}^{k} u_{iv}^2 / n$$

For a completely fuzzy clustering (all $u_{iv} = 1/k$) this takes on its minimal value $1/k$, whereas a partition (all $u_{iv} = 0$ or 1) yields the maximal value $F_k = 1$. The *normalized version* given by

$$F_k' = \frac{F_k - (1/k)}{1 - (1/k)} = \frac{kF_k - 1}{k - 1}$$

```
                    **********************
                    *                    *
                    *  FUZZY  ANALYSIS   *
                    *                    *
                    **********************

TITLE  : Artificial data set with 22 points

DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 THERE ARE   22 OBJECTS
 LABELS OF OBJECTS ARE NOT READ
 INPUT OF MEASUREMENTS
 SMALL OUTPUT
 GRAPHICAL OUTPUT IS WANTED (SILHOUETTES)
 CLUSTERINGS ARE CARRIED OUT IN    3 TO    3 CLUSTERS

 THERE ARE    2 VARIABLES IN THE DATA SET,
  AND    2 OF THEM WILL BE USED IN THE ANALYSIS
 THE LABELS OF THESE VARIABLES ARE :
         x-coordina    (POSITION :  1)
         y-coordina    (POSITION :  2)
 THE MEASUREMENTS WILL NOT BE STANDARDIZED
 EUCLIDEAN DISTANCE WILL BE USED
 THERE ARE NO MISSING VALUES
 THE MEASUREMENTS WILL BE READ IN FREE FORMAT

 YOUR DATA RESIDE ON FILE       : a:22.dat


*********************************
*                               *
*  NUMBER OF CLUSTERS     3     *
*                               *
*********************************

ITERATION     OBJECTIVE FUNCTION

    1               16.8363
    2               16.0871
    3               16.0744
    4               16.0742
    5               16.0742

FUZZY CLUSTERING
****************

        1      2      3

001   .8677  .0564  .0759
002   .8785  .0551  .0664
003   .9362  .0274  .0364
004   .8606  .0562  .0832
005   .8741  .0549  .0709
006   .4205  .3545  .2250
007   .0849  .8188  .0963
008   .0618  .8718  .0664
009   .0629  .8564  .0807
010   .0596  .8745  .0659
011   .0606  .8614  .0781
012   .0734  .8386  .0880
013   .3553  .2713  .3734
014   .1156  .0853  .7992
015   .0787  .0689  .8524
016   .0972  .1017  .8012
017   .0794  .0617  .8589
018   .0424  .0380  .9196
019   .0687  .0714  .8599
020   .0982  .0796  .8222
021   .0696  .0636  .8668
022   .0873  .0902  .8226

PARTITION COEFFICIENT OF DUNN =    .71
ITS NORMALIZED VERSION        =    .57

CLOSEST HARD CLUSTERING
***********************

CLUSTER NUMBER     SIZE     OBJECTS

        1           6      001 002 003 004 005 006

        2           6      007 008 009 010 011 012

        3          10      013 014 015 016 017 018 019 020 021 022
```

Figure 2 FANNY output for the example of Figure 1.

```
CLUSTERING VECTOR
*****************

                 1  1  1  1  1  1  2  2  2  2  2  2  3  3  3  3  3  3  3  3
                 3  3

                               ****************
                               *              *
                               * SILHOUETTES  *
                               *              *
                               ****************

                          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                          . . . . . . . . . . . . . . . . . . . . . . . . . .
                          0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                          0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0
 CLU  NEIG  S(I)       I +++++++++++++++++++++++++++++++++++++++++++++++++++
                         +                                                  +
  1    3    .73     003+************************************                +
  1    3    .73     002+************************************                +
  1    3    .70     001+***********************************                 +
  1    3    .68     005+**********************************                  +
  1    3    .64     004+********************************                    +
  1    2    .14     006+*******                                             +
                         +                                                  +
  2    3    .83     010+*****************************************           +
  2    3    .82     008+*****************************************           +
  2    3    .80     011+****************************************            +
  2    3    .80     012+****************************************            +
  2    3    .79     009+***************************************             +
  2    3    .75     007+*************************************               +
                         +                                                  +
  3    1    .82     018+*****************************************           +
  3    1    .80     021+****************************************            +
  3    2    .78     019+***************************************             +
  3    1    .78     015+***************************************             +
  3    1    .78     017+***************************************             +
  3    2    .76     022+**************************************              +
  3    1    .76     020+**************************************              +
  3    2    .74     016+*************************************               +
  3    1    .73     014+************************************                +
  3    1    .11     013+*****                                               +
                         +                                                  +
                         ++++++++++++++++++++++++++++++++++++++++++++++++++++
                          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                          . . . . . . . . . . . . . . . . . . . . . . . . . .
                          0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                          0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

      CLUSTER    1 HAS AVERAGE SILHOUETTE WIDTH    .60
      CLUSTER    2 HAS AVERAGE SILHOUETTE WIDTH    .80
      CLUSTER    3 HAS AVERAGE SILHOUETTE WIDTH    .71

      FOR THE ENTIRE DATA SET, THE AVERAGE SILHOUETTE WIDTH IS   .70

 The output is on file : a:22.fan
```

Figure 2 (*Continued*)

always varies from 0 to 1, whatever value of k was chosen. In Figure 2, we see that $F_k = 0.71$ and $F_k' = 0.57$, which lie somewhere between the extremes.

We are also interested in the partition that is closest to our fuzzy clustering, especially when the output contains many membership coefficients. This closest hard clustering is obtained by assigning each object to the cluster in which it has the largest membership. In our example, objects $1, \ldots, 5$ are clearly to be assigned to cluster 1, objects $7, \ldots, 12$ to cluster 2, and objects $14, \ldots, 22$ to cluster 3. However, the intermediate objects also have to be assigned. Object 6 is put in cluster 1 because its membership in that cluster (0.42) is somewhat larger than that in the second cluster (0.35).

The assignment of object 13 is even more doubtful because its membership in the third cluster (0.37) is but slightly larger than its other memberships (0.36 and 0.27). We may conclude that the closest hard clustering does simplify the situation, but that for some objects quite a bit of information may be lost. (Another option, not implemented in FANNY, would be to delete the most fuzzy observations before constructing the hard clustering.)

In the output, the closest hard clustering is listed in the same way as the partitions obtained from PAM and CLARA. Each cluster is identified by its number, followed by its size and the labels of its objects. Also the clustering vector is printed, in which the different clusters are again encountered in ascending order, so the user may easily compare the results with the clusterings obtained from the other programs. (In fact, FANNY first numbers the hard clusters like this before printing the fuzzy clustering, where the clusters are ranked in the same way.)

The last part of the output is the silhouette plot of the hard clustering. In Section 2.2 of Chapter 2 we saw that the silhouettes can be computed for any partition, regardless of the clustering algorithm used (no representative objects are needed). The silhouette plot is constructed from the interobject dissimilarities only. In Figure 2 we see that the first cluster contains five objects with large $s(i)$ values, whereas for object 6 we find $s(i) = 0.14$, which is very low, indicating that this object is not "well-clustered". In the second column (NEIG) we see that the neighbor of object 6 is cluster 2, so object 6 is intermediate between its own cluster and cluster 2. The second cluster is very pronounced because all of its $s(i)$ values are quite large. In the third cluster we see that nine objects are well inside their cluster, whereas object 13 has a very low $s(i)$ of 0.11. [Note that object 13 is listed at the bottom because the $s(i)$ are ranked in decreasing order in each cluster.]

Below the plot some summary values are given. For each cluster the average silhouette width is listed [this is just the average of its $s(i)$ values]. They show that cluster 2 is more pronounced than clusters 1 and 3, both of which are stuck with an outlier. Finally, the average $s(i)$ of the entire data set is listed. The latter value corresponds to the blackness of the plot and assesses the overall quality of the partition. The present value (0.70) is quite high. It is also better than the average silhouette width for other values of k: If we run FANNY again for $k = 2$ we find 0.54 and for $k = 4, \ldots, 10$ we obtain still lower values. This leads us to assume that $k = 3$ is a fair choice for these data. The best average $s(i)$ is called the *silhouette coefficient* (SC). If we compare SC = 0.70 to Table 4 of Chapter 2, we may conclude that a reasonable clustering structure has been found.

If we run PAM on the same data for $k = 3$, we happen to find the same hard clustering and hence the same silhouette plot. Also for $k = 2$ they turn

out to coincide, whereas for $k = 4$, 5, and 6, PAM and FANNY give different results (some better, some worse). It is often instructive to run both programs on the same data sets and to compare the outputs (preferably across different values of k).

3 EXAMPLES

Our first example is a collection of subjective dissimilarities between 12 countries, listed in Table 5 of Chapter 2. FANNY can be applied to these data in exactly the same way as PAM, except that it is no longer allowed to put $k = 1$. Figure 3 shows the output for $k = 3$, for which the algorithm needed 16 iteration steps. The fuzzy clustering does not immediately appeal to the intuition, partly because it still lists the countries in their original (alphabetical) order. None of the membership coefficients is very large, so there is a considerable amount of fuzziness, as is also reflected by the normalized partition coefficient which equals 0.11. The closest hard clustering is easier to interpret because the cluster {BEL, FRA, ISR, USA} contains the Western countries, {BRA, EGY, IND, ZAI} consists of the developing countries, and {CHI, CUB, USS, YUG} contains the Communist countries of this study. In each cluster, the countries are still listed alphabetically. Note that this hard clustering slightly differs from the partition found by PAM (Figure 8 of Chapter 2) in which EGY was added to the first cluster. Also the silhouettes are not quite the same, because in the FANNY output EGY now obtains $s(i) = -0.02$. Without EGY, the first cluster gets smaller within distances, and so USA, FRA, BEL, and ISR now obtain better $s(i)$ values than in the PAM output. The average silhouette width in the FANNY plot becomes 0.34, a little higher than the 0.33 value yielded by PAM. In either case, the structure is relatively weak.

In the silhouette plot, the countries are no longer listed in their original order but ranked according to their $s(i)$. This makes it easy to see that USA is the "best clustered" object in cluster 1, that ZAI ranks highest in cluster 2, and that CUB ranks highest in cluster 3. This is similar to the original fuzzy clustering, because USA had the highest membership (0.63) in cluster 1, ZAI had the highest membership (0.53) in cluster 2, and CUB had the highest membership (0.64) in cluster 3. In the silhouette plot we see that the "worst clustered" object is EGY, for which $s(i)$ is -0.02. Looking at the fuzzy clustering, we note that EGY was about evenly distributed over clusters 1 and 2, with memberships of 0.33 and 0.42.

Let us now try FANNY on the same extreme examples that we considered in Section 3 of Chapter 2. The first data set contains five objects coinciding with one geometrical point and three objects coinciding with

```
*********************************
*                               *
*  NUMBER OF CLUSTERS      3    *
*                               *
*********************************

ITERATION       OBJECTIVE FUNCTION

    1                10.7794
    2                10.0553
    3                 9.9468
    4                 9.9197
    5                 9.9094
    6                 9.9045
    7                 9.9019
    8                 9.9005
    9                 9.8998
   10                 9.8994
   11                 9.8992
   12                 9.8991
   13                 9.8990
   14                 9.8990
   15                 9.8990
   16                 9.8990

FUZZY CLUSTERING
****************

          1       2       3

BEL    .5984   .2400   .1616
BRA    .2602   .5293   .2104
CHI    .2239   .2823   .4939
CUB    .1582   .2058   .6360
EGY    .3318   .4172   .2509
FRA    .5997   .2313   .1690
IND    .2528   .4588   .2884
ISR    .4930   .2931   .2139
USA    .6305   .2243   .1452
USS    .1819   .2170   .6011
YUG    .2339   .2576   .5085
ZAI    .2514   .5345   .2141

PARTITION COEFFICIENT OF DUNN =    .41
ITS NORMALIZED VERSION        =    .11

CLOSEST HARD CLUSTERING
***********************

CLUSTER NUMBER     SIZE     OBJECTS

        1            4      BEL FRA ISR USA

        2            4      BRA EGY IND ZAI

        3            4      CHI CUB USS YUG

CLUSTERING VECTOR
*****************

          1  2  3  3  2  1  2  1  1  3  3  2

                          *****************
                          *               *
                          *  SILHOUETTES  *
                          *               *
                          *****************

                    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                    0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                    0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

 CLU   NEIG   S(I)    I +-------------------------------------------------------+
                        +                                                       +
   1     2    .53    USA+*************************                             +
   1     2    .51    FRA+************************                              +
   1     2    .50    BEL+************************                              +
   1     2    .41    ISR+*********************                                 +
                        +                                                       +
   2     1    .23    ZAI+***********                                           +
   2     1    .20    BRA+***********                                           +
   2     3    .19    IND+*********                                             +
   2     1   -.02    EGY+                                                      +
                        +                                                       +
   3     2    .46    CUB+************************                              +
   3     1    .44    USS+**********************                                +
   3     2    .36    CHI+******************                                    +
   3     1    .31    YUG+***************                                       +
                        +                                                       +
                        +-------------------------------------------------------+

                    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                    0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                    0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

      CLUSTER    1 HAS AVERAGE SILHOUETTE WIDTH    .49
      CLUSTER    2 HAS AVERAGE SILHOUETTE WIDTH    .15
      CLUSTER    3 HAS AVERAGE SILHOUETTE WIDTH    .40

      FOR THE ENTIRE DATA SET, THE AVERAGE SILHOUETTE WIDTH IS    .34

The output is on file : a:country.fan
```

Figure 3 Output of FANNY for the 12 countries data, for $k = 3$.

another. Running FANNY with $k = 2$ yields Figure 4, in which only a single iteration step was necessary to reduce the objective function to 0. The fuzzy clustering is already quite hard, because the objects $1, \ldots, 5$ have a membership of approximately 1 in the first cluster and the objects 6, 7, and 8 have a membership of 1 in the second. Therefore Dunn's partition coefficient becomes 1.00, as well as its normalized version. The closest hard clustering is what it should be and the silhouette plot is the same as that of PAM. The average silhouette width attains its maximal value 1.00, so $k = 2$ is selected.

The second data set contains seven objects with zero dissimilarities to each other and one object which is far away from all of them. This kind of situation occurs when there is a far outlier, which makes all other dissimilarities look small by comparison. FANNY yields Figure 5, with again only a single iteration. The membership coefficients are already hard and they put only object 8 in the second cluster. Dunn's partition coefficient reaches 1.00, as does the normalized version. The clustering vector and silhouette plot correspond to those of PAM, so the overall average silhouette width is again $1 - \frac{1}{8} \approx 0.88$.

In the third data set all dissimilarities between objects are equal, so there is no clustering structure at all. FANNY gives an adequate description of this by putting all memberships equal to $\frac{1}{2}$ (up to numerical accuracy). This is exactly the situation in which Dunn's partition coefficient takes on its minimal value $1/k = \frac{1}{2}$, so its normalized version becomes 0. The output in Figure 6 also contains the closest hard clustering, which is rather arbitrary because no object shows a definite preference for either cluster. Although this hard clustering differs from the one found by PAM, the silhouette plot is again empty because all $s(i)$ remain 0. Therefore, the average silhouette width becomes 0, telling the user that no real clusters have been found.

In one of the first papers on fuzzy clustering, Ruspini (1970) used the data listed in Table 6 of Chapter 2. Their scatterplot (Figure 12 of Chapter 2) clearly contains four groups of points when viewed with the human eye. Group A equals $\{1, \ldots, 20\}$, whereas $B = \{21, \ldots, 43\}$, $C = \{44, \ldots, 60\}$, and $D = \{61, \ldots, 75\}$. If we apply FANNY with $k = 2$, we obtain the clusters $A \cup D$ and $B \cup C$ that were also found by PAM, so the average silhouette width $\bar{s}(k)$ again equals 0.58. Figure 7 shows the silhouette plots produced by FANNY for $k = 2, \ldots, 6$. For $k = 3$ we find A, $B \cup C$, and D, whereas PAM yielded $A \cup D$, B, and C. For $k = 4$ FANNY yields the expected clustering into A, B, C, and D. The corresponding average silhouette width $\bar{s}(k) = 0.74$ is the highest across all values of k, so $k = 4$ is a reasonable choice. Also for $k = 5$ and $k = 6$ FANNY yields hard clusterings that differ from those of PAM: For $k = 5$ the cluster B is split in two, whereas for $k = 6$ the cluster A is bisected. Although FANNY and

```
DISSIMILARITY MATRIX
--------------------

001
002        .00
003        .00       .00
004        .00       .00       .00
005        .00       .00       .00       .00
006       3.60      3.60      3.60      3.60      3.60
007       3.60      3.60      3.60      3.60      3.60       .00
008       3.60      3.60      3.60      3.60      3.60       .00       .00

*********************************
*                               *
*  NUMBER OF CLUSTERS     2     *
*                               *
*********************************

ITERATION     OBJECTIVE FUNCTION
    1                 .0000

FUZZY CLUSTERING
****************

        1       2

001   .9998   .0002
002   .9999   .0001
003   .9999   .0001
004   .9999   .0001
005   .9999   .0001
006   .0000  1.0000
007   .0000  1.0000
008   .0000  1.0000

PARTITION COEFFICIENT OF DUNN =  1.00
ITS NORMALIZED VERSION        =  1.00

CLOSEST HARD CLUSTERING
***********************

CLUSTER NUMBER     SIZE     OBJECTS

        1            5      001 002 003 004 005

        2            3      006 007 008

CLUSTERING VECTOR
*****************

             1  1  1  1  1  2  2  2

                          *****************
                          *               *
                          *  SILHOUETTES  *
                          *               *
                          *****************

                      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                      0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                      0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

 CLU  NEIG  S(I)    I +++++++++++++++++++++++++++++++++++++++++++++++++++++++++
                      +                                                       +
   1     2  1.00    001+*******************************************************+
   1     2  1.00    002+*******************************************************+
   1     2  1.00    003+*******************************************************+
   1     2  1.00    004+*******************************************************+
   1     2  1.00    005+*******************************************************+
                      +                                                       +
   2     1  1.00    006+*******************************************************+
   2     1  1.00    007+*******************************************************+
   2     1  1.00    008+*******************************************************+
                      +                                                       +
                      +++++++++++++++++++++++++++++++++++++++++++++++++++++++++

                      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                      0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                      0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

     CLUSTER    1 HAS AVERAGE SILHOUETTE WIDTH  1.00
     CLUSTER    2 HAS AVERAGE SILHOUETTE WIDTH  1.00

     FOR THE ENTIRE DATA SET, THE AVERAGE SILHOUETTE WIDTH IS  1.00
```

Figure 4 FANNY output for a data set with two tight clusters.

```
DISSIMILARITY MATRIX
--------------------

001
002        .00
003        .00       .00
004        .00       .00       .00
005        .00       .00       .00       .00
006        .00       .00       .00       .00       .00
007        .00       .00       .00       .00       .00       .00
008       3.60      3.60      3.60      3.60      3.60      3.60      3.60

*********************************
*                               *
*  NUMBER OF CLUSTERS      2    *
*                               *
*********************************

ITERATION      OBJECTIVE FUNCTION
    1                  .0000

FUZZY CLUSTERING
****************

         1       2

001   .9998   .0002
002   .9999   .0001
003   .9999   .0001
004   .9999   .0001
005   .9999   .0001
006  1.0000   .0000
007  1.0000   .0000
008   .0000  1.0000

PARTITION COEFFICIENT OF DUNN =  1.00
ITS NORMALIZED VERSION        =  1.00

CLOSEST HARD CLUSTERING
***********************

CLUSTER NUMBER     SIZE     OBJECTS

         1           7      001 002 003 004 005 006 007

         2           1      008

CLUSTERING VECTOR
*****************

             1  1  1  1  1  1  1  2

                          *****************
                          *               *
                          *  SILHOUETTES  *
                          *               *
                          *****************

                     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                     0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                     0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

 CLU  NEIG  S(I)    I +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
                      +                                                           +
   1    2  1.00    001+***********************************************************+
   1    2  1.00    002+***********************************************************+
   1    2  1.00    003+***********************************************************+
   1    2  1.00    004+***********************************************************+
   1    2  1.00    005+***********************************************************+
   1    2  1.00    006+***********************************************************+
   1    2  1.00    007+***********************************************************+
                      +                                                           +
   2    1   .00     008+                                                           1+
                      +                                                           +
                      +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

                     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                     0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                     0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

     CLUSTER    1 HAS AVERAGE SILHOUETTE WIDTH  1.00
     CLUSTER    2 HAS AVERAGE SILHOUETTE WIDTH   .00

     FOR THE ENTIRE DATA SET, THE AVERAGE SILHOUETTE WIDTH IS    .88
```

Figure 5 FANNY output for a data set with an extreme outlier.

```
DISSIMILARITY MATRIX
--------------------

001
002      3.60
003      3.60      3.60
004      3.60      3.60      3.60
005      3.60      3.60      3.60      3.60
006      3.60      3.60      3.60      3.60      3.60
007      3.60      3.60      3.60      3.60      3.60      3.60
008      3.60      3.60      3.60      3.60      3.60      3.60      3.60

********************************
*                              *
*  NUMBER OF CLUSTERS     2    *
*                              *
********************************

ITERATION     OBJECTIVE FUNCTION

    1               6.5880
    2               6.3721
    3               6.3211
    4               6.3064
    5               6.3019
    6               6.3006
    7               6.3002
    8               6.3001
    9               6.3000
   10               6.3000
   11               6.3000

FUZZY CLUSTERING
****************

         1       2

001   .5001   .4999
002   .5000   .5000
003   .4997   .5003
004   .4992   .5008
005   .4999   .5001
006   .5000   .5000
007   .5002   .4998
008   .5006   .4994

PARTITION COEFFICIENT OF DUNN =    .50
ITS NORMALIZED VERSION        =    .00

CLOSEST HARD CLUSTERING
***********************

CLUSTER NUMBER     SIZE     OBJECTS

         1           4      001 006 007 008

         2           4      002 003 004 005

CLUSTERING VECTOR
*****************

          1  2  2  2  2  1  1  1

                                  *****************
                                  *               *
                                  *  SILHOUETTES  *
                                  *               *
                                  *****************

                         0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                         . . . . . . . . . . . . . . . . . . . . . . . . . .
                         0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                         0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

 CLU  NEIG  S(I)     I +++++++++++++++++++++++++++++++++++++++++++++++++++++
                       +                                                   +
  1    2    .00    001+                                                    +
  1    2    .00    006+                                                    +
  1    2    .00    007+                                                    +
  1    2    .00    008+                                                    +
                       +                                                   +
  2    1    .00    002+                                                    +
  2    1    .00    003+                                                    +
  2    1    .00    004+                                                    +
  2    1    .00    005+                                                    +
                       +                                                   +
                       +++++++++++++++++++++++++++++++++++++++++++++++++++++

                         0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
                         . . . . . . . . . . . . . . . . . . . . . . . . . .
                         0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
                         0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

        CLUSTER    1 HAS AVERAGE SILHOUETTE WIDTH    .00
        CLUSTER    2 HAS AVERAGE SILHOUETTE WIDTH    .00

        FOR THE ENTIRE DATA SET, THE AVERAGE SILHOUETTE WIDTH IS    .00
```

Figure 6 FANNY output for a data set without clusters.

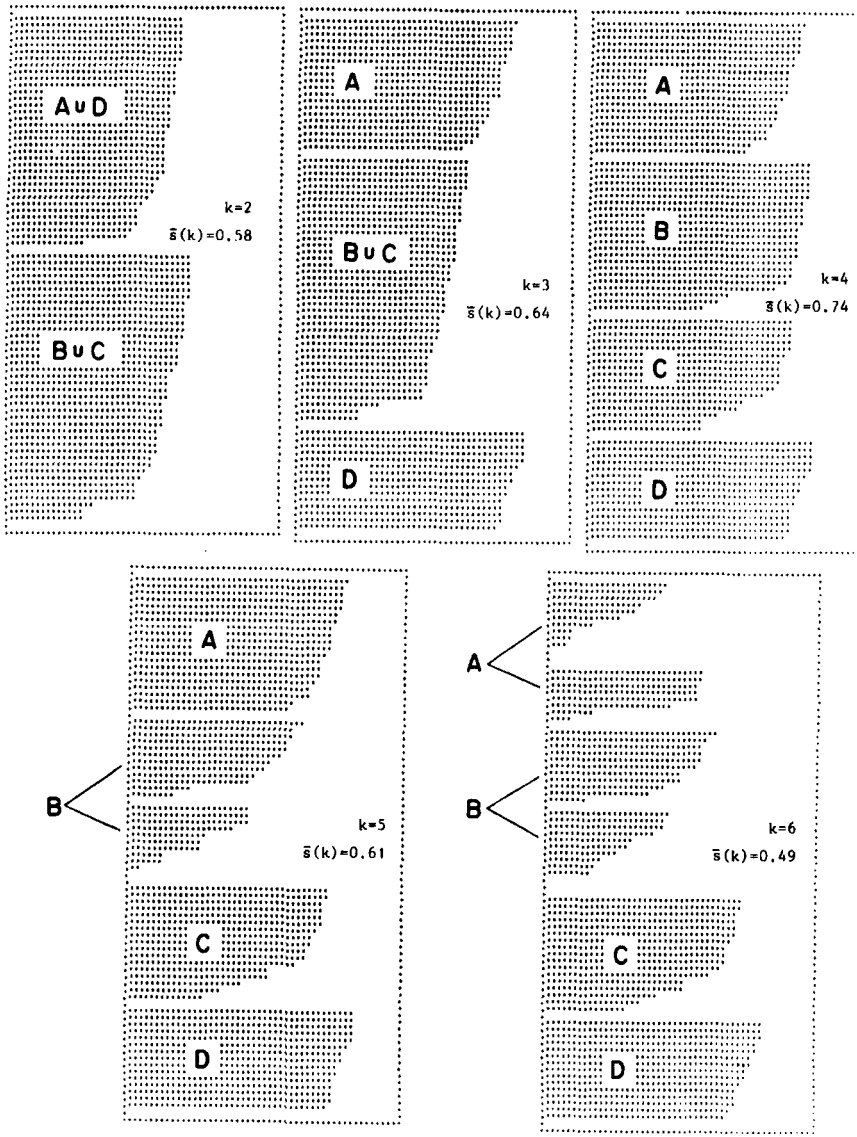


Figure 7 Silhouette plots obtained by running FANNY on the Ruspini data, for k ranging from 2 to 6.

PAM operate quite differently, they both select the natural clustering with $k = 4$ on the basis of the $\bar{s}(k)$.

*4 MORE ON THE ALGORITHM AND THE PROGRAM

4.1 Description of the Algorithm

The fuzzy clustering technique used in this program aims at the minimization of the objective function

$$C = \sum_{v=1}^{k} \frac{\sum_{i,j=1}^{n} u_{iv}^2 u_{jv}^2 d(i,j)}{2\sum_{j=1}^{n} u_{jv}^2} \tag{1}$$

in which the $d(i, j)$ represent the given distances (or dissimilarities) between objects i and j, whereas u_{iv} is the unknown membership of object i to cluster v. Note that each term appears two times in the multiple sum. The factor 2 in the denominator compensates for this duplicity, while assuring the coherence with other algorithms (see Section 5.1). The membership functions are subject to the constraints

$$u_{iv} \geq 0 \quad \text{for } i = 1, \ldots, n;\ v = 1, \ldots, k \tag{2}$$

$$\sum_{v} u_{iv} = 1 \quad \text{for } i = 1, \ldots, n \tag{3}$$

expressing that memberships cannot be negative and that each object has a constant total membership, distributed over the different clusters; by convention this total membership is normalized to 1.

The remainder of this section is a technical description of the numerical algorithm used to minimize (1). Readers wishing to skip this material may continue directly with Section 5.

A characterization of the local optima of (1) can be found from the Lagrange equation

$$L = \sum_{v} \frac{\sum_{ij} u_{iv}^2 u_{jv}^2 d(i,j)}{2\sum_{j} u_{jv}^2} - \sum_{j} \gamma_j \left(\sum_{v} u_{jv} - 1 \right) - \sum_{j} \sum_{v} \psi_{jv} u_{jv} \tag{4}$$

in which the γ_j and the ψ_{jv} are known as Lagrange multipliers. Its derivatives with respect to the membership variables are

$$\frac{\partial L}{\partial u_{iv}} = \frac{2u_{iv}\sum_{j} u_{jv}^2 d(i,j)}{\sum_{j} u_{jv}^2} - \frac{u_{iv}\sum_{h}\sum_{j} u_{jv}^2 u_{hv}^2 d(h,j)}{\left(\sum_{j} u_{jv}^2\right)^2} - \gamma_i - \psi_{iv} \tag{5}$$

Taking into account the objective function and the constraints (2) and (3) of the original minimization problem, we can write down the corresponding Kuhn and Tucker conditions:

$$\psi_{iv} \geq 0 \tag{6}$$

$$\frac{\partial L}{\partial u_{iv}} = 0 \tag{7}$$

$$u_{iv}\psi_{iv} = 0 \tag{8}$$

The relations (7) and (5) can be combined into

$$a_{iv}u_{iv} - \gamma_i - \psi_{iv} = 0 \tag{9}$$

in which

$$a_{iv} = \frac{2\Sigma_j u_{jv}^2 d(i, j)}{\Sigma_j u_{jv}^2} - \frac{\Sigma_h \Sigma_j u_{hv}^2 u_{jv}^2 d(h, j)}{\left(\Sigma_j u_{jv}^2\right)^2} \tag{10}$$

The function a_{iv} can be either positive, zero, or negative. Considering first the nonzero cases, one can divide all terms of Eq. (9) by a_{iv} and upon summation for all values of v, taking into account Eq. (3), one finds

$$\gamma_i = \frac{1 - \Sigma_v(\psi_{iv}/a_{iv})}{\Sigma_v(1/a_{iv})}$$

Replacing this term in (9), one gets

$$u_{iv} = \frac{1/a_{iv}}{\Sigma_w(1/a_{iw})} + \frac{\psi_{iv}}{a_{iv}} - \frac{\Sigma_w(\psi_{iw}/a_{iw})}{a_{iv}\Sigma_w(1/a_{iw})} \tag{11}$$

Considering the conditions (6), the relations (11) can take one of two forms for each object i:

1. $\psi_{iv} = 0$ for $v = 1, \ldots, k$ so that

$$u_{iv} = \frac{1/a_{iv}}{\Sigma_w(1/a_{iw})} \tag{12}$$

Taking into account constraint (2), this set of solutions is only possible for each object i if

$$\frac{1/a_{iv}}{\Sigma_w(1/a_{iw})} \geq 0 \quad \text{for } v = 1, \ldots, k \tag{13}$$

If this condition is not fulfilled, the preceding solution is not valid and we have to consider the alternative form:

2. $\psi_{iv} > 0$ for at least some v. According to (8) and (11) this solution implies that

$$u_{iv} = 0 = \frac{1/a_{iv}}{\Sigma_w(1/a_{iw})} + \frac{\psi_{iv}}{a_{iv}} - \frac{\Sigma_w(\psi_{iw}/a_{iw})}{a_{iv}\Sigma_w(1/a_{iw})} \tag{14}$$

for at least some v. Because Eq. (3) must also be satisfied, it is clear that this solution is not valid for all v of one object i. Hence let us define the partition:

$$\begin{aligned} V- &= \{v;\ u_{iv} = 0\} \\ V+ &= \{v;\ u_{iv} > 0 \Rightarrow \psi_{iv} = 0\} \neq \varnothing \end{aligned} \tag{15}$$

If one can exclude the case where $1/a_{iv} = 0$, solution (14) implies

$$\psi_{iv} = \frac{\Sigma_w(\psi_{iw}/a_{iw})}{\Sigma_w(1/a_{iw})} - \frac{1}{\Sigma_w(1/a_{iw})} \quad \text{for } v \in V- \tag{16}$$

In Eq. (16) the right-hand term is independent of v; hence all ψ_{iv} are identical for all $v \in V-$ (but may differ for different i). Solution (16) can hence be written:

$$\psi_{iv} = -\frac{1}{\Sigma_{w \in V+}(1/a_{iw})} \quad \text{for } v \in V- \tag{17}$$

As for $v \in V+$, (11) becomes

$$u_{iv} = \frac{1/a_{iv}}{\Sigma_w(1/a_{iw})} - \frac{\Sigma_w(\psi_{iw}/a_{iw})}{a_{iv}\Sigma_w(1/a_{iw})} \tag{18}$$

Introducing (17) in (18) provides, after some transformation,

$$u_{iv} = \frac{1/a_{iv}}{\Sigma_{w \in V+}(1/a_{iw})} \tag{19}$$

which is analogous to (12).

Equations (15), (17), and (19) are, according to Kuhn and Tucker, necessary conditions for a local minimum, but in general they are not sufficient conditions. Actually it can be seen that these equations also describe local maxima and saddle points.

In fact, the local minima will be reached for

$$u_{iv} = 0 \quad \text{for } v \in V- \tag{20}$$

and

$$u_{iv} = \frac{1/a_{iv}}{\sum_{w \in V+}(1/a_{iw})} \quad \text{for } v \in V+ \tag{21}$$

where

$$V- = \left\{ v;\ \frac{1/a_{iv}}{\sum_{w}(1/a_{iw})} \leq 0 \right\} \tag{22}$$

and

$$V+ = \left\{ v;\ \frac{1/a_{iv}}{\sum_{w}(1/a_{iw})} > 0 \right\} \tag{23}$$

As for the degenerate case where $1/a_{iv} = 0$, it can be seen from (10) that it corresponds to $\sum_i u_{iv}^2 = 0$, meaning that some cluster v has no membership at all: Again it can be shown that this solution is not a minimum.

The fact that (13) is not always satisfied implies that a_{iv} can be either positive or negative. Therefore one must also consider the possibility that a_{iv} be zero, which invalidates expression (11). However, this particular case can be solved by regarding it as the limiting solution for a_{iv} being any positive or negative small value, and it can be seen that both limits render $u_{iv} = 1$.

The system of Eqs. (20) and (21) does not provide a straightforward analytical solution to the problem of minimizing the objective function (1), because the right-hand term of (21) still contains all the unknowns. However, it does provide a way to find the solutions iteratively. Indeed, having some initial values for all u_{iv}, one can compute all a_{iv} according to (10) and calculate new u_{iv} from (20) and (21), and so on. Hence the iterative algorithm can take the following form:

A1 Initialize the membership functions as

$$^0u_{iv} \quad \text{for all } i = 1, \ldots, n \quad \text{and all } v = 1, \ldots, k$$

taking into account constraints (2) and (3). Calculate the objective function ${}^{0}C$ by (1). (Note that the left superscripts stand for the number of the iteration step.)

A2 Compute for each $i = 1, \ldots, n$ the following quantities:

A2.1 Compute for each $v = 1, \ldots, k$

$$
{}^{m}a_{iv} = \frac{2\left(\sum_{j=1}^{i-1} {}^{m+1}u_{jv}^2\, d(i,j) + \sum_{j=i}^{n} {}^{m}u_{jv}^2\, d(i,j)\right)}{\sum_{j=1}^{i-1} {}^{m+1}u_{jv}^2 + \sum_{j=i}^{n} {}^{m}u_{jv}^2}
$$

$$
- \frac{\sum_{j=1}^{i-1}\sum_{h=1}^{i-1} {}^{m+1}u_{jv}^2\, {}^{m+1}u_{hv}^2\, d(i,j) + \sum_{j=1}^{i-1}\sum_{h=i}^{n} {}^{m+1}u_{jv}^2\, {}^{m}u_{hv}^2\, d(i,j)}{\sum_{j=1}^{i-1} {}^{m+1}u_{jv}^2 + \sum_{j=i}^{n} {}^{m}u_{jv}^2}
$$

$$
+ \frac{\sum_{j=i}^{n}\sum_{h=1}^{i-1} {}^{m}u_{jv}^2\, {}^{m+1}u_{hv}^2\, d(i,j) + \sum_{j=i}^{n}\sum_{h=i}^{n} {}^{m}u_{jv}^2\, {}^{m}u_{hv}^2\, d(i,j)}{\sum_{j=1}^{i-1} {}^{m+1}u_{jv}^2 + \sum_{j=i}^{n} {}^{m}u_{jv}^2}
$$

A2.2 Compute for each $v = 1, \ldots, k$:

$$
A_v = \frac{1/{}^{m}a_{iv}}{\sum_{w}(1/{}^{m}a_{iw})}
$$

A2.2.1 if $A_v \leq 0 \Rightarrow V- = V- \cup \{v\}$

A2.2.2 if $A_v > 0 \Rightarrow V+ = V+ \cup \{v\}$

A2.3 Put for all $v \in V-$

$$
{}^{m+1}u_{iv} = 0
$$

A2.4 Compute for all $v \in V+$

$$
{}^{m+1}u_{iv} = \frac{1/{}^{m}a_{iv}}{\sum_{w \in V+}(1/{}^{m}a_{iw})}
$$

A2.5 Put $V- = V+ = \varnothing$ and restart from A2.1 with the next i.

A3 Calculate the new objective function value ${}^{m+1}C$ by (1). If $({}^{m}C/{}^{m+1}C - 1) < \varepsilon$, then go to A2; otherwise stop.

The rather cumbersome calculations of A2.1 can be simplified by keeping track of intermediate results and by limiting the computations to the updating of the partial sums at each step.

The preceding algorithm has always shown good convergence performance. However, if ever some convergence problems might arise, it is still possible to improve on the iteration steps by applying some ade-

quate converging method, such as the steepest descent method, the Newton–Raphson method, or a similar technique.

Any fuzzy solution found by the preceding algorithm satisfies the general constraints (2) and (3). The corresponding constraints for a hard solution, obtained by replacing the u_{iv} by w_{iv}, would require (2) and (3) to be changed into

$$w_{iv} = 0 \text{ or } 1 \quad \text{for } i = 1, \ldots, n \quad \text{and } v = 1, \ldots, k$$

$$\sum_{v} w_{iv} = 1 \quad \text{for } i = 1, \ldots, n$$

In a fuzzy clustering the membership coefficients of each object can all be strictly positive, provided their sum over all clusters is 1. On the contrary, in a hard cluster solution each object must have one and only one nonzero membership coefficient, which necessarily takes the value 1.

The hard clustering solutions are hence limiting cases of fuzzy ones. How far off a fuzzy solution is from a hard clustering can be evaluated by Dunn's partition coefficient (1976), which is defined as the sum of squares of all the membership coefficients, divided by the number of objects, i.e.,

$$F_k(U) = \sum_{i=1}^{n} \sum_{v=1}^{k} u_{iv}^2 / n \tag{24}$$

in which U is the matrix of all memberships:

$$U = \begin{array}{c} \\ 1 \\ \vdots \\ n \end{array} \begin{array}{c} \begin{array}{ccc} 1 & \cdots & k \end{array} \\ \begin{pmatrix} & u_{iv} & \end{pmatrix} \end{array}$$

It can be seen that for a partition (u_{iv} restricted to 0s and 1s) $F_k(U)$ gets the maximum value of 1, whereas it takes on the minimum value of $1/k$ when all $u_{iv} = 1/k$. This coefficient can thus be normalized to vary from 1 (hard clusters) to 0 (entirely fuzzy), independently of the number of clusters, by the following transformation:

$$F_k'(U) = \frac{F_k(U) - (1/k)}{1 - (1/k)} = \frac{kF_k(U) - 1}{k - 1} \tag{25}$$

This normalized coefficient has sometimes been called "nonfuzziness index" (Roubens, 1982).

It is often interesting to translate a fuzzy clustering allocation to a hard one. By definition, the *closest hard clustering corresponding to a fuzzy one* is given by putting $w_{iq} = 1$ for the cluster q with largest u_{iv}. In case of ties an (arbitrary) choice is made.

This transformation can be used to compare fuzzy solutions to hard ones and for the evaluation of the fuzziness of solutions (see Section 5.3). It should however be appreciated that the fact that no optimal fuzzy cluster remains empty does not preclude the preceding fuzzy-to-hard transformation to produce less than k hard clusters. This occurrence has actually been observed in some special cases.

4.2 Structure of the Program

The structure of the program FANNY is very similar to that of the former programs; the main difference is the actual clustering subroutine, which in the present case is called FUZZY. This subroutine constructs an initial allocation of the objects to the k clusters and it performs the iterations until convergence is reached. It calculates and prints Dunn's partition coefficient (24) as well as its normalized version (25).

The numerical output subroutine is CADDY, which gives both the fuzzy clustering output and the closest hard clustering. It first renumbers the clusters as in the other programs.

The optional graphical output is made by the subroutine FYGUR, which yields the silhouettes (see Chapter 2) that are based on the closest hard clustering.

All these subroutines are called from the main program, which is otherwise identical to that of the other programs except for a slightly different way of storing the dissimilarities in a one-dimensional array.

Table 2 lists some computation times on an IBM/XT with an 8087 accelerator. The same computer and the same data were used as in Table 7 of Chapter 2. It seems that the extra information provided by FANNY (as

Table 2 Computation Times (in minutes) on an IBM / XT with 8087 Accelerator, for Some Randomly Generated Data

Objects	Variables	Clusters	Time
20	2	5	1.35
40	2	5	6.88
60	2	5	11.95
80	2	5	34.57
100	2	5	27.30

compared to the hard clustering yielded by PAM) is obtained at the expense of a substantial increase of computation time. Note that the computation time for 100 objects is less than that for 80 objects, because FANNY needed only 14 iteration steps in the experiment with 100 objects, whereas 29 iterations were necessary to cluster the smaller data set with 80 objects. In general, the computation time of FANNY is hard to predict because the number of iteration steps depends on the actual data.

*5 RELATED METHODS AND REFERENCES

5.1 Fuzzy *k*-Means and the MND2 Method

One of the first fuzzy clustering techniques was the well known *fuzzy k-means* method proposed by Dunn (1974) and Bezdek (1974). This method is based on the minimization of the objective function

$$\sum_i \sum_v u_{iv}^2 \|x_i - m_v\|^2 = \sum_i \sum_v u_{iv}^2 \sum_{f=1}^{p} (x_{if} - m_{vf})^2 \qquad (26)$$

in which m_v is the center of the cluster v, calculated for each variable f by

$$m_{vf} = \frac{\sum_i u_{iv}^2 x_{if}}{\sum_i u_{iv}^2} \qquad (27)$$

and the norm $\|x_i - m_v\|$ is the Euclidean distance between an object x_i and the center of cluster v. Part of the popularity of this approach certainly rests on the fact that it generalizes the classical k-means approach of hard clustering (described in Section 5.3 of Chapter 2).

Implicit in the fuzzy k-means approach is the assumption that the different objects are given by means of coordinates in a p-dimensional space. This is a restrictive condition in comparison with FANNY, for which no such representation of the objects is needed, because only the distances or dissimilarities between objects are required.

Note that, when the data do consist of measurements, it is possible to make a direct comparison between the two methods. In order to do so it is

sufficient to replace m_v in (26) by its value from (27). Hence

$$\sum_i \sum_v u_{iv}^2 \sum_f (x_{if} - m_{vf})^2$$

$$= \sum_i \sum_v u_{iv}^2 \sum_f \left(x_{if} - \frac{\sum_j u_{jv}^2 x_{jf}}{\sum_j u_{jv}^2} \right)^2$$

$$= \sum_v \sum_f \left[\sum_i u_{iv}^2 x_{if}^2 - 2 \frac{\sum_i u_{iv}^2 x_{if} \sum_j u_{jv}^2 x_{jf}}{\sum_j u_{jv}^2} + \frac{\left(\sum_j u_{jv}^2 x_{jf}\right)^2}{\sum_j u_{jv}^2} \right]$$

$$= \sum_v \sum_f \left[\sum_j u_{jv}^2 x_{jf}^2 - \frac{\left(\sum_j u_{jv}^2 x_{jf}\right)^2}{\sum_j u_{jv}^2} \right] = \sum_v \sum_f \frac{\sum_j u_{jv}^2 \sum_i u_{iv}^2 x_{if}^2 - \sum_i \sum_j u_{iv}^2 u_{jv}^2 x_{if} x_{jf}}{\sum_j u_{jv}^2}$$

$$= \sum_v \sum_f \frac{\sum_i \sum_j u_{iv}^2 u_{jv}^2 (x_{if} - x_{jf})^2}{2 \sum_j u_{jv}^2} = \sum_v \frac{\sum_i \sum_j u_{iv}^2 u_{jv}^2 \|x_i - x_j\|^2}{2 \sum_j u_{jv}^2} \qquad (28)$$

The last expression is exactly the objective function of FANNY, apart from the fact that the distances are squared, which is a variant of the current L_1 form of our program. This demonstrates the possible equivalence between FANNY and fuzzy k-means, for objects described by a set of measurements. (It would suffice to enter a dissimilarity matrix consisting of *squared* Euclidean distances into FANNY, without changing the program.)

The equivalence of the two techniques not only concerns their objective functions: The algorithms can be so constructed that each iteration produces the same result with both programs. The only difference is that within each iteration cycle FANNY performs a loop over all pairs of objects, whereas fuzzy k-means loops for each object over the measurement variables. Because the number of objects is usually larger than twice the number of variables, the FANNY algorithm will be somewhat slower than fuzzy k-means, but with the computation speed of modern computers this should only be a minor drawback.

Another program that shows some resemblance to FANNY is the *MND2* algorithm of Roubens (1978), with the objective function

$$\sum_v \sum_{ij} u_{iv}^2 u_{jv}^2 d(i, j) \qquad (29)$$

Although (29) looks similar to the FANNY objective (1), it is their difference that is most important and that explains why FANNY was preferred to MND2. The importance of this difference, the denominator $\sum_j u_{jv}^2$, can best be explained by reference to a hard clustering: In that case,

with all u_{jv} either 0 or 1, this denominator is equal to the number of objects in each cluster. Hence FANNY minimizes a fuzzy equivalent of a sum of error functions for each cluster, whereas MND2 does the same with a sum of products of the number of objects times the error functions. It can be shown that the MND2 minimization tends to bias the result toward clusters of more equal number of objects and error functions than does FANNY. This systematic bias is the main reason for preferring FANNY to MND2.

5.2 Why Did We Choose FANNY?

As seen above, the exponent of the distance term in the objective function can be 1 or 2. Putting the distance exponent equal to 2 corresponds to fuzzy k-means, so the latter is an L_2 method. (Already the classical k-means approach was of the least squares type because its objective was to minimize an error sum of squares.) Putting the exponent of the distance equal to 1 yields FANNY, which is therefore a fuzzy L_1 method. It was shown by Trauwaert (1987) that our fuzzy L_1 method has some definite advantages over fuzzy L_2: a lower sensitivity to outliers or otherwise erroneous data and a better recognition of nonspherical clusters.

Not only the exponents of the distances can vary, but also those of the membership functions u_{iv} and u_{jv}. This possibility was already implemented by Bezdek (1974) in fuzzy k-means and by Libert and Roubens (1982) in MNDR. The same potential exists of course for FANNY; attention must, however, be paid to the fact that the described algorithm needs membership exponents strictly larger than 1 in order to converge properly. This is also the case for the other two algorithms. Recent convergence results for fuzzy k-means with a general membership exponent are given by Hathaway and Bezdek (1988).

Changing the exponent of the memberships in FANNY has some influence on the allocation of the objects in the clustering, although it is not easy to describe this effect. What is certain is that decreasing the exponent will yield higher values of the largest membership functions, i.e., the clusters will appear less fuzzy. However, because the aim of fuzzy clustering is to use the particular features of fuzziness, one should not go too far in that direction. Moreover, exponent values near 1 cause the algorithm to converge more slowly. Therefore, exponents equal to 2 seem to be a reasonable choice, as is confirmed by actual clustering analyses.

5.3 Measuring the Amount of Fuzziness

It has been seen in Section 4.1 how a fuzzy clustering solution can be transformed into a hard one, allowing the results to be compared to

partitions obtained by hard clustering methods, such as the technique described in Chapter 2.

However, by this transformation, a lot of information contained in the membership functions gets lost. This fuzzy information could be of value in all sorts of comparisons between fuzzy solutions, such as:

Comparison between different fuzzy algorithms.

Comparison between solutions for various numbers of clusters.

Comparisons between:

- membership function exponents
- distance function exponents
- varying positions of one or a few objects
- varying choices of distances

and so on.

Although the effect of some of these variations could show up in the hard clusterings, this representation is not as sensitive as the fuzzy one. In the latter case, with membership values for each object and each cluster, the problem is rather to summarize the situation. For this purpose, different coefficients have been proposed by various authors. One of these coefficients was already defined in Section 4.1. However, considering the $k \times n$ elements of matrix U, the reduction to only one value $[F_k(U)]$ is probably too drastic a condensation to be able to express the most important features.

Taking into account a second function of U, defined as

$$D_k(U) = \sum_i \sum_v (w_{iv} - u_{iv})^2/n, \tag{30}$$

one obtains a wider basis for the evaluation of a fuzzy clustering. In this definition, W is the closest hard representation of the fuzzy U, as derived in Section 4.1. Hence $D_k(U)$ represents the average squared error of a fuzzy clustering with respect to the closest hard clustering. It can be shown to vary between 0 (hard clustering) and $1 - (1/k)$ (completely fuzzy).

Normalizing this function (in the same way as Dunn's partition coefficient), we obtain

$$D'_k(U) = D_k(U)/(1 - (1/k)) = k D_k(U)/(k - 1) \tag{31}$$

It is possible to represent each fuzzy clustering as a point in the (D'_k, F'_k) system shown in Figure 8 (Trauwaert, 1988). These points have to stay inside a certain region. The points on the lower boundary correspond to a

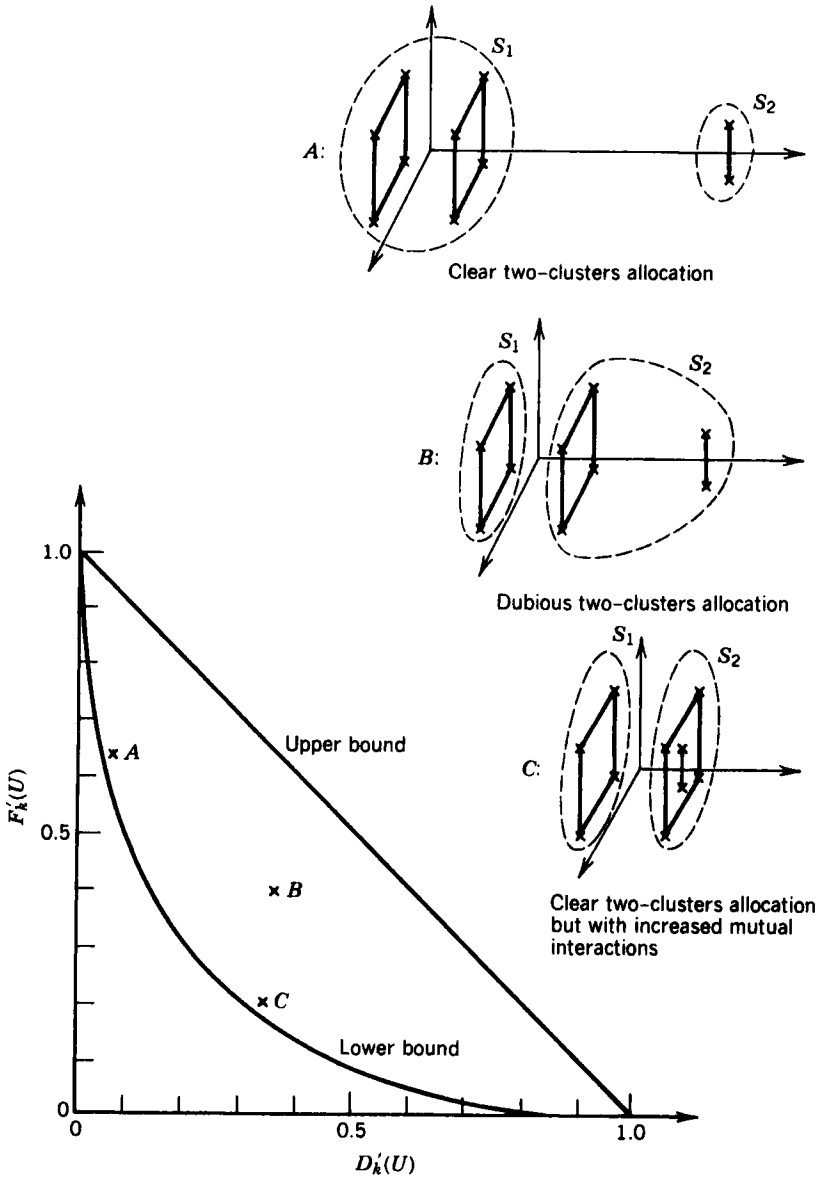


Figure 8 Representation of some fuzzy clusterings (with $n = 10$ and $k = 2$) in a partition coefficient diagram.

membership matrix of the form

$$U = \begin{matrix} \\ 1 \\ \vdots \\ n \end{matrix} \begin{matrix} \begin{matrix} 1 & \cdots & k-1 & k \end{matrix} \\ \begin{pmatrix} \dfrac{\beta}{k-1} & \cdots & \dfrac{\beta}{k-1} & 1-\beta \end{pmatrix} \end{matrix} \quad \text{with } 0 \le \beta \le (k-1)/k \tag{32}$$

where each object is primarily attributed to one of the clusters, with a membership $(1 - \beta)$, and for all other clusters it has a lower membership of $\beta/(k - 1)$. Points on the upper boundary correspond to a membership matrix of the form

$$U = \begin{matrix} \\ 1 \\ \vdots \\ n \end{matrix} \begin{matrix} \begin{matrix} 1 & \cdots\cdots & k \end{matrix} \\ \begin{pmatrix} \overbrace{\frac{1}{v}\ \frac{1}{v} \quad \cdots \quad \frac{1}{v}}^{v} & 0 \quad \cdots \quad 0 \end{pmatrix} \end{matrix} \tag{33}$$

indicating that each object is uniformly distributed over some clusters and not at all present in the others.

In terms of the quality of the clustering, a point at or near the upper boundary indicates that, apart from the well-defined clusters, some objects are bridges or outliers to a number of clusters. On the other hand, a point at or near the lower boundary means that all objects show a definite preference for one cluster, with however some constant membership to all other clusters. It is as if some background noise is added to an otherwise fairly well-defined clustering. This background noise could be due to the algorithm itself.

Moreover, a point near the upper left edge of the diagram corresponds to a fairly hard clustering, whereas on the lower right edge the clusters are completely fuzzy.

From this two-dimensional representation one gets a much better image of a fuzzy clustering than from $F_k'(U)$ alone. It appears clearly from this diagram that the higher values of $F_k'(U)$ do not necessarily indicate a better classification.

A variant of the nonfuzziness index (25) was provided by Libert and Roubens (1982). It is defined as

$$L_k(U) = \left(\sum_i u_{iq}/n + \min_i u_{iq} \right) / 2$$

with normalized version

$$L'_k(U) = \frac{L_k(U) - (1/k)}{1 - (1/k)} = \frac{kL_k(U) - 1}{k - 1}$$

in which q is the cluster for which u_{iv} is maximal.

5.4 A Graphical Display of Fuzzy Memberships

The primary output of FANNY is a list of membership coefficients, which may contain many numbers and therefore becomes difficult to visualize. To summarize this mass of information, Rousseeuw et al. (1989) proposed computing the principal components of the membership coefficients. One merely applies a standard principal components program (as available in SPSS, BMDP, SAS, etc.) to the memberships, in the same way that it is usually applied to measurements. The number of nondegenerate principal components is the number of fuzzy clusters minus 1 (because the sum of memberships is a constant, for each object). For instance, applying FANNY with $k = 3$ to the 12 countries data yielded the fuzzy memberships in Figure 3. Because there are three fuzzy clusters, we obtain two principal components, the scores of which are plotted in Figure 9. The vertical

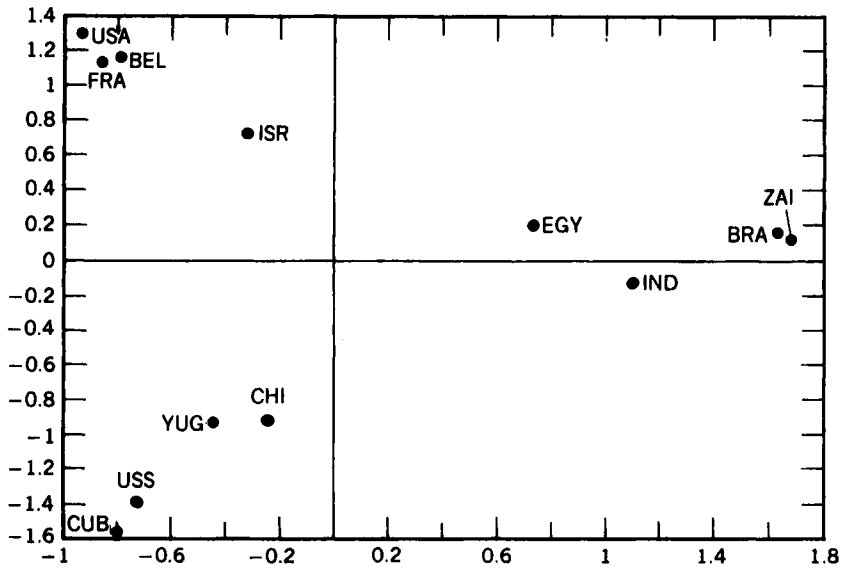


Figure 9 Principal components of memberships of 12 countries in three fuzzy clusters.

component can be interpreted as the countries' political orientation, whereas the horizontal component seems to correspond to the degree of industrialization. In this plot we clearly see the three clusters (consisting of Capitalist, developing, and Communist countries) as well as the fact that Egypt holds an intermediate position.

Because this method is based on the memberships only, the original data need not consist of measurements (indeed, the 12 countries example was based on dissimilarities). The idea to compute the principal components of the memberships did not appear to be in the literature yet.

Let us now look at some special cases. When there are only two fuzzy clusters, only one nondegenerate component will be left. It is then sufficient to plot the membership u_{i1} of each object in the first cluster, because its membership in the second cluster can then be read from right to left as $u_{i2} = 1 - u_{i1}$.

When there are three fuzzy clusters, each object has memberships (u_{i1}, u_{i2}, u_{i3}). The possible combinations fill an equilateral triangle in three-dimensional space. Principal components recover this triangle (as in Figure 9), but one can also plot the memberships directly by means of barycentric coordinates (also called trilinear coordinates). For instance, one could plot

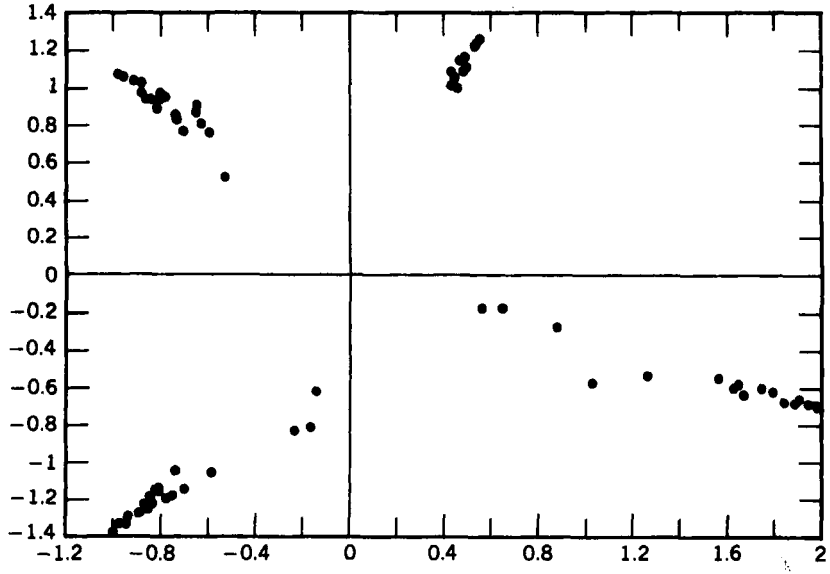


Figure 10 First two principal components of memberships of the Ruspini data in four fuzzy clusters.

$u_{i3}\sqrt{3}/2$ versus $u_{i2} + u_{i3}/2$ for each object, thereby using an equilateral triangle with vertices $(0,0)$, $(1,0)$, and $(1/2, \sqrt{3}/2)$.

When there are more than three fuzzy clusters, there will be more than two principal components. We then follow the customary practice of displaying the two components with largest eigenvalues, thereby "explaining" the largest portion of the variability. An example is given in Figure 10, displaying the two main components of the memberships of the Ruspini data in four fuzzy clusters (as given by FANNY). Sometimes one will want to make a three-dimensional plot or perhaps draw several plots in which each component is plotted versus every other component.

The plot can also be refined by adding "ideal" objects, corresponding to the clusters themselves. Indeed, each cluster can be represented by an object with membership 1 to that cluster and zero membership to all others. By transforming these "membership coordinates" in the same way as the actual objects, the plot will be enriched by as many additional points as there are clusters. In this way the final plot contains both objects and clusters (in the same way that correspondence analysis yields plots containing both objects and variables).

EXERCISES AND PROBLEMS

1. Carefully examine the membership coefficients shown in Table 1, in particular the differences between memberships of objects belonging to the same cluster. Explain these differences by the positions of the objects in Figure 1.

2. Run the program FANNY on the data set of Figure 1. Use the same options as in Section 2.1 but with the number of clusters varying between 2 and 5. Then select a value of k with the silhouettes.

3. Apply FANNY to the sciences data in Table 6 of Chapter 2. Check that Dunn's normalized partition coefficient and the silhouettes yield different choices of k.

4. Apply FANNY to the data in Table 1 of Chapter 2, for $k = 2$. Which object is most fuzzy?

5. Apply FANNY with $k = 2$ to the dissimilarity matrix in Figure 12 of Chapter 5, concerning nine diseases. What do you think of the cluster-

ing quality of these data based on (a) the memberships, (b) Dunn's normalized partition coefficient, and (c) the average silhouette width?

6. A possible nonfuzziness index is the average difference between the largest and the second largest membership for each object. (Observe that this index can take all values between 0 and 1.) Calculate this index for the clusterings in Exercises 4 and 5.

7. Consider the bacteria data in Exercise 1 of Chapter 2. Cluster these data into 2 and 3 clusters using the program FANNY and compare the results with those obtained from the program PAM.

8. Show that the exact minimum of the objective function (1) is a decreasing function of the number of clusters.

9. Compute the fuzzy k-means clustering (with $k = 3$) of the data of Figure 1 by entering the matrix of *squared* Euclidean distances as input to FANNY. Compare the result with Table 1.

10. Consider the dissimilarities between 12 countries listed in Table 5 of Chapter 2. Calculate the coefficients $D_k(U)$ and $D_k'(U)$ for the FANNY clustering with $k = 3$ and draw a plot in which this fuzzy clustering is represented by the point (D_k', F_k').

11. Compute both principal components of the memberships in Table 1 (this can be done by means of any standard software package). Compare the resulting bivariate plot with the original data in Figure 1.

Finding Groups in Data: An Introduction to Cluster Analysis
Leonard Kaufman and Peter J. Rousseeuw

CHAPTER 5

Agglomerative Nesting (Program AGNES)

In the preceding chapters we have seen methods for partitioning a data set with n objects into a fixed number k of clusters. Whatever the data set is like, these methods will come up with k clusters, some of which might not be natural. By varying the number k and studying the resulting clustering characteristics and graphical representations, one can then often decide on a "most suitable" value of k.

In the present chapter, as well as in the two subsequent ones, a completely different approach is adopted. The user does not specify a value of k, but instead the algorithm constructs a tree-like *hierarchy* which implicitly contains all values of k. On the one end of this hierarchy, there are n clusters each containing a single object, and on the other end there is only one cluster containing all n objects. There are basically two types of hierarchical methods. The *agglomerative methods*, treated in this chapter, start with n clusters and proceed by successive fusions until a single cluster is obtained containing all the objects. On the other hand, the *divisive methods* of Chapters 6 and 7 proceed by splitting the data set into smaller and smaller clusters until each object belongs to a separate cluster.

1 SHORT DESCRIPTION OF THE METHOD

The algorithm described in this chapter can be used on exactly the same data sets as those of Chapters 2, 4, and 6. That is, one has n cases (sometimes called objects, entities, or individuals) for which either p interval-scaled variables are given, or for which one has a complete set of dissimilarities between objects. For instance, the interval-scaled variables

may be measurements of objective quantities such as height, length, weight, etc. Dissimilarity coefficients between objects may be obtained from the computation of distances, such as the Euclidean distance

$$d(i, j) = \sqrt{(x_{i1} - x_{j1})^2 + \cdots + (x_{ip} - x_{jp})^2} \tag{1}$$

or the Manhattan distance

$$d(i, j) = |x_{i1} - x_{j1}| + \cdots + |x_{ip} - x_{jp}| \tag{2}$$

between the objects with measurements $x_{i1}, x_{i2}, \ldots, x_{ip}$ and $x_{j1}, x_{j2}, \ldots, x_{jp}$. Dissimilarity coefficients can also arise from a more complicated computation based on variables of different types (binary, nominal, ordinal, interval) by means of the program DAISY of Chapter 1. Sometimes people use *similarities* $s(i, j)$ taking values between 0 and 1, but in this book it is always assumed that the user starts by transforming them into dissimilarities. In cases where one wants to perform cluster analysis on a set of *variables* which have been observed on some population, one can use the (parametric or nonparametric) correlation coefficient $R(f, g)$ of two variables for determining a dissimilarity coefficient $d(f, g)$ between them. These transformations are all discussed in Chapter 1 and can be performed by means of the program DAISY.

When the objects to be clustered are characterized by only two variables, as in the case of Table 1, it is possible to make a plot of the data as in Figure 1. Because the data set can be represented in two dimensions, we can discover its structure visually. In this data set there are clearly two rather isolated clusters of objects, and we expect any reasonable clustering method to recover this fact.

Table 1 A Data Set Consisting of Seven Objects for Which Two Variables Were Measured

Object	Variable 1	Variable 2
1	2.00	2.00
2	5.50	4.00
3	5.00	5.00
4	1.50	2.50
5	1.00	1.00
6	7.00	5.00
7	5.75	6.50

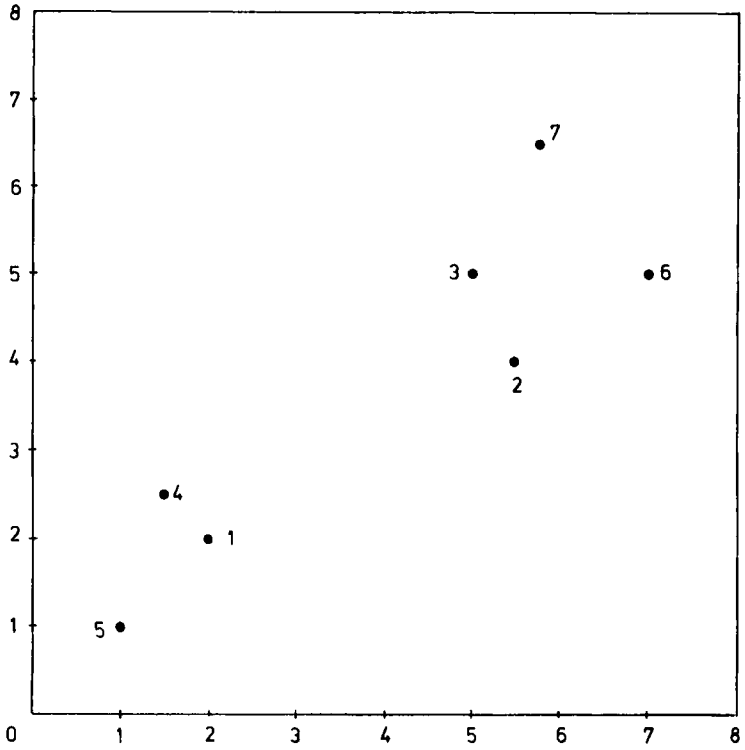


Figure 1 Plot of the data of Table 1.

It is possible to compute a dissimilarity matrix from these data, for instance by calculating Euclidean distances between objects [Eq. (1)]. This yields

$$
\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \end{array}
\begin{array}{c}
\begin{array}{ccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{array} \\
\left[\begin{array}{ccccccc}
0.0 & 4.0 & 4.2 & 0.7 & 1.4 & 5.8 & 5.9 \\
4.0 & 0.0 & 1.1 & 4.3 & 5.4 & 1.8 & 2.5 \\
4.2 & 1.1 & 0.0 & 4.3 & 5.7 & 2.0 & 1.7 \\
0.7 & 4.3 & 4.3 & 0.0 & 1.6 & 6.0 & 5.8 \\
1.4 & 5.4 & 5.7 & 1.6 & 0.0 & 7.2 & 7.3 \\
5.8 & 1.8 & 2.0 & 6.0 & 7.2 & 0.0 & 2.0 \\
5.9 & 2.5 & 1.7 & 5.8 & 7.3 & 2.0 & 0.0
\end{array}\right]
\end{array}
\qquad (3)
$$

The dissimilarity between object 6 and object 2 can be found at the intersection of row 6 and column 2 of the matrix, yielding 1.8. [Note that

the matrix (3) is symmetric and its diagonal elements are 0, so it would suffice to give only the lower triangular half.] When the data are represented in this form, the structure we saw so easily in Figure 1 is rather hidden from visual inspection.

However, we would like to have a clustering method that only makes use of the information contained in such a dissimilarity matrix. Indeed, it can happen that the data simply consist of a dissimilarity matrix that has been given to us, without any measurement values (perhaps the dissimilarities have been computed from some unknown number of variables, or there have never been any variables and the dissimilarities were obtained in some other way, for example as subjective assessments). For instance, suppose we have been given the dissimilarity matrix

$$\begin{array}{c} \\ a \\ b \\ c \\ d \\ e \end{array} \begin{array}{c} \begin{array}{ccccc} a & b & c & d & e \end{array} \\ \left[\begin{array}{ccccc} 0.0 & 2.0 & 6.0 & 10.0 & 9.0 \\ 2.0 & 0.0 & 5.0 & 9.0 & 8.0 \\ 6.0 & 5.0 & 0.0 & 4.0 & 5.0 \\ 10.0 & 9.0 & 4.0 & 0.0 & 3.0 \\ 9.0 & 8.0 & 5.0 & 3.0 & 0.0 \end{array}\right] \end{array} \tag{4}$$

It is often difficult to spot a structure in a data set by merely looking at its dissimilarity matrix. Even in this extremely small example, some kind of clustering algorithm would be useful.

In this chapter we shall apply a method that proceeds by a series of successive fusions of the objects and which we therefore refer to as *agglomerative nesting*. In the beginning (at step 0) all objects are apart, so we could say that each object forms a small cluster by itself. At the first step, the two "closest" or "most similar" objects are joined to form a cluster of two objects (while all other objects remain apart). What we have to do is to find the smallest entry of the dissimilarity matrix and join the corresponding objects (when there are several pairs of objects with minimal dissimilarity, we pick one at random). In matrix (4) the smallest dissimilarity (not on the diagonal) is 2.0, so objects a and b will be joined to form cluster $\{a, b\}$.

The first step leaves us with four clusters: $\{a, b\}$, $\{c\}$, $\{d\}$, $\{e\}$. In the second step (and in all subsequent steps) we will want to merge the two closest *clusters*. But in order to select these, we must first say what we mean by the dissimilarity between two *clusters*, because so far we have only used dissimilarities between *objects*. This is the crucial point, because there are many agglomerative algorithms (see Section 5.1) which only differ from each other in this respect. For several reasons, which will be discussed in Section 5, we have decided to use the *group average method* of Sokal and

Michener (1958), which is sometimes called "unweighted pair-group average method" and abbreviated as "UPGMA". Its definition is very simple. Take two clusters R and Q, and let $|R|$ and $|Q|$ denote their number of objects. Then the dissimilarity $d(R, Q)$ between the clusters R and Q is defined as the average of all dissimilarities $d(i, j)$, where i is any object of R and j is any object of Q. More formally,

$$d(R, Q) = \frac{1}{|R|\,|Q|} \sum_{\substack{i \in R \\ j \in Q}} d(i, j) \tag{5}$$

[Actually, Sokal and Michener only used Eq. (5) when one of the clusters consisted of a single object. The present version of the definition is due to Lance and Williams (1966b).] As a special case of (5), the dissimilarity between the clusters $\{a\}$ and $\{b\}$ containing only a single object simply equals $d(a, b)$. In Figure 2, we give an impression of how the group average rule (5) works for general clusters.

In our example,

$$d(\{a, b\}, \{c\}) = \tfrac{1}{2}[d(a, c) + d(b, c)] = 5.5$$
$$d(\{a, b\}, \{d\}) = \tfrac{1}{2}[d(a, d) + d(b, d)] = 9.5$$
$$d(\{a, b\}, \{e\}) = \tfrac{1}{2}[d(a, e) + d(b, e)] = 8.5$$

This means we can now construct a new dissimilarity matrix that gives all dissimilarities between the four clusters $\{a, b\}$, $\{c\}$, $\{d\}$, and $\{e\}$. [As we are only interested in the off-diagonal entries, we simply put the diagonal entries equal to 0, although (5) would not always yield $d(R, R) = 0$.] We

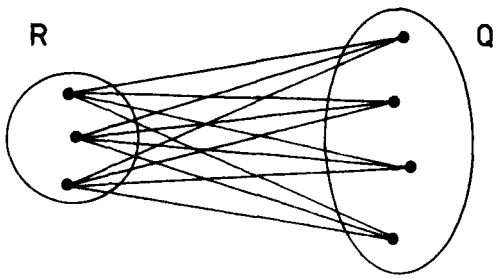


Figure 2 The straight lines indicate the dissimilarities between the objects of the cluster R and the objects of the cluster Q. The group average dissimilarity $d(R, Q)$ is defined as the average of all these dissimilarities.

obtain

$$\begin{array}{c} \\ \{a,b\} \\ \{c\} \\ \{d\} \\ \{e\} \end{array} \begin{array}{c} \begin{array}{cccc} \{a,b\} & \{c\} & \{d\} & \{e\} \end{array} \\ \begin{bmatrix} 0.0 & 5.5 & 9.5 & 8.5 \\ 5.5 & 0.0 & 4.0 & 5.0 \\ 9.5 & 4.0 & 0.0 & 3.0 \\ 8.5 & 5.0 & 3.0 & 0.0 \end{bmatrix} \end{array} \tag{6}$$

Of course, the dissimilarities between the clusters $\{c\}$, $\{d\}$, and $\{e\}$ have remained unchanged.

In this new matrix (6) the smallest off-diagonal entry is 3.0, which means that in the second step $\{d\}$ and $\{e\}$ will be merged to form the cluster $\{d, e\}$. We now need the dissimilarities of $\{d, e\}$ to the other clusters. Using the group average rule,

$$d(\{d,e\},\{c\}) = \tfrac{1}{2}[d(d,c) + d(e,c)] = 4.5$$

$$d(\{d,e\},\{a,b\}) = \tfrac{1}{4}[d(d,a) + d(d,b) + d(e,a) + d(e,b)] = 9.0$$

This yields the following dissimilarity matrix between the clusters $\{a, b\}$, $\{c\}$, and $\{d, e\}$:

$$\begin{array}{c} \\ \{a,b\} \\ \{c\} \\ \{d,e\} \end{array} \begin{array}{c} \begin{array}{ccc} \{a,b\} & \{c\} & \{d,e\} \end{array} \\ \begin{bmatrix} 0.0 & 5.5 & 9.0 \\ 5.5 & 0.0 & 4.5 \\ 9.0 & 4.5 & 0.0 \end{bmatrix} \end{array} \tag{7}$$

The smallest off-diagonal entry of the matrix (7) is 4.5, so the clusters $\{c\}$ and $\{d, e\}$ will be merged in step 3. Using formula (5),

$$\begin{aligned} &d(\{c,d,e\},\{a,b\}) \\ &\quad = \tfrac{1}{6}[d(c,a) + d(c,b) + d(d,a) + d(d,b) + d(e,a) + d(e,b)] \\ &\quad = \tfrac{47}{6} \cong 7.83 \end{aligned}$$

Therefore, the final dissimilarity matrix between the two remaining clusters becomes

$$\begin{array}{c} \\ \{a,b\} \\ \{c,d,e\} \end{array} \begin{array}{c} \begin{array}{cc} \{a,b\} & \{c,d,e\} \end{array} \\ \begin{bmatrix} 0.00 & 7.83 \\ 7.83 & 0.00 \end{bmatrix} \end{array} \tag{8}$$

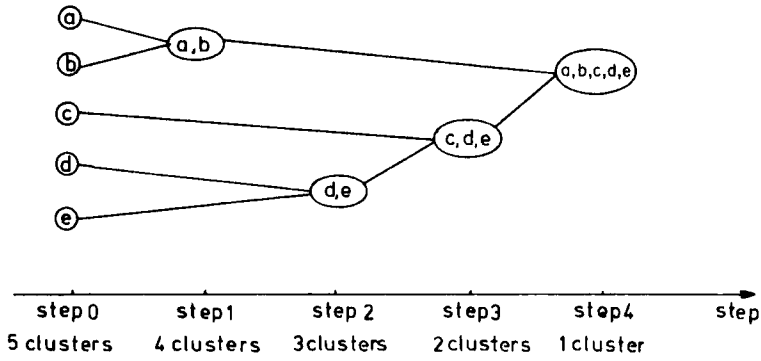


Figure 3 Fusions obtained when clustering the data of matrix (4) with the group average algorithm.

The fourth step simply consists of joining these last two clusters into one single cluster $\{a, b, c, d, e\}$ containing all objects.

We have now seen the agglomerative approach in action. In order to visualize this series of fusions, we need some kind of schematic summary as in Figure 3. The numbering of the steps (on the horizontal axis) shows the direction of time. Clearly, objects a and b join in the first step, objects d and e in the second step, etc.

Figure 3 displays the order in which the objects come together, but does not give any idea of the relative magnitude of the dissimilarities involved. For instance, Figure 3 would remain unaltered if the dissimilarity between objects a and b had been only 0.1 instead of 2.0.

At this point it is worthwhile to note a property of the group average method: The dissimilarity between merging clusters is monotone. By this we mean the following. In the example we are looking at, the first fusion (that of $\{a\}$ with $\{b\}$) joins clusters with dissimilarity 2.0, the second joins clusters with dissimilarity 3.0, the third with dissimilarity 4.5, and the fourth with dissimilarity 7.83. The numbers 2.0, 3.0, 4.5, and 7.83 form a nondecreasing sequence, and it will be seen in Section 4.1 that this is generally true. This property makes it possible to replace Figure 3 by another diagram which still shows the order in which the clusters are merged, but which gives more information. Indeed, Figure 4 actually displays the critical dissimilarities (which we call *levels*) on the horizontal axis.

Two important points should be noted here. First, everything we have said about the construction of the group average hierarchy and its graphical representation only makes use of the dissimilarity matrix, and not of any

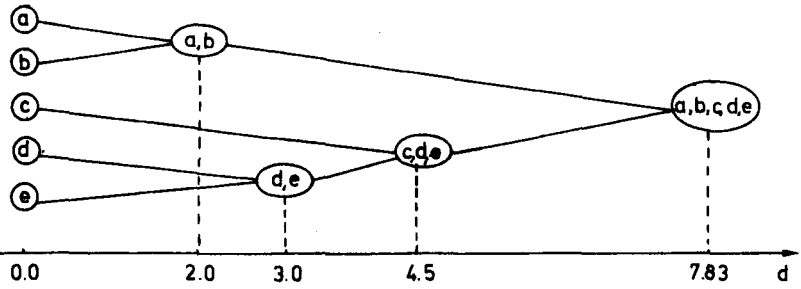


Figure 4 Display showing the same hierarchy as in Figure 3, but also containing the level of each fusion.

measurements. Second, making diagrams like Figure 3 or 4 is not as easy as it looks, because the algorithm often has to change the order of the objects to avoid crossing lines. This could even be done in different ways, as noted by Gower (1968, Section 7), Gruvaeus and Wainer (1972), Kraus et al. (1980), and Critchley and Heiser (1988). At any rate, it is the task of the clustering program to sort the objects into their appropriate sequence.

Figure 4 is very appealing, but becomes cumbersome when the number of objects increases to, say, 50. Another disadvantage is that this kind of display can only be produced automatically by means of good plotting equipment. At the present time, computer graphics are far from standardized, so we prefer portable programs that only use an ordinary line printer (which is usually available).

Therefore, we decided to use another kind of graphical representation, which is called a *banner* (Rousseeuw, 1986). Its name stems from the fact that for many examples it looks like a waving flag. This display is a variant of the icicle plot of Kruskal and Landwehr (1983). (The connections with the latter method will be treated in Section 5.3, together with other displays such as dendrograms.) The banner of Figure 5 contains exactly the same information as Figure 4.

A banner consists of stars and stripes. The stars indicate linking of objects and the stripes are repetitions of the labels of these objects. In the case of agglomerative clustering, the (vertical) flagstaff can be imagined on the right, whereas in the case of divisive clustering (Chapters 6 and 7) the flagstaff is on the left. A banner is always read from left to right, just like Figures 3 and 4.

Let us look at Figure 5. The white space in the left part indicates the original stage where all the objects are separate entities. Then, at the level

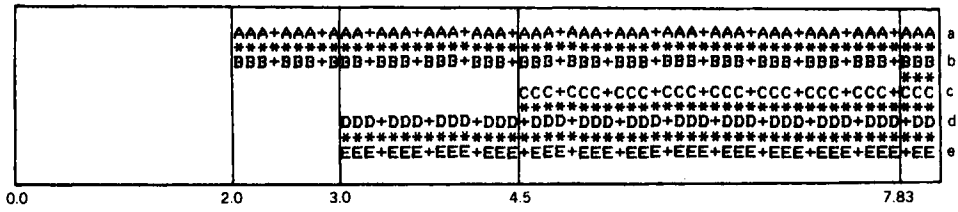


Figure 5 A banner containing the same information as Figure 4.

2.0, we see the beginning of a strip containing three lines. The first of these lines reads $AAA + AAA + \cdots$ which is simply a repetition of the three-character label AAA standing for object a, separated by the symbol $+$. (Any three-character label could be inserted; when no natural label is available, one can always take the number of the object, writing 038 for object number 38.) The label BBB on the third line denotes object b. The second line is a row of stars * * * * * indicating that the two objects in question are joined, starting from level 2.0. Because we are working with an agglomerative method, objects that have once come together will always stay together. The next event is the linking of objects d (with label DDD) and e (with label EEE) at the level 3.0. At the level 4.5, we see that object c joins this cluster. Finally, at the extreme right, we see that the clusters $\{a, b\}$ and $\{c, d, e\}$ are merged at the level 7.83. If we were to move further to the right, nothing would change any more, because the five objects stay together. Therefore, the banner is not drawn any further, but stops at the highest clustering level 7.83 (at the flagstaff).

A word of caution is necessary here. The white space at the left of the banner seems to conceal the objects $\{a\}$, $\{b\}$, $\{c\}$, $\{d\}$, and $\{e\}$, which are separated from each other prior to level 2.0. It would have been possible to draw the lines containing the labels (like $AAA + AAA + \cdots$) starting from the left margin, keeping the stars where they are now. This would seem more logical, the absence of stars indicating the fact that the objects are not yet linked. However, it turns out that our eye can see the pattern much more easily when the unlinked labels are deleted, especially when the data set contains many objects.

The banner allows us to investigate easily the structure of the data set at a given level. Suppose we want to know what the situation looks like at the level 6.0: By this we mean the result of the interrupted agglomerative procedure where all mergers have been executed for which the clusters to be merged were at most 6.0 apart. To find this out, we draw a vertical line at the level 6.0 and note immediately that there are two clusters $\{a, b\}$ and

$\{c, d, e\}$. It is easy to see this because the object labels are actually in the display. In order to find the clustering into three groups, we can make a cut at the level 4.0. This yields the clusters $\{a, b\}$ and $\{d, e\}$ and the singleton $\{c\}$, the label of the latter being suppressed in the banner because object c is still unlinked at this stage.

In order to extract a partitioning from a hierarchy, we have to choose an appropriate level. For this purpose, Mojena (1977) considers stopping rules which select a suitable number of clusters based on the distribution of a clustering criterion.

2 HOW TO USE THE PROGRAM AGNES

The group average clustering algorithm can be applied by using the program AGNES (this name is abbreviated from AGglomerative NESting), which runs on IBM-PC and compatible microcomputers. Because the program AGNES has several parts in common with the program DIANA discussed in the next chapter, we decided to combine them into a larger program, called TWINS, in order to save space on floppy disk. This program accepts the same data types as do PAM (Chapter 2) and FANNY (Chapter 4), and the input dialogue is nearly identical. Therefore, it is very easy to run PAM, FANNY, AGNES, and DIANA on the same data and then to compare the results.

2.1 Interactive Use and Input

In order to run AGNES we merely have to put the floppy with the file TWINS.EXE in drive A and type

A:TWINS

The program then responds with the following screen:

```
HIERARCHICAL CLUSTERING

DO YOU WANT AGGLOMERATIVE NESTING (AGNES)
OR DIVISIVE ANALYSIS (DIANA) ?
PLEASE ENTER YOUR CHOICE (A OR D) : A
```

If we choose agglomerative nesting, we obtain

```
AGGLOMERATIVE NESTING
```

```
DO YOU WANT TO ENTER MEASUREMENTS ? (PLEASE ANSWER M)
OR DO YOU PREFER TO GIVE DISSIMILARITIES ? (THEN ANSWER D) : M
```

and the remainder of the interactive dialogue is the same as in the programs PAM or FANNY, except that the number of clusters is no longer asked for. Also the treatment of missing values is identical.

2.2 Output

The first three parts of the output correspond to the parts a, b, and c of the output of PAM, as they were described in Section 2.2 of Chapter 2:

Identification of the program and the data set.
Data specifications and chosen options.
Dissimilarities and standardized measurements.

If we run AGNES on the dissimilarity data (4) we obtain Figure 6, in which these three parts are immediately recognized. However, the cluster results and the banner are new.

Cluster Results

This part of the output contains two sequences of numbers: the final ordering of the n objects and the dissimilarities between clusters. To understand the importance of these numbers, let us look back to Figure 4. On the left, there is a vertical ordering of the objects: a, b, c, d, e. When the objects are listed in this order, the diagram can be drawn without crossing lines. (In this particular example, the final ordering happens to coincide with the original ordering of the objects, but this is rarely the case.) On the horizontal axis of Figure 4, the dissimilarities between joining clusters are plotted. Looking at Figure 4 from top to bottom, we encounter the dissimilarities 2.0 (between $\{a\}$ and $\{b\}$), 7.83 (between $\{a, b\}$ and $\{c, d, e\}$), 4.5 (between $\{c\}$ and $\{d, e\}$), and 3.0 (between $\{d\}$ and $\{e\}$). Therefore, these numbers 2.0, 7.83, 4.5, and 3.0 are listed in the same order in Figure 6. (Note that the number of dissimilarities recorded is one less than the number of objects n, because there are $n - 1$ fusions.)

```
                    ****************************
                    *                          *
                    *  AGGLOMERATIVE NESTING   *
                    *                          *
                    ****************************

TITLE : Dissimilarity matrix of display (4)
DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 THERE ARE     5 OBJECTS
 LABELS OF OBJECTS ARE READ
 INPUT OF DISSIMILARITIES
 LARGE OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (BANNER)
 THE DISSIMILARITIES WILL BE READ IN FREE FORMAT
 YOUR DATA RESIDE ON FILE        : a:example.dat

DISSIMILARITY MATRIX
--------------------

AAA
BBB        2.00
CCC        6.00       5.00
DDD       10.00       9.00       4.00
EEE        9.00       8.00       5.00       3.00


CLUSTER RESULTS
---------------

THE FINAL ORDERING OF THE OBJECTS IS
       1              2              3              4              5

THE DISSIMILARITIES BETWEEN CLUSTERS ARE
             2.000          7.833          4.500          3.000

                            ************
                            *          *
                            *  BANNER  *
                            *          *
                            ************

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

                    AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA
                    ***********************************************************
                    BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB
                                                                          ***
                                                  CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC
                                                  *******************************
                            DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DD
                            *******************************************************
                            EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EE

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0


THE ACTUAL HIGHEST LEVEL IS                  7.8333330000

THE AGGLOMERATIVE COEFFICIENT OF THIS DATA SET IS     .63

THE OUTPUT IS WRITTEN ON FILE : a:example.agn
```

Figure 6 Output obtained by running AGNES on the data of matrix (4).

On the other hand, we claim that these two sequences of numbers are sufficient to reconstruct Figure 4 or any equivalent display, such as the banner or one of the diagrams discussed in Section 5.3 (dendrogram, icicle plot, ...). Indeed, consider the two rows

1	2	3	4	5
2.0	7.83	4.5	3.0	

The upper numbers give us the order in which to list the objects. In the lower sequence we start by looking up the smallest value, 2.0, which is directly under the numbers 1 and 2. This means that the objects with numbers 1 and 2 will be joined first, at the level 2.0. The second smallest value is 3.0, under the entries 4 and 5, so the objects 4 and 5 will be joined next. The third value is 4.5 under 3 and 4, but at this point we have to recollect that 4 was already joined with 5, so this means a merger of $\{3\}$ with $\{4, 5\}$. The largest value is 7.83 under 2 and 3, meaning that $\{1, 2\}$ and $\{3, 4, 5\}$ join in the last step. We conclude that the entire hierarchy can be described by these two sequences of length n and $n - 1$.

Banner

Finally, the results of the calculations are summarized in a banner. (The banner in Figure 6 was already shown and explained in Figure 5.) For practical reasons, there are fixed scales above and below the banner, going from 0.00 to 1.00 with steps of size 0.04. Here, 0.00 indicates a dissimilarity of 0, and 1.00 stands for the largest dissimilarity encountered, that is, the dissimilarity between the two clusters merged in the last step. This actual highest level (which equals 7.83 in the present example) is listed below the banner. The approximate level for a merger can easily be estimated as follows: Just look above or below the beginning of the string of * * * * *, read off the scale at that point, and multiply with the actual highest level. For instance, $\{d\}$ and $\{e\}$ meet at about 0.37 on the scale, so the real level is approximately $0.37 \times 7.83 \cong 2.90$ (indeed, the true value is 3.0).

The overall width of the banner is very important because it gives an idea of the amount of structure that has been found by the algorithm. Indeed, when the data possess a clear cluster structure, the between-cluster dissimilarities (and hence the highest level) will become much larger than the within-cluster dissimilarities, and as a consequence the black lines in the banner become longer. For each object i, we look at the line containing its label and measure its length $l(i)$ on the 0-1 scale above or below the

banner. The *agglomerative coefficient* (AC) of the data set is then defined as

$$\mathrm{AC} = \frac{1}{n} \sum_{i=1}^{n} l(i) \tag{9}$$

The AC is a dimensionless quantity between 0 and 1, because all the $l(i)$ lie between 0 and 1. It is simply the average width of the banner (or, if you will, the fraction of "blackness" in the plot) and it does not change when all the original dissimilarities are multiplied by a constant factor. (This means that we are assuming that the dissimilarities are on a ratio scale.) In Figure 6, AC = 0.63, which points to a reasonable structure.

In order to obtain some intuition about the meaning of the agglomerative coefficient, the reader is advised to look at the examples in Section 3. Generally speaking, the AC describes the strength of the clustering structure that has been obtained by group average linkage. However, the AC tends to become larger when n increases, so it should not be used to compare data sets of very different sizes. For the divisive method of Chapter 6 there exists a similar *divisive coefficient* (DC) that typically takes on slightly larger values when applied to the same data sets. The AC can also be compared to the silhouette coefficient (SC) of Chapters 2, 3, and 4.

```
                    **************************
                    *                        *
                    *  AGGLOMERATIVE NESTING *
                    *                        *
                    **************************

TITLE : Data set of Table 1
DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 THERE ARE     7 OBJECTS
 LABELS OF OBJECTS ARE NOT READ
 INPUT OF MEASUREMENTS
 LARGE OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (BANNER)

 THERE ARE     2 VARIABLES IN THE DATA SET
  AND    2 OF THEM WILL BE USED IN THE ANALYSIS
 THE LABELS OF THESE VARIABLES ARE :
          x
          y
 THE MEASUREMENTS WILL NOT BE STANDARDIZED
 EUCLIDEAN DISTANCE IS USED
 THERE ARE NO MISSING VALUES
 THE MEASUREMENTS WILL BE READ IN FREE FORMAT

 YOUR DATA RESIDE ON FILE        : a:seven.dat


DISSIMILARITY MATRIX
--------------------

001
002      4.03
003      4.24      1.12
004      3.21      4.27      4.30
005      1.41      5.41      5.66      1.58
006      5.83      1.80      2.00      6.04      7.21
007      5.86      2.51      1.68      5.84      7.27      1.95
```

Figure 7 Output obtained by running AGNES on the data of Table 1.

When the AC, DC, or SC are very small, the corresponding method has not found a natural structure, which can be expressed by saying that no clusters have been found, or rather that the data consists of one big cluster. On the other hand, a value of the AC, DC, or SC close to 1 means that a very clear clustering structure has been identified. We must stress that this does not necessarily mean that the "right" clustering has been found: For instance, the AC, DC, and SC all become very large when one bad outlier is added to any data set. However, the graphical display will clearly expose the outlier and thereby pinpoint the cause. The use of a quality coefficient like the AC (or, say, the coefficient of determination in regression analysis) must always be accompanied by a look at the graphical output (the banner) and an analysis of the structure that has been obtained.

```
CLUSTER RESULTS
---------------

THE FINAL ORDERING OF THE OBJECTS IS
       1              4              5              2              3
       6              7

THE DISSIMILARITIES BETWEEN CLUSTERS ARE
           .707          1.498          5.496          1.118          1.901
          2.047


                                  ************
                                  *          *
                                  *  BANNER  *
                                  *          *
                                  ************

0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
.  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .
0  0  0  1  1  2  2  2  3  3  4  4  4  5  5  6  6  6  7  7  8  8  8  9  9  0
0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0

         001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+0
         *********************************************************************
         004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+0
                    **********************************************************
                    005+005+005+005+005+005+005+005+005+005+005+005+005+005+00
                                                                           ***
               002+002+002+002+002+002+002+002+002+002+002+002+002+002+002+002
               ***************************************************************
               003+003+003+003+003+003+003+003+003+003+003+003+003+003+003+003
                         *****************************************************
                         006+006+006+006+006+006+006+006+006+006+006+006+006+0
                           ***************************************************
                           007+007+007+007+007+007+007+007+007+007+007+007+007

0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
.  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .
0  0  0  1  1  2  2  2  3  3  4  4  4  5  5  6  6  6  7  7  8  8  8  9  9  0
0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0


THE ACTUAL HIGHEST LEVEL IS                5.4964090000

THE AGGLOMERATIVE COEFFICIENT OF THIS DATA SET IS     .76

THE OUTPUT IS WRITTEN ON FILE : a:seven.agn
```

Figure 7 (*Continued*)

Let us now consider another example. Figure 7 contains the output for the data of Table 1. We now also have the specifications concerning measurements (there are two variables, the measurements will not be standardized, Euclidean distance is used, there are no missing values). Labels of objects have not been read, so that the program has produced the labels $001, 002, \ldots, 007$, which are printed at the left of the dissimilarity matrix. The final ordering of the objects is now $1, 4, 5, 2, 3, 6, 7$: This is how the object labels are ranked in the banner (looking from top to bottom). The smallest entry in the dissimilarity matrix is 0.707, indicating that objects 004 and 001 will be joined first. Indeed, the banner string of * * * * * extending furthest to the left corresponds to this couple. The second match is of 002 with 003, at the level 1.118, which can also easily be detected in the dissimilarity matrix. The other numbers in the "dissimilarities between clusters" list are the result of applying the group average rule (5), and can also be traced back in the banner. The agglomerative coefficient of this data set is 0.76, indicating a more pronounced clustering structure than in Figure 6. Indeed, the banner consists of two solid strips which are relatively long, thereby conveying an impression of two tight clusters that are clearly separated from each other, as was to be expected from Figure 1.

3 EXAMPLES

In our first example we analyze the 12 countries data given in Table 5 of Chapter 2, which were already clustered by means of the program PAM in Section 3 of Chapter 2, and with the program FANNY in Section 3 of Chapter 4.

Figure 8 contains the output obtained by running AGNES on these data. The first half of the output is almost identical to Figure 7 of Chapter 2, except for the heading "agglomerative nesting" and the fact that the line "clusterings are carried out in 1 to 3 clusters" has disappeared. Indeed, the agglomerative nesting algorithm computes a complete hierarchy, from n clusters to 1 cluster, so it does not need a prespecified number of clusters. The lower triangular half of the dissimilarity matrix is reproduced in the output because the large output option was selected.

The second half of the output contains the final ordering of the objects, which have been considerably reshuffled (only the first object has remained where it was, but this is *always* true for AGNES and DIANA). Then the critical dissimilarities are listed, the smallest of which is 2.17 between Belgium and France. Indeed, 2.17 is also the smallest off-diagonal element of the original dissimilarity matrix (it is the first entry of the fifth line). The

```
*************************
*                       *
*  AGGLOMERATIVE NESTING *
*                       *
*************************

TITLE : Subjective dissimilarities between 12 countries
DATA SPECIFICATIONS AND CHOSEN OPTIONS
---------------------------------------
 THERE ARE   12 OBJECTS
 LABELS OF OBJECTS ARE READ
 INPUT OF DISSIMILARITIES
 LARGE OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (BANNER)
 THE DISSIMILARITIES WILL BE READ IN FREE FORMAT

 YOUR DATA RESIDE ON FILE       : a:country.dat


DISSIMILARITY MATRIX
--------------------

BEL
BRA   5.58
CHI   7.00   6.50
CUB   7.08   7.00   3.83
EGY   4.83   5.08   8.17   5.83
FRA   2.17   5.75   6.67   6.92   4.92
IND   6.42   5.00   5.58   6.00   4.67   6.42
ISR   3.42   5.50   6.42   6.42   5.00   3.92   6.17
USA   2.50   4.92   6.25   7.33   4.50   2.25   6.33   2.75
USS   6.08   6.67   4.25   2.67   6.00   6.17   6.17   6.92
      6.17
YUG   5.25   6.83   4.50   3.75   5.75   5.42   6.08   5.83
      6.67   3.67
ZAI   4.75   3.00   6.08   6.67   5.00   5.58   4.83   6.17
      5.67   6.50   6.92
```

Figure 8 Output of AGNES for the 12 countries data.

critical dissimilarities of the other three couples, Brazil–Zaire (3.00), Egypt–India (4.67), and Cuba–USSR (2.67) can also easily be detected in the original dissimilarity matrix. The other dissimilarities between clusters have been computed by means of the group average rule.

The banner looks remarkably similar to a mirror image of the silhouettes for $k = 3$ obtained from PAM (Figure 8 of Chapter 2) or from FANNY (Figure 3 of Chapter 4). We can again easily distinguish three groups of four countries: Western, developing, and Communist. The first and third clusters appear to be quite pronounced because their banner sections are the widest and have only a single top, whereas the developing countries cluster grows from two different poles: the Brazil–Zaire link and the Egypt–India link, the latter being formed in a relatively late stage of the process. These results visualize the combined subjective views of the students, summarizing some 66 dissimilarity coefficients.

Our overall impression of the banner is that it is merely of medium width, meaning that the clustering structure is not very strong, and indeed the agglomerative coefficient equals 0.50. (This confirms the medium silhouette coefficient of PAM and FANNY.) On the other hand, some clustering structure is definitely present, also because many features are confirmed by the application of PAM, FANNY, and DIANA.

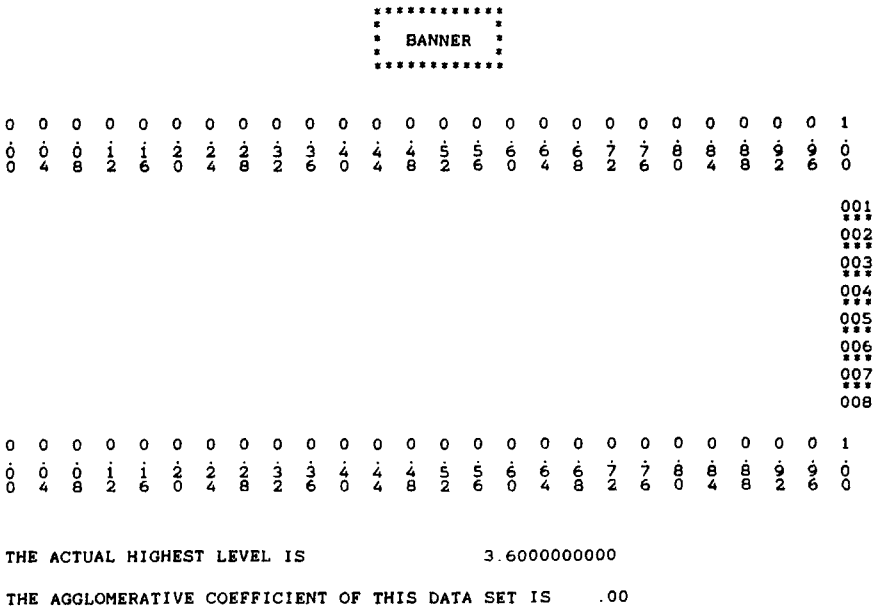
```
CLUSTER RESULTS
---------------

THE FINAL ORDERING OF THE OBJECTS IS

      1        6        9        8        2
     12        5        7        3        4
     10       11

THE DISSIMILARITIES BETWEEN CLUSTERS ARE

          2.170    2.375    3.363    5.532    3.000
          4.977    4.670    6.417    4.193    2.670
          3.710

                    ************
                    *          *
                    *  BANNER  *
                    *          *
                    ************

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

                                BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+B
                                FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+F
                                USA+USA+USA+USA+USA+USA+USA+USA+USA+USA+USA+USA+USA
                                                ISR+ISR+ISR+ISR+ISR+ISR+ISR+ISR+ISR+ISR
                                BRA+BRA+BRA+BRA+BRA+BRA+BRA+BRA+BRA+BRA+BRA+BRA
                                ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZAI
                                                EGY+EGY+EGY+EGY+EGY+EGY+
                                                IND+IND+IND+IND+IND+IND+
                                                CHI+CHI+CHI+CHI+CHI+CHI+CHI+C
                                CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB
                                USS+USS+USS+USS+USS+USS+USS+USS+USS+USS+USS+USS
                                                YUG+YUG+YUG+YUG+YUG+YUG+YUG+YUG+YUG

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

THE ACTUAL HIGHEST LEVEL IS                  6.4171880000

THE AGGLOMERATIVE COEFFICIENT OF THIS DATA SET IS     .50

THE OUTPUT IS WRITTEN ON FILE : a:country.agn
```

Figure 8 (*Continued*)

Why would the agglomerative coefficient indicate anything? The white part of the banner begins from the left, at zero dissimilarity, and ends when the objects get linked, the plotted line of * * * * * starting at the corresponding dissimilarity. The dark part of the banner ends at the right (the flagstaff), at the highest level where all objects come together. The width of the banner for any given object, measured as the length of its label line

$XYZ + XYZ + XYZ + \cdots$ with respect to the 0-1 scale above and below the banner, therefore equals the fraction of the total evolution where this object was linked to another object. The width of the white part equals the level of first linking divided by the final level, so it corresponds to the bachelor part of the object's life span. (Because of this formulation, the AC does not depend on the ordering of the objects and may be defined independently of the banner itself.)

When the banner is narrow, and therefore the agglomerative coefficient given by Eq. (9) is low, this means that most objects remain unlinked for a relatively long time and that therefore the data set does not contain very natural clusters which would have been formed sooner. Of course, this is merely a heuristic reasoning. However, let us look at some extreme cases. On the one hand, suppose we have eight objects for which the off-diagonal entries of the dissimilarity matrix are all equal to the same positive constant, say 3.6. (In the case of Euclidean distances, this can happen when you have at least seven variables: In general one can take the n vertices of a regular simplex in $n - 1$ dimensions.) In this case, the objects stay apart until the very end, when they all join at the level 3.6. The resulting banner is displayed in Figure 9 and shows that there is indeed no clustering structure



THE ACTUAL HIGHEST LEVEL IS 3.6000000000

THE AGGLOMERATIVE COEFFICIENT OF THIS DATA SET IS .00

Figure 9 Agglomerative banner constructed from eight objects, with the same dissimilarity between any two objects.


```
0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
0  0  0  1  1  2  2  2  3  3  4  4  4  5  5  6  6  6  7  7  8  8  8  9  9  0
0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0

001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+00
002+002+002+002+002+002+002+002+002+002+002+002+002+002+002+002+002+002+002+00
003+003+003+003+003+003+003+003+003+003+003+003+003+003+003+003+003+003+003+00
004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+00
005+005+005+005+005+005+005+005+005+005+005+005+005+005+005+005+005+005+005+00
006+006+006+006+006+006+006+006+006+006+006+006+006+006+006+006+006+006+006+00
007+007+007+007+007+007+007+007+007+007+007+007+007+007+007+007+007+007+007+00
008+008+008+008+008+008+008+008+008+008+008+008+008+008+008+008+008+008+008+00

0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
0  0  0  1  1  2  2  2  3  3  4  4  4  5  5  6  6  6  7  7  8  8  8  9  9  0
0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0  4  8  2  6  0

THE ACTUAL HIGHEST LEVEL IS                    3.6000000000

THE AGGLOMERATIVE COEFFICIENT OF THIS DATA SET IS   1.00
```

Figure 10 Agglomerative banner constructed from eight objects that make up two very tight clusters.

in the data: No linking is more natural than any other.The agglomerative coefficient equals 0.00, as well as the divisive coefficient of Chapter 6. [Note that the silhouettes also have zero width in this case, for any clustering partition, so the silhouette coefficient (SC) of Chapters 2 and 4 also equals 0.00 for this data set.]

On the other hand, suppose that the objects are divided into some very tight clusters that are far away from each other. For instance, assume that five objects coincide with one geometrical point and the other three coincide with another geometrical point at a distance of, say, 3.6. This is an extremely sharp clustering structure, and the resulting banner of Figure 10 is as wide as possible. Therefore, the AC attains its maximal value of 1.00, and the same holds for the divisive coefficient of Chapter 6. (The silhouettes for $k = 2$ look exactly like the banner, and therefore the silhouette coefficient also attains its maximal value 1.00.)

Another extreme example is a tight cluster plus one outlier. For instance, suppose seven objects have dissimilarities of nearly 0 to each other and all have large dissimilarities (say, 3.6) to the eighth object, which is an outlier. The resulting banner then looks like Figure 11, clearly separating object 8 from the rest. The agglomerative coefficient equals $1 - \frac{1}{8} = 0.875$, which is

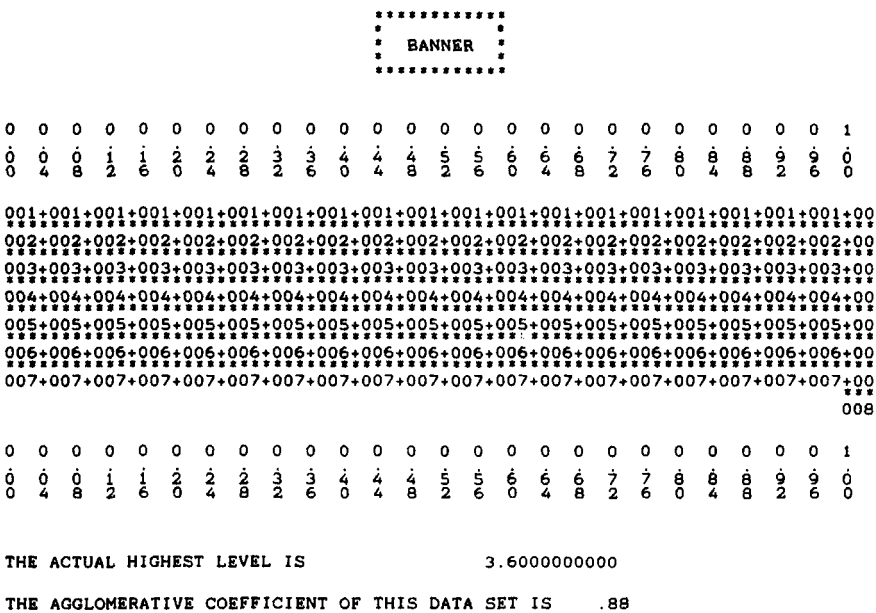


Figure 11 Agglomerative banner constructed from eight objects, one of which is a distant outlier.

very high. The same value is obtained for the divisive coefficient and the silhouette coefficient (which is attained at $k = 2$). In general, when a distant outlier is present in any data set, all three coefficients will tend to $1 - 1/n$ (where n is the sample size) because a distant outlier will make the remaining data look like a tight cluster. Therefore, one should never merely accept a high value of either coefficient, but look at the graphical output to find out what caused it. (Such an outlier usually deserves further investigation, and sometimes its origin can be traced back. In many applications, one may delete the outlier and cluster the remaining data again.)

In Figures 10 and 11, the "good" clusters correspond to a long strip of the banner and only have a very short link to each other near the flagstaff. When there are more than two natural clusters, usually not all clusters are at the same dissimilarity from each other, so they have links of varying length. For instance, in Figure 8 the developing countries have a larger link with (are closer to) the Western countries than to the Communist ones. The banner strips corresponding to the three clusters are also shorter, meaning that the clusters are less tight. In Figures 9, 10, and 11, the banner parts have very flat left ends because the dissimilarities within each cluster are very homogeneous. On the other hand, in Figure 8 the left ends are quite

```
DISSIMILARITY MATRIX
--------------------

001
002   .99
003   .92   1.03
004  1.13   1.18   1.06
005   .82    .65    .74   1.26
006   .94    .76    .95   1.29    .82
007   .92   1.17   1.04    .71   1.15    .95
008  1.05    .69    .82    .74    .87    .86   1.22
009   .95    .86   1.03    .98    .84    .96    .67    .90

CLUSTER RESULTS
---------------

THE FINAL ORDERING OF THE OBJECTS IS

  1     2     5     6     3
  4     8     7     9

THE DISSIMILARITIES BETWEEN CLUSTERS ARE

      .918  .650  .790  .907  1.004
      .740  .952  .670

            ************
            *          *
            *  BANNER  *
            *          *
            ************

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

                                                001+001+00
                                                **********
                                  002+002+002+002+002+002+002+00
                                  **********************
                                  005+005+005+005+005+005+005+00
                                                **********
                                        006+006+006+006+006
                                        **********
                                              003+003+003
                                              ***
                                        004+004+004+004+004+004
                                        **********************
                                        008+008+008+008+008+008
                                              ******
                                  007+007+007+007+007+007+007+
                                  ***************************
                                  009+009+009+009+009+009+009+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0 0 0 1 1 2 2 2 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 9 9 0
0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0 4 8 2 6 0

THE ACTUAL HIGHEST LEVEL IS                    1.0040000000

THE AGGLOMERATIVE COEFFICIENT OF THIS DATA SET IS     .25
```

Figure 12 Agglomerative clustering of nine diseases.

ragged because the dissimilarities within a cluster are far from constant (for instance, the dissimilarity between USSR and China is 4.25, but between USSR and Cuba it is only 2.67).

Let us now look at some real data with a very bad clustering quality, which were provided by Nini Vrijens of the State University of Antwerp. The occurrence of nine diseases in the female population of 43 Belgian communities was recorded over several years. Figure 12 shows the corresponding dissimilarity matrix and the group average linkage results. The banner is very narrow because there are no clear links, as all dissimilarities between objects are of the same order of magnitude. The agglomerative coefficient is only 0.25. The situation resembles that of Figure 9. In conclusion, we cannot say that we have found any groups in this particular data set.

*4 MORE ON THE ALGORITHM AND THE PROGRAM

4.1 Description of the Algorithm

In Section 1 we saw the definition of the group average linkage method of Sokal and Michener (1958), and the algorithm was illustrated step by step on the data of matrix (4). After each fusion a new dissimilarity matrix was obtained by applying the group average rule (5) to the newly formed clusters, leading to matrices (6), (7), and (8). However, we shall see that these computations can be performed in a more efficient way. Whereas in the description of Section 1 one always has to return to the original dissimilarity matrix (4), it is also possible to apply an update mechanism in order to drastically reduce the number of calculations.

Indeed, assume we have at one step joined the clusters A and B to form a new cluster R. In the next step we will need the dissimilarity $d(R, Q)$ of R to any other cluster Q. By formula (5),

$$
\begin{aligned}
d(R,Q) &= \frac{1}{|R||Q|} \sum_{\substack{i \in R \\ j \in Q}} d(i,j) \\
&= \frac{1}{|R||Q|} \sum_{\substack{i \in A \\ j \in Q}} d(i,j) + \frac{1}{|R||Q|} \sum_{\substack{i \in B \\ j \in Q}} d(i,j) \\
&= \frac{|A|}{|R|} \left(\frac{1}{|A||Q|} \sum_{\substack{i \in A \\ j \in Q}} d(i,j) \right) + \frac{|B|}{|R|} \left(\frac{1}{|B||Q|} \sum_{\substack{i \in B \\ j \in Q}} d(i,j) \right)
\end{aligned}
$$

Hence

$$d(R,Q) = \frac{|A|}{|R|}\,d(A,Q) + \frac{|B|}{|R|}\,d(B,Q) \tag{10}$$

Note that the dissimilarities $d(A,Q)$ and $d(B,Q)$ are available from the matrix of the previous step and that the dissimilarities not involving R remain unaltered. Therefore, it is no longer necessary to go back to matrix (4); indeed matrix (6) is sufficient to compute matrix (7) and matrix (7) is sufficient to obtain matrix (8). For instance, in order to construct matrix (8) it suffices to apply formula (10) as follows:

$$\begin{aligned} d(\{c,d,e\},\{a,b\}) &= \tfrac{1}{3}\,d(\{c\},\{a,b\}) + \tfrac{2}{3}\,d(\{d,e\},\{a,b\}) \\ &= \tfrac{5.5}{3} + 2\tfrac{9.0}{3} = \tfrac{23.5}{3} \cong 7.83 \end{aligned}$$

in which we only need the entries of matrix (7). From the point of view of the computer, this means that only one dissimilarity matrix must be stored at any given time, and it is possible to devise the program in such a way that the same memory spaces are being used again in all steps (by overwriting the altered values over the old ones). But the main advantage of the update formula (10) lies in its simplicity, because only *two* dissimilarities (between A and Q and between B and Q) must be looked up, instead of *all* dissimilarities between objects of R and objects of Q (there are $|R|\,|Q|$ such dissimilarities, a number which may become very large for increasing cluster sizes). Therefore, formula (10) reduces the computation time.

We can also use the update formula (10) for showing that the critical dissimilarities form a monotone sequence, a fact we already used in Section 1 to represent the hierarchy in Figures 4 and 5. Indeed, suppose we have merged clusters A and B in the previous step, which means that $d(A,B)$ was the smallest off-diagonal entry of the dissimilarity matrix at that stage. Let us denote this critical dissimilarity by d, from which it follows that all off-diagonal entries of that dissimilarity matrix were larger than or equal to d. After the merger of A and B into some new cluster called R, we have to construct the new dissimilarity matrix. All dissimilarities not involving R remain unaltered and hence are at least equal to d. The dissimilarities that do involve R can be computed according to (10), and for these it holds that

$$\begin{aligned} d(R,Q) &= \frac{|A|}{|R|}\,d(A,Q) + \frac{|B|}{|R|}\,d(B,Q) \\ &\geq \frac{|A|}{|R|}\,d + \frac{|B|}{|R|}\,d = d \end{aligned} \tag{11}$$

Hence they are also at least d. Therefore, all off-diagonal entries of the new dissimilarity matrix are at least as large as d. The critical dissimilarity of the next merger equals the smallest off-diagonal entry of this matrix, so it cannot be smaller than d. Applying this reasoning to the consecutive steps of the amalgamation process, it follows that the critical dissimilarity is monotone.

4.2 Structure of the Program

The program TWINS consists of:

a main unit
subroutine ENTR
subroutine QYN
function MEET
subroutine NWLAB
subroutine STAND
subroutine DYSTA
subroutine AVERL
subroutine BANAG
subroutine SPLYT
subroutine SUPCL
subroutine BANDY

The main unit is similar to that of program PAM, so we refer to Section 4.2 of Chapter 2 for its description, as well as for ENTR, QYN, MEET, NWLAB, STAND, and DYSTA.

At the end of the main unit, subroutine AVERL is called which actually performs the AVERage Linkage. This subroutine operates on four arrays, the first of which is DYS which in the beginning contains the $n(n-1)/2$ entries of the dissimilarity matrix (as in Figure 14 of Chapter 2). In later stages of the computation, new dissimilarities are obtained from the group average recipe (10). These dissimilarities between clusters then replace some of the original numbers in DYS. To keep track of things, at each step the number of objects of every cluster is counted and stored in the array KWAN. The third and fourth arrays are NER, which contains the ordering of the objects, and BAN, in which the dissimilarities between merging clusters are stored. The final contents of NER and BAN are printed under the heading "cluster results" (see Section 2.2). During the computation, NER is continuously adapted to the merging process. This is done in such a way as to change the original ordering of the objects as little as possible; as

Table 2 Computation Times (in minutes) on an IBM-XT with 8087 Coprocessor, for a Set of Randomly Generated Problems of Increasing Sizes Clustered Using the Program AGNES

Objects	Variables	Time
20	2	0.15
40	2	0.35
60	2	0.85
80	2	1.75
100	2	3.50

a consequence, object 1 will always remain the first object in the list. (The same goal was pursued in DIANA and a very similar approach was adopted for the numbering of the clusters in PAM and FANNY, making it easier to compare the results of these four programs on the same data set.) At each step, the changes in NER also induce permutations in BAN. Finally, the two arrays BAN and NER are used by subroutine BANAG to produce the banner of the agglomerative hierarchy.

The last three subroutines (SPLYT, SUPCL, and BANDY) are not used at all in the case of agglomerative nesting, but they are needed for the divisive method described in the next chapter.

As an indication of the speed of agglomerative nesting, Table 2 lists some computation times for data sets of different sizes. The same computer and the same data sets were used as for Table 7 of Chapter 2. The times in the latter table were about twice as large, and they were needed for five clusters, whereas Table 2 gives the times necessary for obtaining a complete hierarchy. This means that agglomerative nesting is really much faster than partitioning into a fixed number k of clusters. [A particularly fast agglomerative program was constructed by van Zomeren (1985).] On the other hand, agglomerative procedures suffer from the defect that a "wrong" fusion can never be repaired in subsequent steps, whereas for a fixed number of clusters a program like PAM will try to find a near-optimal solution. The choice between a hierarchical and a nonhierarchical method depends mainly on the purpose of the investigation: For instance, in biological applications one usually wants a hierarchical classification.

*5 RELATED METHODS AND REFERENCES

5.1 Other Agglomerative Clustering Methods

In the last decades, a large number of agglomerative techniques have been used. We will give a survey of the most popular ones and say something

about their properties. Other aspects can be found in Anderberg (1973), Bock (1974), Gordon (1981), Hartigan (1975), and Späth (1980).

a. Single Linkage

The *single linkage algorithm*, which is the oldest and simplest agglomerative method, was introduced by Florek et al. (1951) and Sneath (1957b). It works exactly as the algorithm we described in Section 1, only the dissimilarity between two clusters is not defined by formula (5) but by

$$d(R, Q) = \min_{\substack{i \in R \\ j \in Q}} d(i, j) \tag{12}$$

This corresponds to a commonly used definition in pure mathematics, where the distance between two sets is often taken to be the minimum (or, more generally, the infimum) of all pairwise distances. In this book all clusters are of course finite, so (12) corresponds to finding a pair of points, one in R and one in Q, with the smallest possible dissimilarity. Therefore, single linkage is also often called the *nearest neighbor method*. As in the group average method, the single linkage dissimilarity also can be computed by means of an updating formula. When clusters A and B have joined to form a new cluster R, all dissimilarities between R and other clusters Q can be obtained from

$$\begin{aligned} d(R, Q) &= \min\{d(A, Q), d(B, Q)\} \\ &= \tfrac{1}{2}(d(A, Q) + d(B, Q)) - \tfrac{1}{2}|d(A, Q) - d(B, Q)| \end{aligned} \tag{13}$$

The updating algorithm using the first equation was already applied by Johnson (1967). The second equation looks slightly artificial, but is used to fit (13) into a more general framework of equations we shall describe later on at the end of this subsection. The program AGNES could be turned into a single linkage program by replacing the seven consecutive lines

```
TA = KWAN(LA)
TB = KWAN(LB)
FA = TA / (TA + TB)
FB = TB / (TA + TB)
NAQ = MEET(LA, LQ)
NBQ = MEET(LB, LQ)
DYS(NAQ) = FA*DYS(NAQ) + FP*DYS(NBQ)
```

of subroutine AVERL by the following ones:

```
NAQ = MEET(LA, LQ)
NBQ = MEET(LB, LQ)
```

```
DNEW = DYS(NAQ)
IF(DYS(NBQ).LT.DNEW)DNEW = DYS(NBQ)
DYS(NAQ) = DNEW
```

Similar small modifications could be made to implement the other methods discussed in this section. For the understanding of these program parts, note that TA = $|A|$, TB = $|B|$, FA = $|A|/|R|$, FB = $|B|/|R|$, and DYS(NBQ) = $d(B, Q)$. The expression DYS(NAQ) first stands for $d(A, Q)$, but in the end its meaning changes to $d(R, Q)$, as the array DYS is being overwritten to save memory space. More efficient algorithms, based on minimum spanning trees, are discussed by Gower and Ross (1969).

When the original dissimilarities between objects are transformed by a strictly monotone function (such as a square root), the single linkage hierarchy remains the same (Johnson, 1967; Sibson, 1972). However, the levels of the fusions will be transformed accordingly, so the banner (and the agglomerative coefficient) may change a lot.

Formula (12) already shows the main weakness of the single link algorithm. When two clusters, however large and clearly distinct, come close to each other at even a single point, the method will not be able to keep them apart. In other words, a single link between two clusters is sufficient to connect them. This leads to the notorious *chaining effect*, by which poorly separated clusters are chained together. The resulting clusters can be drawn out or even linear, instead of the usual ball-shaped ones. Of course, in certain fields drawn out clusters do occur, in which case single linkage may prove useful. But on the whole, we do not recommend this method. Baker (1974) shows that single linkage suffers from a lack of robustness. Also many other authors reject single linkage on the basis of empirical studies (Milligan and Isaac, 1980). Wishart (1969a) considered a variant that tries to eliminate the objects in sparsely populated regions before applying single linkage, in order to inhibit chain building. Jardine (1969) and van Rijsbergen (1970) propose searching the result of single linkage for L- and L^*-clusters (for a definition of L and L^*, see Section 2.2 in Chapter 2).

b. Complete Linkage

The *complete linkage algorithm* is exactly the opposite of single linkage (one might even say it falls into the other extreme). The dissimilarity between two clusters is now defined as the *largest* dissimilarity between an object of the one cluster and an object of the other. For this reason, complete linkage is often referred to as the *furthest neighbor* method. Formally,

$$d(R, Q) = \max_{\substack{i \in R \\ j \in Q}} d(i, j) \tag{14}$$

This method was described by McQuitty (1960), Sokal and Sneath (1963) and Macnaughton-Smith (1965). The updating equation now becomes

$$d(R,Q) = \max\{d(A,Q), d(B,Q)\}$$
$$= \tfrac{1}{2}(d(A,Q) + d(B,Q)) + \tfrac{1}{2}|d(A,Q) - d(B,Q)| \quad (15)$$

Like single linkage, complete linkage also yields an invariant hierarchy under strictly monotone transformations of the original dissimilarities (but again, the banner may change). Whenever the algorithm joins clusters A and B to form a new cluster R, the dissimilarity between A and B equals the diameter of R [this can easily be shown by induction, as in Theorem 39.3 of Bock (1974)].

In order to run complete linkage on the computer, we merely have to replace the above seven lines of subroutine AVERL by

```
NAQ = MEET(LA, LQ)
NBQ = MEET(LB, LQ)
DNEW = DYS(NAQ)
IF(DNEW.LT.DYS(NBQ))DNEW = DYS(NBQ)
DYS(NAQ) = DNEW
```

Defay (1977) and Hansen and Delattre (1978) have constructed some efficient algorithms for complete linkage.

Whereas single linkage usually leads to too few clusters which are drawn out, often complete linkage yields the opposite effect: many clusters with small within-cluster dissimilarities. Indeed, a couple of clusters containing at least one remote pair of objects will only be joined at a late stage. As a consequence, relatively similar objects will often stay in different clusters for a long time (dissection effect), hence complete linkage is sometimes said to be *space dilating*. On the other hand, single linkage will often bring rather dissimilar objects into the same cluster due to the chaining effect, and is therefore said to be *space contracting*. The necessity to compromise between these two extremes has lead to group average linkage and other methods discussed in this section, which are *space conserving*.

c. Centroid Method

The centroid method (Sokal and Michener, 1958; Lance and Williams, 1966a, b; Gower, 1967) is intended for data consisting of interval-scaled measurements (in principle without missing values). We denote by x_{if} the fth measurement of the ith object x_i, where i ranges from 1 to n and f

ranges from 1 to p. The *centroid* of a cluster R is then the point

$$\bar{x}(R) = \left(\bar{x}_1(R), \bar{x}_2(R), \ldots, \bar{x}_p(R)\right)$$

having for its fth coordinate

$$\bar{x}_f(R) = \frac{1}{|R|} \sum_{i \in R} x_{if} \tag{16}$$

for $f = 1, \ldots, p$. When all the points making up cluster R have the same physical mass, the centroid $\bar{x}(R)$ is simply the center of gravity of R. In what follows, we shall use the fact that the squared Euclidean distance between two objects is also the squared norm of their difference:

$$\begin{aligned} d^2(u, v) &= \|u - v\|^2 = (u - v) \cdot (u - v) \\ &= u \cdot u - v \cdot u - u \cdot v + v \cdot v = \|u\|^2 + \|v\|^2 - 2u \cdot v \end{aligned} \tag{17}$$

where $\cdot$ denotes the dot product of vectors

$$\begin{aligned} u \cdot v &= (u_1, u_2, \ldots, u_p) \cdot (v_1, v_2, \ldots, v_p) \\ &= u_1 v_1 + u_2 v_2 + \cdots + u_p v_p \end{aligned}$$

When merging clusters A and B to form cluster R, the centroid of R can be written as a function of those of A and B:

$$\bar{x}(R) = \frac{|A|}{|R|}\bar{x}(A) + \frac{|B|}{|R|}\bar{x}(B) \tag{18}$$

where $|R| = |A| + |B|$. The following identity will be useful further on:

$$\begin{aligned} &|A|\,\|\bar{x}(A) - \bar{x}(R)\|^2 + |B|\,\|\bar{x}(B) - \bar{x}(R)\|^2 \\ &\quad = |A| \left\| \bar{x}(A) - \left(\frac{|A|}{|R|}\bar{x}(A) + \frac{|B|}{|R|}\bar{x}(B) \right) \right\|^2 \\ &\qquad + |B| \left\| \bar{x}(B) - \left(\frac{|A|}{|R|}\bar{x}(A) + \frac{|B|}{|R|}\bar{x}(B) \right) \right\|^2 \\ &\quad = |A| \left\| \frac{|B|}{|R|}\bar{x}(A) - \frac{|B|}{|R|}\bar{x}(B) \right\|^2 + |B| \left\| \frac{|A|}{|R|}\bar{x}(B) - \frac{|A|}{|R|}\bar{x}(A) \right\|^2 \\ &\quad = \frac{|A|\,|B|^2}{|R|^2}\|\bar{x}(A) - \bar{x}(B)\|^2 + \frac{|B|\,|A|^2}{|R|^2}\|\bar{x}(A) - \bar{x}(B)\|^2 \\ &\quad = \frac{|A|\,|B|}{|R|}\|\bar{x}(A) - \bar{x}(B)\|^2 \end{aligned} \tag{19}$$

In the centroid method (also called *centroid linkage* or *centroid sorting*), the dissimilarity between two clusters is defined as the *Euclidean* distance between their centroids:

$$d(R,Q) = \|\bar{x}(R) - \bar{x}(Q)\| \tag{20}$$

The update equation is more complicated:

$$d^2(R,Q) = \frac{|A|}{|R|}d^2(A,Q) + \frac{|B|}{|R|}d^2(B,Q) - \frac{|A||B|}{|R|^2}d^2(A,B) \tag{21}$$

Note that this equation contains squares, so the final value of $d(R,Q)$ is the square root of the right-hand side of (21). By means of identity (19) it is possible to prove this update equation, starting with the right-hand side:

$$\begin{aligned}
&\frac{|A|}{|R|}\|\bar{x}(A) - \bar{x}(Q)\|^2 + \frac{|B|}{|R|}\|\bar{x}(B) - \bar{x}(Q)\|^2 - \frac{|A||B|}{|R|^2}\|\bar{x}(A) - \bar{x}(B)\|^2 \\
&= \frac{|A|}{|R|}\|(\bar{x}(A) - \bar{x}(R)) + (\bar{x}(R) - \bar{x}(Q))\|^2 \\
&\quad + \frac{|B|}{|R|}\|(\bar{x}(B) - \bar{x}(R)) + (\bar{x}(R) - \bar{x}(Q))\|^2 \\
&\quad - \left(\frac{|A|}{|R|}\|\bar{x}(A) - \bar{x}(R)\|^2 + \frac{|B|}{|R|}\|\bar{x}(B) - \bar{x}(R)\|^2\right) \\
&= \frac{|A|}{|R|}\left\{\|\bar{x}(A) - \bar{x}(R)\|^2 + \|\bar{x}(R) - \bar{x}(Q)\|^2\right. \\
&\qquad \left. + 2(\bar{x}(R) - \bar{x}(Q)) \cdot (\bar{x}(A) - \bar{x}(R)) - \|\bar{x}(A) - \bar{x}(R)\|^2\right\} \\
&\quad + \frac{|B|}{|R|}\left\{\|\bar{x}(B) - \bar{x}(R)\|^2 + \|\bar{x}(R) - \bar{x}(Q)\|^2\right. \\
&\qquad \left. + 2(\bar{x}(R) - \bar{x}(Q)) \cdot (\bar{x}(B) - \bar{x}(R)) - \|\bar{x}(B) - \bar{x}(R)\|^2\right\} \\
&= \frac{|A| + |B|}{|R|}\|\bar{x}(R) - \bar{x}(Q)\|^2 \\
&\quad + 2(\bar{x}(R) - \bar{x}(Q)) \cdot \left[\frac{|A|}{|R|}(\bar{x}(A) - \bar{x}(R)) + \frac{|B|}{|R|}(\bar{x}(B) - \bar{x}(R))\right] \\
&= \|\bar{x}(R) - \bar{x}(Q)\|^2 + 2(\bar{x}(R) - \bar{x}(Q)) \cdot (\bar{x}(R) - \bar{x}(R)) \\
&= \|\bar{x}(R) - \bar{x}(Q)\|^2
\end{aligned}$$

The centroid algorithm can be implemented by using the following lines:

```
TA = KWAN(LA)
TB = KWAN(LB)
FA = TA / (TA + TB)
FB = TB / (TA + TB)
FC = -FA*FB
NAQ = MEET(LA, LQ)
NBQ = MEET(LB, LQ)
NAB = MEET(LA, LB)
D = FA*DYS(NAQ)*DYS(NAQ) + FB*DYS(NBQ)*DYS(NBQ)
D = D + FC*DYS(NAB)*DYS(NAB)
DYS(NAQ) = SQRT(D)
```

instead of the original seven lines in subroutine AVERL.

Although this algorithm is intended for Euclidean distances, it is of course possible to apply the update equation (21) to any kind of dissimilarity measures, with or without the squares. However, this may lead to strange results which lack interpretation (Anderberg, 1973; Steinhausen and Langer, 1977) and is therefore not recommended. This restricts the centroid method to measurement data. Another problem lies in the fact that the dissimilarities are no longer monotone, even when Euclidean distances are used. That is, it may happen that the dissimilarity of a given fusion is strictly smaller than that of a previous fusion, making it very difficult to represent the results in a meaningful way (see Anderberg, 1973, Section 6.2.5). For instance, the banner can no longer be used.

d. Ward's Method

Like centroid linkage, the method of Ward (1963) is intended for interval-scaled measurements and makes use of Euclidean distances. The dissimilarity between two clusters is again based on the Euclidean distance between their centroids, but now multiplied by a factor:

$$d^2(R, Q) = \frac{2|R||Q|}{|R| + |Q|} \| \bar{x}(R) - \bar{x}(Q) \|^2 \qquad (22)$$

The actual value of $d(R, Q)$ is the square root of (22). The factor 2 in (22) is necessary to retain the original Euclidean distance between objects, when both clusters consist of a single object. Definition (22) does not appeal to the intuition at first, but is the result of a statistical reasoning based on the idea of least squares, like the variance minimization techniques discussed in

Section 5.3 of Chapter 2. The *error sum of squares* of a cluster C is defined as the sum of squared Euclidean distances between the objects of the cluster and its centroid:

$$\mathrm{ESS}(C) = \sum_{i \in C} \|x_i - \bar{x}(C)\|^2 \tag{23}$$

and is used as a measure of the tightness of a cluster.

At each level of the hierarchy we consider the total ESS, which is the sum of all $\mathrm{ESS}(C)$ over all clusters C at this level. With the fusion of two clusters A and B to form a new cluster R at the next level, their ESS can only increase (or remain the same in very rare cases). As the ESS of all other clusters remain unchanged, the increment in total ESS is

$$\begin{aligned}
\Delta\mathrm{ESS} &= \mathrm{ESS}(R) - \mathrm{ESS}(A) - \mathrm{ESS}(B) \\
&= \sum_{i \in R} \|x_i - \bar{x}(R)\|^2 - \sum_{i \in A} \|x_i - \bar{x}(A)\|^2 - \sum_{i \in B} \|x_i - \bar{x}(B)\|^2 \\
&= \sum_{i \in A} \left(\|x_i - \bar{x}(R)\|^2 - \|x_i - \bar{x}(A)\|^2\right) \\
&\quad + \sum_{i \in B} \left(\|x_i - \bar{x}(R)\|^2 - \|x_i - \bar{x}(B)\|^2\right)
\end{aligned}$$

Making use of $\|u\|^2 - \|v\|^2 = (u + v) \cdot (u - v)$ this becomes

$$\begin{aligned}
&= \left[\sum_{i \in A} (x_i - \bar{x}(R) + x_i - \bar{x}(A))\right] \cdot (\bar{x}(A) - \bar{x}(R)) \\
&\quad + \left[\sum_{i \in B} (x_i - \bar{x}(R) + x_i - \bar{x}(B))\right] \cdot (\bar{x}(B) - \bar{x}(R))
\end{aligned}$$

Using the fact that $\sum_{i \in A} x_i = |A|\bar{x}(A)$ and identity (19) this yields

$$\begin{aligned}
&= |A|(\bar{x}(A) - \bar{x}(R) + \bar{x}(A) - \bar{x}(A)) \cdot (\bar{x}(A) - \bar{x}(R)) \\
&\quad + |B|(\bar{x}(B) - \bar{x}(R) + \bar{x}(B) - \bar{x}(B)) \cdot (\bar{x}(B) - \bar{x}(R)) \\
&= |A|\,\|\bar{x}(A) - \bar{x}(R)\|^2 + |B|\,\|\bar{x}(B) - \bar{x}(R)\|^2 \\
&= \frac{|A|\,|B|}{|R|}\|\bar{x}(A) - \bar{x}(B)\|^2
\end{aligned}$$

Making use of formula (22), we finally conclude that

$$\Delta\text{ESS} = \tfrac{1}{2} d^2(A, B) \tag{24}$$

Ward (1963) originally constructed an algorithm by requiring that ΔESS be as small as possible at each step. The idea to introduce the dissimilarity measure (22) in order to establish (24) is due to Wishart (1969b). Because of this last result, Ward's method simply amounts to merging those clusters A and B between which the dissimilarity $d(A, B)$ is minimal. Therefore, Ward's algorithm can be carried out in exactly the same way as the previously discussed ones. In the computation, we can use the update equation

$$d^2(R, Q) = \frac{|A| + |Q|}{|R| + |Q|} d^2(A, Q) + \frac{|B| + |Q|}{|R| + |Q|} d^2(B, Q) - \frac{|Q|}{|R| + |Q|} d^2(A, B) \tag{25}$$

To prove it, use formula (18) to write the left-hand side of (25) as

$$\begin{aligned}
&\frac{2|R||Q|}{|R| + |Q|} \|\bar{x}(R) - \bar{x}(Q)\|^2 \\
&\quad = \frac{2|R||Q|}{|R| + |Q|} \left\| \left(\frac{|A|}{|R|} \bar{x}(A) + \frac{|B|}{|R|} \bar{x}(B) \right) - \bar{x}(Q) \right\|^2 \\
&\quad = \frac{2|R||Q|}{|R| + |Q|} \left\| \frac{|A|}{|R|} (\bar{x}(A) - \bar{x}(Q)) + \frac{|B|}{|R|} (\bar{x}(B) - \bar{x}(Q)) \right\|^2 \\
&\quad = \frac{2|R||Q|}{|R| + |Q|} \left\{ \frac{|A|^2}{|R|^2} \|\bar{x}(A) - \bar{x}(Q)\|^2 + \frac{|B|^2}{|R|^2} \|\bar{x}(B) - \bar{x}(Q)\|^2 \right. \\
&\qquad \left. + 2 \frac{|A|}{|R|} \frac{|B|}{|R|} (\bar{x}(A) - \bar{x}(Q)) \cdot (\bar{x}(B) - \bar{x}(Q)) \right\}
\end{aligned}$$

and transform the last term using $2u \cdot v = \|u\|^2 + \|v\|^2 - \|u - v\|^2$,

obtaining

$$= \frac{2|Q|}{(|R| + |Q|)|R|}\Big\{|A|^2\|\bar{x}(A) - \bar{x}(Q)\|^2 + |B|^2\|\bar{x}(B) - \bar{x}(Q)\|^2$$

$$+|A||B|\Big(\|\bar{x}(A) - \bar{x}(Q)\|^2 + \|\bar{x}(B) - \bar{x}(Q)\|^2 - \|\bar{x}(A) - \bar{x}(B)\|^2\Big)\Big\}$$

$$= \frac{2|Q||A|}{|R| + |Q|}\frac{|A| + |B|}{|R|}\|\bar{x}(A) - \bar{x}(Q)\|^2$$

$$+ \frac{2|Q||B|}{|R| + |Q|}\frac{|B| + |A|}{|R|}\|\bar{x}(B) - \bar{x}(Q)\|^2$$

$$- \frac{|Q|}{|R| + |Q|}\frac{2|A||B|}{|R|}\|\bar{x}(A) - \bar{x}(B)\|^2$$

Both factors $(|A| + |B|)/|R|$ vanish and we find the right-hand side of formula (25).

By means of this update equation, we can easily adapt program AGNES to Ward's method using the lines

```
TA = KWAN(LA)
TB = KWAN(LB)
TQ = KWAN(LQ)
FA = (TA + TQ) / (TA + TB + TQ)
FB = (TB + TQ) / (TA + TB + TQ)
FC = -TQ / (TA + TB + TQ)
NAQ = MEET(LA, LQ)
NBQ = MEET(LB, LQ)
NAB = MEET(LA, LB)
D = FA*DYS(NAQ)*DYS(NAQ) + FB*DYS(NBQ)*DYS(NBQ)
D = D + FC*DYS(NAB)*DYS(NAB)
DYS(NAQ) = SQRT(D)
```

instead of the original ones.

The methods discussed until now (group average, single linkage, complete linkage, centroid, Ward) were all based on an inherent definition of the dissimilarity between any pair of clusters, from which update equations were derived. The next three methods (weighted average, Gower, flexible strategy) are of a different type, because they *only* have update equations.

Hence, the dissimilarity between clusters is defined recursively and can only be computed among clusters occurring at the same level of the hierarchy. As we shall see, this may even lead to contradictions. Therefore, we do not recommend these methods, but merely describe them for the sake of completeness.

e. Weighted Average Linkage

Weighted average linkage (Sokal and Sneath, 1963) is a variant of the group average method used in this chapter. One starts with the original dissimilarities between objects (which need not be Euclidean distances, but may be of any type) and at each merger of clusters A and B, forming some new cluster R, the dissimilarities are updated by

$$d(R, Q) = \tfrac{1}{2} d(A, Q) + \tfrac{1}{2} d(B, Q) \tag{26}$$

This recipe is very simple, but does not correspond to any inherent definition of dissimilarity between clusters. Indeed, in some situations contradictions will occur. Consider a set of four objects $\{a, b, c, d\}$ with the dissimilarity matrix

$$\begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \left[\begin{array}{cccc} 0.0 & 10.0 & 10.0 & 24.0 \\ 10.0 & 0.0 & 15.0 & 20.0 \\ 10.0 & 15.0 & 0.0 & 28.0 \\ 24.0 & 20.0 & 28.0 & 0.0 \end{array}\right] \end{array} \tag{27}$$

In the first step, one can choose arbitrarily whether to join a with b or with c. In the second step, the cluster $\{a, b, c\}$ is formed. However, let us now consider $d(\{a, b, c\}, \{d\})$. If a was first joined with b, we find

$$\begin{aligned} d(\{a, b, c\}, \{d\}) &= \tfrac{1}{2} d(\{a, b\}, \{d\}) + \tfrac{1}{2} d(\{c\}, \{d\}) \\ &= \tfrac{1}{2}\left[\tfrac{1}{2} d(a, d) + \tfrac{1}{2} d(b, d)\right] + \tfrac{1}{2} d(c, d) = 25.0 \end{aligned}$$

but if a was first joined with c we obtain

$$\begin{aligned} d(\{a, b, c\}, \{d\}) &= \tfrac{1}{2} d(\{a, c\}, \{d\}) + \tfrac{1}{2} d(\{b\}, \{d\}) \\ &= \tfrac{1}{2}\left[\tfrac{1}{2} d(a, d) + \tfrac{1}{2} d(c, d)\right] + \tfrac{1}{2} d(b, d) = 23.0 \end{aligned}$$

These different results also affect the banner, because $d(\{a, b, c\}, \{d\})$ is the level of the last step. The same kind of example can even be constructed using Euclidean distances.

Implementation of the weighted average linkage method is very simple, because one only has to insert the lines

```
NAQ = MEET(LA, LQ)
NBQ = MEET(LB, LQ)
DYS(NAQ) = (DYS(NAQ) + DYS(NBQ)) / 2.Ø
```

instead of the original ones.

The name "weighted average linkage" at first sight appears rather strange, because there are no weights in formula (26). However, imagine a large cluster A being merged with a small cluster B. In this case, the *objects* of B will carry a much larger weight than those of A in the dissimilarity (26). On the other hand, the group average method assigns to all pairs of *objects* the same weight by formula (5) and is therefore sometimes called *unweighted average linkage*, notwithstanding the weights in the update equation (10). This situation has lead to some confusion between the terms weighted and unweighted, but calling the latter method *group average* (Lance and Williams, 1966b) has largely resolved this ambiguity.

f. Gower's Method

The method of Gower (1967) is a variant of the centroid method previously described and its interpretation is also restricted to measurement data and Euclidean distances. When clusters A and B join, the centroid $\bar{x}(R)$ of the new cluster R is given by formula (18). Thus $\bar{x}(R)$ lies on the straight line segment between $\bar{x}(A)$ and $\bar{x}(B)$, and it is closer to the centroid of the cluster containing the largest number of objects. This is part of the "unweighted" principle, which assigns the same importance to all *objects*, making large clusters more influential than small ones. Gower argued that there are situations in which it is more sensible to attach equal importance to all *clusters*, regardless of their number of objects (as in weighted average linkage). As a consequence, he did not work with the real centroid but with something we shall call the *center* $c(A)$ of a cluster. In the case of clusters containing only a single object, the center equals this object. When joining clusters A and B, Gower argued that the center of the new cluster should be the midpoint of the previous centers,

$$c(R) = \tfrac{1}{2}c(A) + \tfrac{1}{2}c(B) \tag{28}$$

instead of (18). Unfortunately, this implies that the center of a cluster is not always uniquely defined, because it depends on the order in which the cluster was assembled. The dissimilarity of cluster R to any other cluster Q

is now defined as the Euclidean distance between their centers:

$$d(R, Q) = \|c(R) - c(Q)\| \tag{29}$$

It turns out that $d(R, Q)$ is measured along the median line passing through $c(Q)$ of the triangle spanned by $\{c(A), c(B), c(Q)\}$, and for this reason Gower's approach has often been referred to as the *median method* (Lance and Williams, 1966b). It is not difficult to obtain the update equation for the dissimilarity (29) because one only has to note that (28) is a special case of (18) when $|A| = |B|$. Therefore, we can simply repeat the reasoning leading to (21), substituting $|R| = 2|A| = 2|B|$ in the latter equation, which yields

$$d^2(R, Q) = \tfrac{1}{2} d^2(A, Q) + \tfrac{1}{2} d^2(B, Q) - \tfrac{1}{4} d^2(A, B) \tag{30}$$

Gower's algorithm may be applied by means of the lines

```
NAQ = MEET(LA, LQ)
NBQ = MEET(LB, LQ)
NAB = MEET(LA, LB)
D = (DYS(NAQ)*DYS(NAQ) + DYS(NBQ)*DYS(NBQ)) / 2.Ø
D = D - (DYS(NAB)*DYS(NAB))/4.Ø
DYS(NAQ) = SQRT(D)
```

It looks as if (29) provides a solid explicit definition of a dissimilarity between clusters, but this is not the case because the centers of the clusters may not be uniquely defined. As in the case of weighted average linkage, application of the update equation (30) may lead to contradictions [this happens for the example of (27)].

g. Flexible Strategy

Lance and Williams (1966b) introduced an algorithm depending on a parameter α which can be specified by the user. They start from an arbitrary set of dissimilarities between objects (which may be Euclidean distances, squared Euclidean distances, Manhattan distances, or whatever) and use the update equation

$$d(R, Q) = \alpha d(A, Q) + \alpha d(B, Q) + (1 - 2\alpha)\, d(A, B) \tag{31}$$

where α is a strictly positive constant. This update equation does not come from any inherent definition of dissimilarity between clusters, and indeed

contradictions can occur. [For instance, the matrix (27) provides such an example for weighted average linkage, Gower's method and the flexible strategy.] The flexible method can be applied by means of the lines

```
NAQ = MEET(LA, LQ)
NBQ = MEET(LB, LQ)
NAB = MEET(LA, LB)
D = ALPHA*(DYS(NAQ) + DYS(NBQ))
DYS(NAQ) = D + (1.Ø-2.Ø*ALPHA)*DYS(NAB)
```

provided the user has assigned a value to ALPHA earlier in the subroutine, for instance by inserting the line

```
ALPHA = Ø.625
```

The behavior of this clustering algorithm depends strongly on the specified value of α. For $\alpha = \frac{1}{2}$ one obtains weighted average linkage. When α tends to 0 the method becomes space contracting, leading to long-shaped clusters. When α grows larger than $\frac{1}{2}$ the method becomes space dilating, yielding a large number of compact clusters in the first stages of the hierarchy. Lance and Williams themselves proposed taking a value of α slightly larger than $\frac{1}{2}$, so that $1 - 2\alpha$ becomes a small negative number.

Lance and Williams (1966b) were the first to consider a unified framework for the commonly used agglomerative methods. Indeed, all update equations we have seen in this chapter are of the form

$$D(R, Q) = \alpha_A D(A, Q) + \alpha_B D(B, Q) + \beta D(A, B) + \gamma |D(A, Q) - D(B, Q)| \tag{32}$$

where D sometimes stands for an arbitrary dissimilarity and sometimes for squared Euclidean distance. Equation (32) is now generally called the *Lance–Williams formula*. The idea is to start from the original dissimilarities between objects and then to use (32) where the α_A, α_B, β, and γ may be either fixed constants or depend on $|A|$, $|B|$, and $|Q|$. The fact that Ward's method also falls into this category was proven by Wishart (1969b). Some mathematical properties of (32) were investigated by DuBien and Warde (1979).

There exist several agglomerative algorithms that cannot be fitted into the Lance–Williams framework, such as Delattre and Hansen's (1980) bicriterion analysis, which compromises between single linkage and com-

plete linkage. However, a discussion of this or other methods falls beyond the scope of this book. Bock (1974) and Gordon (1981) contain some references to techniques not covered here.

5.2 Comparing Their Properties

In this chapter we have described eight agglomerative methods: group average linkage, single linkage, complete linkage, centroid sorting, Ward's method, weighted average linkage, Gower's method, and the flexible strategy. These methods are usually considered together because they all fit into the Lance–Williams formalism (32) and can therefore easily be implemented with the same computer program. The user of such a program has to face a perplexing multitude of methods to choose from (also because the parameter α of the flexible strategy may be selected arbitrarily).

Of course, there is no single "best" clustering procedure, and some methods will work better for a particular application than others, as was illustrated by Dubes and Jain (1976). For instance, a user expecting long-shaped clusters will apply single linkage or the flexible strategy with small α, but when one searches for compact clusters, of which no two objects are far apart, one will run complete linkage or the flexible strategy with large α. Most often people are looking for roughly spherical clusters, in which case they will use one of the other methods. It is also possible to compare the results of different algorithms on the same data (Fowlkes and Mallows, 1983).

A good understanding of the properties of these algorithms is important because to a certain extent they impose their own structure on the data (this is especially true for the space-contracting and space-dilating methods). Jardine and Sibson (1968, 1971) and Sibson (1970, 1971) introduced some mathematical conditions in an axiomatic framework. For instance, they required that permutation of the objects or multiplication with a constant scale factor should not change the clustering in an essential way. Taken together, their axioms are only satisfied by the single linkage method. The crucial axiom seems to be the restriction to classifications that are (in a certain mathematical sense) *continuous* functions of the data. Several workers (Cormack 1971, 1980; Gower 1971b) argue that this continuity condition is too severe. [A similar point was made by Rousseeuw (1983a, Remark 2) showing that the only *continuous* affine equivariant central point of a cluster is its centroid, notwithstanding the sensitivity to outliers noted in Section 5.3 of Chapter 2.] A more versatile approach is due to Fisher and Van Ness (1971). They made up a list of useful properties one might be interested in having and then verified which clustering techniques satisfy these (so-called *admissibility*) conditions. For instance, the result of a

clustering technique is *image admissible* if the data cannot be clustered in another way (in which each cluster has the same number of objects as in the original clustering) that is uniformly better (in the sense that within-cluster dissimilarities are not larger than before and between-cluster dissimilarities are not smaller, with strict improvement for at least one dissimilarity). *Cluster omission admissibility* means that upon omitting a cluster and restarting the procedure, the remaining clusters will again be found. Van Ness (1973) extended this work by investigating more clustering algorithms and adding two admissibility properties. It turns out that single linkage satisfies the largest number of conditions.

At this point, we feel we should say something about the "optimality" of single linkage. Because it is the oldest and most simple method, it has gathered the largest collection of mathematical properties. This situation resembles the position of the least squares estimator in regression, which was also the oldest technique and the easiest one to compute. Afterward, many mathematicians produced nice conditions and optimality criteria especially tailored to suit the least squares estimator. Some of these justifications were plainly circular, such as the use of quadratic loss functions or the argument that least squares is optimal under the Gaussian distribution; indeed, Gauss himself constructed the distribution carrying his name in order to fit the least squares estimator (Gauss, 1821). Even now that the dangers of the least squares estimator are becoming well known, especially its extreme sensitivity to outliers, many people still hang on to its nice mathematical properties (although robust methods are available; see Rousseeuw and Leroy, 1987).

The same kind of self-justification mechanism has been going on for the single linkage method. Many criteria have been invented to make single linkage come out best. In our opinion, its most useful property (shared with complete linkage and some more recent techniques, such as nearest q-neighbors) is that monotone transformations on the dissimilarities do not change the clustering, which is important for ordinal dissimilarities. However, many other criteria have been devised (which do not take the negative aspects of single linkage into account, such as the chaining effect) in order to recommend single linkage in *all* situations. For instance, the axioms of Jardine and Sibson (1971), taken together, are only satisfied by the single linkage method. The same thing has been done over and over again for the least squares estimator, the real advantage of which was its algorithmic simplicity (the estimate can be obtained explicitly), making it the only computationally feasible method in the precomputer age. Similarly, the simplicity of single linkage has made it possible to construct very efficient algorithms (Sibson, 1973) that can technically run on large data sets. Ironically, many people have therefore *recommended* single linkage for

large data sets, when the very nature of the method makes it inappropriate because the clusters then tend to stick to each other due to the building of chains connecting them.

To show that the mathematical respectability of a method depends on who is writing down the criteria, we shall in this subsection consider a set of three simple conditions leading to the selection of the group average method among the eight techniques considered, following Rousseeuw (1985).

The first condition is that *the dissimilarity between merging clusters be monotone*. We already saw in Section 1 that this condition is necessary for us to be able to represent the clustering graphically, because we can then talk about the *level* of a merger. For group average linkage we saw in Section 4.1 that this condition is satisfied. We proved this by formula (11) which followed from the update equation (10). Let us now consider more general agglomerative procedures defined by the Lance–Williams update equation (32). It is well known that the resulting dissimilarity D is monotone whenever $\alpha_A \geq 0$, $\alpha_B \geq 0$, $\gamma = 0$, and $(\alpha_A + \alpha_B + \beta) \geq 1$. To see this, we merely have to repeat the reasoning involving formula (11):

$$\begin{aligned} D(R,Q) &= \alpha_A D(A,Q) + \alpha_B D(B,Q) + \beta D(A,B) \\ &\geq \alpha_A D + \alpha_B D + \beta D = (\alpha_A + \alpha_B + \beta) D \geq D \end{aligned}$$

These constraints on α_A, α_B, β, and γ hold for group average linkage, Ward's method, weighted average linkage, and the flexible strategy. The constraint $\gamma = 0$ does not hold for single linkage or complete linkage, but for these methods the monotonicity follows from

$$d(R,Q) = \min\{d(A,Q), d(B,Q)\} \geq \min\{d, d\} = d$$

and

$$d(R,Q) = \max\{d(A,Q), d(B,Q)\} \geq \max\{d, d\} = d$$

The constraint $(\alpha_A + \alpha_B + \beta) \geq 1$ does not hold for centroid sorting nor for Gower's method, and for these cases counterexamples are easily constructed. Hence, graphical representations of these methods may be very misleading. [In a dendrogram, exceptions to the monotonicity lead to so-called *reversals* discussed by Anderberg (1973).] We conclude that only centroid sorting and Gower's method do not satisfy the first condition.

For the second condition, we require that *the dissimilarities between clusters be unambiguous*. In particular, we do not want contradictions as in the case of weighted average linkage applied to (27), where two equivalent choices lead to different dissimilarities between the same clusters. Also

Gower's method and the flexible strategy suffer from this defect. On the other hand, there is no problem for the group average rule, single linkage, and complete linkage, because for them the dissimilarity between two clusters is defined explicitly in terms of the original interobject dissimilarities, by (5), (12), and (14). The same can be said about centroid sorting and Ward's method when the objects are characterized by interval measurements, that is, when they can be described by points in some Euclidean space, because then we only have to compute the Euclidean distance between cluster centroids. Therefore, only weighted average linkage, Gower's method, and the flexible strategy do not satisfy the second condition.

The third condition imposes that *the dissimilarities between clusters be statistically consistent*. In sampling situations, we want the dissimilarity between groups to be meaningful when the sample becomes larger. For instance, consider a one-, two-, or multidimensional Euclidean space. Take two statistical distributions F and G on this space, and sample a large number of points from both. When the two densities are fairly well-separated, two clusters will be visible in the resulting data set. What does the dissimilarity between these samples tend to, when the number of observations increases? Clearly, there is no point in considering methods that were already excluded by the second condition. On the other hand, the centroid method does satisfy the third condition, because the dissimilarity (20) tends to the Euclidean distance between the means of the underlying distributions. In mathematical notation, the limit is

$$\left\| \int x \, dF(x) - \int y \, dG(y) \right\|$$

For the group average method the limit is also meaningful because we obtain

$$\iint \|x - y\| \, dF(x) \, dG(y)$$

(Note that neither limiting formula is a distance in the strict sense. Also note that the average dissimilarity of points to their medoids, which is the objective to be minimized in Chapter 2, is statistically consistent as well. Therefore, average dissimilarities were used again in Chapter 3 for clustering large data sets.) However, Ward's method runs into trouble because the factor $|R|\,|Q|/(|R| + |Q|)$ in formula (22) makes the dissimilarity blow up to infinity. (Indeed, in many real data sets we have noticed that the final level of Ward's clustering was much larger than the largest dissimilarity between any two objects.) The dissimilarity (12) of single linkage will tend

to 0: The more points you draw from two strictly positive densities, the closer will be their nearest neighbors. For any two such densities, their limiting dissimilarity becomes 0. Complete linkage (14) suffers from the opposite defect: The more points you draw, the more their furthest neighbors will be apart. Like Ward's method, complete linkage will also lead to an infinite limiting dissimilarity. Consequently, only group average linkage and centroid sorting satisfy the third condition. Probably some people will say that this condition is too severe. However, we feel that for a statistician it is perfectly natural to expect that more observations yield more accurate results, or a sharper image of what is going on, instead of something completely blurred. In our opinion the third condition is not strong at all, because it only concerns the dissimilarity between groups known in advance and does not even ask whether the "right" groups were actually uncovered by the algorithm. In the case of single linkage, often the "right" groups are not found because large samples lead to chains of intermediate objects connecting one cluster to another. The question of consistency of the clustering itself was addressed by Degens and Federkiel (1978) who found that complete linkage is not consistent in one dimension.

Combining all three conditions, only the group average method remains. Of course, we do not claim that group average is the only reasonable agglomerative clustering method. Nevertheless, we do think that group average linkage is a good technique which performs well in practice. We also like it because it is easy to understand and to explain, and can be used on data that are not restricted to Euclidean distances. This is why we only implemented the group average method in AGNES. For similar reasons, average dissimilarities are used in many other parts of this book.

Another way to compare the various clustering methods is by means of simulation studies. The general idea is to generate data with *known* structure and then to see if the clustering techniques can recover it. However, this leads to a similar problem as in the case of mathematical conditions, because generating different types of data will make different clustering methods look best. For instance, when spherical multivariate normal distributions are used, Ward's method is excellent (Kuiper and Fisher, 1975), which is only natural because this method is based on a sum of squares criterion. Similar results were obtained by Blashfield (1976) and Bayne et al. (1980). However, it must be noted that Ward's method only performs well if an equal number of objects is drawn from each population and that it has difficulties with clusters of unequal diameters. Moreover, Everitt (1977) showed that Ward's method often leads to misclassifications when the clusters are distinctly ellipsoidal rather than spherical, that is, when the

variables are correlated within a cluster. On the other hand, Cunningham and Ogilvie (1972) considered a wide variety of sampling situations and clustering methods, and found that group average linkage was usually the most effective technique. Also Sneath (1966) and Milligan and Isaac (1980) concluded that group average linkage ranked first. It appears that this method is suitable for many situations and possesses a certain robustness with respect to slight distortions. Virtually all authors agreed that single linkage was least successful in their studies.

5.3 Graphical Displays

There are many ways to represent the result of a hierarchical clustering algorithm graphically. After applying group average linkage to the data of matrix (4) we first constructed Figure 3, which visualizes the order in which the clusters are assembled. Because the dissimilarity between merging clusters turns out to be monotone for this clustering method (a fact we proved in Section 4.1), it was possible to replace Figure 3 by Figure 4, which contains all the details of the amalgamation process. In Section 2.2 we explained how all this information can be stored in just two sequences of numbers, the one containing the final ordering of the objects (array NER) and the other consisting of the levels at which the clusters are merged (array BAN). For practical reasons, we decided to use the banner (Figure 5) instead of Figure 4, because the production of a banner requires no sophisticated plotting machinery, but merely a line printer, and it can therefore be implemented in portable programs.

Let us now describe the historical origin of the banner and its relation to the icicle plot. Basically, there are two roots, the first of them being the display proposed by Ward (1963). Figure 13 shows a Ward-type display describing the same hierarchy as in Figures 3, 4, and 5.

Unlike the banner, Figure 13 is to be read from right to left, at least if one wants to follow the order in which the calculations have taken place. The number of groups is given from left to right, whereas the number of the amalgamation step would go from right to left. In Ward's display, the dotted arrows indicate separation, and white space between objects stands for linking: Therefore, white space has opposite meanings in this display and the banner. The labels of the objects are repeated within the display, even when the object is the only element of a cluster (in which case said label is suppressed in the banner). The length of the dotted arrows depends on the number of steps and not on the actual level of the merger, which is listed at the bottom of the figure. [Actually, Ward himself did not enter the level but the total error sum of squares ESS given by formula (23), which is

Object	Number of Groups				
	1	2	3	4	5
a	a	a	a	a	a
b	b	b	b	b	b
c	c	c	c	c	c
d	d	d	d	d	d
e	e	e	e	e	e
level	7.83	4.5	3.0	2.0	0.0

Figure 13 A Ward-type display of the group average linkage clustering of the data of matrix (4).

basic to the method he was proposing; the dissimilarity between merging clusters essentially appears as the sequence of first differences ΔESS given by (24), which he lists too.]

The second root of both banner and icicle plot is Johnson's (1967) display, which we have constructed in Figure 14 for the same data.

This display is read from top to bottom. The dissimilarity between merging clusters is given in the leftmost column, for each computation step. (In Johnson's application a coefficient of *similarity* was used, which decreases from top to bottom.) Again, the scale of the diagram is in terms of the number of the amalgamation step, in this case going from 0 to 4, and not in terms of the actual level. The object labels are printed only once, at the top of the picture. The dots in the main part of the diagram denote objects that are still unlinked at a certain stage, but as soon as the object joins at least one other object it is depicted by the letter *X*. Also the links

Dissimilarity	Objects				
	a	b	c	d	e
0.00	.	.	.	.	.
2.00	X	X	X	.	.
3.00	X	X	X	.	X X X
4.50	X	X	X	X	X X X X
7.83	X	X	X	X	X X X X X

Figure 14 A Johnson-type display of the group average linkage clustering of the data of matrix (4).

```
                A   B   C   D   E
                A   B   C   D   E
                A   B   C   D   E

4     7.83      A = B = C = D = E
3     4.50      A = B   C = D = E
2     3.00      A = B       D = E
1     2.00      & = &
```

Figure 15 Icicle plot of the group average linkage clustering of the data of matrix (4).

between clusters are denoted by X's, whereas white space now separates clusters. Johnson's display is contained in the output of HICLUS, in the MDS(X) series of multidimensional scaling programs (Davies and Coxon, 1983). Quite similar displays were also used by Wirth, Estabrook, and Rogers (1966) and Hartigan (1975, Tables 8.2, 8.6, and 8.7).

The banner is closely related to the icicle plot of Kruskal and Landwehr (1983), displayed in Figure 15 for the same data set. Its name stems from its resemblance to a row of icicles hanging from the eaves. This display is to be read from bottom to top. The leftmost column contains the number of the amalgamation step and the second column lists the level of each merger. Again the diagram is scaled by the number of the step and not by the level. (However, Kruskal and Landwehr also consider a variant that is regularly spaced in terms of the *logarithm* of the level.) The object labels can be read off vertically above the plot as well as in it, where they are separated by the character "&". The idea to reproduce the labels within the plot stems from Ward's display, whereas the deletion of labels corresponding to singleton clusters was inherited from Johnson's diagram. Linking is now denoted with an equal sign and white space indicates nonlinking.

The resemblance between the icicle plot and the banner is very large. The different characters for linking clusters (* instead of =) and for separating labels (+ instead of &) are only a matter of taste. However, there are two differences. First, the banner lists the objects vertically, whereas the icicle plot lists them horizontally. Therefore, the banner can always be printed as a whole, whatever the size of the data set, whereas the icicle plot is limited by the width of the printing paper. As a consequence, except for small data sets the icicle plot must be printed in sections, which makes the program more complicated, and then the user has to tape or paste the parts together. (It recently came to our attention that the package SPSS-X also provides a vertical version of the icicle plot.) The second and more essential difference is the scaling. The banner uses the actual level of each merger, which to us seems more natural (for instance, imagine what would happen to Figures 9, 10, and 11 if the number of the step were used). This provides a better impression of relative magnitudes of dissimilarities (at least with a space-

conserving method like group average linkage). As an additional advantage, the average width of the banner gives a quick impression of the cluster quality of the data, which can be summarized by the agglomerative coefficient AC. All this holds for divisive clustering too, only then the banner floats in the opposite direction.

Most users of agglomerative clustering have been displaying their results by means of *dendrograms*. In Figure 16 two types of dendrograms are illustrated, but many other variants exist. Type (a) is probably most familiar and descends clearly from the tree diagram in Figure 4. This dendrogram is read from left to right, and the labels are listed only once in the column on the left. The horizontal scale is proportional to the actual level of the mergers. Type (b) is very similar, but the vertical line specifying each cluster now extends over all its objects: For instance, the vertical line at level 4.5 extends over *c*, *d*, and *e* (see Kruskal and Landwehr, 1983). Some people feel that a dendrogram is more aesthetically pleasing than a

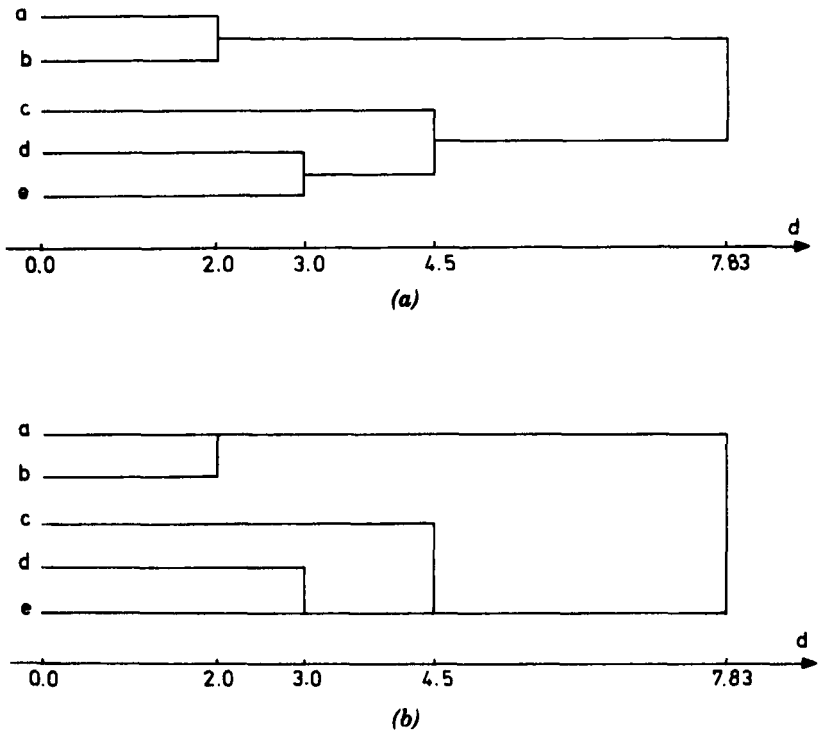


Figure 16 Two types of dendrogram, applied to the group average linkage clustering of the data of matrix (4).

banner, but we think that the latter display is more practical in actual data analysis because the labels are within the plot and because—at least to us —it gives a better overall insight into cluster structure and data quality.

The dendrograms in Figure 16 proceed from left to right, but often the picture is rotated 90° so it has to be read from bottom to top. In many cases the axis containing the levels is omitted.

Dendrograms can be prepared in many ways. Figure 16 was made by hand, but dendrograms very much like these can be produced by automatic plotting equipment. However, this depends strongly on the computer system at hand. Therefore, several programs are available which display dendrograms on a line printer, making them look considerably less beautiful. Program BMDP2M (Engelman, 1977) prints dendrograms that are to be read from top to bottom, making use of the characters I, −, and +. This limits the number of objects by the width of the paper, making it necessary to print the dendrogram in several sections that must be pasted together. BMDP2M can also produce a skewed dendrogram if desired. (It also provides a shaded dissimilarity matrix, as described in Section 5.6 of Chapter 2). On the other hand, the program of Anderberg (1973) prints dendrograms in the same direction as Figure 16, only making use of the characters − and I. Therefore, the dendrograms are always printed as a whole. Whereas BMDP scales its dendrograms by the number of the amalgamation step, Anderberg uses the actual level of each merger. Because a line printer offers only a discrete set of possibilities, Anderberg starts by segmenting the dissimilarities into 25 equally spaced classes between the smallest and the largest. (In the banner, we used 75 classes between 0 and the largest dissimilarity.) The package CLUSTAN (Wishart, 1978) provides similar horizontal dendrograms which are scaled by the actual level, starting from 0. Other CLUSTAN options include vertical dendrograms resembling those of BMDP2M and horizontal tables in which the tree may be sketched by hand.

Recently, Kent (1984) proposed a display with some characteristics of both dendrograms and icicle-type diagrams. Figure 17 illustrates this display for the data of matrix (4). At the left we find the labels and the numbers of the objects. The diagram is scaled by the number of clusters, as is Ward's display (Figure 13). To understand the main part of Kent's display, we must read our previous diagrams in the "wrong" direction, that is, Figures 3, 4, 5, and 16 from right to left, Figure 13 from left to right, Figure 14 from bottom to top, and Figure 15 from top to bottom. We first look at the final stage of the clustering, when all objects have come together. We call this cluster 1, and write "1" in a vertical line extending over all objects. The last merger was of clusters $\{a, b\}$ and $\{c, d, e\}$, so Kent calls $\{c, d, e\}$ cluster 2 and puts "2" in a vertical line next to *CCC*, *DDD*, and

LABEL	NO	1	2	3	4	5
AAA	1	1				
BBB	2	1				5
CCC	3	1	2			
DDD	4	1	2	3		
EEE	5	1	2	3	4	

Figure 17 A Kent-type display of the group average linkage clustering of the data of matrix (4).

EEE. The merger before that one was of $\{c\}$ and $\{d, e\}$, so Kent calls $\{d, e\}$ cluster 3 and writes "3" next to *DDD* and *EEE*. Before that, $\{d\}$ and $\{e\}$ came together, so singleton $\{e\}$ is called cluster 4. In the very first merger $\{a\}$ and $\{b\}$ were joined, so $\{b\}$ is called cluster 5. Kent's display allows a backward reconstruction of the clustering. Its main advantage is that it takes less space than the other displays. However, we think it is needlessly compressed (a simple printout of the numbers in the arrays NER and BAN contains even more information in a still smaller space). Kruskal and Landwehr (1984) pointed out the main weakness of Kent's display: Because at each divisive step only the lower cluster is numbered, half of the clusters are not displayed at all and may easily be forgotten by the data analyst. The vertical lines of digits correspond to some of the vertical lines of Figure 16(b), but not to all of them: In our example, there is no counterpart to the vertical line next to cluster $\{a, b\}$.

All the displays considered until now (Figures 3 to 5 and 13 to 17) can be constructed from the two arrays NER and BAN in program AGNES. Indeed, NER lists the final ordering of the objects, which is the same for all displays, and BAN shows the level of each merger (and hence the order in which the mergers take place, up to some arbitrariness in the case of equal levels). Therefore, it is possible to replace the subroutine BANAG by a different subroutine which plots any of the other displays.

There exists still another type of display, for which more information about the original data is needed. In Figure 18, the group average linkage clustering of the data in Table 1 is described by a *loop plot*. Here the original data is two-dimensional, so it can easily be plotted as in Figure 1. The loop plot can then be formed by adding nested loops to this picture which indicate the clusters that were obtained. The resulting diagram is pretty and instructive, especially when the loops are smooth. In more complicated situations, which are no longer two-dimensional, loop plots may still be used (Shepard, 1974). In general, one has to place the object

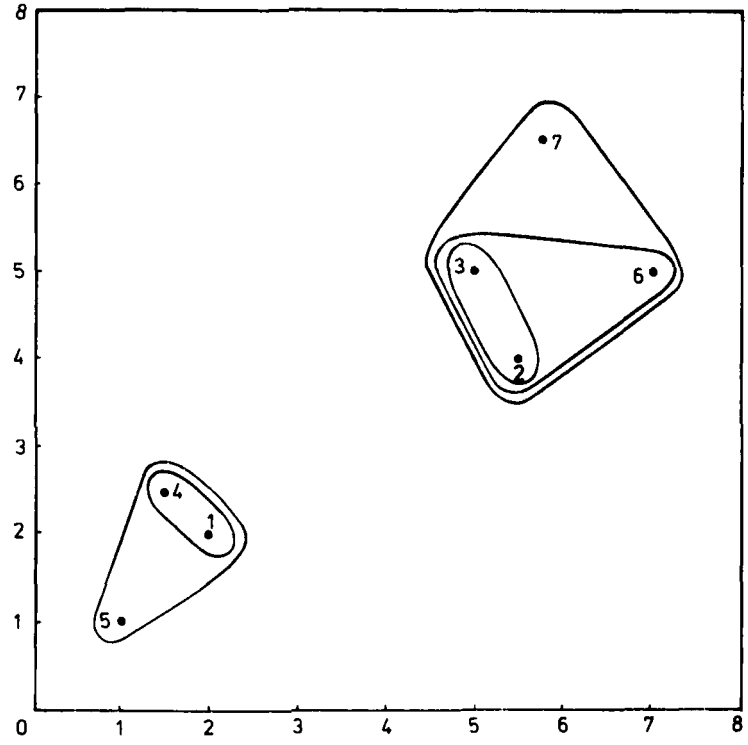


Figure 18 Loop plot of the group average linkage clustering of the data of Table 1.

labels in suitable positions in the plane so that the loops are well-shaped and do not intersect; this could be done by trial and error. When the data consist of points in higher dimensions, one could try plotting the first two principal coordinates, perhaps adjusting the position of the object labels manually in order to permit well-formed loops. In case of general dissimilarity matrices such as matrix (4), multidimensional scaling techniques can be used. Bertin (1967, p. 270) also experimented with three-dimensional versions of loop plots.

We think that loop plots are very useful tools for interpreting the results of cluster analysis. The main problem is in obtaining them; to date they are only made by hand. The most difficult part is to find a suitable configuration of points in the plane, which allows the drawing of nice loops. Especially when the number of cases increases, this can become a cumbersome task. However, it is hoped that the current boom in interactive computer graphics will provide efficient ways to construct loop plots.

A similar two-dimensional display was proposed by Fowlkes et al. (1976). Starting from a dendrogram, some important clusters are selected by means of certain criteria. These clusters are then represented by circles that are connected by a series of horizontal and vertical lines.

Other people have used agglomerative clustering techniques to construct general-purpose graphical displays for multivariate data. Kleiner and Hartigan (1981) apply a hierarchical clustering algorithm to the p variables and then represent each object by a tree or a castle. Kent (1985) uses the minimum spanning tree (which corresponds to single linkage clustering) to construct a new coordinate axis against which the objects are plotted.

On the other hand, it is also possible to extend the theory of hierarchical clustering to allow for overlapping clusters. Diday (1985) introduced so-called *pyramids* as a visual representation of such a clustering.

EXERCISES AND PROBLEMS

1. Repeat the group average clustering of (4), but change $d(a, b)$ from 2.0 to 0.1. Check that all subsequent levels remain the same as before and that Figure 3 is unaltered.

2. Chandon and Pinson (1981) give the following dissimilarity matrix between four mammals:

	Camel	Monkey	Cow	Pig
Camel	0	5.0	5.6	7.2
Monkey	5.0	0	4.6	5.7
Cow	5.6	4.6	0	4.9
Pig	7.2	5.7	4.9	0

   Construct an agglomerative hierarchy on this data set by means of the group average clustering method.

3. Apply the program AGNES to cluster the data concerning the 11 sciences in Table 6 of Chapter 1.

4. Use the data in Table 7 of Chapter 1 to examine the effect of a noninformative variable on the clustering of objects. First apply AGNES to all four variables, and then to the same data without the variable "month."

5. Apply AGNES to the data on 47 stars in Table 1 of Chapter 6, without standardization and using Euclidean distance. Check whether the resulting partition with $k = 2$ separates the giants from the main sequence stars.

6. **(a)** Apply AGNES to the bacteria data in Exercise 1 of Chapter 2. Does the clustering into two clusters correspond to the result of PAM?

(b) When a data set consists of two L^*-clusters (in the sense of Section 2.2 of Chapter 2) show that AGNES always recovers these groups.

7. The critical dissimilarities of successive mergers can be used to define a new dissimilarity between objects. This new dissimilarity, denoted by $u(i, j)$, is the critical dissimilarity encountered when forming the first cluster containing both objects i and j.

(a) Show that the $u(i, j)$ possess the *ultrametric property*

$$u(i, j) \leq \max\{u(i, h), u(h, j)\} \quad \text{for every } i, j, h$$

(b) Construct the matrix of dissimilarities $u(i, j)$ from the clustering of the 12 countries data in Section 3.

8. Prove the equalities in (13) and (15):

$$\begin{aligned}\min\{d(A, Q), d(B, Q)\} &= \tfrac{1}{2}(d(A, Q) + d(B, Q)) \\ &\quad - \tfrac{1}{2}|d(A, Q) - d(B, Q)| \\ \max\{d(A, Q), d(B, Q)\} &= \tfrac{1}{2}(d(A, Q) + d(B, Q)) \\ &\quad + \tfrac{1}{2}|d(A, Q) - d(B, Q)|\end{aligned}$$

9. An alternative to the group average method is to replace (5) by another dissimilarity between clusters, defined by

$$d(R, Q) = \underset{\substack{i \in R \\ j \in Q}}{\text{median}}\, d(i, j)$$

where the median is over all pairs of i and j, of which there are $|R|\,|Q|$. The median is defined by sorting the $d(i, j)$ from smallest to largest. When the number of values is odd, the median is the middle value.

When their number is even, we define the median as the highest of the two middle values.

(a) Show that the dissimilarity between merging clusters is monotone.

(b) Show that the dissimilarity between clusters is unambiguous and statistically consistent in the sense of Section 5.2.

(c) Show that monotone transformations on the dissimilarities between objects do not change the clustering (and, in fact, the levels of the mergers are transformed in the same way).

10. Another alternative method is based on the dissimilarity

$$d(R, Q) = \max\left\{ \max_{i \in R} \left[\min_{j \in Q} d(i, j) \right], \max_{j \in Q} \left[\min_{i \in R} d(i, j) \right] \right\}$$

which is again uniquely defined and symmetric in R and Q.

(a) Show that this dissimilarity transforms properly under monotone transformations of the interobject dissimilarities $d(i, j)$.

(b) As opposed to the group average dissimilarity (5), now the dissimilarity of a cluster to itself is 0.

(c) Assuming that $d(i, j) = 0$ implies $i = j$, it even follows that

$$d(R, Q) = 0 \quad \text{implies} \quad R = Q$$

which is not true for any other method we considered, not even for single linkage or the centroid method.

Finding Groups in Data: An Introduction to Cluster Analysis
Leonard Kaufman and Peter J. Rousseeuw

CHAPTER 6

Divisive Analysis (Program DIANA)

1 SHORT DESCRIPTION OF THE METHOD

Divisive clustering techniques are hierarchical in nature. Their main difference with the agglomerative methods of Chapter 5 is that they proceed in the inverse order. At each step, a divisive method splits up a cluster into two smaller ones, until finally all clusters contain only a single element. This means that the hierarchy is again built in $n - 1$ steps when the data set contains n objects.

In the literature, divisive methods have been largely ignored. (In fact, when people talk about hierarchical clustering, they often mean agglomerative clustering.) Most books on cluster analysis pay little attention to divisive techniques, and many software packages do not include divisive algorithms at all. The main reason for this appears to be the computational aspect. In the first step of an agglomerative algorithm all possible fusions of two objects are considered, leading to

$$C_n^2 = \frac{n(n-1)}{2} \tag{1}$$

combinations. This number grows quadratically with n, so it does become large, but the computations are still feasible. A divisive algorithm based on the same principle would start by considering all divisions of the data set into two nonempty subsets, which amounts to

$$2^{n-1} - 1 \tag{2}$$

possibilities. The latter number grows exponentially fast and soon exceeds the current estimate of the number of atoms in the universe. Even for medium-sized data sets, such a complete enumeration approach is computationally prohibitive.

Nevertheless, it is possible to construct divisive methods that do not consider *all* divisions, most of which would be totally inappropriate anyway. In this chapter we will use an algorithm based on the proposal of Macnaughton-Smith et al. (1964). This algorithm can be applied to exactly the same types of data as in Chapters 2, 4, and 5. All data sets that can be clustered by means of the agglomerative nesting approach of the preceding chapter can also be analyzed in a divisive way. In most examples the computation time is merely increased by a factor of 2, so the algorithm is still faster than the nonhierarchical methods of Chapters 2 and 4.

To illustrate the divisive analysis algorithm, we cluster the same example that we used in Section 1 of Chapter 5 to explain the agglomerative approach. The data consist of a matrix of dissimilarities

	a	*b*	*c*	*d*	*e*
a	0.0	2.0	6.0	10.0	9.0
b	2.0	0.0	5.0	9.0	8.0
c	6.0	5.0	0.0	4.0	5.0
d	10.0	9.0	4.0	0.0	3.0
e	9.0	8.0	5.0	3.0	0.0

between the objects a, b, c, d, and e. Being divisive, the algorithm assumes that the objects initially form a single cluster $\{a, b, c, d, e\}$.

In the first step, the algorithm has to split up the data set into two clusters. This is not done by considering all possible divisions, but rather by means of a kind of iterative procedure. The mechanism somewhat resembles the way a political party might split up due to inner conflicts: First the most discontented member leaves the party and starts a new one, and then some others follow him until a kind of equilibrium is attained. So we first need to know which member disagrees most with the others. Translated back to the algorithm, we look for the object that is most dissimilar to all other objects. To make this precise, we have to define the dissimilarity between an object and a group of objects. As in Chapters 2, 3, and 5, we use the *average dissimilarity* for this purpose, so we look for the object for which the average dissimilarity to all other objects is largest. (When there are two such objects, we have to pick one at random.) In our example, we

obtain

Object	Average Dissimilarity to the Other Objects
a	$(2.0 + 6.0 + 10.0 + 9.0)/4 = 6.75$
b	$(2.0 + 5.0 + 9.0 + 8.0)/4 = 6.00$
c	$(6.0 + 5.0 + 4.0 + 5.0)/4 = 5.00$
d	$(10.0 + 9.0 + 4.0 + 3.0)/4 = 6.50$
e	$(9.0 + 8.0 + 5.0 + 3.0)/4 = 6.25$

so object a is chosen to initiate the so-called *splinter group*. At this stage we have the groups $\{a\}$ and $\{b, c, d, e\}$, but we don't stop here. For each object of the larger group we compute the average dissimilarity with the remaining objects, and compare it to the average dissimilarity with the objects of the splinter group:

Object	Average Dissimilarity to Remaining Objects	Average Dissimilarity to Objects of Splinter Group	Difference
b	$(5.0 + 9.0 + 8.0)/3 \approx 7.33$	2.00	5.33
c	$(5.0 + 4.0 + 5.0)/3 \approx 4.67$	6.00	−1.33
d	$(9.0 + 4.0 + 3.0)/3 \approx 5.33$	10.00	−4.67
e	$(8.0 + 5.0 + 3.0)/3 \approx 5.33$	9.00	−3.67

On the political scene, some party members are secretly asking themselves whether they disagree more (on average) with the people remaining in the old party than with the splinter group. The politician for whom this difference is largest will be the next to move. In our example the difference is largest for object b, which lies much further from the remaining objects than from the splinter group. Therefore object b changes sides, so the new splinter group is $\{a, b\}$ and the remaining group becomes $\{c, d, e\}$. When we repeat the computations we find

Object	Average Dissimilarity to Remaining Objects	Average Dissimilarity to Objects of Splinter Group	Difference
c	$(4.0 + 5.0)/2 = 4.50$	$(6.0 + 5.0)/2 = 5.50$	−1.00
d	$(4.0 + 3.0)/2 = 3.50$	$(10.0 + 9.0)/2 = 9.50$	−6.00
e	$(5.0 + 3.0)/2 = 4.00$	$(9.0 + 8.0)/2 = 8.50$	−4.50

At this stage, all the differences have become negative. Returning to our political analogy, the remaining party members have more quarrels with the splinter group than with each other. Therefore, no further moves are made. The process stops and we have completed the first divisive step, which splits the data into the clusters $\{a, b\}$ and $\{c, d, e\}$.

In the next step we divide the biggest cluster, that is, the cluster with the largest diameter. (As before, the diameter of a cluster is just the largest dissimilarity between two of its objects.) The diameter of $\{a, b\}$ is 2.0, and for $\{c, d, e\}$ we find 5.0. Therefore, the above procedure will be applied to the cluster $\{c, d, e\}$, with dissimilarity matrix

	c	d	e
c	0.0	4.0	5.0
d	4.0	0.0	3.0
e	5.0	3.0	0.0

To find the rebel to start the splinter group with, we compute

Object	Average Dissimilarity to the Other Objects
c	$(4.0 + 5.0)/2 = 4.50$
d	$(4.0 + 3.0)/2 = 3.50$
e	$(5.0 + 3.0)/2 = 4.00$

and obtain object c. Afterward, we find

Object	Average Dissimilarity to Remaining Objects	Average Dissimilarity to Objects of Splinter Group	Difference
d	3.0	4.00	−1.00
e	3.0	5.00	−2.00

and the process stops because all differences are negative. Therefore, our second step divides $\{c, d, e\}$ into $\{c\}$ and $\{d, e\}$, so we are left with the clusters $\{a, b\}$, $\{c\}$, and $\{d, e\}$. The cluster $\{c\}$ is called a singleton because it contains only one object.

In the third step we must decide which of these clusters to split. Obviously, the singleton $\{c\}$ cannot be divided any further (also note that its diameter is 0). The cluster $\{a, b\}$ has diameter 2 and that of $\{d, e\}$ is 3.

Therefore, we have to divide the cluster $\{d, e\}$ with dissimilarity matrix

$$\begin{array}{c} \\ d \\ e \end{array} \begin{array}{c} \begin{array}{cc} d & e \end{array} \\ \begin{bmatrix} 0.0 & 3.0 \\ 3.0 & 0.0 \end{bmatrix} \end{array}$$

To start the splinter group, we calculate very little:

Object	Average Dissimilarity to the Other Objects
d	3.00
e	3.00

Because the average dissimilarities are the same, we may choose either object to begin the splinter group with. Let us choose object d, so we obtain $\{d\}$ and $\{e\}$. It is clear that object e, being the last remnant, cannot join the splinter group. Therefore, step 3 divides $\{d, e\}$ into the singletons $\{d\}$ and $\{e\}$. (Note that the same result would be obtained if we had picked object e to start the splinter group with.) Step 3 leaves us with four clusters: $\{a, b\}$, $\{c\}$, $\{d\}$, and $\{e\}$.

In the fourth step we have to split up the cluster $\{a, b\}$, because all the others contain only a single object. As in the third step, $\{a, b\}$ is divided into the singletons $\{a\}$ and $\{b\}$. After this fourth step we only have singleton clusters $\{a\}$, $\{b\}$, $\{c\}$, $\{d\}$, and $\{e\}$, so the algorithm stops.

The resulting hierarchy may be displayed as in Figure 1, in which the horizontal axis contains the step number. At step 0 there is still a single

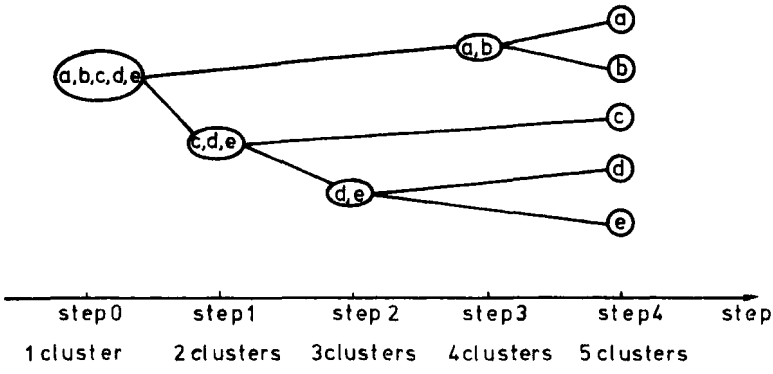


Figure 1 Graphical display of a divisive hierarchy.

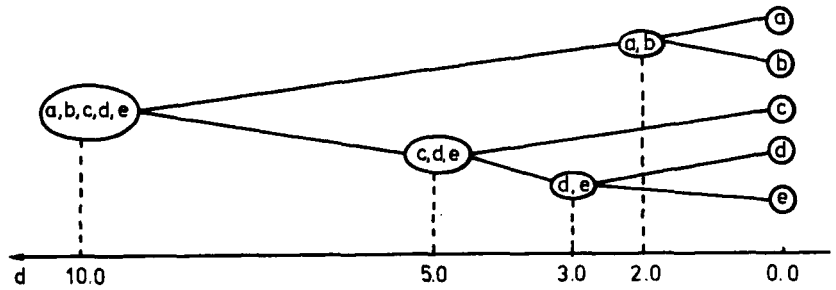


Figure 2 Diagram showing the same hierarchy as in Figure 1, but also displaying the level of each division.

cluster with all the objects, while at step 4 all objects are apart (in this example the objects retain their original ranking, but of course this need not be true in general).

It is possible to construct a more informative version of this diagram. Rather than just displaying the order in which the divisions take place, we could also indicate the diameter of the clusters involved, because we know that the bigger clusters are divided first. For this purpose, in Figure 2 each cluster is plotted versus its diameter. This diameter is a monotone function of the step number, because when a cluster has been split into two subclusters, neither can have a larger diameter than the original one. Also note that everything we have done only depends on the dissimilarity matrix, so the data need not consist of measurements. (When they do consist of measurements, we begin by computing dissimilarities, as will be illustrated in some examples.)

Instead of Figure 2, which was drawn by hand, it is possible to construct a display by means of an ordinary line printer. Figure 3 shows a banner (Rousseeuw, 1986) that contains the same information as Figure 2. At the extreme left (where the flagstaff can be imagined) all objects still stick together and the diameter is 10.0. The first split produces two clusters. The

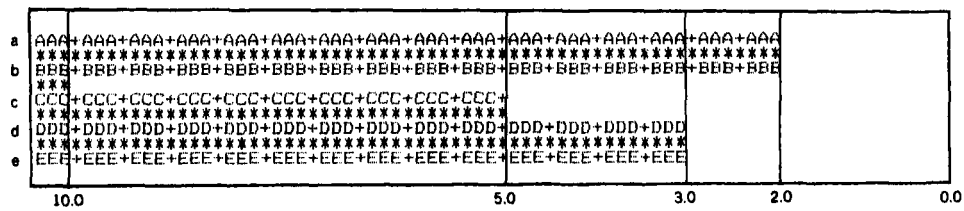


Figure 3 A divisive banner containing the same information as Figure 2.

first cluster is $\{a, b\}$, the objects of which are denoted by the labels *AAA* and *BBB*, and linked by a row of asterisks. The second cluster is $\{c, d, e\}$. Next, $\{c, d, e\}$ is split (at the level 5.0) into $\{c\}$ and $\{d, e\}$. Note that the label *CCC* is no longer continued after that, because $\{c\}$ is a singleton. The third step divides $\{d, e\}$ into $\{d\}$ and $\{e\}$ at the level 3.0 and the last step splits $\{a, b\}$ at the level 2.0.

Note that the representations in Figures 1, 2, and 3 are very similar to those of an agglomerative hierarchy, described in Section 1 of Chapter 5. The main difference is the direction of the algorithm, so the present displays look like mirror images of the previous ones. Also their interpretations are alike. For instance, one may again draw a vertical line through the banner to find the clustering corresponding to a certain level. However, the divisive algorithm is not the *exact* counterpart of the agglomerative one, so in general the resulting hierarchies do not coincide.

2 HOW TO USE THE PROGRAM DIANA

To apply this algorithm we use the program DIANA (from DIvisive ANAlysis), which was combined with the program AGNES described in Chapter 5. Both programs accept the same data sets. To run DIANA, we have to insert the floppy with the file TWINS.EXE in drive *A* and type

A:TWINS

which yields the screen

```
HIERARCHICAL CLUSTERING

DO YOU WANT AGGLOMERATIVE NESTING (AGNES)
OR DIVISIVE ANALYSIS (DIANA) ?
PLEASE ENTER YOUR CHOICE (A OR D) : D
```

By typing *D* we select the divisive algorithm. After that, the remaining input is exactly the same as for AGNES.

When we apply DIANA to the example treated in Section 1, we obtain the output shown in Figure 4. The first part is identical to the corresponding output of AGNES (Figure 6 of Chapter 5), but the cluster results and the banner are different. The program begins by telling us that in the first step the five objects are divided into two objects and three objects. This is useful because the first step of a divisive algorithm is very important. Indeed, the objects separated in the first step will stay apart throughout the

```
                              ***********************
                              *                     *
                              *  DIVISIVE ANALYSIS  *
                              *                     *
                              ***********************

TITLE : Dissimilarities between five objects
DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 THERE ARE    5 OBJECTS
 LABELS OF OBJECTS ARE READ
 INPUT OF DISSIMILARITIES
 LARGE OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (BANNER)
 THE DISSIMILARITIES WILL BE READ IN FREE FORMAT
 YOUR DATA RESIDE ON FILE       : a:example.dat


DISSIMILARITY MATRIX
--------------------

AAA
BBB        2.00
CCC        6.00      5.00
DDD       10.00      9.00      4.00
EEE        9.00      8.00      5.00      3.00


CLUSTER RESULTS
---------------

AT THE FIRST STEP THE   5 OBJECTS ARE DIVIDED INTO
     2 OBJECTS AND   3 OBJECTS

THE FINAL ORDERING OF THE OBJECTS IS

       1              2              3              4              5

THE DIAMETERS OF THE CLUSTERS ARE

            2.000          10.000          5.000          3.000


                                    ************
                                    *          *
                                    *  BANNER  *
                                    *          *
                                    ************

  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .
  0  9  9  8  8  8  7  7  6  6  6  5  5  4  4  4  3  3  2  2  2  1  1  0  0  0
  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0

AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA
***************************************************************
BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB
***
CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+
****************************************
DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD
*******************************************************
EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE

  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .
  0  9  9  8  8  8  7  7  6  6  6  5  5  4  4  4  3  3  2  2  2  1  1  0  0  0
  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0

THE ACTUAL DIAMETER OF THIS DATA SET IS          10.0000000000

THE DIVISIVE COEFFICIENT OF THIS DATA SET IS    .70

THE OUTPUT IS WRITTEN ON FILE : a:example.dia
```

Figure 4 DIANA output for the example of Section 1.

hierarchy, in which both clusters are divided further. We can easily identify the clusters found in the initial step because they consist of the first two and the last three objects in the "final ordering of the objects" list. The diameters of the clusters are listed below this ordering.

The final ordering and the diameters were already encountered in Figure 2. In fact, these two sequences of numbers together characterize the whole hierarchy. In this example, they are

1	2	3	4	5
2.0	10.0	5.0	3.0	

In the bottom row we first look up the largest diameter, 10.0, which stands

```
**********************
*                    *
*  DIVISIVE ANALYSIS *
*                    *
**********************

TITLE : Data set of Table 1 of Chapter 5

DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 THERE ARE     7 OBJECTS
 LABELS OF OBJECTS ARE NOT READ
 INPUT OF MEASUREMENTS
 LARGE OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (BANNER)

 THERE ARE     2 VARIABLES IN THE DATA SET,
  AND     2 OF THEM WILL BE USED IN THE ANALYSIS
 THE LABELS OF THESE VARIABLES ARE :
        x
        y
 THE MEASUREMENTS WILL NOT BE STANDARDIZED
 EUCLIDEAN DISTANCE IS USED
 THERE ARE NO MISSING VALUES
 THE MEASUREMENTS WILL BE READ IN FREE FORMAT

 YOUR DATA RESIDE ON FILE        : a:seven.dat

DISSIMILARITY MATRIX
--------------------

001
002       4.03
003       4.24      1.12
004        .71      4.27      4.30
005       1.41      5.41      5.66      1.58
006       5.83      1.80      2.00      6.04      7.21
007       5.86      2.51      1.68      5.84      7.27      1.95

CLUSTER RESULTS
---------------

AT THE FIRST STEP THE    7 OBJECTS ARE DIVIDED INTO
     3 OBJECTS AND    4 OBJECTS

THE FINAL ORDERING OF THE OBJECTS IS

      1                 4                 5                 2                 3
      6                 7

THE DIAMETERS OF THE CLUSTERS ARE

            .707              1.581             7.267             1.118             2.000
          2.512
```

Figure 5 DIANA output for the data in Table 1 of Chapter 5.

between two numbers of the upper row. This means that the whole data set will be split at the level 10.0, yielding a cluster with the objects 1 and 2 (standing to the left of 10.0) and a cluster with the objects 3, 4, and 5 (standing to the right of 10.0). The second largest diameter is 5.0, indicating that $\{3,4,5\}$ is to be split into $\{3\}$ and $\{4,5\}$ at that level. Continuing in this way, one can immediately reconstruct Figure 2.

The last part of the output is the banner that we already saw in Figure 3. It looks like the agglomerative banner in the AGNES output, but it floats in the opposite direction. Also the scales that surround it are plotted differently because they *decrease* from 1.00 to 0.00. Here, 0.00 indicates a zero diameter (corresponding to singletons) and 1.00 stands for the actual diameter of the data set (which is printed immediately below the banner). Again the overall width of the banner reflects the strength of the clustering: A very pronounced structure implies that the diameter of the entire data set is much larger than the diameters of the individual clusters, leading to a wide banner. As in the case of agglomerative nesting, we may summarize the blackness of the banner in a coefficient. For each object i we measure the length $l(i)$ of its line in the banner, with respect to the normalized scale. Therefore all $l(i)$ lie between 0 and 1, so the same holds for the *divisive*

```
                              ************
                              *          *
                              *  BANNER  *
                              *          *
                              ************

 1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .
 0  9  9  8  8  8  7  7  6  6  6  5  5  4  4  4  3  3  2  2  2  1  1  0  0  0
 0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0

001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+001+00
**********************************************************************
004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+004+00
************************************************************
005+005+005+005+005+005+005+005+005+005+005+005+005+005+005+0
***
002+002+002+002+002+002+002+002+002+002+002+002+002+002+002+002+00
******************************************************************
003+003+003+003+003+003+003+003+003+003+003+003+003+003+003+003+00
************************************************************
006+006+006+006+006+006+006+006+006+006+006+006+006+006+0
*****************************************************
007+007+007+007+007+007+007+007+007+007+007+007+007+

 1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .  .
 0  9  9  8  8  8  7  7  6  6  6  5  5  4  4  4  3  3  2  2  2  1  1  0  0  0
 0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0


THE ACTUAL DIAMETER OF THIS DATA SET IS               7.2672210000

THE DIVISIVE COEFFICIENT OF THIS DATA SET IS     .81

THE OUTPUT IS WRITTEN ON FILE : a:seven.dia
```

Figure 5 (*Continued*)

coefficient (DC) defined by

$$\mathrm{DC} = \frac{1}{n} \sum_{i=1}^{n} l(i) \tag{3}$$

The DC can be seen as the average width of the divisive banner, so it is the counterpart of the agglomerative coefficient (AC) defined in Section 2 of Chapter 5. Also the DC does not change when all the original dissimilarities are multiplied by a constant factor, nor does it depend on the ordering of the objects in the banner [because the $l(i)$ only depend on the actual hierarchy]. In Figure 4, the DC equals 0.70, which is quite good.

Of course, DIANA can also deal with data consisting of interval-scaled measurements. To illustrate this, we analyze the data listed in Table 1 of Chapter 5. When running DIANA, we specify that there are seven objects and two variables, which we decide not to standardize. We also instruct the program to compute Euclidean distances. Figure 5 contains the resulting output, which again looks very similar to the corresponding AGNES output in Figure 7 of Chapter 5. In the first (and most important) step, the data are split up into the clusters $\{1, 4, 5\}$ and $\{2, 3, 6, 7\}$, as could be anticipated from the scatterplot (Figure 1 of Chapter 5). The second largest value in the "diameters of the clusters" list is 2.512, so $\{2, 3, 6, 7\}$ is divided into $\{2, 3, 6\}$ and $\{7\}$ in the second step (note that all these diameters are dissimilarities between two objects, so they can always be traced back in the dissimilarity matrix). Because the diameter of the entire data set (7.267) is much larger than those of the clusters, the banner becomes rather wide, yielding a DC of 0.81. The ordering of the objects in the banner corresponds to that in Figure 7 of Chapter 5. This is partly due to the particular implementation of AGNES and DIANA, because in all our programs we have strived to modify the original ordering as little as possible to enable the user to compare the results of different methods.

3 EXAMPLES

Let us look at some examples to gain a better insight into the divisive approach. Applying DIANA to the 12 countries data in Table 5 of Chapter 2 yields Figure 6. (The first part of the output is identical to that produced by AGNES, so only the second part is shown here.) The first step divides the 12 objects into the clusters {BEL, FRA, USA, ISR, BRA, ZAI, EGY, IND} and {CHI, CUB, USS, YUG}, which means that the Communist countries are split off first. In the second step, the remainder

```
CLUSTER RESULTS
---------------

AT THE FIRST STEP THE  12 OBJECTS ARE DIVIDED INTO
     8 OBJECTS AND    4 OBJECTS

THE FINAL ORDERING OF THE OBJECTS IS

      1               6               9               8               2
     12               5               7               3               4
     10              11

THE DIAMETERS OF THE CLUSTERS ARE

          2.170           2.500           3.920           6.420           3.000
          5.080           4.670           8.170           4.500           2.670
          3.750

                          ************
                          *          *
                          *  BANNER  *
                          *          *
                          ************

  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  0  9  9  8  8  8  7  7  6  6  6  5  5  4  4  4  3  3  2  2  2  1  1  0  0  0
  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0

BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BEL+BE
**********************************************************
FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FRA+FR
**********************************************************
USA+USA+USA+USA+USA+USA+USA+USA+USA+USA+USA+USA+USA+USA
**************************************************
ISR+ISR+ISR+ISR+ISR+ISR+ISR+ISR+ISR+ISR+IS
******************************************
BRA+BRA+BRA+BRA+BRA+BRA+BRA+BRA+BRA+BRA+BRA+BRA+BR
**************************************************
ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZAI+ZA
**********************************************
EGY+EGY+EGY+EGY+EGY+EGY+EGY+EGY+EGY
**********************************
IND+IND+IND+IND+IND+IND+IND+IND
*******************************
CHI+CHI+CHI+CHI+CHI+CHI+CHI+CHI+CHI+
*************************************
CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB+CUB+C
******************************************************
USS+USS+USS+USS+USS+USS+USS+USS+USS+USS+USS+USS+USS+U
******************************************************
YUG+YUG+YUG+YUG+YUG+YUG+YUG+YUG+YUG+YUG+YUG

  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  0  9  9  8  8  8  7  7  6  6  6  5  5  4  4  4  3  3  2  2  2  1  1  0  0  0
  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0  6  2  8  4  0

THE ACTUAL DIAMETER OF THIS DATA SET IS                8.1700000000

THE DIVISIVE COEFFICIENT OF THIS DATA SET IS     .60

THE OUTPUT IS WRITTEN ON FILE : a:country.dia
```

Figure 6 Output of DIANA for the 12 countries data.

is divided into {BEL, FRA, USA, ISR}, the Western countries, and {BRA, ZAI, EGY, IND}, the developing ones. (This may be seen from the cluster results or from the banner.) As usual, the most important information is provided by the first few steps of the divisive algorithm.

This clustering of the 12 countries is very similar to the results we obtained in previous chapters by means of PAM, FANNY, and AGNES.

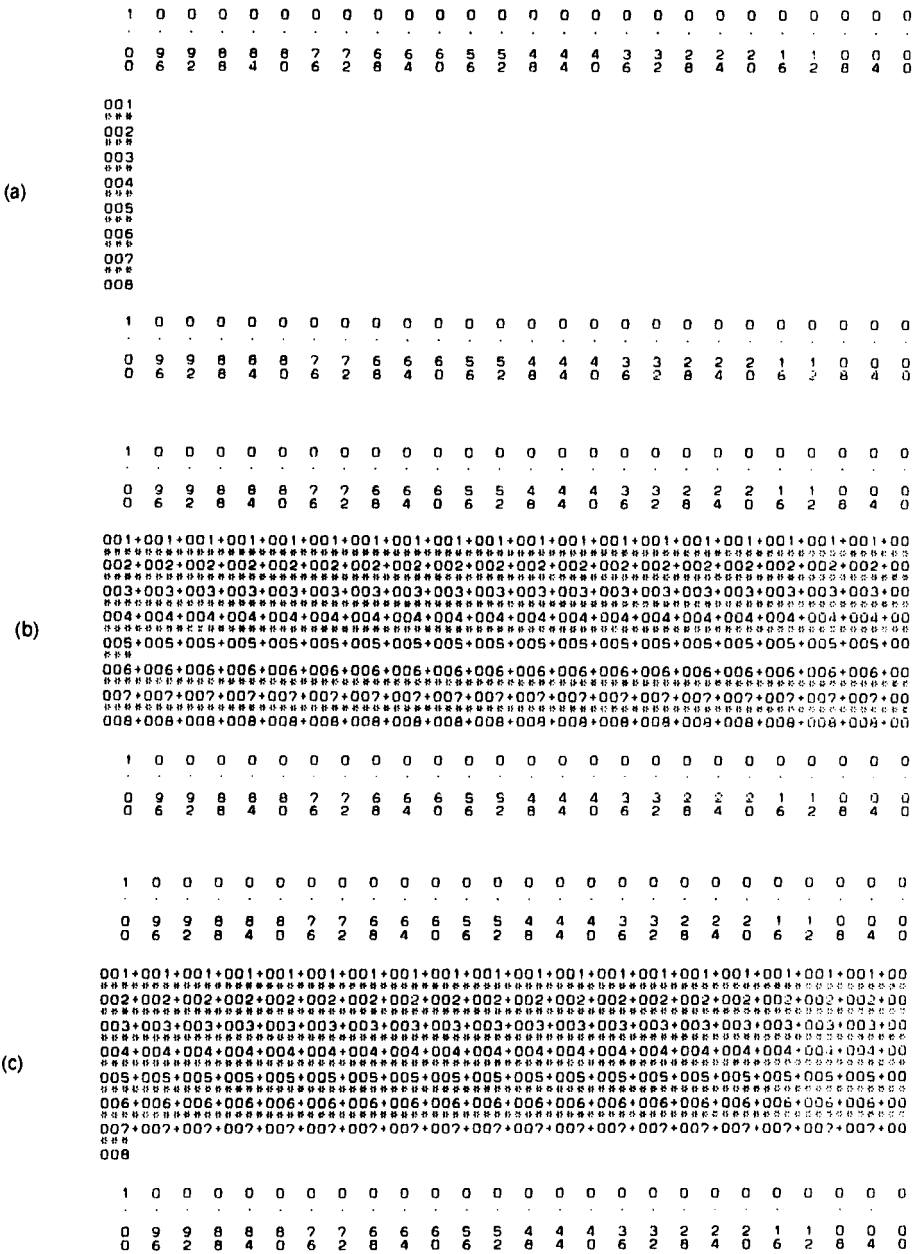


Figure 7 Divisive banners of some extreme examples, with (a) no clustering structure, (b) two very tight clusters, and (c) one distant outlier.

Table 1 Logarithmic Surface Temperature (x) and Logarithmic Light Intensity (y) of 47 Stars

i	x_i	y_i
1	4.37	5.23
2	4.56	5.74
3	4.26	4.93
4	4.56	5.74
5	4.30	5.19
6	4.46	5.46
7	3.84	4.65
8	4.57	5.27
9	4.26	5.57
10	4.37	5.12
11	3.49	5.73
12	4.43	5.45
13	4.48	5.42
14	4.01	4.05
15	4.29	4.26
16	4.42	4.58
17	4.23	3.94
18	4.42	4.18
19	4.23	4.18
20	3.49	5.89
21	4.29	4.38
22	4.29	4.22
23	4.42	4.42
24	4.49	4.85
25	4.38	5.02
26	4.42	4.66
27	4.29	4.66
28	4.38	4.90
29	4.22	4.39
30	3.48	6.05
31	4.38	4.42
32	4.56	5.10
33	4.45	5.22
34	3.49	6.29
35	4.23	4.34
36	4.62	5.62
37	4.53	5.10
38	4.45	5.22
39	4.53	5.18
40	4.43	5.57
41	4.38	4.62
42	4.45	5.06

Table 1 (*Continued*)

i	x_i	y_i
43	4.50	5.34
44	4.45	5.34
45	4.55	5.54
46	4.45	4.98
47	4.42	4.50

Source: Rousseeuw and Leroy (1987).

The main features are found in all four analyses. The DC = 0.60, so it is somewhat larger than the AC, as is often the case.

To illustrate the interpretation of the divisive banner and the DC, we turn to the same extreme examples that were considered in Section 3 of the preceding chapter. Figure 7a is the banner of the situation where all dissimilarities between objects equal the same positive constant. It clearly tells us that the data have no clustering structure, hence the DC is 0. Figure 7b corresponds to two very tight and well-separated clusters, yielding the widest possible banner with DC = 1.00. When the data contain an extreme outlier, we obtain the banner in Figure 7c, with DC = $1 - 1/n \approx 0.88$. All

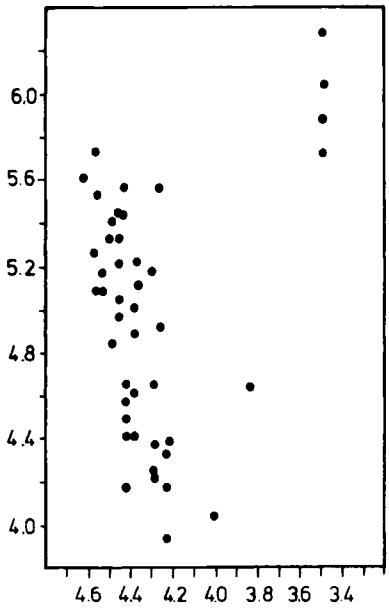


Figure 8 Scatterplot of the data in Table 1.

three banners are mirror images of those produced by AGNES, so the results of both hierarchical methods are consistent with each other.

The data in Table 1 are about the star group denoted by CYG OB1, which consists of 47 stars in the direction of Cygnus. This set of real data was given to us by C. Doom (personal communication). The variable x stands for the logarithm of the star's surface temperature (as measured from its spectrum) and y is the logarithm of its light intensity. In astronomy it is common practice to draw the so-called Hertzsprung–Russell diagram (Figure 8), which is simply a scatterplot of y versus x (but note that x is plotted from right to left).

In Figure 8, our eyes see two rather distinct clusters. Most of the points lie close to a steep band, whereas four points sit in the upper right corner of the plot. These regions of the Hertzsprung–Russell diagram are well known: The 43 stars belong to the so-called main sequence, whereas the four remaining ones (numbers 11, 20, 30, and 34) are giant stars. Running DIANA yields the banner of Figure 9, in which the first step does distinguish the main sequence from the giants. In subsequent steps the algorithm then splits up both clusters until all points are isolated. Also when the data are standardized, DIANA finds the "right" clusters in the first step. By means of AGNES we obtain a similar (though reversed) picture. Note that this example is not easy, because the first cluster is much larger and contains many more objects than the second, from which it is not clearly separated. For this reason, many algorithms have difficulties with these data. For instance, PAM yields two other clusters when $k = 2$, but it does isolate the giants for $k = 3$. One may also apply a totally different approach: Because the largest cluster (the main sequence) is nearly linear, it may be identified by means of a robust regression technique, as done by Rousseeuw and Leroy (1987, p. 28) who apply the least median of squares method of Rousseeuw (1984).

Our last example is the data set of Ruspini (Table 6 of Chapter 2) that was already analyzed in Chapters 2 and 4. In the scatterplot (Figure 12 of Chapter 2) four natural groups were indicated, namely $A = \{1, \ldots, 20\}$, $B = \{21, \ldots, 43\}$, $C = \{44, \ldots, 60\}$, and $D = \{61, \ldots, 75\}$. When we apply DIANA we obtain the banner of Figure 10. In the first step, the data are divided into $A \cup D$ on the one hand and $B \cup C$ on the other. In step 2 the cluster $A \cup D$ is split into A and D, and in step 3 also $B \cup C$ is divided into B and C. In step 4 the trio $\{46, 47, 48\}$ is taken out of C, whereas step 5 bisects A (but note that steps 4 and 5 occur at a much lower level, so it would seem reasonable to stop after step 3). This whole process corresponds exactly to the partitions obtained by PAM for 2, 3, 4, 5, and 6 clusters, the silhouettes of which are shown in Figure 13 of Chapter 2. Apparently the natural structure is sufficiently clear-cut to be uncovered by very different clustering algorithms.

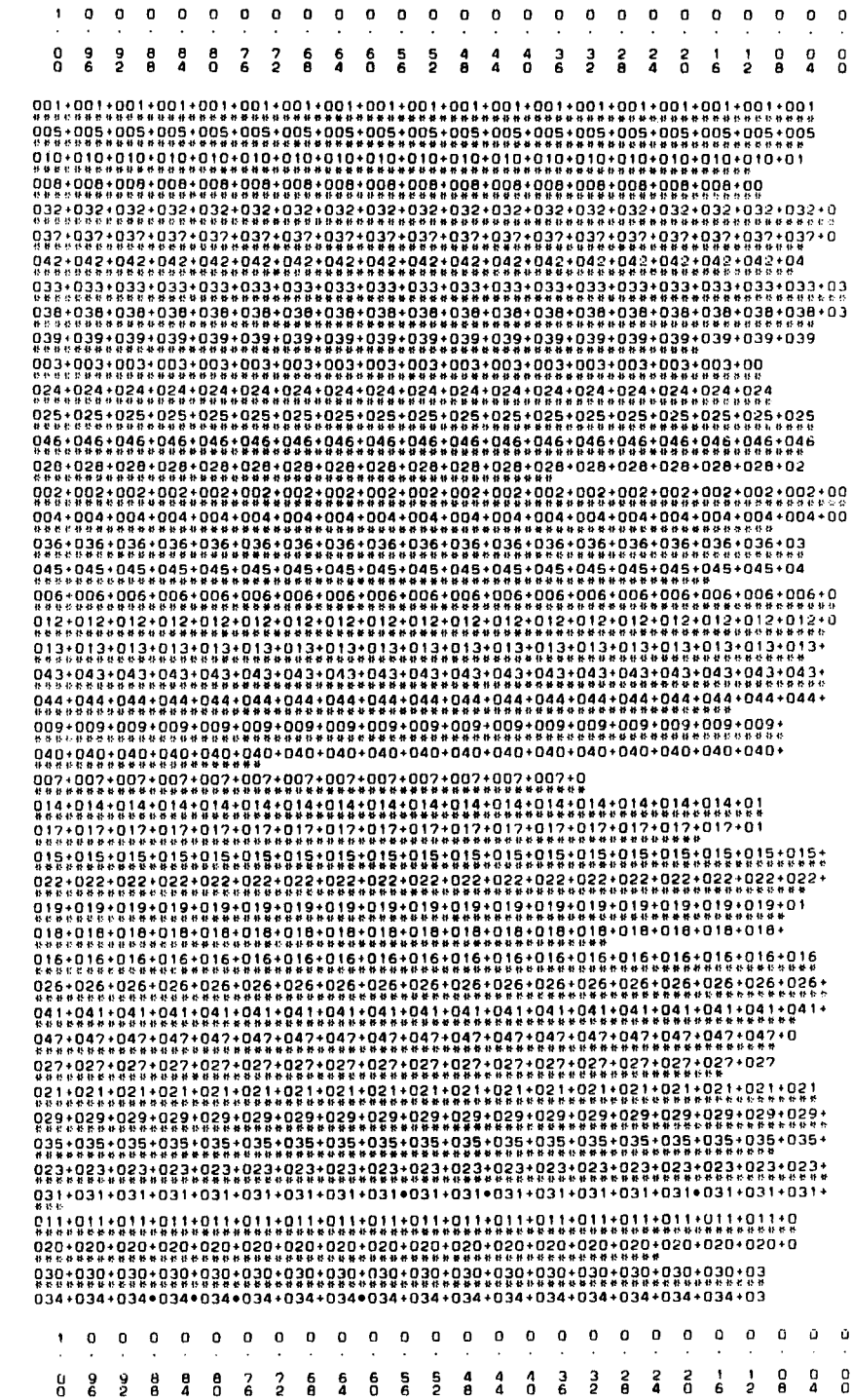


Figure 9 Divisive banner of the data in Table 1.

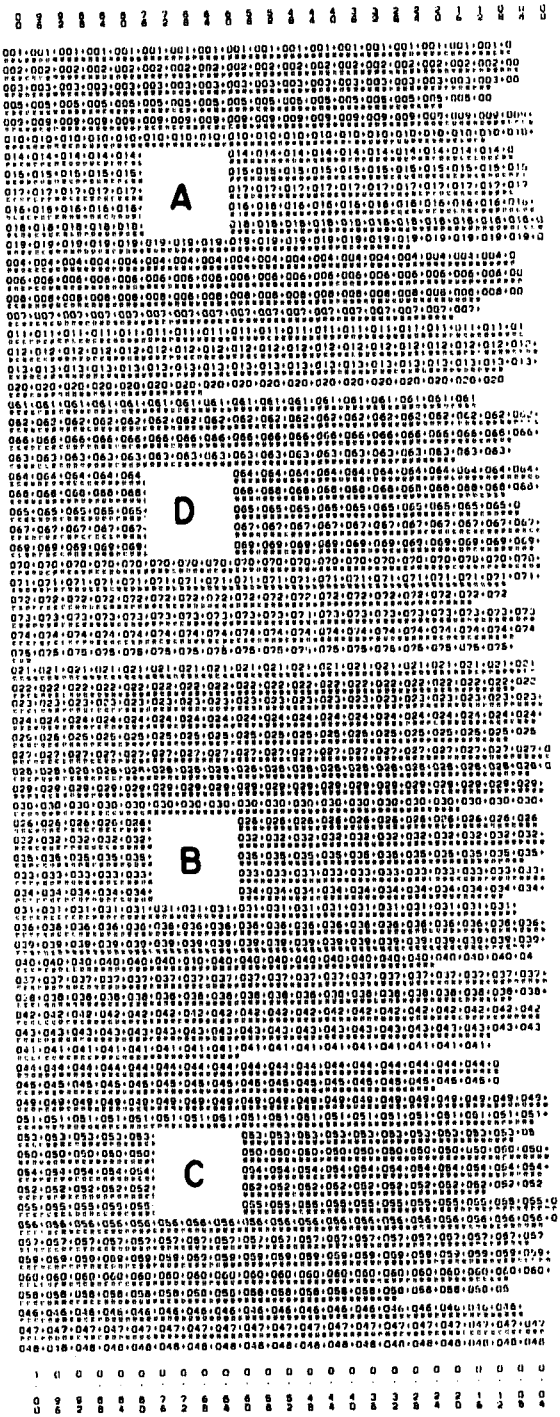


Figure 10 Divisive banner of the Ruspini data.

*4 MORE ON THE ALGORITHM AND THE PROGRAM

4.1 Description of the Algorithm

A divisive analysis proceeds by a series of successive splits. At step 0 (before starting the algorithm) all objects are together in a single cluster. At each step a cluster is divided, until at step $n - 1$ all objects are apart (forming n clusters, each with a single object).

Each step divides a cluster, let us call it R, into two clusters A and B. This is done according to the iterative method of Macnaughton-Smith et al. (1964) that was illustrated in Section 1. Initially, A equals R and B is empty. In a first stage, we have to move one object from A to B. (Naturally, it is assumed here that A contains more than one object, or there is nothing to split.) For each object i of A, we compute the average dissimilarity to all other objects of A:

$$d(i, A \setminus \{i\}) = \frac{1}{|A| - 1} \sum_{\substack{j \in A \\ j \neq i}} d(i, j) \tag{4}$$

The object i' for which (4) attains its maximal value will be moved, so we put

$$\begin{aligned} A_{\text{new}} &= A_{\text{old}} \setminus \{i'\} \\ B_{\text{new}} &= B_{\text{old}} \cup \{i'\} \end{aligned} \tag{5}$$

In the next stages, we look for other points to move from A to B. As long as A still contains more than one object, we compute

$$d(i, A \setminus \{i\}) - d(i, B) = \frac{1}{|A| - 1} \sum_{\substack{j \in A \\ j \neq i}} d(i, j) - \frac{1}{|B|} \sum_{h \in B} d(i, h) \tag{6}$$

for each object i of A and we consider the object i'' that maximizes this quantity. When the maximal value of (6) is strictly positive, we move i'' from A to B as in (5) and then look in the new A for another object that might be moved. On the other hand, when the maximal value of (6) is negative or 0 we stop the process and the division of R into A and B is completed.

At each step of the divisive algorithm we also have to decide which cluster to split. For this purpose we compute the diameter

$$\operatorname{diam}(Q) = \max_{\substack{j \in Q \\ h \in Q}} d(j, h) \tag{7}$$

for each cluster Q that is available after the previous step, and choose the cluster for which (7) is largest. This value of (7) is also used as the level for representing the division of Q in the banner. We can do this because (7) is *monotone*:

$$A \subset R \quad \text{implies} \quad \text{diam}(A) \leq \text{diam}(R) \tag{8}$$

from which it follows that the levels of the successive steps form a nonincreasing sequence.

4.2 Structure of the Program

A list of subroutines and functions of the program TWINS was already given in Section 4.2 of Chapter 5. When we ask the program to perform a divisive analysis, the subroutines AVERL and BANAG (corresponding to agglomerative nesting) are no longer used, but instead SPLYT, SUPCL, and BANDY are activated.

The subroutine SPLYT divides a cluster by means of (4) to (6), except when the cluster has only two objects, because it can then be split without these computations. At each step the array NER, which contains the ordering of the objects, is updated in such a way as to disturb the original ranking as little as possible. (This implies that the splinter group B may either be listed as the first or as the second subcluster, depending on the situation.) The diameter (7) of a cluster is computed in subroutine SUPCL and afterward stored in the array BAN, which is updated accordingly. When the algorithm is finished, the numbers in NER ("final ordering of the objects") and BAN ("diameters of the clusters") are printed. Finally, the subroutine BANDY combines the arrays BAN and NER to draw the banner of the divisive hierarchy.

Table 2 lists some computation times for various values of n. In order to compare the speed of DIANA with that of AGNES, we used the same data

Table 2 Computation Times of DIANA (in minutes on an IBM-XT with 8087 coprocessor) for Increasing Numbers of Objects

Objects	Variables	Time
20	2	0.20
40	2	0.60
60	2	1.50
80	2	3.45
100	2	6.65

as in Table 2 of Chapter 5. It turns out that DIANA consumes about twice as much time as AGNES, which is perfectly feasible. In fact, DIANA is still faster than the nonhierarchical algorithms of Chapters 2 and 4, because a single run of DIANA yields partitions for all $k = 1, 2, \ldots, n$.

*5 RELATED METHODS AND REFERENCES

5.1 Variants of the Selected Method

In their very concise article, Macnaughton-Smith et al. (1964) describe how a cluster may be split in two by means of (4) to (6). Instead of (4), they also consider other measures of dissimilarity between clusters, particularly for binary data. They argue that divisive methods are safer than agglomerative ones, because "wrong" decisions in the early stages of an agglomerative analysis cannot be corrected later on, and one is mostly interested in the large clusters. Also, they note that it is infeasible to consider all possible divisions, of which there are $2^{n-1} - 1$. One could, of course, restrict attention to *monothetic* methods, that make each split according to a single variable, whereas *polythetic* methods use all variables simultaneously. (Our own point of view is to give preference to methods that only depend on interobject distances or dissimilarities, such as the algorithms of Chapters 2, 4, 5, and 6. Such methods are necessarily polythetic.) The method of Macnaughton-Smith et al. combines the three advantages of being divisive rather than agglomerative, polythetic rather than monothetic, and computationally manageable even for large n. To demonstrate the latter property, Rousseeuw (1983b) implemented this technique on an Apple II microcomputer in a way to minimize the use of memory. The implementation in DIANA takes somewhat more memory but less computation time.

Lance and Williams (1966a) investigated the computational complexity of several hierarchical methods. They found that the number of operations needed for the first step of the Macnaughton-Smith technique varies with the evenness of the division it produces. When the data set is divided into two clusters with n' and $n - n'$ objects, the number of operations was $(n' + 1)(2n - 1) - n$. In the worst case, when $n' = n/2$, this is of the order of n^2. In the best case, when $n' = 1$, it reduces to $3n - 2$. Therefore, the actual computation time depends on the course of the analysis, as in many iterative methods (such as our programs PAM and FANNY). But at any rate, the worst-case computation time of the Macnaughton-Smith technique remains feasible.

In order to reduce the amount of computation, Macnaughton-Smith et al. (1964) also considered the following variant of their procedure.

Provided that $d(i, A \setminus \{i\}) - d(i, B) > 0$, they chose the object i minimizing $d(i, B)$ instead of maximizing (6). It seems that this version might lead to a good internal cohesion in the splinter group B, but maybe not in the remaining cluster A.

Another variant that we might think of would be to start as in (4) and (5), and at each following stage move the object i that maximizes the group average dissimilarity

$$d(A \setminus \{i\}, B \cup \{i\}) \tag{9}$$

A possible stopping rule would be to halt the process as soon as $d(A_{\text{new}}, B_{\text{new}})$ no longer increases. Note that this procedure is internally consistent, because (4) is a special case of (9). Unfortunately, it takes somewhat more computation time than the Macnaughton-Smith method.

Chandon and Pinson (1981, p. 122) go even further when they propose to divide the data into any clusters A and B maximizing $d(A, B)$. This is a complete enumeration approach in which all $2^{n-1} - 1$ possible divisions must be considered, making the method extremely time-consuming [although much more elegant from a theoretical point of view, because it is dual to the group average method described in Chapter 5, in which $d(A, B)$ is minimized at each agglomerative step].

It appears that divisive clustering is only computationally feasible when performed in some iterative way. However, one aspect of the Macnaughton-Smith technique one might object to is its asymmetric treatment of the two clusters A and B, one of which arises as a splinter group whereas the other may be a rather loose collection of remaining objects. Therefore, one may prefer to grow the clusters from *two* kernel objects, instead of the single object i determined in (4). One proposal (Hubert, 1973, p. 51) would be to start with the objects i and j with the largest interobject dissimilarity $d(i, j)$. Afterward one could assign the remaining objects to i or j, whichever is nearer, or apply an iterative procedure in which the objects are assigned one at a time, taking into account their average dissimilarities to the clusters being formed. The main problem with this method appears to be its lack of robustness, as both i and j may be outliers.

A more robust approach would be to begin with two objects i and j that are centrally located in the clusters they determine. For instance, one might select i and j so as to maximize $d(A, B)$ where A contains all objects that are nearer to i than to j and B contains all objects that are nearer to j than to i. Note that this is similar to the k-medoid partition (for $k = 2$) described in Chapter 2. Indeed, one could also carry out a 2-medoid

clustering at each step and obtain another divisive hierarchy. However, these methods would also require more computation time.

Until now, we have only discussed *how* to split up a cluster. In the original method of Macnaughton-Smith et al. (1964) this was sufficient because at each step they split all available clusters. However, in our concept of a divisive hierarchy we want to split one cluster at a time, so we also need to know *which* cluster to split next. Leaving aside trivial solutions (such as making an arbitrary choice or splitting the cluster with the largest number of objects) this begs for the definition of a *level*. For instance, one may use a dispersion measure of the cluster to be split, or a kind of average dissimilarity between the two subclusters. Such a level must be meaningful (in relation to the interobject dissimilarities) and *monotone*, which means that neither subcluster may have a larger level than the original one. For some of the divisive methods sketched above the choice of a level is quite natural, but for the Macnaughton-Smith technique it is not so simple. We have tried out many definitions, but most of them were not monotone in all data sets (sometimes monotonicity could be proved for the splinter group but not for the remaining subcluster). This left us with the diameter, which is always monotone by (8) but not very satisfactory otherwise because of its sensitivity to outliers and its lack of consistency when n goes to infinity.

The program DIANA uses diameters for displaying the divisive hierarchy (as we did in Figures 2 and 3), which is better than just plotting the number of the divisive step (as in Figure 1) because it may happen that two clusters are split at the same level, in which case their step number would be arbitrary. Moreover, the step number always ranges from 1 to $n - 1$, so it does not reflect the particular clustering structure of the data. When a continuous level is plotted, the user may notice when a data set has been split into two clusters with much smaller levels than the original one (as in Figure 7b), leading to a wide banner and thus a large DC, whereas a banner merely displaying the step number would not have revealed the strength of the clustering structure.

The graphical displays that were considered in Section 5.3 of Chapter 5, such as those of Ward and Johnson as well as icicle plots and dendrograms, may also be used to describe a divisive hierarchy. It suffices to draw these displays in the inverse direction. Note that the DC does not depend on the type of display or the ranking of the objects in it.

5.2 Other Divisive Techniques

The methods reviewed in Section 5.1 only needed a matrix of distances or dissimilarities between the objects. Some other divisive methods are more

restrictive, in that they need a matrix of objects by variables. In this subsection we discuss some polythetic divisive methods, whereas monothetic divisive methods will be treated in Chapter 7.

The most well-known polythetic divisive method is that of Edwards and Cavalli-Sforza (1965). It assumes that the n objects are characterized by p interval-scaled variables. It is basically a least squares (L_2) method, just like minimum variance partitioning (Section 5.3 of Chapter 2) and Ward's agglomerative method (Section 5.2 of Chapter 5). Everything is based on the error sum of squares

$$\mathrm{ESS}(R) = \sum_{i \in R} \| x_i - \bar{x}(R) \|^2 \tag{10}$$

where $\bar{x}(R)$ is the centroid of the cluster R, with coordinates

$$\bar{x}_f(R) = \frac{1}{|R|} \sum_{i \in R} x_{if} \quad \text{for } f = 1, \ldots, p$$

Edwards and Cavalli-Sforza divide the cluster R into two subclusters A and B in such a way that the objective function

$$\mathrm{ESS}(A) + \mathrm{ESS}(B) \tag{11}$$

is minimized. In Section 5.2 of Chapter 5 [between (23) and (24), in connection with Ward's method] we proved that

$$\mathrm{ESS}(R) = \mathrm{ESS}(A) + \mathrm{ESS}(B) + \frac{|A||B|}{|R|} \| \bar{x}(A) - \bar{x}(B) \|^2$$

This means that the total sum of squares $\mathrm{ESS}(R)$ can be written as the *within* sum of squares $\mathrm{ESS}(A) + \mathrm{ESS}(B)$ plus the *between* sum of squares

$$\frac{|A||B|}{|R|} \| \bar{x}(A) - \bar{x}(B) \|^2 \tag{12}$$

Therefore, minimizing (11) is equivalent to maximizing (12), and the latter objective function is somewhat easier to compute. Unfortunately, the method of Edwards and Cavalli-Sforza still imposes a computational burden because *all* possible divisions of R into some clusters A and B must be tried out. A simplified sequential algorithm was announced, but not described. Such an approximate algorithm was, however, proposed by Gower (1967, p. 632). Gower advised against the exhaustive method of Edwards

and Cavalli-Sforza because it is computationally impracticable and because the centroid is not always a desirable measure of the location of a cluster. When comparing this method with agglomerative nesting and a monothetic divisive method, he recommended the agglomerative technique. Also Lance and Williams (1966a) dismissed the method of Edwards and Cavalli-Sforza because of the large number of dichotomous choices that would have to be examined. Steinhausen and Langer (1977, p. 100) decided not to pursue such divisive methods, because they consume more computation time than agglomerative methods and at the same time yield less satisfactory results than partitioning techniques. Roux (1985, pp. 86–87) independently rediscovered the Edwards and Cavalli-Sforza criterion (12) and proposed another heuristic algorithm yielding an approximate solution.

Edwards and Cavalli-Sforza split all available clusters at each step. MacQueen (1967) proposed a variant of this method in which at each step only the cluster with the largest error sum of squares (10) is divided, so that there are again $n - 1$ steps. This algorithm may be considered as a divisive counterpart to Ward's agglomerative method. Instead of making the splits by total enumeration, it is also possible to apply the k-means algorithm (Section 5.3 of Chapter 2) with $k = 2$ to find approximate solutions for some or all steps.

The reasons why we did not select any of these variance minimization techniques are similar to our objections to k-means clustering and Ward's method. First of all, we prefer clustering techniques that only need a collection of dissimilarities because measurements are not always available, and second, methods based on sums of squares are generally nonrobust to the presence of outliers.

EXERCISES AND PROBLEMS

1. Draw a diagram as in Figure 2 for the divisive clustering of the countries in Section 3.

2. Show that for a three object cluster, the final splinter group consists of the object for which the average dissimilarity to the other two objects is maximal.

3. Run DIANA again on the 47 stars in Table 1, but select the option to standardize the data first.

4. Apply DIANA to the nine diseases in Figure 12 of Chapter 5, and compare the results with those of AGNES.

5. Apply DIANA to cluster the 11 sciences in Table 6 of Chapter 1. Compare the results with those obtained by running AGNES.

6. Run DIANA to cluster the objects of the artificial data set of Figure 1 in Chapter 4. (The actual data are listed in Section 2.1 of that chapter.) Do not standardize the measurements, and use Euclidean distance. What does DIANA do with the intermediate objects 6 and 13?

7. As suggested in Section 5.1, splitting a cluster into two subclusters could be done with the program PAM. (Note that for $k = 2$ the algorithm in PAM is exact, so this approach should lead to a tight clustering.) Apply this method (repeatedly!) to the dissimilarity matrix in Section 1 and compare the results with those of DIANA.

8. Often agglomerative and divisive algorithms yield similar clustering results. To show that this is not always the case, consider the following bivariate data set with 18 points:

$$\begin{array}{cccccccccc} (0,0) & (0,2) & (0,4) & (2,0) & (2,2) & (2,4) & (4,0) & (4,2) & (4,4) \\ (5,5) & (5,7) & (5,9) & (7,5) & (7,7) & (7,9) & (9,5) & (9,7) & (9,9) \end{array}$$

   (a) Make a scatterplot of this data set.
   (b) Use both the agglomerative and divisive options of the program TWINS to cluster the data.
   (c) Indicate on the plot the clusterings into two clusters, obtained with both methods.

9. (a) Apply DIANA to the bacteria data in Exercise 1 of Chapter 2. Does the clustering into two clusters correspond to the result of PAM?
   (b) When a data set consists of two L^*-clusters (in the sense of Section 2.2 of Chapter 2) show that DIANA always recovers these groups. (Note that AGNES also finds the same groups by Exercise 6 of Chapter 5.)

10. Show that the number of possible partitions of n objects into two nonempty subsets is $2^{n-1} - 1$ (either directly, or by means of binomial coefficients, or as a special case of Stirling's result for a general number of subsets).

11. At each step of the algorithm, a cluster R is split into two subclusters A and B. The level of this division is presently defined as the diameter of R, which is monotone in the sense that the diameters of A and B are smaller than that of R. One could think of several alternative definitions of a level, to be used with the same splitting method. Show that the following variants, although intuitively appealing, are not always monotone:

(a) $$\operatorname*{average}_{\substack{i,\, j \in R \\ i \neq j}} d(i, j)$$

(b) $$\max_{i \in R} \operatorname*{average}_{\substack{j \in R \\ j \neq i}} d(i, j)$$

(c) $$\operatorname*{average}_{\substack{i \in A \\ j \in B}} d(i, j)$$

Finding Groups in Data: An Introduction to Cluster Analysis
Leonard Kaufman and Peter J. Rousseeuw

CHAPTER 7

Monothetic Analysis (Program MONA)

1 SHORT DESCRIPTION OF THE METHOD

In the social sciences one often encounters binary variables. They take only two values, 0 and 1, corresponding to the presence or absence of some attribute. An example of such a data set is shown in Table 1.

There are several ways to cluster such data. Most of the algorithms described in the previous chapters use a matrix of dissimilarities between objects. In the case of binary variables, such dissimilarities can be computed by means of the program DAISY described in Chapter 1. Then one can apply one of the programs of Chapters 2, 4, 5, or 6 to the resulting dissimilarity matrix.

In the program MONA an approach of a quite different nature is adopted. The basic idea is to select one of the variables and to divide the set of objects into those objects with and those without the corresponding attribute. In each of the two subsets, one of the remaining variables is selected and used in the same way to divide this subset into two smaller groups. (Note that it is not necessary to use the same second variable in both subsets.) The process is continued until either the subset contains a single object (it is then called a singleton) or until the remaining variables cannot separate the subset any further. This last situation only occurs when each variable remains constant for all objects of this subset. (For example, objects *CCC* and *DDD* in Table 1 cannot be separated.)

Because the set of objects is divided into subsets and this process is continued inside each subset, the algorithm is hierarchical. To be more precise, it is divisive. Furthermore, because each separation is carried out

Table 1 Example of a Data Set with Binary Variables

	Variables					
Objects	1	2	3	4	5	6
AAA	1	1	0	1	1	0
BBB	1	1	0	0	0	1
CCC	1	1	1	1	1	0
DDD	1	1	1	1	1	0
EEE	0	0	0	1	0	1
FFF	0	0	0	0	0	0
GGG	0	0	1	1	0	1
HHH	0	0	1	1	1	0

using a single variable, it is called *monothetic*. Methods such as the divisive analysis of Chapter 6, which use all variables simultaneously, are called *polythetic*.

The most important part of the algorithm is how to choose the variable to separate a subset. The idea is to select the variable for which the sum of "similarities" to all the other variables is as large as possible, i.e., the variable which is the most centrally located. Several measures of association have been proposed to define the similarity between binary variables, some of which will be discussed in Section 5.

In MONA we have opted for a quite simple measure of association between two variables, which uses the number of objects for each combination of values that the two variables can take. The product of the number of objects for which the two variables take on the value 0 and the number for which they take on the value 1 is calculated. Then the number of objects for which the first variable is 0 and the second is 1 is multiplied with the number of objects for which the two variables take on opposite values. The measure of association (similarity) is defined as the absolute value of the difference between these two products. As an example, consider the measurements of Table 1. The variables 1 and 2 are identical and should therefore show a high association value. The two products are 16 (4×4) and 0 (0×0), so the measure of association becomes $|16 - 0| = 16$. The variables 1 and 3 are quite different from each other, and indeed their association value is $|(2 \times 2) - (2 \times 2)| = 0$. The measure of association between two variables can be calculated from a two-by-two contingency table. In Figure 1a a general contingency table is shown and Figure 1b corresponds to the variables 1 and 3 of Table 1.

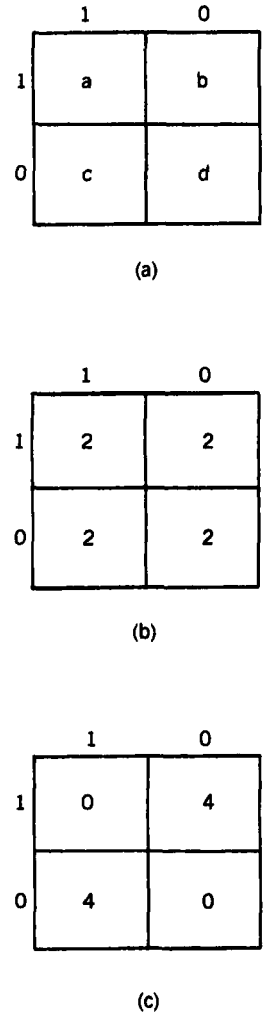


Figure 1 (a) General two-by-two contingency table. (b) Table for the variables 1 and 3 of Table 1. (c) Table for two variables with opposing values for all objects.

The measure of association just defined expresses whether two variables provide similar divisions of the set of objects. The variables 1 and 3 give quite different information and are therefore not at all similar (their measure of association is 0). However, if two variables have different values for all objects of a data set, they give identical information and the measure of association is very large (see, for example, Figure 1c). It should be noted that the measure of association closely resembles the chi-squared statistic for the two-by-two table.

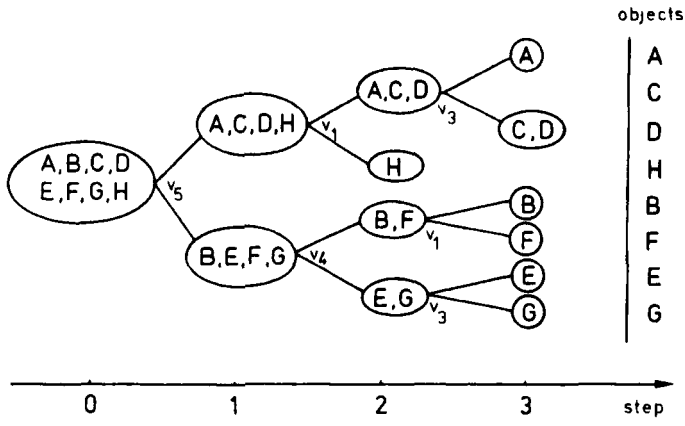


Figure 2 Example of the results of applying the program MONA.

Because we are searching for the variable that is most similar to all other variables, we *maximize* the sum of its associations to all other variables. Because we are looking at a sum of absolute values, this criterion bears resemblance to the one used in Chapters 2 and 3 (for finding representative *objects*) as well as those of Chapters 5 and 6. It falls in line with one of the aims of this book, which is to advocate the use of robust criteria in clustering algorithms.

An example of the results of MONA is shown in Figure 2. In the beginning of the algorithm (the left side of the figure), all objects belong to a single cluster. During the first step, variable 5 is used to separate this cluster into two subsets. The separation steps are continued until either a cluster consists of a single object, or until the remaining variables cannot be used to split it up. This last situation occurs for the cluster $\{CCC, DDD\}$.

2 HOW TO USE THE PROGRAM MONA

Like the techniques of previous chapters, the clustering method described in Section 1 was programmed in Fortran for an IBM-PC or compatible computer (with at least 256 K of internal storage). In Section 2.1 we will describe an interactive session (which is similar to previous chapters), and in Section 2.2 we will explain the output. In Section 3 some examples will be examined. In Section 4 some limitations of the program are described, and the Appendix contains more details on its implementation.

2.1 Interactive Use and Input

In order to run the program, the first thing to do is to insert the diskette containing the file MONA.EXE and to type MONA. This starts an interactive session, an example of which follows.

```
MONOTHETIC ANALYSIS

THE PRESENT VERSION OF THE PROGRAM CAN HANDLE UP TO 200 OBJECTS.
(IF MORE ARE TO BE CLUSTERED, THE ARRAYS INSIDE THE PROGRAM MUST BE ADAPTED.)
HOW MANY OBJECTS ARE TO BE CLUSTERED ?
PLEASE GIVE A NUMBER BETWEEN 3 AND 200 : 8

DO YOU WANT TO ENTER LABELS OF OBJECTS ?
PLEASE ANSWER YES OR NO ..... YES

EACH LABEL MAY CONSIST OF AT MOST 3 CHARACTERS

OBJECT          LABEL
----------------↓↓↓
NUMBER 1 :      AAA
NUMBER 2 :      BBB
NUMBER 3 :      CCC
:
:

THE PRESENT VERSION OF THE PROGRAM ALLOWS TO ENTER UP TO 200 VARIABLES, OF WHICH AT MOST 100 CAN BE USED IN THE ACTUAL COMPUTATIONS.
(IF MORE ARE NEEDED, THE ARRAYS INSIDE THE PROGRAM MUST BE ADAPTED)
AT LEAST THREE VARIABLES ARE NECESSARY FOR ASSOCIATION ANALYSIS.
IF LESS ARE AVAILABLE A DIFFERENT CLUSTERING STRATEGY SHOULD BE USED.
(FOR EXAMPLE, RUN THE PROGRAM DAISY TO COMPUTE A DISSIMILARITY MATRIX.)

WHAT IS THE TOTAL NUMBER OF VARIABLES IN YOUR DATA SET ?
------------------------------------------------

PLEASE GIVE A NUMBER BETWEEN 3 AND 200 : 6

HOW MANY VARIABLES DO YOU WANT TO USE IN THE ANALYSIS ?
------------------------------------------------

PLEASE GIVE A NUMBER BETWEEN 3 AND 6 : 5

DO YOU WANT TO ENTER LABELS OF VARIABLES ? PLEASE ANSWER
YES OR NO ..... YES
```

```
VARIABLE TO BE USED :     POSITION     LABEL (AT MOST 3
                                       CHARACTERS)
                          ↓ ↓ ↓ ↓      ↓ ↓ ↓
NUMBER 1 :                    1        v1
NUMBER 2 :                    3        v3
NUMBER 3 :                    4        v4
NUMBER 4 :                    5        v5
NUMBER 5 :                    6        v6
```

PLEASE ENTER A TITLE FOR THE OUTPUT (AT MOST 60 CHARACTERS)

Data of Table 1

DO YOU WANT LARGE OUTPUT ? (PLEASE ANSWER YES)
OR. IS SMALL OUTPUT SUFFICIENT ? (THEN ANSWER NO)
(IN THE FORMER CASE MEASUREMENT VALUES AND DETAILED INFORMATION ON EACH SEPARATION STEP ARE PROVIDED. IF THE PROGRAM FINDS MISSING VALUES, THE ESTIMATES ARE ALSO GIVEN.) . . . . . YES

DO YOU WANT GRAPHICAL OUTPUT (BANNER) ? PLEASE ANSWER YES OR NO . . . . . YES

DO YOU WANT TO READ THE DATA IN FREE FORMAT ?

THIS MEANS THAT YOU ONLY HAVE TO INSERT BLANK(S) BETWEEN MEASUREMENTS.
(NOTE: WE ADVISE USERS WITHOUT KNOWLEDGE OF FORTRAN FORMATS TO ANSWER YES.)
MAKE YOUR CHOICE (YES / NO) : NO

PLEASE ENTER A FORTRAN FORMAT.
THIS FORMAT MAY CONTAIN AT MOST 60 CHARACTERS AND SHOULD BE PUT BETWEEN BRACKETS, e.g. (10(2X,F1.0)).
ONLY F AND E FORMATS ARE ALLOWED (THIS DOES NOT MEAN THAT YOUR MEASUREMENTS MUST CONTAIN DECIMAL POINTS, BUT IT ENABLES YOU TO HANDLE MIXED DATA FILES).
(6(2X,F1.0))

The only measurement values allowed by the program are 0 and 1. All other values will be treated as missing measurements. (In Section 4.2 it is shown how the program can be adapted to allow other values.)

PLEASE GIVE THE NAME OF THE FILE CONTAINING THE DATA (e.g. A:EXAMPLE.DAT) OR TYPE KEY IF YOU PREFER TO ENTER THE DATA BY KEYBOARD.
WHAT DO YOU CHOOSE ? KEY

DO YOU WANT TO SAVE YOUR DATA ON A FILE ?
PLEASE ANSWER YES OR NO : YES

ON WHICH FILE DO YOU WANT TO SAVE YOUR DATA ?
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME
NAME THEN THE OLD FILE WILL BE OVERWRITTEN.)
TYPE e.g. B:SAVE.DAT .....TEST.DAT

WHERE DO YOU WANT YOUR OUTPUT ?

TYPE CON IF YOU WANT IT ON THE SCREEN
OR TYPE PRN IF YOU WANT IT ON THE PRINTER
OR TYPE THE NAME OF A FILE (e.g. B:EXAMPLE.OUT)
(WARNING : IF THERE ALREADY EXISTS A FILE WITH THE SAME
NAME THEN THE OLD FILE WILL BE OVERWRITTEN.)
WHAT DO YOU CHOOSE ? .....TEST.RES

DATA SPECIFICATIONS AND CHOSEN OPTIONS

TITLE : Data of Table 1
THERE ARE 8 OBJECTS
LABELS OF OBJECTS ARE READ
LABELS OF VARIABLES ARE READ
LARGE OUTPUT IS WANTED
GRAPHICAL OUTPUT IS WANTED (BANNER)

THERE ARE 6 VARIABLES IN THE DATA SET,
AND 5 OF THEM WILL BE USED IN THIS ANALYSIS

THE INPUT FORMAT FOR THE MEASUREMENTS IS
(6(2X,F1.0))
THE DATA WILL BE READ FROM THE KEYBOARD
THE DATA WILL BE SAVED ON FILE : TABLE 1.DAT
YOUR OUTPUT WILL BE WRITTEN ON : TABLE 1.RES

ARE ALL THESE SPECIFICATIONS OK ? YES OR NO : YES

PLEASE ENTER YOUR DATA FOR EACH OBJECT

THE 6 MEASUREMENTS FOR OBJECT AAA :
1 1 0 1 1 0
THE 6 MEASUREMENTS FOR OBJECT BBB :
1 1 0 0 0 1
THE 6 MEASUREMENTS FOR OBJECT CCC :
1 1 1 1 1 0
THE 6 MEASUREMENTS FOR OBJECT DDD :
1 1 1 1 1 0

THE 6 MEASUREMENTS FOR OBJECT EEE :
0 0 0 1 0 1
THE 6 MEASUREMENTS FOR OBJECT FFF :
0 0 0 0 0 0
THE 6 MEASUREMENTS FOR OBJECT GGG :
0 0 1 1 0 1
THE 6 MEASUREMENTS FOR OBJECT HHH :
0 0 1 1 1 0

Note that only the variables 1, 3, 4, 5, and 6 are to be used in this particular analysis.

2.2 Output

In this section the output generated by MONA is described and illustrated with the output from the data set of Table 1. This output can be divided into several parts.

a. Data Specifications and Measurement Values

In Figure 3, an example is given of part a of the output corresponding to the input described in Section 2.1.

b. Missing Measurements

If there are no missing measurements (all measurement values are 0 or 1), a message is given indicating this.

If there are missing measurements, a message is printed in the following situations:

- the number of missing measurements for some variable is at least half the number of objects
- all measured values are identical for some variable
- each variable lacks at least one measurement

If any of these situations arises, the program stops after all variables have been examined.

Inventory of the variables for which some measurements are lacking, the number of missing measurements for each of these variables, and the total number of missing measurements.

After all the missing measurements have been filled in, the revised data are outputted (only if large output was requested).

```
**********************************
*                                *
*      MONOTHETIC ANALYSIS       *
*                                *
**********************************

DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 TITLE : Data of Table 1
 THERE ARE       8 OBJECTS
 LABELS OF OBJECTS ARE READ
 LABELS OF VARIABLES ARE READ
 LARGE OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (BANNER)

 THERE ARE     6 VARIABLES IN THE DATA SET,
  AND     5 OF THEM WILL BE USED IN THE ANALYSIS
 THESE VARIABLES ARE :
          v1    (POSITION :  1)
          v3    (POSITION :  3)
          v4    (POSITION :  4)
          v5    (POSITION :  5)
          v6    (POSITION :  6)
 THE INPUT FORMAT FOR THE MEASUREMENTS IS
 (6(2X,F1.0))

 YOUR DATA RESIDE ON FILE        : TABLE1.DAT


INPUT DATA
**********


       V V V V V
       1 3 4 5 6

AAA    1 0 1 1 0
BBB    1 0 0 0 1
CCC    1 1 1 1 0
DDD    1 1 1 1 0
EEE    0 0 1 0 1
FFF    0 0 0 0 0
GGG    0 1 1 0 1
HHH    0 1 1 1 0

 THERE ARE NO MISSING VALUES
```

Figure 3 Parts a and b of the MONA output for the example of Section 2.1.

In Section 3 an example is discussed with missing measurements. The estimation of missing measurements is explained in Section 4.

c. Detailed Clustering Information

While the algorithm is being carried out, and if large output was requested, the following information is provided for each step:

1. The subset to be separated: The objects of the subset are given in the order obtained after separation.
2. The number of objects in each of the two subsets.
3. The variable used for the separation.

```
STEP NUMBER      1
*****************

THE CLUSTER   AAA CCC DDD HHH BBB EEE FFF GGG
IS DIVIDED INTO      4 AND      4 OBJECTS, USING VARIABLE       v5

STEP NUMBER      2
*****************

THE CLUSTER   AAA CCC DDD HHH
IS DIVIDED INTO      3 AND      1 OBJECTS, USING VARIABLE       v1

THE CLUSTER   BBB FFF EEE GGG
IS DIVIDED INTO      2 AND      2 OBJECTS, USING VARIABLE       v4

STEP NUMBER      3
*****************

THE CLUSTER   AAA CCC DDD
IS DIVIDED INTO      1 AND      2 OBJECTS, USING VARIABLE       v3

THE CLUSTER   BBB FFF
IS DIVIDED INTO      1 AND      1 OBJECTS, USING VARIABLE       v1

THE CLUSTER   EEE GGG
IS DIVIDED INTO      1 AND      1 OBJECTS, USING VARIABLE       v3

STEP NUMBER      4
*****************

THE CLUSTER   CCC DDD
CANNOT BE SEPARATED BY THE REMAINING VARIABLES

FINAL RESULTS
*************

THE FINAL ORDERING OF THE OBJECTS IS
        AAA     CCC     DDD     HHH     BBB     FFF     EEE     GGG
THE SEPARATION STEP IS
             3       0       2       1       3       2       3
THE VARIABLE USED IS
             v3              v1      v5      v1      v4      v3


                          ************
                          *          *
                          *  BANNER  *
                          *          *
                          ************

       0                       1                       2                       3
  v3 AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+AAA+
     ***********************************************************************************
     CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+CCC+
     DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+DDD+
  v1 ***********************************************
     HHH+HHH+HHH+HHH+HHH+HHH+HHH+HHH+HHH+HHH+HHH+HHH+H
  v5 ***************************
     BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+BBB+
  v1 ***********************************************************************************
     FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+FFF+
  v4 ***********************************************
     EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+EEE+
  v3 ***********************************************************************************
     GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+GGG+
       0                       1                       2                       3

The output is on file : TABLE1.RES
```

Figure 4 Parts c, d, and e of the MONA output for the example of Section 2.1.

An example of this output is:

> The cluster AAA CCC DDD HHH BBB EEE FFF GGG
> is divided into 4 and 4 objects using the variable v5

The two new clusters are {AAA, CCC, DDD, HHH} and {BBB, EEE, FFF, GGG}.

d. Final Results

The first array in the final results contains the objects, ordered as on the vertical axis to the right in Figure 2. In the second array the separation steps are listed: Note, for example, that the 1 in this array appears between objects HHH and BBB, because at the *first* step the set of objects starting with BBB (i.e., objects BBB, FFF, EEE, and GGG) are separated from the other objects. This separation was carried out using the variable v5, which is why v5 appears at the same place in the third array. By the way, note that a 0 in the array of separation steps means that the objects above it could not be separated. This is the case for objects CCC and DDD in the example.

e. Banner

Finally, the results of the algorithm are summarized in a banner, which is quite similar to the banners used in Chapters 5 and 6. Figure 4 contains the banner for the data of Table 1.

Each object of the data set corresponds to a horizontal line in the banner. These horizontal lines are ordered in the same way as in the first array of the final results. The end of a row of stars * * * * * indicates a separation between clusters. (If two or more lines representing objects are stuck together this means that these objects cannot be divided; see, for example, the rows of objects CCC and DDD in Figure 4.) The length of a row of stars is proportional with the step number at which the separation was carried out. The variable used for the separation is shown to the left of the row of stars. When the row of an object does not continue to the right-hand side of the banner, this means that at the corresponding step it became a singleton cluster. For example, object HHH became a singleton at step 2.

3 EXAMPLES

The first example is the family data described in Table 9 of Chapter 1. It consists of 10 binary variables measured on 8 persons (the objects). Only 0s and 1s appear in the data, so that there are no missing measurements.

The analysis carried out on these data uses all variables. The large output option and the banner are both selected. The labels of the objects are the first three letters of each name, and for each variable a three-letter code was chosen as label.

Figure 5 contains the output of MONA with these options. This output was directed to the printer (by entering option PRN for output). Below the data specifications and chosen options, the input data are shown. The program then searches for missing data (values different from 0 and 1). As none are found, this is mentioned and the actual algorithm can be carried out. In the first step of the calculations the variable MAR was selected as the most representative, and therefore as the most adequate for dividing the data set into two clusters. The actual split can be seen in Figure 5 under "step number 1." In the output, the first object of a cluster is the one which appears first in the data matrix. Then all objects are given that have the same value for the separation variable. In the example, the first person (object) is ILA, who is not married. He is followed by KIM, TAL, and TIN. After this first cluster, the objects are given that have the opposite value; in the example they are JAC, LIE, LEO, and PET. Note that in both clusters the objects appear in the same order as in the data matrix. The algorithm is constructed so that the final ordering is as close as possible to the original ranking. This was done in all programs, in order to facilitate comparisons of outputs for the same data.

It is interesting to observe that in this example the variable used for the first division is intuitively the most important, because it distinguishes between the children and the adults.

In the second step, both clusters are separated using one of the remaining variables. The cluster of children is separated on the basis of the color of hair, while for the adults the variable SEX is the most centrally located.

In the third step the following clusters are examined: {ILA, KIM}, {TAL, TIN}, {JAC, LIE}, and {LEO, PET}. The first of these clusters can only be separated using the variables SEX and LFT. (The other variables take the same value for both children, so they will no longer be considered.) The similarity between SEX and LFT will be calculated using the following table:

		LFT 1	LFT 0
SEX	1	0	1
	0	1	0

```
                    **********************************
                    *                                *
                    *       MONOTHETIC ANALYSIS      *
                    *                                *
                    **********************************


DATA SPECIFICATIONS AND CHOSEN OPTIONS
--------------------------------------
 TITLE : Binary family data
 THERE ARE       8 OBJECTS
 LABELS OF OBJECTS ARE READ
 LABELS OF VARIABLES ARE READ
 LARGE OUTPUT IS WANTED
 GRAPHICAL OUTPUT IS WANTED (BANNER)

 THERE ARE    10 VARIABLES IN THE DATA SET,
  AND ALL OF THEM WILL BE USED IN THE ANALYSIS
 THESE VARIABLES ARE :
         sex    (POSITION :  1)
         mar    (POSITION :  2)
         hai    (POSITION :  3)
         eye    (POSITION :  4)
         gla    (POSITION :  5)
         fac    (POSITION :  6)
         pes    (POSITION :  7)
         eve    (POSITION :  8)
         one    (POSITION :  9)
         lft    (POSITION : 10)
 THE MEASUREMENTS WILL BE READ IN FREE FORMAT

 YOUR DATA RESIDE ON FILE        : FAMIMONA.DAT


INPUT DATA
**********

      s m h e g f p e o l
      e a a y l a e v n f
      x r i e a c s e e t

Ila   1 0 1 1 0 0 1 0 0 0
Jac   0 1 0 0 1 0 0 0 0 0
Kim   0 0 1 0 0 0 1 0 0 1
Lie   0 1 0 0 0 0 0 1 1 0
Leo   1 1 0 0 1 1 0 1 1 0
Pet   1 1 0 0 1 0 1 1 0 0
Tal   0 0 0 1 0 1 0 0 0 0
Tin   0 0 0 1 0 1 0 0 0 0

 THERE ARE NO MISSING VALUES


 STEP NUMBER      1
 *****************

 THE CLUSTER   Ila Kim Tal Tin Jac Lie Leo Pet
 IS DIVIDED INTO       4 AND      4 OBJECTS, USING VARIABLE      mar
```

Figure 5 MONA output for the binary family data.

```
STEP NUMBER     2
****************

THE CLUSTER   Ila Kim Tal Tin
IS DIVIDED INTO      2 AND     2 OBJECTS, USING VARIABLE     hai

THE CLUSTER   Jac Lie Leo Pet
IS DIVIDED INTO      2 AND     2 OBJECTS, USING VARIABLE     sex


STEP NUMBER     3
****************

THE CLUSTER   Ila Kim
IS DIVIDED INTO      1 AND     1 OBJECTS, USING VARIABLE     sex

THE CLUSTER   Tal Tin
CANNOT BE SEPARATED BY THE REMAINING VARIABLES

THE CLUSTER   Jac Lie
IS DIVIDED INTO      1 AND     1 OBJECTS, USING VARIABLE     gla

THE CLUSTER   Leo Pet
IS DIVIDED INTO      1 AND     1 OBJECTS, USING VARIABLE     fac


FINAL RESULTS
*************

THE FINAI ORDERING OF THE OBJECTS IS

       Ila    Kim    Tal    Tin    Jac    Lie    Leo    Pet

THE SEPARATION STEP IS

            3      2      0      1      3      2      3

THE VARIABLE USED IS

          sex    hai           mar    gla    sex    fac
```


```
      0                    1                    2                    3

    Ila+Ila+Ila+Ila+Ila+Ila+Ila+Ila+Ila+Ila+Ila+Ila+Ila+Ila+Ila+Ila+Ila+
sex ********************************************************************************
    Kim+Kim+Kim+Kim+Kim+Kim+Kim+Kim+Kim+Kim+Kim+Kim+Kim+Kim+Kim+Kim+Kim+
hai ********************************************
    Tal+Tal+Tal+Tal+Tal+Tal+Tal+Tal+Tal+Tal+Tal+Tal+T
    Tin+Tin+Tin+Tin+Tin+Tin+Tin+Tin+Tin+Tin+Tin+Tin+T
mar ************************
    Jac+Jac+Jac+Jac+Jac+Jac+Jac+Jac+Jac+Jac+Jac+Jac+Jac+Jac+Jac+Jac+Jac+
gla ********************************************************************************
    Lie+Lie+Lie+Lie+Lie+Lie+Lie+Lie+Lie+Lie+Lie+Lie+Lie+Lie+Lie+Lie+Lie+
sex ********************************************
    Leo+Leo+Leo+Leo+Leo+Leo+Leo+Leo+Leo+Leo+Leo+Leo+Leo+Leo+Leo+Leo+Leo+
fac ********************************************************************************
    Pet+Pet+Pet+Pet+Pet+Pet+Pet+Pet+Pet+Pet+Pet+Pet+Pet+Pet+Pet+Pet+Pet+

      0                    1                    2                    3
```

Figure 5 (*Continued*)

The similarity between the two variables equals $|0 \times 0 - 1 \times 1| = 1$, which is also the *total* similarity for each variable. In a situation where several variables yield the same total similarity, the one that appears first in the data matrix is chosen for the separation. This is of course an arbitrary choice. Note that when there are two objects in a cluster, the first variable is selected which takes different values in them.

The next cluster to be considered in step 3 is {TAL, TIN}. Because all remaining variables take the same values for these two children, they cannot be separated. In such a situation this cluster will no longer be considered in subsequent steps. Observe that the objects of such a cluster are identical for *all* variables of the data set, not only for the remaining ones. Indeed, because they are in the same cluster they are also identical for the variables used to *obtain* this cluster.

The remaining clusters {JAC, LIE} and {LEO, PET} are separated by the variables GLA and FAC, as these are the first variables for which the objects have different values.

When small output is requested, the detailed clustering information is not given. In this case the hierarchical structure yielded by the algorithm can be deduced from the final results. These start with the final ordering of the objects, which can be different from the original one. (However, as in the other programs, the first object has remained where it was.) Then, between each pair of objects the separation step is printed, indicating when the clusters to which these objects belong were formed. For example, the number 1 between objects TIN and JAC indicates that the clusters to which TIN and JAC belong (clusters {ILA, KIM, TAL, TIN} and {JAC, LEO, LIE, PET}) have been separated during the first step. The variable used for this separation (MAR) is shown in the third array, right underneath the number of the step. Sometimes a 0 is given for the separation step. This means that the adjacent objects (between which the 0 is lying) cannot be separated. In the example this is the case for persons TAL and TIN.

Finally, the results are summarized in the banner. The first split, using the variable MAR, divides the data into the clusters {ILA, KIM, TAL, TIN} and {JAC, LIE, LEO, PET}. In the first of these clusters the variable HAI is used for the next division, and in the second one it is the variable SEX. The variables used in the third step are of less importance. However, note that the cluster {TAL, TIN} cannot be separated, which is why their label lines were printed right below each other.

In the banner, the end of a row of stars * * * * * indicates a separation. The shorter the row, the earlier the separation was carried out in the algorithm. However, the banner does not provide a *quantitative* measure of the importance of a separation. In the graphical output of the other

programs of this book this is the case, making it possible to deduce the quality of the clustering from the fullness of the graphical representation. The banner of MONA cannot be used in this way because the length of a row of stars is proportional to the number of the separation step, not to the tightness of the clusters.

An alternative way of investigating this binary data set is to start by computing a dissimilarity matrix with the program DAISY and then to cluster the objects using either AGNES or DIANA. (See Exercise 4.)

Let us now look at a data set with missing values and see how the missing attributes are estimated by the program. Six 0-1 attributes were considered for 20 animals. The six attributes are

WAR : 1 = warm-blooded		0 = cold-blooded
FLY : 1 = can fly		0 = cannot fly
VER : 1 = vertebrate		0 = invertebrate
END : 1 = endangered		0 = not endangered
GRO : 1 = live in groups		0 = do not live in groups
HAI : 1 = have hair		0 = do not have hair

```
INPUT DATA
**********

      W F V E G H
      A L E N R A
      R Y R D O I

ant   0 0 0 0 1 0
bee   0 1 0 0 1 1
cat   1 0 1 0 0 1
cpl   0 0 0 0 0 1
chi   1 0 1 1 1 1
cow   1 0 1 0 1 1
duc   1 1 1 0 1 0
eag   1 1 1 1 0 0
ele   1 0 1 1 1 0
fly   0 1 0 0 0 0
fro   0 0 1 1 9 0
her   0 0 1 0 1 0
lio   1 0 1 9 1 1
liz   0 0 1 0 0 0
lob   0 0 0 0 9 0
man   1 0 1 1 1 1
rab   1 0 1 0 1 1
sal   0 0 1 0 9 0
spi   0 0 0 9 0 1
wha   1 0 1 1 1 0

   2 VARIABLES HAVE MISSING VALUES

 VARIABLE END HAS     2 MISSING VALUES
 VARIABLE GRO HAS     3 MISSING VALUES

   5 MISSING VALUES HAVE BEEN ESTIMATED
```

Figure 6 First part of the output for the animal data.

The following animals were selected (in a rather arbitrary way): ant, bee, cat, caterpillar, chimpanzee, cow, duck, eagle, elephant, fly, frog, herring, lion, lizard, lobster, man, rabbit, salmon, spider, and whale. For the variables WAR, FLY, VER, and HAI information was available for all animals. But for the variables END and GRO there was some doubt for, respectively, two and three animals. Therefore we decided to consider the corresponding measurements as missing. These values were identified by the program, and in Figure 6 the input data are followed by an inventory of the missing values for each variable.

After the identification of missing measurements, a procedure is carried out for estimating their values. In this procedure each variable containing missing values is considered in turn. Each time the algorithm looks for the most similar complete variable and then uses the latter for filling in the missing values. In our example END has two missing values. The similarities between this variable and the complete variables are given in Figure 7.

The variable WAR has the highest similarity with END and is therefore the most appropriate for estimating the missing values of END. The two

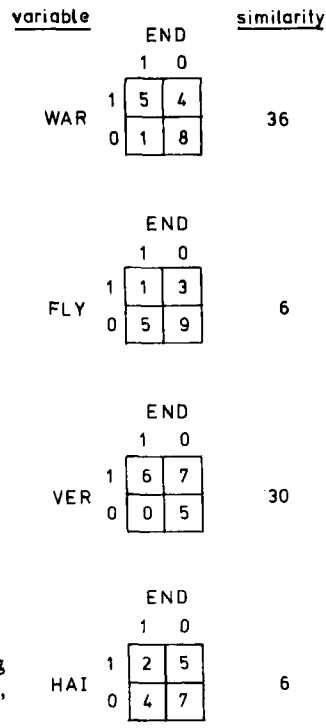


Figure 7 Similarities between a variable with missing values (END) and all variables without missing values, in the animal data set.

```
REVISED DATA
************

        W F V E G H
        A L E N R A
        R Y R D O I

ant     0 0 0 0 1 0
bee     0 1 0 0 1 1
cat     1 0 1 0 0 1
cpl     0 0 0 0 0 1
chi     1 0 1 1 1 1
cow     1 0 1 0 1 1
duc     1 1 1 0 1 0
eag     1 1 1 1 0 0
ele     1 0 1 1 1 0
fly     0 1 0 0 0 0
fro     0 0 1 1 0 0
her     0 0 1 0 1 0
lio     1 0 1 1 1 1
liz     0 0 1 0 0 0
lob     0 0 0 0 0 0
man     1 0 1 1 1 1
rab     1 0 1 0 1 1
sal     0 0 1 0 0 0
spi     0 0 0 0 0 1
wha     1 0 1 1 1 0



 STEP NUMBER     1
 ****************


 THE CLUSTER   ant bee cpl fly fro her liz lob sal spi cat chi cow duc eag
               ele lio man rab wha
 IS DIVIDED INTO     10 AND    10 OBJECTS, USING VARIABLE     WAR


 STEP NUMBER     2
 ****************


 THE CLUSTER   ant bee cpl fly lob spi fro her liz sal
 IS DIVIDED INTO      6 AND     4 OBJECTS, USING VARIABLE     VER


 THE CLUSTER   cat chi cow ele lio man rab wha duc eag
 IS DIVIDED INTO      8 AND     2 OBJECTS, USING VARIABLE     FLY


 STEP NUMBER     3
 ****************


 THE CLUSTER   ant cpl lob spi bee fly
 IS DIVIDED INTO      4 AND     2 OBJECTS, USING VARIABLE     FLY


 THE CLUSTER   fro her liz sal
 IS DIVIDED INTO      1 AND     3 OBJECTS, USING VARIABLE     END


 THE CLUSTER   cat cow rab chi ele lio man wha
 IS DIVIDED INTO      3 AND     5 OBJECTS, USING VARIABLE     END


 THE CLUSTER   duc eag
 IS DIVIDED INTO      1 AND     1 OBJECTS, USING VARIABLE     END
```

Figure 8 Some results for the animal data.

animals for which the attribute END is missing (lion and spider) have values 1 and 0 for WAR. They are given the same value for END, as can be seen in Figure 8 in the revised data matrix. Figure 8 also contains the first three steps of the algorithm.

In the first separation step (which is usually the most important) the two clusters of warm-blooded and cold-blooded species are found. In Figure 8 we can see that after this first separation, different variables are used for further divisions. In the cold-blooded group the next separation is between vertebrate and invertebrate animals, while in the warm-blooded cluster the attribute of being able to fly is the most centrally located. Observe that the attribute "vertebrate" cannot be used in the warm-blooded cluster because all animals in this group are vertebrate. Analogously, in the third step, the cluster {cat, cow, rabbit, chimpanzee, elephant, lion, man, whale} is separated into {cat, cow, rabbit} and the others. It should be noted that the separation variables used after step 3 are not very significant because the total similarities found are often the same for several variables, yielding an arbitrary choice of the separating variable (in such a case the first variable is chosen, which implies that another ranking of the variables would result in a different choice).

Another example can be obtained by applying MONA to the binary variables of a mixed data set, such as the flower data in Table 12 of Chapter 1 (see Exercise 6a).

*4 MORE ON THE ALGORITHM AND THE PROGRAM

4.1 Description of the Algorithm

The clustering algorithm used in MONA assumes that there are no missing measurements. However, in many situations not all data can be obtained. Therefore, the program has a provision for filling in missing data. The program starts by identifying all values different from 0 and 1 as missing. The actual filling in is done by examining, one at a time, those variables for which some of the measurements are missing. When investigating such a variable (with index f), each variable is considered for which all measurements are available. Let us call g one of these complete variables. Note that there exists at least one complete variable (because if all variables have missing measurements, a message is given and the program stops). The following measure of association is then calculated between f and g:

$$A_{fg} = |a_{fg}d_{fg} - b_{fg}c_{fg}|$$

where the values a_{fg}, b_{fg}, c_{fg}, and d_{fg} are obtained from the following

contingency table:

Variable f	Variable g: 1	Variable g: 0
1	a_{fg}	b_{fg}
0	c_{fg}	d_{fg}

Note that $a_{fg} + b_{fg} + c_{fg} + d_{fg}$ is the total number of nonmissing values of the variable f. After calculating A_{fg} for each complete variable g, the variable t is determined for which the association with the variable f is maximal:

$$A_{ft} = \max_g A_{fg}$$

If the same maximal association is found for several complete variables, t is chosen as the first in the list.

Because the variable t has the largest association with the variable f, it is used for filling in missing measurements of f. How this is done depends on the sign of $a_{ft}d_{ft} - b_{ft}c_{ft}$. If it is positive, a missing value x_{if} of the variable f is simply replaced by the value x_{it} of the variable t. On the other hand, if $a_{ft}d_{ft} - b_{ft}c_{ft}$ is negative, the variable f is actually most similar to the *complementary* variable of t. In this case, a missing value x_{if} is replaced by $1 - x_{it}$.

After a complete data matrix has been obtained, MONA starts the actual clustering algorithm. The algorithm used is of the hierarchical divisive type. At each separation step it selects one of the variables and divides the set of objects being considered into objects for which the selected variable equals 0 and objects for which it equals 1. The selection of a variable is also based on the association between variables. For each variable f, the association measures with all other variables are added, giving the total measure

$$A_f = \sum_{g \neq f} A_{fg}$$

The variable t for which this sum is maximal is then determined:

$$A_t = \max_f A_f$$

Again, if the same maximal value is found for several variables, t is chosen as the one appearing first.

The association between variables can be considered as a kind of similarity between them. Indeed, the association between a variable and itself is usually very large. (The reason for this is that b_{ff} and c_{ff} are both 0. Note that the association between a variable and itself can be 0 in the extreme case that either a_{ff} or d_{ff} is 0. However, in this case f cannot be used for separating the set of objects.) On the other hand, if the two variables provide quite different information (see, for example, the variables 1 and 3 in Table 1), their association is very small. (Strictly speaking, this association measure is not a real similarity because it may take values exceeding 1.)

The variable selected for the separation is the one for which the total association with all other variables is as large as possible. Therefore it can be argued that the total dissimilarity with other variables is as small as possible. This variable can thus be considered as a medoid of the variables. (See Section 1 of Chapter 2 for the definition of a medoid of *objects*.)

The association measure does not depend on the coding of the variables. Indeed, if (for example) for variable g all zeroes are replaced by 1s and all 1s by 0s, the association measure $A_{fg'}$ is given by

$$A_{fg'} = |b_{fg}c_{fg} - a_{fg}d_{fg}|$$

which is equal to the original A_{fg}. This implies that the criterion treats all binary variables as if they were symmetric. It should be observed that a variable with many more 0s than 1s (or many more 1s than 0s) is likely to yield small association measures. As an illustration, compare the measures obtained from the two tables in Figure 9.

The association for the contingency table of Figure 9a equals 24. The table of Figure 9b was obtained by changing three-quarters of the 0s of the variable f to 1s. The association then becomes 6. If only half the 0s had been changed, a value of 12 would have been obtained. This example

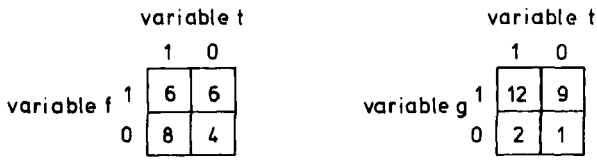


Figure 9 Contingency tables for calculating the measure of association between: (a) a balanced variable f and a variable t; (b) a strongly unbalanced variable g and the same variable t.

Table 2 Example of a Data Set in Which an Arbitrary Choice is Made for the Selection of a Separation Variable

V1	V2	V3
1	1	1
0	0	0
1	1	1
0	0	0
0	1	1
1	0	0

illustrates why strongly unbalanced variables are unlikely to be selected for separations, because they are located far away from most variables.

After the first separation of the objects into two subsets, the process is repeated within each of these. Of course the variable used for the first separation must not be considered any further, because it takes identical values for all objects of the same subset. Also, the separation of each subset is carried out independently.

The separation steps are continued until either a subset consists of a single object or until the remaining variables cannot be used for its separation (because all of its objects have the same values for these variables). In the latter situation the subset is kept as a whole.

The separation step relies heavily on the association between remaining variables. The way in which these associations are calculated implies that only a limited number of different values can be obtained. This is particularly the case during the latter stages of the algorithm. As an illustration, consider Table 2 in which there are six remaining objects and three variables that can be used for their separation.

For the measurements of Table 2 the following values are obtained: $A_{12} = 3$, $A_{13} = 3$, and $A_{23} = 9$. Variables 2 and 3 will both yield a total measure of 12 and an arbitrary choice will be made between them. In most applications similar situations occur when there are just a few remaining variables and/or objects. In particular, this happens when there are just two variables remaining for the separation of a subset. In this case, the choice is always arbitrary.

4.2 Structure of the Program

The program MONA is written in Fortran and consists of approximately 800 statement lines. Besides the main unit, the program contains one

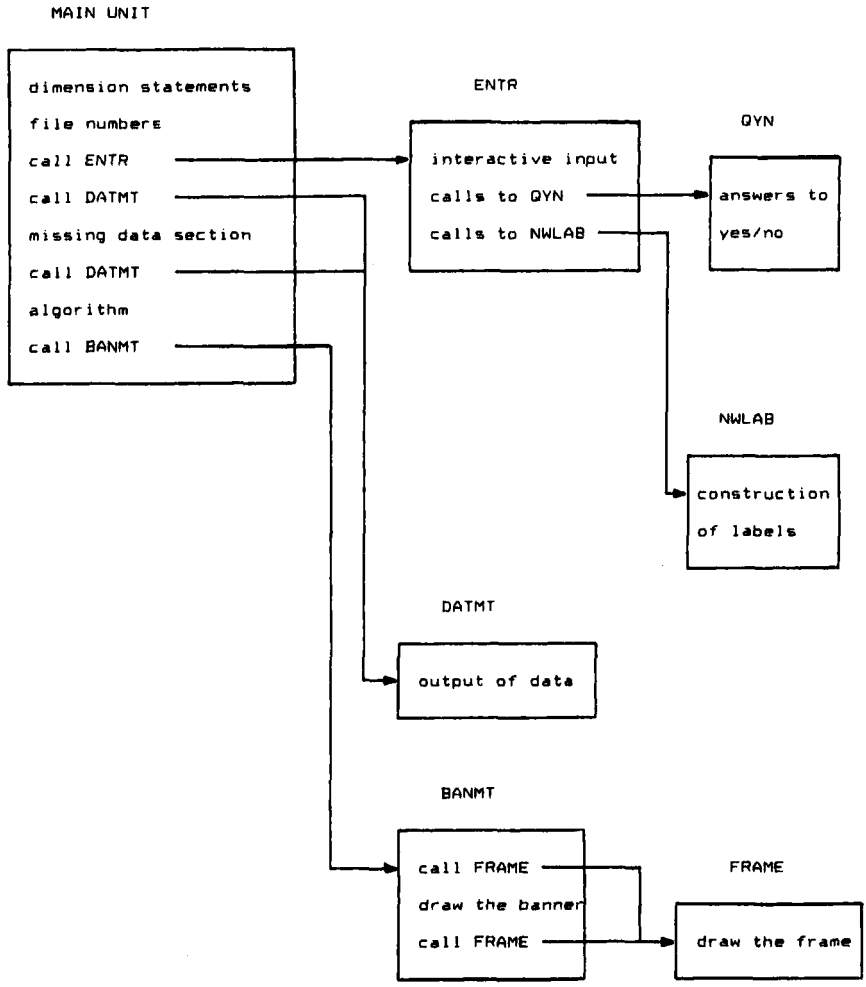


Figure 10 Structure of the program MONA.

function and six subroutines. The structure of the program is shown in Figure 10.

The program starts with dimension and character statements. After these statements, values are given to MAXNN, MAXTT, and MAXPP, making it possible to cluster data sets of different sizes. MAXNN and MAXTT are the maximum numbers of objects and variables, and MAXPP is the maximum number of variables that can be used in the actual computations. In the compiled version of the program they were given the following

values:

MAXNN = 200
MAXTT = 200
MAXPP = 100

The values of MAXNN, MAXTT, and MAXPP can be changed by the user who then must also adapt the dimensions of the arrays (both in the dimension and character statements). These changes only have to be made in the main program and not in the subroutines. However, it should be noted that the values cannot be changed arbitrarily because this has an effect on the size of the EXE file obtained after compilation.

MONA considers all measurement values different from 0 or 1 as missing. In order to change the symbols used to denote measurements, two situations can be considered. If other real values are wanted, instead of 0.0 and 1.0, it is sufficient to adapt the assignment statements situated at the beginning of the main program (right after the statements for MAXNN, MAXTT, and MAXPP):

ABSL = −0.001
ABSH = 0.001
PRSL = 0.999
PRSH = 1.001

All values of a measurement between ABSL and ABSH will be interpreted as the 0 state and all values between PRSL and PRSH as the 1 state. All other values will be considered as corresponding to a missing measurement. If the user requires characters instead of reals, he must change the type of some Fortran variables to characters and also adapt the type of the array HULP (both in the main program and in the subroutine ENTR).

Another possible adaptation of the program concerns the symbols used in the banner. The use of other symbols is discussed in the Appendix. Finally, the user might want to know the value of the objective function A_t for the variable (t) used to separate a cluster. This can easily be achieved by adding the following statements just before statement 395 NBAN(KM) = NPASS in the main program:

```
      WRITE (LUB,9097)LAMA
9097 FORMAT('The value of the objective function is ',I7)
```

when the user wishes this information.

*5 RELATED METHODS AND REFERENCES

The monothetic divisive algorithm in MONA is a variant of a method called *association analysis*, which was introduced by Williams and Lambert (1959). In Section 5.1 association analysis and several other variants are discussed and compared. These methods are all based on the chi-squared statistic. The use of other statistics has led to different monothetic divisive algorithms for binary data (Section 5.2). In Section 5.3 some polythetic methods for binary data and monothetic divisive methods for continuous data are described.

5.1 Association Analysis

A well-known result from probability theory is that for a two-by-two contingency table (as in Figure 1), the statistic

$$K = \frac{(ad - bc)^2 n}{(a + b)(a + c)(b + d)(c + d)} \tag{1}$$

has approximately a chi-squared distribution with 1 degree of freedom. This result is widely used for testing the hypothesis of independence between the two variables used to construct the table. A corollary is that the value of K can be used as a measure of the association between the two variables. A small value of K implies that the two variables are unrelated and in a sense provide different information on the set of objects. This can be expressed as a large distance between the two variables. A similar argument shows that a large value of K implies that the two variables are very related (with either positive or negative dependence).

The position of a variable f with respect to all other variables can be measured by calculating the sum of the K_{fg} for all variables g:

$$K_f = \sum_{g \neq f} K_{fg} \tag{2}$$

A large value of K_f indicates that f is centrally located in the set of variables.

Association analysis (Williams and Lambert, 1959) is based on the selection of the variable f that maximizes K_f. The method starts by dividing the set of objects into those for which x_f is 0 and those for which x_f is 1. After this splitting the same operation is repeated on each of the two subsets, and subsequently on smaller and smaller subsets. When

calculating K_f, Williams and Lambert only consider significant K_{fg} values (at the 5% level of significance). When for a given subset none of the K_{fg} values are significant, this subset is not divided any further. Also, these authors have suggested two variants of this method. In the first, the Yates correction is applied to the K_{fg} values, and in the second the following objective function is maximized:

$$\sum_g \sqrt{K_{fg}/n} \tag{3}$$

Lance and Williams (1965) also consider (3) and justify its use by observing the following relationship between K_{fg} and the Pearson correlation coefficient:

$$|R_{fg}| = \sqrt{K_{fg}/n}$$

This follows from

$$R_{fg} = \frac{n\Sigma_i x_{if} x_{ig} - (\Sigma_i x_{if})(\Sigma_i x_{ig})}{\sqrt{n\Sigma_i x_{if}^2 - (\Sigma_i x_{if})^2}\sqrt{n\Sigma_i x_{ig}^2 - (\Sigma_i x_{ig})^2}}$$

where

$$\sum_i x_{if} = \sum_i x_{if}^2 = a + b$$

$$\sum_i x_{ig} = \sum_i x_{ig}^2 = a + c$$

$$\sum_i x_{if} x_{ig} = a$$

Hence

$$\begin{aligned} R_{fg} &= \frac{na - (a+b)(a+c)}{\sqrt{\left(n(a+b) - (a+b)^2\right)\left(n(a+c) - (a+c)^2\right)}} \\ &= \frac{(a+b+c+d)a - (a+b)(a+c)}{\sqrt{(c+d)(a+b)(b+d)(a+c)}} \\ &= \frac{ad - bc}{\sqrt{(a+b)(c+d)(a+c)(b+d)}} \end{aligned}$$

so finally

$$nR_{fg}^2 = \frac{(ad - bc)^2 n}{(a + b)(c + d)(a + c)(b + d)}$$

This result implies that the original objective (2) is equivalent to maximizing $\Sigma_g nR_{fg}^2$ or also $\Sigma_g R_{fg}^2$.

A computer program for association analysis was implemented by Williams and Lambert (1960). Lance and Williams (1965) also discuss computer programs for association analysis, as well as for the variants using the objective functions

$$\sum_g |R_{fg}| \tag{4}$$

$$\sum_g (a_{fg}d_{fg} - b_{fg}c_{fg})^2 \tag{5}$$

$$\sum_g |a_{fg}d_{fg} - b_{fg}c_{fg}| \tag{6}$$

They showed that the use of (2) as a basis of splitting approaches the maximum information split (see the next subsection). However, they also remark that it has the disadvantage of fragmenting the clustering process by splitting off outliers at an initial stage of the algorithm. On the other hand, (4) appears to lead to more even splits and therefore preserves more of the structure in the data set through the initial part of the analysis. In their opinion (which to our knowledge is not accompanied by strong empirical or mathematical evidence), this last criterion provides the best general-purpose solution.

The program MONA uses objective (6), which differs from (2) in three respects:

1. The factor n has been removed because it has no effect on the clustering.
2. The marginal totals $(a + b)$, $(a + c)$, $(b + d)$, and $(c + d)$ are not considered, which has the computational advantage of not having to worry about any of these values being 0.
3. The absolute value is taken instead of the square of expression $ad - bc$; this has the general advantage of being a more robust value.

Finally it should be noted that association analysis has been widely applied in biology and particularly in plant ecology. For more information

the reader is advised to consult the series of papers by Williams and Lambert (1959, 1960, 1961), by Lambert and Williams (1962, 1966), and by Williams, Lambert, and Lance (1966).

5.2 Other Monothetic Divisive Algorithms for Binary Data

It has been noted by Macnaughton-Smith (1965) that association analysis yields a near-optimum information split. Lance and Williams (1968) give the following definition of the information content of a population of n objects characterized by p binary variables:

$$I = pn \log n - \sum_{f=1}^{p} \left(a_f \log a_f + (n - a_f) \log (n - a_f) \right)$$

where a_f is the number of objects for which attribute f is present (takes value 1):

$$a_f = \sum_{i=1}^{n} x_{if}$$

If a population X is divided into two groups, A and B, they define the information fall by:

$$I_{AB,X} = I_X - I_A - I_B$$

This coefficient can be considered as a measure for the importance of a splitting variable. The greater the information fall, the smaller the information remaining after the splitting. Therefore, the algorithm selects the variable for which the corresponding division yields a maximal information fall, and as in association analysis this variable is used to dichotomize the population. Lance and Williams note that since the information content falls monotonically (if $A \subset B$, then $I_A \leq I_B$) the hierarchy yielded by the method can be plotted with the I value as hierarchical level. This is not possible in association analysis, in which reversals of K_f are frequent.

Crawford and Wishart (1967) describe a rapid clustering method called *group analysis* which is based on the potential of a variable for determining a cluster.

The Clustan package (see Wishart, 1978) contains a general monothetic algorithm that can be used with a large number of intercluster dissimilarity coefficients.

In view of constructing a technique particularly suited for clustering large data sets, Openshaw (1980) has compared 17 methods using 24 data

sets with known cluster structure. Four of these methods are variants of association analysis, one is group analysis, and the general monothetic algorithm is considered with 12 intercluster dissimilarity coefficients. Combining the criteria of quality and computation time, Openshaw concluded that the error sum dissimilarity coefficient was best suited for clustering large data sets. The main idea he introduced to improve the performance of the algorithm is to use a sparse matrix technique to store only the nonzero measurements. According to Openshaw, his method makes it possible to cluster data sets of 50,000 to 400,000 objects with 50 variables into 35 groups in times going from 170 to 800 CPU seconds on an IBM 370/168. Openshaw also proposes a relocation method to improve the resulting clustering.

5.3 Some Other Divisive Clustering Methods

The methods discussed so far in this chapter are all divisive and monothetic, and specifically designed for handling binary data. The divisive methods of Chapter 6 are of the polythetic type and intended for clustering continuous data. However, those methods can also be used for binary data, as we will see further on. In this section two additional situations will be investigated: monothetic methods for quantitative measurement data and polythetic methods for binary data.

Gower (1967) proposed a variant of association analysis in which the separation variable is the one that maximizes the multiple correlation coefficient R^2 instead of maximizing the sum of simple correlation coefficients (see Section 5.1). As in association analysis, each variable is considered in turn and a multiple linear regression is carried out with the other $p - 1$ variables as explanatory variables. Normally, this would require a matrix inversion for each variable. However, Gower also gives a way to replace all these matrix inversions by a single one, thus considerably reducing the amount of calculation.

As Gower remarks, his variant is also suited for quantitative data, provided a rule is added for splitting the set of objects using the selected variable. Gower suggests using a cutoff point q that maximizes the difference between the mean values of the selected variable in both subgroups. The set is then split into objects for which the selected variable is less than q and objects for which it exceeds q. Another monothetic method for quantitative measurements is to start by determining cutoff values for all variables (possibly in the same way as suggested by Gower) and then to replace all values below the cutoff value by 0 and the values above it by 1. Subsequently, the clustering can be carried out using MONA. This approach can also be used for mixed data sets.

The *projection pursuit* algorithm of Friedman and Tukey (1974) is similar to monothetic clustering because it also uses a single variable for the splitting at each iteration. (However, because the variable is a linear combination of the original variables, their algorithm is closer to the polythetic methods.) The CART approach to discrimination and regression analysis (Breiman et al., 1984) uses the same kind of tree structure.

When investigating binary data, and if one does not absolutely require a monothetic classification, a natural approach is to construct a matrix of dissimilarities between the objects and subsequently to apply one of the polythetic divisive algorithms. This can be achieved by using DAISY for the dissimilarity matrix and then running DIANA in which the option of dissimilarity input is selected. This approach has the additional advantage of also allowing other clustering methods, such as agglomerative nesting or partitioning, based on this dissimilarity matrix.

Another algorithm in this category of polythetic methods for binary data was proposed by Macnaughton-Smith et al. (1964). This much cited method is a variant of their algorithm for quantitative data. The splitting of a cluster X proceeds by the construction of a splinter group, to which objects are assigned one at a time. Suppose the dissimilarity between two clusters A and B is denoted by $d(A, B)$. Let us denote the splinter group found so far by X_0 and investigate the transfer of an object x_i to the splinter group. One then calculates the dissimilarity between object x_i and the remaining objects:

$$d(X \setminus X_0 \setminus \{x_i\}, \{x_i\})$$

and the dissimilarity between x_i and the splinter group:

$$d(X_0, \{x_i\})$$

If the difference between these two dissimilarities

$$d(X \setminus X_0 \setminus \{x_i\}, \{x_i\}) - d(X_0, \{x_i\})$$

is positive, object x_i is a candidate for joining the splinter group. All objects remaining in X are considered, and the object is transferred for which the computed difference is maximal. If all the differences are negative, the separation of this cluster stops. For binary data Macnaughton-Smith et al. (1964) propose the dissimilarity

$$d(A, B) = \sum_f \left[(\bar{x}_{Af} - \bar{x}_{Bf})^2 \sum_{g \neq f} \chi^2_{fg} \right]$$

where $\bar{x}_{Af}$ and $\bar{x}_{Bf}$ denote the proportions of objects possessing the attribute f in the clusters A and B. In order to reduce the amount of calculation, the χ^2_{fg} values are calculated in the cluster X which is to be divided, and not recalculated in the successive groups ($X \setminus X_0$ and X_0) along the way.

EXERCISES AND PROBLEMS

1. Consider the data set of Table 1. Compute the total similarity between variable 1 and all other variables. Repeat this computation for variable 2, and so on. Which variable yields the largest total similarity?

2. The animals data were listed in Figure 7 of Section 3. Cluster this data set with MONA, after dropping the animals for which not all measurements are available. Compare the results with those obtained in Section 3. In particular, the order in which the variables are selected should be considered in both outputs.

3. Extend the animal data set given in Figure 7 by adding data on 10 more animals. Cluster the entire data set using MONA. Compare the results with those obtained for the original data.

4. Consider the family data clustered in Section 3. Compute a dissimilarity matrix between objects with the program DAISY (considering all binary variables to be symmetric) and apply DIANA to it. Compare the resulting hierarchy with the MONA results in Section 3.

5. Repeat the preceding exercise for the data set of animals in Figure 6, again considering all binary variables to be symmetric.

6. Consider the mixed data set of flowers listed in Table 12 of Chapter 1.
   (a) Apply MONA to the data set obtained by considering only the binary variables.
   (b) Transform the other variables into binary variables by grouping values, and then apply MONA to the entire data set.

7. The program MONA can also be used to cluster a set of binary *variables*. For this purpose the data matrix must first be transposed. Apply this approach to cluster the variables of the family data described in Section 3. Check that another clustering may be obtained

when some of the original variables are coded differently (that is, by interchanging 0 and 1).

8. **(a)** Which values can be taken by the association measure between a variable and itself? In which situation is this similarity maximized?

(b) Consider a clustering algorithm, similar to the one used in MONA, in which the selection of a variable is based on the sum of similarities to *all* variables (including the variable itself). Which variables will be favored by such an algorithm?

9. Compute upper and lower bounds on the similarity used in MONA, for a data set containing n objects. Suggest a way of transforming the similarity between variables into a dissimilarity. Such a dissimilarity can then be used as input for PAM, FANNY, AGNES, and DIANA to cluster the variables.

10. Construct a divisive monothetic algorithm for binary data, where the data are split according to the variable with smallest total Manhattan distance (computed from the transposed data matrix) to all other variables. Apply this algorithm to the data set of Table 1 and compare the results with Figure 4.

Finding Groups in Data: An Introduction to Cluster Analysis
Leonard Kaufman and Peter J. Rousseeuw

Appendix

The purpose of this appendix is to provide additional information about the programs described in this book. Besides giving a better understanding of the implementation of the various techniques and algorithms, this information should allow the reader to use the programs efficiently and to adapt them to his or her particular requirements when needed. Moreover, Section 4 describes a new program called CLUSPLOT, by which a graphical representation of a partition can be obtained.

1 IMPLEMENTATION AND STRUCTURE OF THE PROGRAMS

The programs of Chapters 1 to 7 were written in Fortran. In an effort to make the programs as portable as possible we have decided to impose several restrictions:

Many statements that are not used in the same way by all compilers or that may make it difficult to modify the programs were excluded, such as COMMON, DATA, EQUIVALENCE, EXTERNAL, REAL, INTEGER, and DOUBLE PRECISION.

The only inline functions were ABS and SQRT.

Names of variables and routines were limited to five alphabetical characters. To avoid confusion, the characters I, O, 1, and 0 were not used.

The first versions of the programs were written for a mainframe computer. These were extensively tested for portability using the PFORT verifier (Ryder, 1974) and ran without problems on many different machines, using either Fortran IV or Fortran 77 compilers. However, when the IBM-PC standard for personal computers came in general use, we decided

to switch to the PC and to make all the programs interactively operated. Although this was done at the expense of some of the portability, this original aim was withheld whenever possible. Adapting the programs to various compilers has proven to be very straightforward. Even the adaptations necessary to run CLARA on a parallel computer system (see Section 5.3 of Chapter 3) were minimal.

The way the logical names of input and output files are assigned in the programs also serves the purpose of making them portable. The numbers of the input and output files are given in the main program unit, right after the dimension statements. In all programs, except DAISY and CLARA, the following statements are used:

LUA = 1 (input file containing the data set)
LUB = 2 (output file containing the clustering results)
LUC = 3 (file used for saving the data set if it was entered from the keyboard).

The program DAISY may open up to three new files: LUB contains information on the variables and the missing values, LUC is the file used for saving the data set if it was entered from the keyboard, and the dissimilarity matrix computed by the program is sent to LUD. In CLARA, which can only be used to process large data sets, the data always must be read from an existing file, so LUC is not used there. In all programs the actual numbers may of course be adapted to the user's hardware.

The names of all input and output files are entered during the interactive dialogue at the beginning of each run. The variables used for these names are FNAMEA, FNAMEB, and FNAMEC. They consist of up to 30 characters and may contain a drive and a path. In all programs except CLARA the data may also be entered from the keyboard, provided the user types KEY in answer to the relevant question. This instructs the program to assign the characters CON to the variable FNAMEA. The name of the output file can be given as CON (if the output should be shown on screen), as PRN (if it should be directed to the printer), or the name of a disk file may be given.

2 RUNNING THE PROGRAMS

The programs described in this book all run on an IBM-PC, XT, AT or any compatible computer with at least 256 K of storage. A printer is not mandatory, but if one is available the output can be sent to it. In order to make this output easy to interpret, it was decided to make all of its lines at most 80 characters long, so that it fits on any screen or printer. The first character of any output line is always left blank.

The correspondence between programs, techniques, and chapters is shown in the following table:

Program	Purpose	Chapter
DAISY	Computing dissimilarities	1
PAM	Partitioning by means of the *k*-medoid method	2
CLARA	Partitioning large data sets	3
FANNY	Fuzzy partitioning	4
TWINS	Agglomerative and divisive clustering (it combines the programs AGNES and DIANA)	5 and 6
MONA	Monothetic analysis of binary data	7

Each program can be run by simply typing its name and hitting the return key. This starts an interactive dialogue during which the user may select certain options by responding to a series of questions. The program checks each answer to see whether it is a valid option or specification. If this is not the case, a message is given and the question is reiterated. For example, when entering the number of objects in PAM (and in most other programs), the following dialogue is possible:

```
THE PRESENT VERSION OF THE PROGRAM CAN HANDLE UP TO 100 OBJECTS.
(IF MORE ARE TO BE CLUSTERED, THE ARRAYS INSIDE THE PROGRAM MUST BE ADAPTED)

HOW MANY OBJECTS ARE TO BE CLUSTERED ?
-------------------------------------
PLEASE GIVE A NUMBER BETWEEN 3 AND    100 : 2

AT LEAST 3 OBJECTS ARE NEEDED FOR CLUSTER ANALYSIS,
PLEASE FORESEE MORE OBJECTS

HOW MANY OBJECTS ARE TO BE CLUSTERED ?
-------------------------------------
PLEASE GIVE A NUMBER BETWEEN 3 AND    100 : 120

NOT ALLOWED ! PLEASE ENTER YOUR CHOICE AGAIN :

HOW MANY OBJECTS ARE TO BE CLUSTERED ?
-------------------------------------
PLEASE GIVE A NUMBER BETWEEN 3 AND    100 : 12
```

Many options take the form of a yes/no question. Only the first character of the answer is read. Both y and Y are interpreted as yes, and both n and N are taken to mean no. All other characters will cause the question to be asked again, as in the following excerpt:

```
DO YOU WANT GRAPHICAL OUTPUT (SILHOUETTES) ?
PLEASE ANSWER YES OR NO : u
NOT ALLOWED ! PLEASE ENTER YOUR CHOICE AGAIN : y
```

Because such questions occur very often, a special subroutine was written for this purpose.

Provisions similar to those for yes/no questions were made for other situations, such as the choice between measurement input (m) and input of dissimilarities (d). Sometimes options are numbered, such as 1, 2, 3, and 4 at the beginning of DAISY. In such case all other characters are rejected.

When the name of an input file is entered, the program verifies whether it exists. If it cannot be found on the disk, the program states this and asks for the name once again. However, the program does *not* check whether a file specified for *output* already exists. If it does, it will be overwritten by the new file. For both input and output files, the program does verify the correctness of the file name syntax. A mistake will be signaled by the program, which will then ask for another name.

For the input of the data, the programs allow the choice between free and fixed format. The free format, which is the easiest to use, supposes that the data all consist of numbers separated by blanks. If some data stick together or if some of it is not numerical (even if these variables are not used for the clustering), the user must supply an input format. Because the Fortran variables used for the data are real, only F and E formats are allowed. The general structure of an F format is Fw.d where w denotes the total number of characters (including the decimal point) and d is the number of digits after the decimal point. If the number to be read does not contain a decimal point, it may occupy all w positions. In this case, the rightmost d digits are interpreted as following the decimal point. (However, decimal points that occur at the "wrong" place take precedence over the format specifications.) Examples of F formats are F15.7 and F8.0. E formats are written as Ew.d. Also here, w is the total number of characters in the field and d is the number of digits after the decimal point. The number may also contain an exponent that is either a sign followed by an integer or an E followed by an optional sign followed by an integer. Note that the data may also contain an exponent when an F format is used. If the same E or F format is appropriate for several variables, it can be preceded by a repetition factor (as for example in 8F10.2).

```
D                   (input of dissimilarities)
12                  (number of objects)
1                   (initial number of clusters)
3                   (final number of clusters)
Country data set    (title for output)
N                   (small output is wanted)
Y                   (graphical output is wanted)
N                   (no object labels will be entered)
Y                   (data will be read in free format)
COUNTRY.DAT         (name of the file containing the data)
COUNTRY.PAM         (name of the output file)
Y                   (all entered specifications are OK)
```

Figure 1 Input file to be used with the program PAM: Its use replaces the interactive dialogue.

To make it possible to disregard one or more positions on the input line, an X format may be used. For example, the format 10X ensures that 10 positions are skipped. Such a format is necessary if this field contains nonnumerical characters. Finally, one or several / make it possible to employ several input lines for the same object. Each time a / is encountered, the program moves to the next input line.

Apart from the usual interactive input of options and parameters as described in each chapter, it is also possible to use an input file containing all the answers and options that are otherwise entered by keyboard. Figure 1 shows an example of such an input file for PAM. The meaning of each line is shown between brackets.

In order to use such an input file (instead of typing the options and parameters on the keyboard), the input to the program must be redirected. This is possible by using a "less than" sign in the command. Suppose the input file depicted in Figure 1 is named OPTIONS.DAT and that it should be used with PAM. This is achieved by typing the instruction

```
PAM < OPTIONS.DAT
```

assuming that the file OPTIONS.DAT is on the current disk.

3 ADAPTING THE PROGRAMS TO YOUR NEEDS

In the course of an application it may be necessary or desirable to modify a program. The most frequent type of modification is due to the size of the data set to be clustered. All of the programs begin by assigning values to the maximum dimensions of problems that can be processed. For example, in PAM, FANNY, AGNES, and DIANA the following upper limits are

set:

```
MAXNN = 100  (maximum number of objects)
MAXTT = 80   (maximum number of variables in the data set)
MAXPP = 20   (maximum number of variables that
              can be used for the clustering)
```

In order to adapt these values, both the assignment statements and the DIMENSION and CHARACTER statements located at the beginning of the main unit must be changed. However, no changes are necessary in the subroutines because the upper limits are passed on as arguments in the calling sequences. It should of course be noted that a modification of the dimensions of the arrays has implications on the compilation of the programs. The characteristics of the compiler should be considered when carrying out any changes. For example, if MS Fortran is used it might be necessary to add a $LARGE metacommand at the beginning of a program to accommodate large arrays.

Sometimes the user might want to change the algorithm used by the program. This is most likely to be the case for AGNES (Chapter 5) because of the popularity of a variety of agglomerative clustering methods. As was explained in Section 5.1 of Chapter 5, a slight alteration in the subroutine AVERL makes it possible to replace the group average method by one of six other agglomerative techniques. In CLARA, the algorithm can be (slightly) modified by changing either the number or the size of the samples that are clustered. In the beginning of the main program unit the statements

```
NRAN = 5
NSAM = 40 + 2*KK
```

are used to determine the number of samples and their size. Both statements may be altered.

Finally, the user may also change the appearance of the graphical output of all the clustering programs by modifying the following assignment statement that is to be found in the subroutine ENTR:

```
NUM ='0123456789* + '
```

Changing the last two characters * and + will alter the graphical output considerably, because these characters make up the silhouettes and the banners.

4 THE PROGRAM CLUSPLOT

The graphical output of the partitioning programs (PAM, CLARA, and FANNY) consists of the so-called silhouettes. These provide a visual representation of each cluster, together with some statistics (the average silhouette width for each cluster and for the entire data set). Apart from this representation it seemed instructive to have a display containing both the objects and the clusters. Such a drawing can picture the size and shape of the clusters and their relative position in space. (Note that this information is partially provided by the neighbor of each object, as shown in the silhouette plot.)

CLUSPLOT is a menu driven PASCAL program that uses output from a partitioning algorithm to visualize the objects and clusters in a two-dimensional plot. The input data structure can either be a matrix of objects by measurements or a dissimilarity matrix. The program also requires the input of a clustering vector, containing the cluster number of each object. The number of clusters drawn by CLUSPLOT is the number of different entries found in the clustering vector.

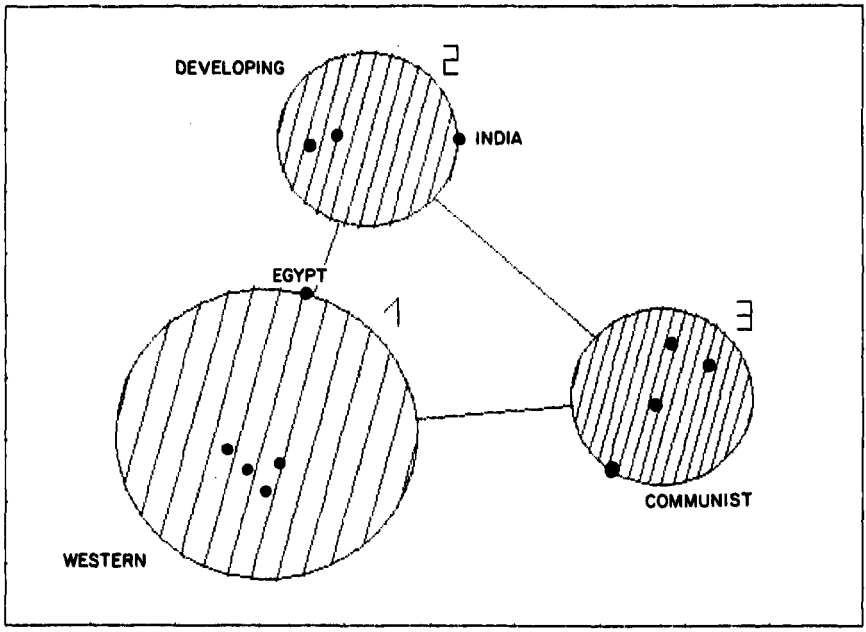


Figure 2 Example of a CLUSPLOT output.

If a dissimilarity matrix is used as input, CLUSPLOT begins by converting the data to two-dimensional coordinates by means of multidimensional scaling. The same technique is used if the data consist of a matrix of measurements with more than two variables.

In the plot, clusters are indicated by circles or ellipses. The program has options allowing the rotation and intersection of the clusters, in order to use the screen area in an optimal way. Further options make it possible to draw the individual points, number the clusters, plot the coordinate axes, shade the clusters, and draw lines between them. Also, the plot can be saved in a file for a quick reproduction on a later occasion.

Figure 2 is a plot showing the results of PAM, obtained by clustering the 12 countries data set into three clusters. The partition itself was discussed in Section 3 of Chapter 2.

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