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AN EVALUATION OF CLUSTER ANALYSIS AND RELATED MULTIVARIATE TECHNIQUES FOR OPERATIONAL RESEARCH

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LIST OF SYMBOLS USED CONSISTENTLY THROUGHOUT

N , n	the number of observations or objects
M , m	the number of variables
S , s	any similarity measure, unless otherwise specified
S(a,b)	the similarity between the objects or sets a and b
D	any dissimilarity measure
D(a,b)	the dissimilarity between the objects or sets a and b
d	a dissimilarity measure, usually constrained to be in a lower dimensioned space than D

D

ORDINATION METHODS

1. General Discussion
2. Explanation of Methods
3. Discussion and Comparison of Methods
4. Conclusions

D.1 GENERAL DISCUSSION

Ordination methods differ from clustering in that the final product - a low dimensional configuration - is not normally an end in itself, and the information which comes out of this technique is normally from the user's visual analysis of the ordination. For example the extraction of labels for dimensions, the discovery of sub-groups within the objects, etc., are all left to user control. In cluster analysis the technique produces an answer, rather than a simplified question as in ordination.

Despite the apparent vagueness of the interpretation of the end product, the aim of the method is clear - to reduce dimensionality in a 'best' way. As in cluster analysis which forms 'optimal' groups, the diversity of methods arises from the definition of a 'best' way.

Ordination methods are thus very varied, and also difficult to categorize into types. Even the division into metric and non-metric methods is not clear-cut, since methods can be devised which attempt to preserve both the rank order and the magnitude of the original distances. However most current methods may be divided on the basis of metric or non-metric properties. A metric method is based on the numerical sizes of the interpoint distances, which are preserved in a 'best' way, in a lower dimension. A non-metric method is one which attempts to preserve only the rank order of these distances in the lower space. For

further categorization of the methods we can suggest five classes into which most current methods may be grouped. These are as follows:

Non-metric methods

1. Stress minimization
2. Manual calculation

Metric methods

1. Dimension elimination
2. Stress minimization
3. Manual calculation

Stress minimization methods begin with a space (usually Euclidean) of specified dimension and in that space find the configuration of points which gives an optimal approximation of some kind, to the original points. Stress is the term used in the method by Kruskal (1964) for a particular function, but here we use it as a general term for any measure of distortion of data in producing a lower dimensioned space.

Non-metric stress minimization is often termed multidimensional scaling, and we have adopted Anderson's (1971) terminology of minimization of loss functions for the metric case. Both these terms could easily be applied to all stress minimization methods, but we shall continue with their now conventional use. In all these cases the ordination procedure is carried out for several dimensions, and in each case the minimization is performed by hill-climbing methods such as the method of steepest descent.

The non-metric manual methods are the psychological scaling methods, which were the forerunners of the current multidimensional scaling techniques. These include the unfolding methods due to Hays and Bennett (1961). These methods are quite lengthy when performed by hand calculation, involving logical steps leading from a raw data matrix to a final ordination which gives only a rank order of the observations on each axis and not exact co-ordinates, so inter-point distances have no meaning in the configuration. This type of method which has both non-metric input and output is called fully non-metric.

In comparison the metric manual methods are more heuristic than their non-metric counterparts. This is because they lack the rationale of methods based on a foundation of psychological theory, as the early unfolding methods had. These metric methods often proceed by progressively fitting points into their 'best' position in a two-dimensional space, and do not utilize the full distance matrix.

Dimension elimination methods are different from other methods in that they do not try to distort the objects into a certain number of dimensions, but rather rotate the configuration of points so that a maximum amount of information lies in as few dimensions as possible. Thus these methods discard dimensions which are of less value. Principal components analysis is perhaps the best example of this type of method - the rotation which takes place involves

no changes in inter-point distance, and the final step of dimension truncation is left to user control.

Seriation methods which we have discussed in Section B.4 can be considered as a separate type of ordination method. As was brought out in the previous discussion on seriation, the limitation to one dimension is dangerously restrictive, and the supposition that time is the major dimension in archaeological data can lead to serious error. The only advantage that seriation possesses is speed, and it could be that these methods would be of some use as a quick test, if they were used with a stress measure. It is also possible that they could be used as a good initial configuration for the stress minimization methods. It should be noted that seriation methods normally proceed from metric input to non-metric output.

The methods discussed in Section B.4 as pure seriation methods will not be analysed further in this section, as they are seen to have little value outside (and possibly in) archaeological dating.

Under the classification discussed above we shall examine several methods, as follows:

Non-Metric

Stress minimization	- Shepard/Kruskal
	- Torgerson & Young
	- Guttman & Lingoes
	- McGee
	- Carroll & Chang
Manual calculation	- Hays Unfolding Model

Metric

Dimension reduction	- Principal Component Analysis
	- Factor Analysis
	- Principal Co-ordinate Analysis
Stress minimization	- Loss functions
Manual calculation	- Bray & Curtis
	- Orloci

The metric methods above have developed virtually independently under the three classes - the dimension reduction methods originally in psychology, and the other methods mainly in ecology. The non-metric methods also had origins in psychology, surprisingly almost independently of the dimension reduction methods. The non-metric stress methods are all fairly similar and arose from the early unfolding work, and re-initiated by Shepard's work in 1962.

We proceed in the next section to explain the methods referred to above.

D.2 EXPLANATION OF METHODS

1. Principal component and factor analyses

2. Principal co-ordinate analysis

3. Bray and Curtis' method

4. Orloci's method

4a. Alternative to Orloci's method

5. Hays' multidimensional unfolding method

6. The Shepard/Kruskal method (MD-SCAL)

7. Torgerson and Young's TORSCA

8. Guttman and Lingoe's smallest space analysis

9. The elastic distance method of McGee

10. Carroll and Chang's INDSCAL and MDPREF models

11. Loss functions

1. Principal Component and Factor Analyses

These methods have been discussed earlier. They were the first ordination methods to be used and have been applied in many fields. The procedures are fast and readily available. The methods produce an optimum and give a measure of fit. The reduction to fewer variables is virtually assured by these methods without significant loss of information, but the reduction to say 2 or 3 axes cannot normally be achieved without large information loss. The methods do not attempt to preserve inter-point distance and a useful addition to the method is to connect the points by their minimum spanning tree in order to give a better picture of the relationship between points. This technique may be employed with any ordination, but seems particularly useful in the cases where inter-point distance is not considered in the optimization procedure. Because principal components produces an ordination very quickly and its solution will be fairly similar to other ordinations, it is sometimes employed as an initial configuration which is iteratively improved upon to attempt to minimize another objective function. Principal components analysis and factor analysis are both fully metric - they require metric input data and produce metric output.

2. Principal Co-ordinates Analysis

This procedure is due to Gower (1966, 1967a). It is very much related to principal components but more generalized. It begins with a distance matrix with elements d_{ij} and then forms the matrix with elements $-\frac{1}{2}d_{ij}^2$ which is

centred by subtracting row and column means and adding the overall mean. From this Gower shows that the k^{th} latent vector of this matrix, normalized so that its sum of squares is equal to the k^{th} latent root gives the co-ordinates along the k^{th} principal axis. The method will thus give identical results with principal components analysis if Euclidean distance is used, but the Gower procedure can be used with any distance measure. In order for real co-ordinates to exist the centred matrix above must have non-negative roots. This is a necessary and sufficient condition which many distance measures comply with. Thus the input data may be non-metric to this procedure. The method has been used by Rayner (1969) in pedology.

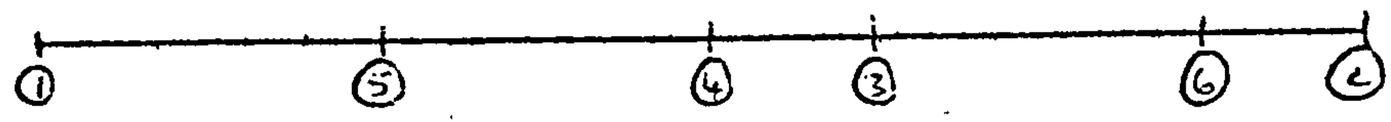
3. Bray and Curtis' Method

This method was an early heuristic attempt at ordination, arising from the need in ecology to understand large data sets. It was introduced by Bray and Curtis (1957) and has been used almost exclusively in ecology, and mainly in America. The authors were forced to reject the use of factor analysis in their study of forest plant life as being too heavy computationally, also they did not wish to use correlations because of its sensitivity at low values where error played a large part.

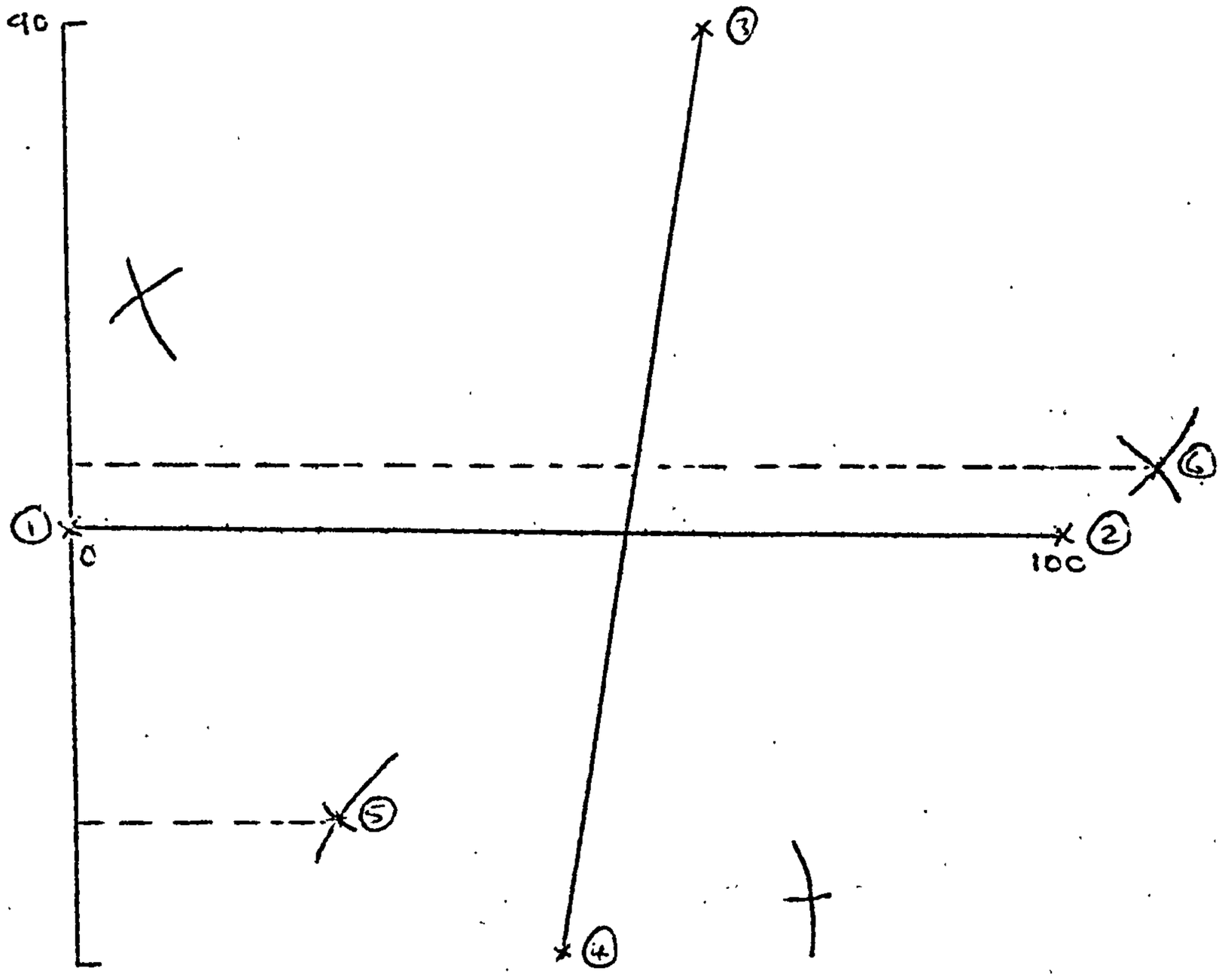
Their method begins with a distance matrix. Suppose we have the following matrix:

1	X					
2	100	X				
3	90	75	X			
4	80	80	90	X		
5	40	80	85	30	X	
6	90	25	60	70	75	X
	1	2	3	4	5	6

The furthest two points are selected as reference points and are placed at either end of the x axis. All other points are projected onto this line. This can be performed rapidly using compass and ruler. This, in the above example, gives the one-dimensional ordination:



A second axis is constructed by selecting another pair of reference points which are close together on the first axis, but yet still separated by a large distance - e.g., points 3 and 4 in the example. Both of the points are fixed by their distances from the first two reference points. The y axis is constructed perpendicular to the x axis and scaled so that the second pair of reference points 3 and 4 are d_{34} apart on this axis. So in our example we have:



Other points are projected onto the y axis, using compass and ruler by their distances from the second reference pair. Of the two possible positions for point 5 the one which is chosen depends on the nearness of 5 to points 1 and 2; this gives the position 5 in the above diagram. The y co-ordinate is the projection of this point on to the y axis. Similarly other points such as 6 are given a y co-ordinate. A z co-ordinate can be constructed in a similar manner. The method has the advantage that it is very fast and can be executed manually. It has, however, several disadvantages, the major one being that even if the data is two-dimensional, unless the second reference pair have the same x co-ordinate, then the ordination does not give a true configuration. This could be rectified by construction of the second axis parallel with the line joining the second reference pair and having oblique axes.

Other disadvantages are the dependence on a few reference points, which, if subject to error, distort the whole ordination, and there is no measure of fit to determine how good an ordination is.

Users of the method include Gittins (1965), Beals (1965), Gimingham et al (1966), Hole and Hironaka (1960), Kershaw (1958), Swan and Dix (1966) and McIntosh (1965).

4. Orloci's Method

This method (Orloci 1966, Austin and Orloci 1966) is a modified form of the Bray and Curtis method but is mathematically exact. The first axis is obtained and points are positioned on this axis in the same way as in the original paper, which can be stated as:

$$x_{1j} = \frac{D_{1j}^2 + D_{12}^2 - D_{2j}^2}{2D_{12}}$$

The point furthest from the first axis is chosen to initiate the y axis. y-co-ordinates are obtained from the formula:

$$y = \frac{D_{1j}^2 - X_{1j}^2 + D_{13}^2 - X_{13}^2 - D_{3j}^2 + (X_{1j}-X_{13})^2}{2\sqrt{(D_{13}^2-X_{13}^2)}}$$

Similarly other axes can be constructed (Orloci 1966).

A formula is also given for the 'efficiency' of the k^{th} axis in accounting for the original interstand distances, which is simply the ratio of the average inter-point distance on the k^{th} axis to the average inter-point distance in the original matrix.

4a. Alternative to Orloci's Method

Orloci's method gives a perfect ordination of two-dimensional data, but is heavily reliant on the choice of the first 2 reference points, since all other co-ordinates in all dimensions are reliant on these points. This is of obvious advantage if the position of two points is known with little error, in which case it would be better to select those two points in which one has greatest confidence, rather than the two most dissimilar as Orloci employs.

The proposed method follows Bray and Curtis' original suggestion more closely than Orloci's and spreads the 'responsibility' of the early reference points. The first axis is obtained using the procedure of Orloci, but with an option to use other reference points if they are considered more suitable. Two points are selected for the second axis, normally by finding that pair for which $d_{ij} - |d_{1i}-d_{1j}|$ is a maximum. Suppose these points are 3 and 4 then $y_4 = 0$ and $y_3 = (d_{34}^2 - (d_{13}-d_{14})^2)^{\frac{1}{2}}$. The position of all other points (including the first two reference points) is found on this axis in the same manner in which the co-ordinates on the first axis were evaluated. This can be simply extended to more dimensions, and a measure of fit similar to Orloci's may be used.

5. Hays' Multidimensional Unfolding Method

Before proceeding to discuss a particular ordination method in psychology, it will be useful to consider the general field of psychological data analysis, since this is

one of the oldest areas of measurement and scaling usage. Coombs (1964) (see also Coombs et al 1970, Green and Carmone 1970) divides data into four types, firstly according to whether they are based on one or two sets of data (i.e. with one set data - comparisons are only made between stimuli; with two set data - stimuli are rated, and hence the rater is under investigation as well as the stimuli), and secondly according to whether the emphasis is on proximity or dominance (i.e. if we ask if A is taller than B, or if B is taller than A, then we are concerned with dominance on a certain scale, whereas if we ask if A and B are the same height or not then we are concerned with proximity). These differences may at first seem subtle, and indeed a set of data may be classifiable in more than one category, but if we consider the normal type of data obtained in each case the differences should become clearer. Coombs' classification is as follows:

	Dominance matrix	Proximity matrix
Two sets	Quadrant II: Single stimulus	Quadrant I: Preferential choice
One set	Quadrant III: Stimulus comparison	Quadrant IV: Similarities

Typical questions to obtain data for each of the quadrants are as follows:

QI - Preferential Choice. Rank the following in order of preference.

QII - Single Stimulus. Rate the following according to their possession of property x on a scale 1 to 5.

QIII - Stimulus Comparison. Which of the following pair of objects do you think possesses property x the most?

QIV - Similarities. Which pair is more similar? A and B or C and D?

Each type of data lends itself to its own particular kind of analysis. Most of the pre-1960 methods are discussed in Coombs (1964) and Torgerson (1958), we list them here with their original references:

QI Parallelogram analysis (Coombs 1953)
One dimensional unfolding (Coombs 1950, 1953)
Multidimensional unfolding (Bennett and Hays 1960, Hays and Bennett 1961)
Factor analysis (Coombs and Kao 1960a, b)

QII Guttman's scalogram analysis (Guttman 1944, 1950)
Lazarfeld's latent distance model (Lazarfeld 1959)
Categorical judgment model (Torgerson 1958)

QIII Law of comparative judgment (Thurstone 1927)
Bradley, Terry, Luce model (Bradley and Terry 1952, Luce 1959)

PAGE NUMBERING AS ORIGINAL

QIV Multidimensional unfolding (Hays 1954, Coombs 1964)

Factor analysis (Torgerson 1952)

Shepard and Kruskal's MDSCAL (Shepard 1962a, b, Kruskal 1964a, b)

Torgerson and Young's TORSCA (Torgerson 1965, Young and Torgerson 1967, Young 1968)

Guttman and Lingoes' SSAR (Lingoes 1965, Guttman 1967, 1968)

McGee's elastic distances model (McGee 1965, 1966, 1967)

Carroll and Chang's INDSCAL (Carroll and Chang 1970)

Current research in mathematical psychology is currently being directed away from its more traditional QII and QIII data analyses, and towards QI and QIV data, and it is in these areas where ordination is particularly applicable (QII and QIII data may be ordinated, but only after conversion to QI or QIV type).

One of the first psychological methods for producing ordinations was that due to Hays. The method is dealt with at length in Coombs (1964) and Coombs, Dawes and Tversky (1970). It is essentially a hand method, and can be a lengthy procedure. The method is based on the idea that the best one dimensional representation of three points will consist of the two furthest points and the projection of the third point on to the line connecting them. The procedure considers all sets of three points (called triples) in order to determine the best configuration. Firstly the most dissimilar pair is found by constructing a partial order of distances (i.e. if a respondent ranks in order ABCD then $AB < AC < AD$, thus from all respondents a partial order may be constructed). These are selected to define the first axis.

From the similarity matrix can be picked out the rank order which begins with each of this pair. From these a partial order of stimuli is obtained. If all triples are satisfied then this order is the final one, otherwise the order is selected which satisfies the most triples. A second dimension can be constructed using all the unsatisfied triples.

The method is fully non-metric, with both input and output data being rank orders. This means that any monotone transformation could be performed on the axes, and so relative distances are meaningless on the Hays configuration. Also, even if Hays' method in a particular case violates none of the triples in k dimensions, this does not mean that a metric solution can necessarily be obtained with that dimensionality.

6. The Shepard/Kruskal Method

The early work of Shepard (1957, 1958a, b, 1960) was concerned with the relationship between the psychological similarity of stimuli and the representation of this in metric space. He postulated an approximately exponential transformation in one particular case (Shepard 1958b), but observed that one had no reason to suppose that this relationship held for other data, and indeed one is more often concerned with finding the transformation than with the metric configuration itself.

The method he later proposed (1962a, b) was a landmark in multidimensional scaling, combining non-metric input with metric output. The only assumption made about the transformation function is that it should be monotonic. Any n points can be placed in a space of n-1 dimensions so as to preserve the rank order of the interpoint similarities (this has been formally proved by Bennett and Hays 1960, but if we consider four points forming a tetrahedron in three-space, it can be seen that the length of any side can be shortened to zero or lengthened until it is the longest without changing the other lengths). The procedure begins by finding this n-1 dimensional problem by an iterative process. The points are placed equidistant (i.e. at the vertices of a simplex) in the n-1 space, the 'force' on each point from the others trying to move it nearer or further to them to satisfy the rank order is calculated, and each point is moved in the direction of this force, and so on until an optimum is reached. There is no unique solution, and thus the additional requirement of minimum dimensionality is introduced. Principal component analysis is used to reduce the dimensionality, by ignoring dimensions which account for little of the overall variance, this also gives an initial configuration in the reduced space. Iterations take place as before to find an optimum (this may however be a local optimum). In this smaller space it will probably be impossible to satisfy the rank order of distances entirely, and a measure of fit is used - the mean square discrepancy between the original and derived rank orders.

One of the outputs of the method is (what Kruskal called) the Shepard diagram - a graph of similarities against derived distances. This gives a picture of the transformation function. The Shepard diagram is of use in any ordination and can indicate particular points which have not been able to be placed satisfactorily in the ordination.

Kruskal (1964a, b) improved upon Shepard's work by putting his method on a more rigorous basis. The original dissimilarities are first ordered so that:

$$D_1 < D_2 < \ldots\ldots < D_M \qquad (M = n(n-1)/2)$$

We position the n points randomly in a k dimensional space and thus we have associated with these dissimilarities, distances $d_1, \ldots d_M$.

These distances will probably not have the same rank order as the dissimilarities, but associated with each dissimilarity we assume a monotonic function $f(D_i)$ which transforms the dissimilarities into distances $\hat{d}_i$ which thus have the same rank order as the dissimilarities. The extent to which the d_i values vary from the $\hat{d}_i$ is minimized in a normalized least squares expression called <u>stress</u>.

Thus we minimize:

$$S = \sqrt{\frac{\sum(d_{ij}-\hat{d}_{ij})^2}{\sum d_{ij}^2}}$$

subject to $\hat{d}_{ij}$ monotone.

This is accomplished by the method of steepest descent. The method is performed for several dimensions and the 'best'

dimensionality is selected as that which has a low stress and if the dimensionality is decreased by one results in a much higher stress. The method has been subjected to random data to determine what is a 'low' or 'high' stress - see Klahr (1969), Stenson and Knoll (1969) and Wadenaar and Padmos (1971). Additional work is contained in Shepard and Kruskal (1964) and Shepard (1966). A computer program for the method called MDSCAL has been produced which is currently up to version 6MP and is available from Ohio State University.

7. Torgerson and Young's TORSCA

This program is very similar to MDSCAL. It is normally preceded by principal components to obtain an initial configuration in the desired space. (This can be employed in MDSCAL. One may also use p.c.a. on a k+1 dim solution to obtain an initial configuration in k dimensions.)

The measure which is maximized is, with the previous notation:

$$\mathcal{L} = \tfrac{1}{2} + \tfrac{1}{2} \frac{\sum \hat{d}_{ij} d_{ij}}{\sqrt{\sum \hat{d}_{ij}^{2} \sum d_{ij}^{2}}}$$

subject to $\hat{d}_{ij}$ monotone, and where d_{ij} is distance in Minkowski space.

The method yields very similar results to the other computer methods. Torgerson (1965) states "which program is in fact superior will depend upon the particular circumstances involved".

The program is outlined in Young (1968, 1970) and Young and Torgerson (1967) although incorrect objective functions are given. The method has been used extensively by Green and co-workers (Green, Maheshwari and Rao 1969, Green, Carmone and Fox 1969, Green and Maheshwari 1969, Green, Wind and Jain 1972). The program is available from Dr. Young at the University of North Carolina.

8. Guttman and Lingoes' Smallest Space Analysis

This method (Lingoes 1965, 1970, Guttman 1968) minimizes the function:

$$\frac{\sum(d_{ij} - \hat{d}_{ij})^2}{2\sum d_{ij}^2}$$

which is related to Kruskal's stress but $\hat{d}_{ij}$ is defined differently. Here $\hat{d}_{ij}$ is a permutation of the d_{ij} to maintain the rank order of the D_{ij}.

The program (SSA IV) is available from Professor Lingoes at the University of Michigan.

This method has been compared with the previous two by Green and Rao (1971) and show that all three can reproduce known configurations accurately.

9. The Elastic Distance Method of McGee

This method (McGee 1965, 1966, 1968) is somewhat different from the mainstream of non-metric scaling methods since it is concerned with distance as well as rank order.

The method, using an analogy of elastic springs connecting unit masses in space, attempts to minimize the expression:

$$W = \sum_{i<j} c^2 \left(\frac{d_{ij}-D_{ij}}{D_{ij}}\right)^2$$

which is analogous to the summed moduli of elasticity between the points. It allows longer 'springs' to be compressed by a larger percentage than the smaller ones. McGee introduces this into the model because he believes larger distances are more likely to be inaccurate. Gregson and Russell (1967) report experiments where middle-range distances were more subject to error. McGee (1967) replies on a theoretical level, showing his assumption is a direct outcome of Weber's law (a relatively old psychological law which relates the variance in response to the physical magnitude of the stimuli - see Torgerson 1958 and Guilford 1954).

10. Carroll and Chang's INDSCAL and MDPREF Models

If we have a set of responses from a group of individuals and we aggregate the data, then we are over-simplifying, since each individual may be judging on different properties, or properties may be of differing importance to him. Thus if we had a method of analysis which enabled us to identify differences in subjects perspective we could gain information.

This concept was used in Tucker and Messick's (1963) 'points of view analysis', although from the scaling of individuals (called the subject space), they only found clusters of subjects who constituted a 'point of view' and

then each of these was scaled independently. This procedure, especially the final independent scaling has come under some criticism (see Ross 1966) and a new program called INDSCAL (for INdividual Differences SCALing model) was introduced by Carroll and Chang (1970) (see also Carroll 1971, 1972, Wish and Carroll 1971, Wish 1970, 1971).

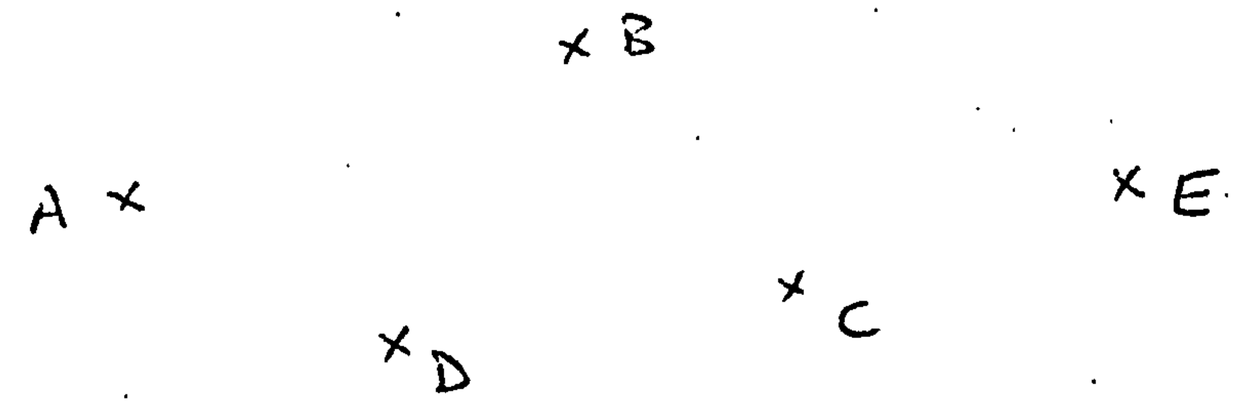
INDSCAL allows for each individual to have his own weighting for each of the axes in the scaling of stimuli (called the stimulus space). The method is analogous to factor analysis, where a representation of objects in space is obtained and also a set of vectors from the original variables, which are in this case individuals.

The procedure in fact is mathematically very similar to factor analysis, using results obtained by Torgerson (1958) for the non-metric case.

The multidimensional scaling methods of Kruskal and McGee have also been adapted to handle these cases of differing perceptions.

A related model, MDPREF, also by Carroll and Chang (see Carroll 1971,'1972), concerns itself with differences in preference rather than perception.

It is concerned with the concept of 'ideal points'. Suppose we had the following configuration showing the similarity of different drinks obtained from the responses of a group of people:



and a particular individual ranked the drinks in the order of preference DACBE. We can assume that his 'ideal' drink would be placed nearest to D in the configuration, and with A its next nearest point, and so on. Thus there exists a point (or area) on the diagram which best represents this rank order of preference. Thus for each individual we can include an 'ideal point' on the diagram.

This concept and a simple method of finding ideal points is used in Bennett and Hays' (1960) unfolding method. Carroll and Chang's method proceeds in a similar way, but enables the rater to view dimensions in differing weights.

11. Loss Functions

Loss functions are very similar to psychological scaling methods except that they try to preserve distance rather than rank order, in a minimum number of dimensions. The dimensionality s is selected and in this space we try to maintain the original distance. Thus we could minimize:

$$\sum |D - d|$$

Since this function is not differentiable at zero we may choose either to split the function or minimize its square:

$$\sum (D - d)^2$$

However, this will tend to maintain larger distances at the expense of smaller ones. Whilst this may be of some

use as a clustering method, it will not give an accurate ordination unless a constant error function is assumed. Thus we minimize:

$$\sum(\frac{D}{d} - 1)^2$$

This is solved by the method of steepest descent.

Other similar functions could be used for optimization. For example:

$\sum (D^2 - d^2)^2$	Thompson and Woodbury (1970)
$1 - \frac{\sum(D-d)^2}{\sum D^2}$	Anderson (1971a)
$1 - \frac{\sum D(D-d)^2}{\sum D^3}$	Anderson (1971a)
$\sum D(D - d)^2$	Anderson (1971b)
$\frac{1}{\sum D}\sum\frac{(D-d)^2}{D}$	Sammon (1969)
$\frac{1}{2}\sum(D - d - c)^2$	Cooper (1972) where c is an additive constant

The functions above can all be generalized to non-metric methods by the incorporation of monotonicity constraints, and similarly non-metric methods may be converted.

The use of loss functions has not been widespread because of the current interest in non-metric methods. The references above contain most of the few applications of loss functions.

D.3 DISCUSSION AND COMPARISON OF METHODS

Ordination methods have only recently come into prominence as multivariate methods, and are at a lower stage of development than cluster analysis. In clustering, most methods have a common aim, which is fairly clear, whereas ordination results require greater investigation by the user, and methods have more diverse objectives. It has thus been easier to perform comparative studies on cluster methods, and more such investigations have been published. The clustering process is also one which is more easily visualized and so the methods have been more widely applied. Green and Carmone (1970) have summed up the current state of non-metric scaling in the following words:

> "...algorithm development has out-stripped application and evaluation techniques.....testing and evaluation will be necessary over the next several years if these procedures are to receive the extent of application that they currently appear to warrant."

Most of the investigations which have been carried out have been into the properties of non-metric stress minimization - in particular, some of the works of Green, Carmone, Kruskal and Shepard. Also, the comparative studies that have been made have usually been between non-metric methods. Because of the computer programs which exist for these methods, and the lack of information on other methods, there has been a preoccupation of ordination users with these, to the exclusion of metric models. Loss functions are a fairly recent addition to ordination (despite their

simplicity relative to non-metric multidimensional scaling), and studies involving these are isolated. It is a difficulty both in clustering and here, that because of the demand for computer packages, that methods which are widely available in this form are used much more than others which are perhaps more suitable. This use of packages as black boxes often leads to an inappropriate method being used, and hence misleading results.

This section, because of the more primitive state of ordination as a technique, is designed to fill in some of the current gaps which exist - in particular in metric models. We have restricted ourselves to a more verbal than experimental comparison. This is partially due to the nature of the ordination methods we have outlined - they have been designed for slightly different purposes, and the choice of technique is to some extent dependent on the input data available and the type of output data required. In this section therefore we will attempt to arrive at decision rules which will simplify the choice of technique in any particular application. We will introduce ordination as an approach to data analysis and not as a cook-book of methods. The sort of items which we will discuss will be such questions as the type of method required by types of data, and for specific purposes, and also the properties and shortcomings of the methods. As we consider this study as a somewhat pioneering work, we shall content ourselves with outlining properties of the methods as a helpful starting point for further research rather than attempting definitive decision rules.

Our discussion will be in three general areas. Firstly a discussion of the existing non-metric method comparisons and evaluations, and the questions which they bring up. The second section will be a consideration of the metric models, and will be more experimentally based. Most of the metric versus non-metric discussion will be left until the third section, where more general topics will be discussed.

Non-Metric Methods

When the Shepard-Kruskal method was first introduced the main question was whether the method could actually give a correct configuration of data that had been monotonically transformed. In the second of Shepard's papers introducing multidimensional scaling (1962b) he gave several examples. Firstly he created a similarity measure $s_{ij} = e^{-1.4d_{ij}}$ from the Euclidean distances d_{ij} between 15 points in 2 dimensions, and his method showed almost perfect recovery of the original configuration. He repeated the experiment with an exponential decay function and an arbitrary monotonic function of line segments, and also a one-dimensional and a three-dimensional data set, all gave very good recoveries. Shepard (1966) analysed a wider range of data sets, using two-dimensional configurations and found the minimum correlation between the original and recovered data in several runs with different data with 3-45 points. The minimum correlation was over .99 for cases with over 10 points, but dropped below .90 for less than 6 points.

Young (1970) obtained results with TORSCA on Shepard's data and compared them with Shepard's results. The most important of his conclusions was:

"If one relies heavily on the stress index, the unfortunate situation exists that as he diligently gathers more and more data about an increasingly larger number of stimuli, he will become less and less confident in the nonmetrically reconstructed configuration, even though it is more accurately describing the structure underlying the data."

Shepard (1962b) also considered the recovery of dimensionality - he used the method of plotting dimension against stress, and looking for a sudden increase in the stress at a certain dimension. We shall call this the elbow method. Considering that the variance of the original points was approximately the same in each dimension, the curve was not as 'elbowed' as one might expect - the curve in the two-dimensional case was very smooth. These results may be due to the actual stress measure used, which was later replaced by Kruskal's stress. In the same paper, Shepard gives several results from real experiments, and it is interesting to note that the transformations from distance to similarity were all simple functions - linear, quadratic, or exponential.

Abelson and Tukey (1963) have shown that, given 4 points in one dimension then if we know the complete ordering of distances, then the minimum r^2 between the real points and any others with the same ordering, is between .91 and .97 depending on the actual order. They also showed that this decreased as the number of points increased, which is contrary to expectation. Shepard and Carroll (1966) suggest that this is due to the measure used, and that perhaps the expected value of r^2 would be a better indication of fit.

Kruskal (1964a) used one of the data sets analysed by Shepard and attempted to recover the configuration after the data had been transformed and a random normal error function added. He achieved almost perfect results. He also showed stress vs. dimension graphs for three sets of random data in 6 dimensions of 20, 15 and 10 points, and the results give two of the data sets 'fair' fits in 3 dimensions and the smallest set gave an 'excellent' fit. Kruskal also suggested 3 dimensions for the sets, but failed to point out that, as the original data was 6 dimensional, then one would have expected to be able to recover this dimensionality. Another point from the real data results that Kruskal gives is that a lot of the stress vs. dimension graphs appear to be very smooth curves.

Wagenaar and Padmos (1971) used Monte Carlo methods to examine how stress varied with dimensions. They used configurations of 8 and 10 points, with equal variance in each dimension, and added various levels of random normal error. Their main conclusions were:

1. Too low a dimensionality does not always cause high stress - for example with three-dimensional data and 8 points, the two-dimensional solutions gave stress of 4-8% for the lower levels of added error (i.e. 'good' fits according to Kruskal's interpretation of stress levels) and with 10 points the levels were 7-12% ('fair').

2. The elbow effect is only found with the lowest error values.

Both points are especially important considering that the data was normalized; if one had, in a real case, dimensions of varying weights, one would expect even better fits in lower dimensions, and less elbow effect.

There are several special cases of data which can give erroneous results under non-metric methods. These are cases where the configuration is under-constrained, and the use of rank order is an oversimplification of the real data. For example, any three points in a two-dimensional space, that form a triangle with a unique longest side, can be scaled by non-metric methods into one dimension with zero stress. If we consider the case where the points form an almost equilateral triangle, slight error could transform the three points into a completely wrong one-dimensional solution with zero stress. This example can be extended to that of a three-dimensional tetrahedron in which the three lines forming any one face are all larger than the other three lines. This will also give a 'perfect' one-dimensional scaling, and this can be further extended to an n-dimensional simplex.

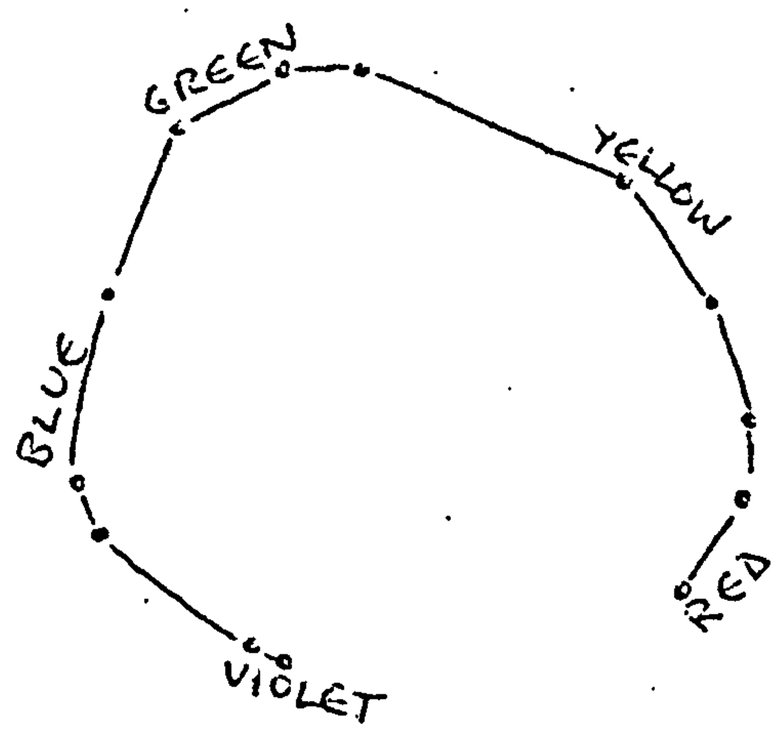
Another instance where misleading results can be obtained is where clusters are present in the data, such that all between cluster distances are larger than all within cluster distances. In this case the input data in rank order form has insufficient information to be able to reconstruct the correct inter-cluster distance, and so the clusters can be a random distance apart in the final ordination.

Shepard (1962b) gives a further instance of possible distortion - that of a smooth arc spanning less than 180^{o}, which will become a 'perfect' one-dimensional scaling. (This may be generalized to several smooth higher dimensioned surves, including some hyperhelices, and also bowl-shaped configurations can be mapped in 2-space without stress.)

Shepard states:

> "...the likelihood that a sufficiently large set of points would fall on the very special kind of curved subspace that will lead to a spuriously flattened solution is probably quite small.....Certainly no such problem seems to have risen in the various applications to real and artificial data presented in the preceding section."

Two pages before this statement Shepard gives an example of the multi-dimensional scaling of people's perception of colours in which he obtains the configuration below:



Here the special type of curve has very nearly occurred, and with the exclusion of five points, would have done. There is also the possibility that the curve might in reality be twisted in a third dimension.

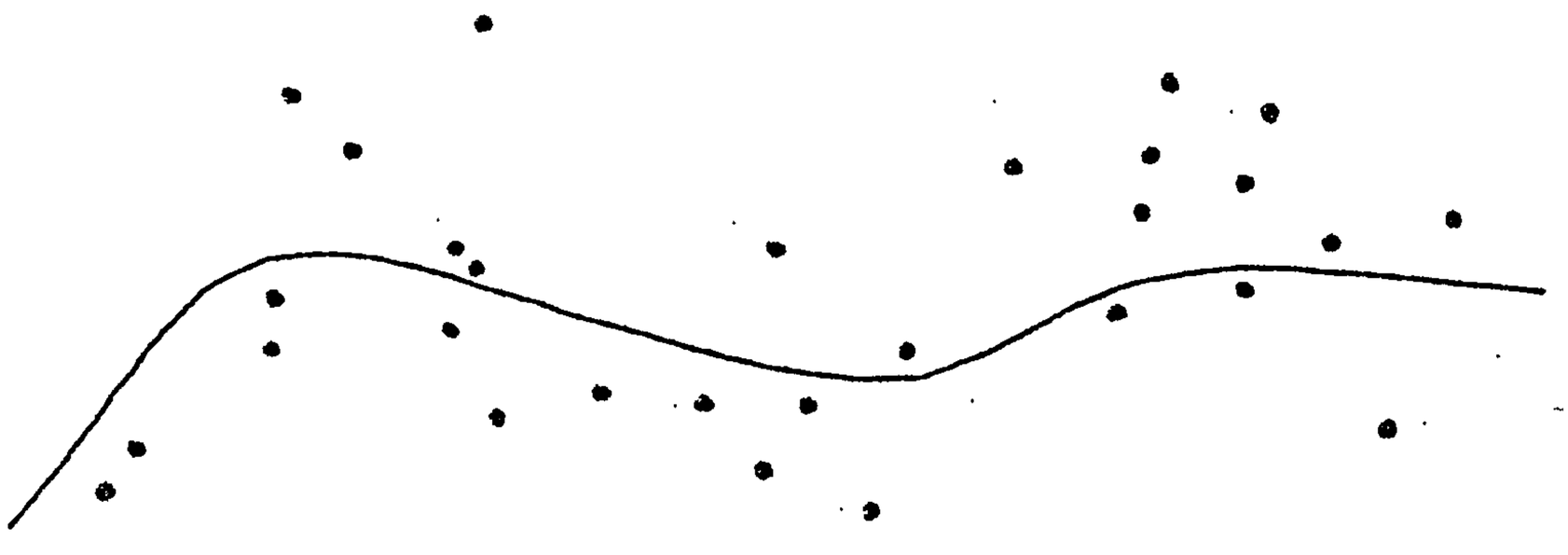
The recovery of metric configurations has been shown to be almost perfect with the non-metric methods for over four points in one dimension and over eight points in two dimensions. Good results have also been obtained with moderate error added to the distance matrix. Certainly rank order information implies a considerable amount of interval information. A point worth mentioning is that some of the examples cited begin with the original configuration as a starting point, and this reduces the chance of finding a local minimum, and in fact, if one is found then it may be closer to the original configuration than the global minimum.

The recovery of dimensionality is a more difficult problem. Most of the graphs of stress that have been published are too smooth for reliable selection of the correct number of dimensions, and these have often been with normalized data, which one would think would be the most difficult to flatten into too few dimensions. It is certainly true, as Torgerson (1965) states, that monotonic distortion gives rise to an increase in dimensionality, but the distortion is difficult to separate from the real values.

We agree with Shepard that in real examples a zero stress configuration in a too low number of dimensions will be unlikely, but consider that there is a fair chance of cases in which false flattening occurs and gives a low enough stress in the lower dimension for this solution to be accepted. In these cases however it might be possible to determine if false flattening has occurred by consideration of the residual matrix of the $(D_{ij} - d_{ij})^2$ terms (- the

error squared for each point). From this any points with high residuals can be found and by comparing this with the ordination result, it is possible that any systematic distortion may be discovered. Some of these statements are equally true for metric stress minimization, and will be considered again later.

Thus given that there is a possibility of over-reducing the number of dimensions, how is an ordination which is forced into a lower space affected by this flattening? The result of an n-dimensional configuration being reduced to (n-1)-space will be the projection of the points on to a 'smooth' hypersurface that will tend to pass through the densest regions of points in the n-space. For example if we consider a two-dimensional space mapped into one, we would map onto a curved line, e.g.

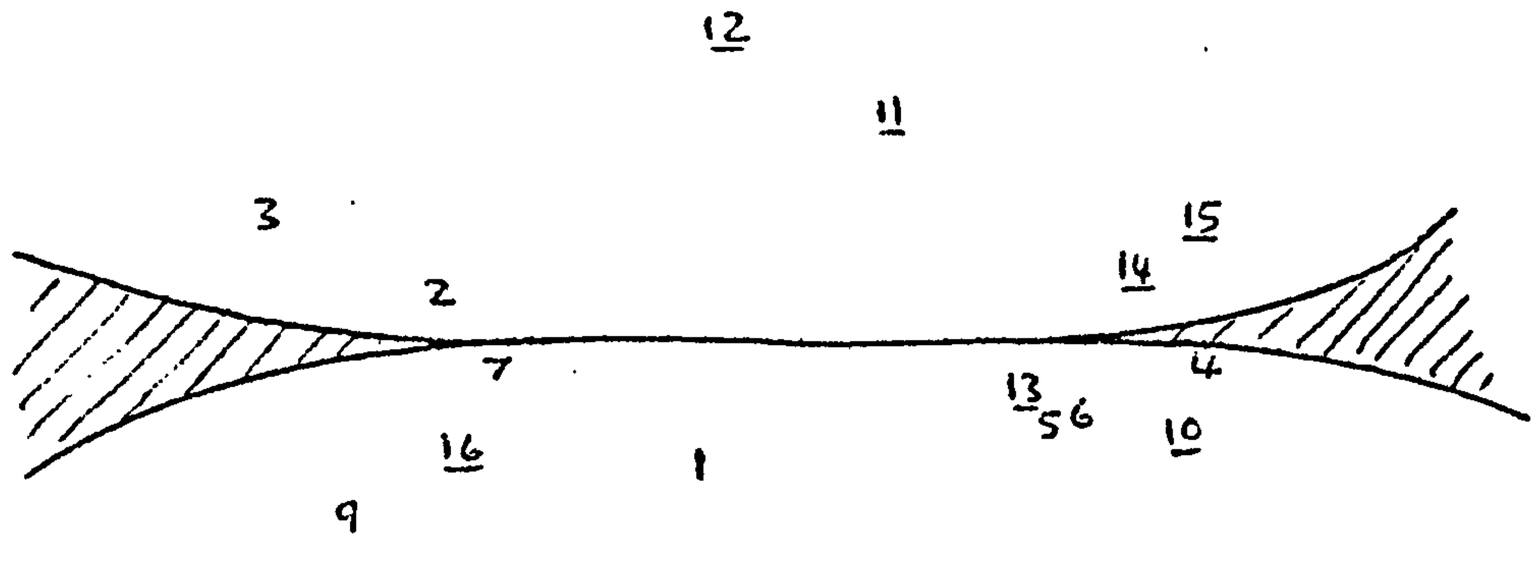


Thus one effect can be the curving of the original dimensions so that they are unrecoverable. If the smooth hypersurface is fairly 'flat' then some of the dimensions of the configuration in (n-1)-dimensions may approximate to some of the 'real' dimensions, which may not be linear in the new

configuration. Shepard (1963) gives three examples of two-dimensional ordinations of the similarity of letters and digits in Morse Code. In all these cases his analysis leads to groups which have boundaries which form curved dimensions. He gives no explanation of how or why the dimensions are curved. Kruskal also refers to one of these examples, and gives the stress curve. The two-dimensional stress is 18% which is not a very good fit, and the curve is very smooth. We therefore suggest that the true configuration is of higher dimensionality, and has been over-reduced to two dimensions. However, it is important to note that the structure of the data was still recoverable, as Shepard's result has a simple interpretation. (We shall discuss the dimensionality of this example later in this section.)

Another point from this example is that the configuration derives from a non-symmetric similarity matrix (from Rothkopf 1957), and Shepard obtains a symmetric matrix by averaging i.e. using $s'_{ij} = s'_{ji} = \frac{1}{2}(s_{ij} + s_{ji})$. However averaging implies that the original data has interval properties, and is not therefore legitimate for non-metric scaling, whereas it would be for metric scaling, which has the underlying assumption of interval data.

If we do over-reduce the dimensionality, we may be able to recover some of the 'real' dimensions, but we are certain to lose at least one (it may well be a less important dimension). If we consider the configuration given by Doran and Hodson (1966) of some archaeological data, obtained using Kruskal's method:



and the corresponding one-dimensional configuration:

3 9 2 16 7 1 12 11 13 5 6 14 10 8 4 15

then the one-dimensional solution is a rough projection of the two-dimensional configuration on to its 1st principal component. The main difference is that points such as 10 and 15 because they are dissimilar from most others (except some in the right group), appear to the right of the one-dimensional solution. The projection is thus on to lines similar to those shown above.

Another effect of this projection is that dissimilar objects (such as 1 and 12) are projected near to each other. This also happens in principal components analysis, but there one is normally given information on all dimensions, so this effect can be noticed. We can conclude that the method does not accurately portray inter-point distance, but more the inter-group distances, in this example (since groups have more 'weight' than single elements thus the distance between cluster centres is more likely to be preserved).

Useful additional information which we suggest can indicate how well positioned objects are in space is the stress of each point - a measure of how well the similarities with each particular object are represented in the configuration.

Another difficult point with scaling methods which obtain metric results is that the 'real nature' of the data may not be Euclidean. It can be shown (see Guttman 1967) that any real symmetric matrix of order n can be represented monotonely as n points in a Euclidean space of at most n-2 dimensions, but this implies nothing as to the adequacy of Euclidean distance for representation of similarity. Kruskal (1964) has analysed Ekmans colours example with several non-metric distance measures and concluded that there was "a hint that distances between colors may be slightly non-Euclidean".

We now move on to discuss the comparisons that have been attempted by other researchers on non-metric methods.

Coombs, Dawes and Tversky (1970) give the ordination of eight points using Hays' unfolding method, Kruskal's and Guttman-Lingoes'. The results were fairly similar although the results from Kruskal's method gave more evenly spaced points than the Guttman-Lingoes ordination. A study by Green and Carmone (1969) gives both Kruskal's and Torgerson and Young's method results. They were very similar, but with local variations - possibly due to the methods being

less accurate at inter-point distances than inter-group distances. A rare chance to compare a metric and non-metric scaling of the same data in published works can be obtained from the ordination obtained by Torgerson and Young's method in Green, Maheshwari and Rao (1969), and a factor analysis result on the same data given in Green and Tull (1970). The two-dimensional configurations given in each case are virtually identical - there being slight local differences.

Green and Carmone (1970) used 27 points in a two-dimensional figure R for the comparison of the methods of Kruskal, Guttman-Lingoes and Torgerson-Young. They transformed the distance matrix by a simple quadratic function and obtained very good recoveries. They all showed some confusion at the point where the oblique line meets the semicircle. The result from Kruskal's method was not as good as the others, although it gave a very low stress (0.9%). The experiment was re-run, this time with an added error term. All three results gave excellent results, with the greatest errors around the same point as before. Torgerson and Young's method probably gave the least best result. All the fit values were 'fair'. The conclusions of Green and Carmone are that the three methods give very similar results and that "the choice of which program to use will depend on the interests of the researcher" and that Kruskal's program "probably represents the most versatile approach".

Green and Rao (1971) also use an R shape - this time of 15 points, INDSCAL, Torgerson-Young and Kruskal's methods.

The configurations were all good representations, but this time Kruskal's method gave stress of 6.4% and still "yielded virtually perfect reproduction". The distance matrix was then turned into binary data by changing the smaller distances into 0 and the larger to 1. The best results were from Torgerson-Young's, INDSCAL, and discriminant analysis, probably in that order. Kruskal's method gave 50% stress and the correlation between the real and obtained distances was slightly negative, indicating that the method had no ability to recover the original configuration at all.

McGee (1966) has tested his elastic scaling model against Kruskal's on a real data set of 8 points and obtained very similar results with each.

From these few results reported above it seems that no significant differences have yet been found between these methods. Two points which we note are the occurrence of local differences between methods, and the unusual behaviour of the stress in the results with Kruskal's method. It seems that the choice between the methods can be largely left to the experimenter, who can choose that minimization function which he thinks is most in accord with the data or theory he is investigating. McGee's method is based on somewhat different theoretical grounds and this method should therefore be easier to accept or reject by a potential user.

We shall now discuss a problem which occurs with a particular kind of data matrix which was discovered by

D. Kendall (1970, 1971), which is called the horse-shoe problem. This problem was found by Kendall in archaeological data, where in this instance similarity was measured between any two graves by the number of artefacts they have in common. This meant with this particular data that a large number of elements in the similarity matrix were zero. This resulted in the two-dimensional scaling result by Kruskal's method not being virtually a straight line, as was expected, but the ends were curved round, forming a horse-shoe shape. This is caused by the large number of zeros, which means that all the points at one end of the line will have the same similarity with all those at the other end, and so the two ends will become parallel in a two-dimensional configuration.

The similarity measure used in this instance was

$$S_{ij} = \sum_k W_k \min(a_{jk}, a_{ik})$$

(where a_{jk} is the number of artefacts k found in grave j, and W_k is the weight given to this artefact).

Kendall's approach was to use a different similarity measure which reduces the number of zero values in the matrix. He uses

$$(S_oS)_{ij} = \sum_h W_h \cdot \min(S_{ih}, S_{jh})$$

where S_{ih} and S_{jh} are the previous similarities as defined above, and W_h are weights. This successfully straighted out the horse-shoe problem, and he suggested that perhaps indices such as $(S_oS)_o(S_oS)$ might be investigated.

This kind of problem has been considered by Shepard and Carroll (1966) who were concerned with trying to 'straighten

out' data which was locally linear, but embedded in a higher space. They used a cut-off point (i.e. only seeking to find a configuration which represented the k smallest dissimilarities) to obtain one-dimensional representations, and proceeded to invent a technique called parametric mapping for more general application. The cut-off procedure should be applicable in the archaeology example - the similarities which are ignored are the zeros, so the problem of where to 'cut' the similarities is not difficult. We suggest that the procedure should be amended so that large dissimilarities are not entirely ignored, but are ignored only when the distances in the new space corresponding to these dissimilarities are larger than a set distance.

We now return to Shepard's ordination of Rothkopf's Morse Code data. Earlier we suggested that the data was really curved in three dimensions. The reason for this curving can be seen from the similarity matrix given by Shepard. The difficulty is the large number of very low similarities, which have given rise to a three-dimensional horse-shoe effect, which has led to a cup-shaped configuration in three dimensions. (The other two sets of data which Shepard investigated had also a large number of zero elements.)

This problem can be alleviated by a change in similarity, like that suggested by Kendall. In this case we would use

$$S_{ij}' = \sum_k (S_{jk} + S_{ik}) \qquad \text{for metric scaling}$$

or $$S_{ij}' = \sum_k \min(S_{jk}, S_{ik}) \qquad \text{for non-metric scaling}$$

Metric Methods

There have been very few works involving the comparison of metric methods. We have found only four such works.

Austin and Orloci (1966) compare principal components, Bray and Curtis' method and Orloci's method on one set of ecological data. They summarize their results saying -

> "the success of simple ordinations (Bray and Curtis, Orloci) is dependent on the position of extreme stands (objects) relative to the point cluster. A better method is principal components analysis of an appropriate similarity coefficient".

They neglect to point out the value of the increased speed of the simple ordinations, or that Bray and Curtis' can be performed by hand. By inspection of the three ordinations they can be seen to be very different - the two simple ordinations being the most similar pair. Austin and Orloci conclude that Bray and Curtis' method gives more evenly spaced ordinations than Orloci's method - this result is borne out by Bannisters' (1968) results on 4 data sets.

Anderson A.J.B. (1971a) discusses principal components, principal co-ordinate analysis, minimization of loss functions (he uses $\sum(D - d)^2$ in his minimization), and Kruskal's method. He compares these three results on a soils example (also comparing them with five clustering methods) and concludes that -

> "the quadratic minimization procedure is to be preferred. It is free from both the difficulties of interpretation inherent in principal components analysis and the computational problems presented

by non-metric scaling. And above all, the criterion to be satisfied seems closest to intuitive ideas about what a co-ordinate representation should provide".

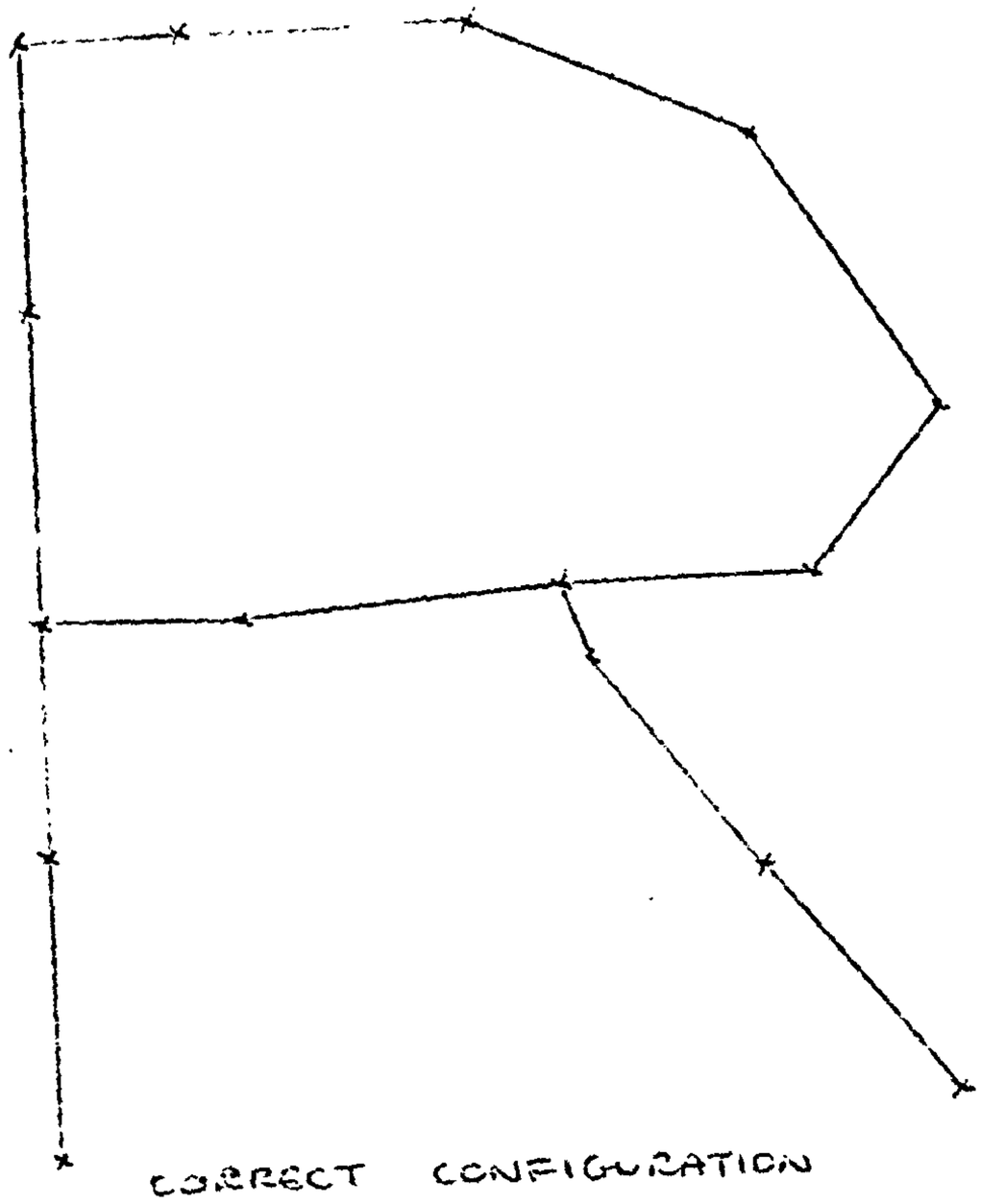
In a later work Anderson (1971b) compares the same methods and also Bray and Curtis' on an ecology example. He states that theoretically the loss function method provides an ordination closest to that required by the ecologist. The loss function and Kruskal methods results are somewhat different despite the fact that the graph of dissimilarity against recovered distance with Kruskal's result is approximately linear. Anderson points out that non-metric methods obscure the presence of outliers and separate small clusters, and that principal components analysis has problems because objects may have high residuals. Bray and Curtis' method is discredited.

The results cited above are too few to draw many conclusions. Simple ordinations appear to come off badly (in particular the method of Bray and Curtis) and loss functions seem to be worth further investigation.

Because of the lack of work on ordination by the minimization of loss functions we will give the results of our own tests of varying kinds of data. We tested three methods - our version of Bray and Curtis method, the method used by Anderson, (minimization of $\sum(D - d)^2$) and the loss function $\sum(\frac{D - d}{d})^2$.

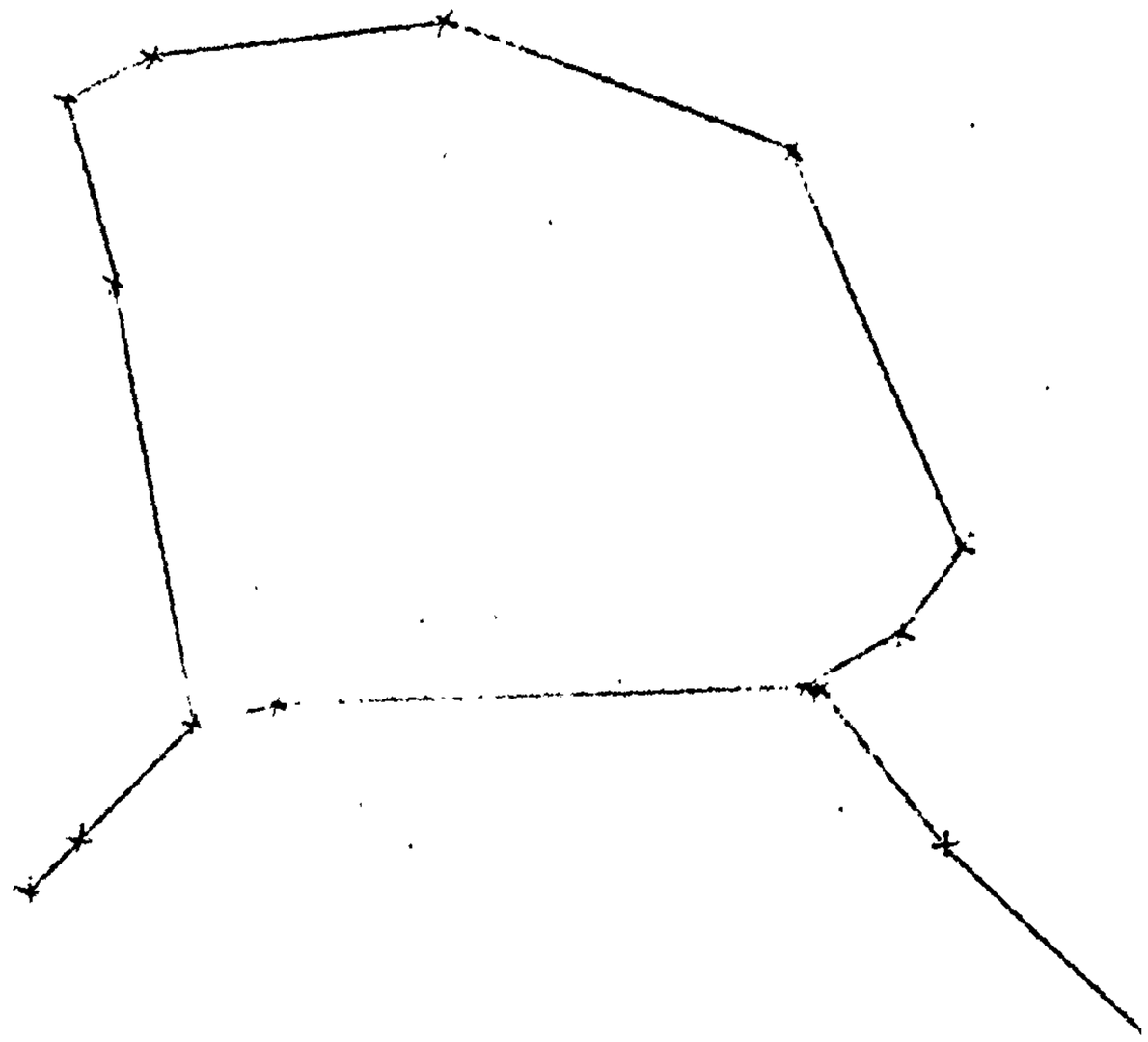
We first considered the recovery of metric from non-metric data. We took our data from the R shaped configuration of 15 points given in Green and Rao (1971). From this we obtained the ranked distance matrix. The original configuration and the results of the three methods are shown in Figures 30 to 33. The similarity of the original configuration and the loss function $\sum(D - d)^2$ is striking. The other two methods performed less well. In the Bray and Curtis result the inter-point distances had been recovered quite well, but the shape was rather distorted. The result with $\sum(\frac{D - d}{d})^2$ showed a contraction of small distances and enlargement of the larger distances.

Our next test was to see how the methods behaved with data which had an included error term. For ease of visual interpretation, we again took a two-dimensional example. We took 25 points arranged in the form of a circle with two orthogonal diameters. The configuration is shown in Figure 34. To this we added three-dimensional error from normally distributed random numbers. The first two dimensions were transformed to the points shown in Figure 34. The results for our three methods are also shown. The recovered configurations are very similar, and almost identical to the original data with two-dimensional error. All three methods are thus capable of eliminating error in other dimensions, but are (not surprisingly) unable to distinguish between the 'real' data and the error in that plane. Note that principal components would give a very



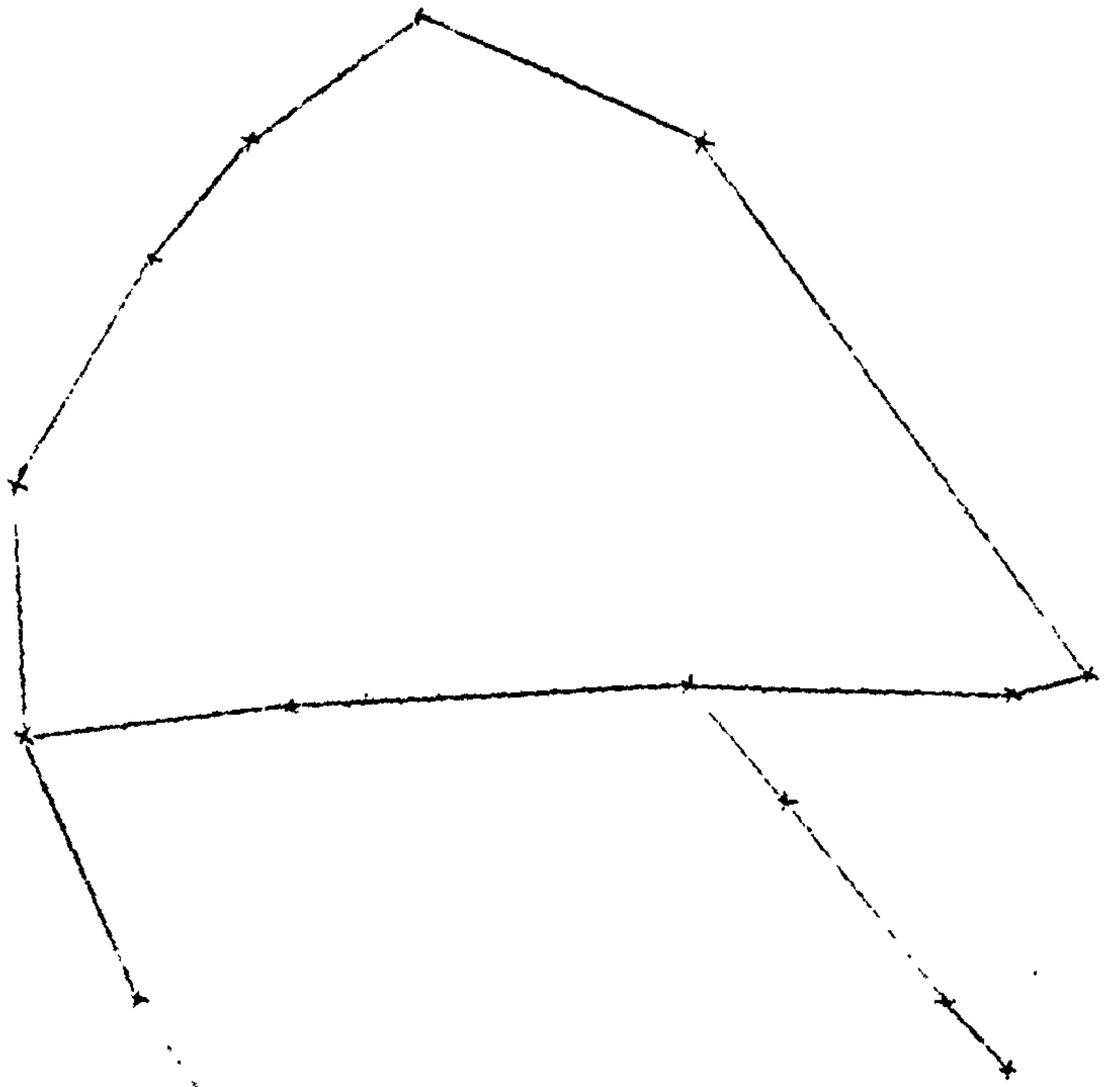
CORRECT CONFIGURATION

FIGURE 30



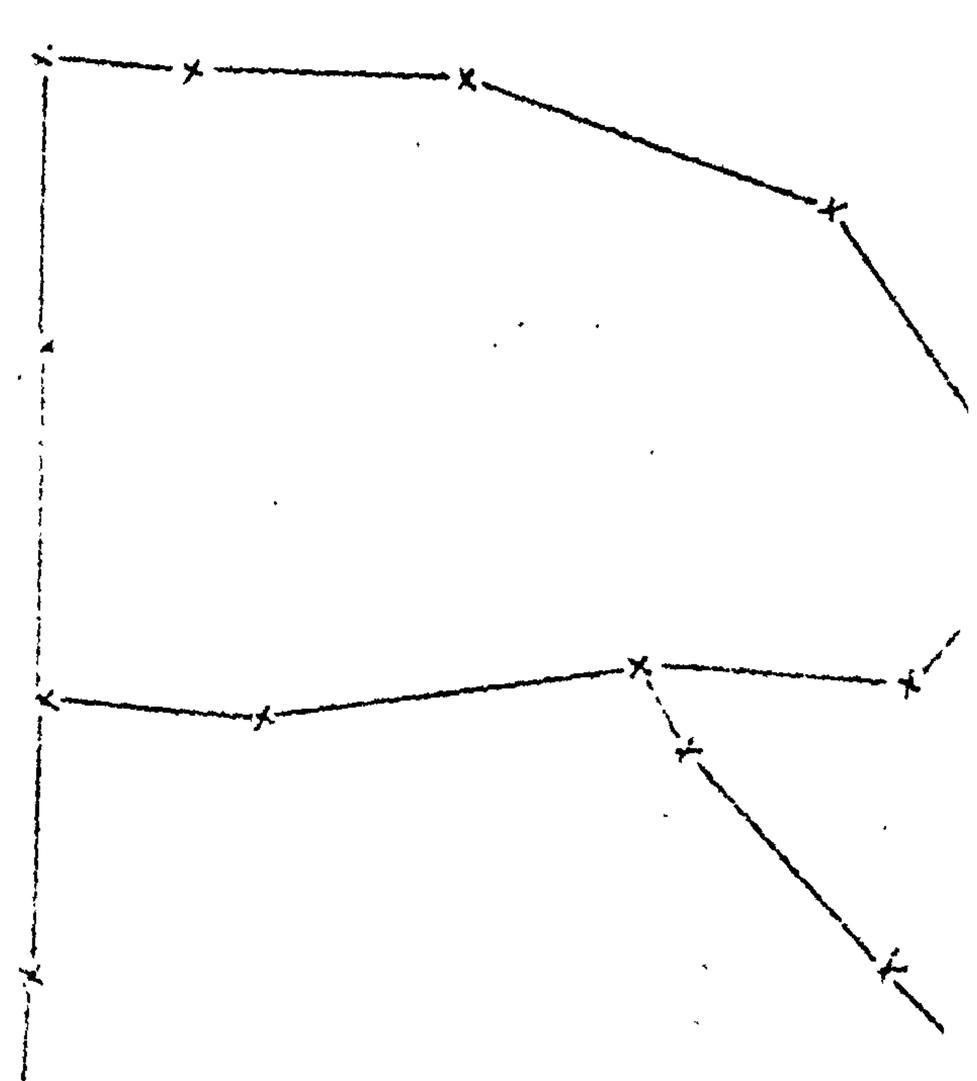
MINIMIZATION OF $\Sigma\left(\frac{D-d}{d}\right)^2$

FIGURE 31



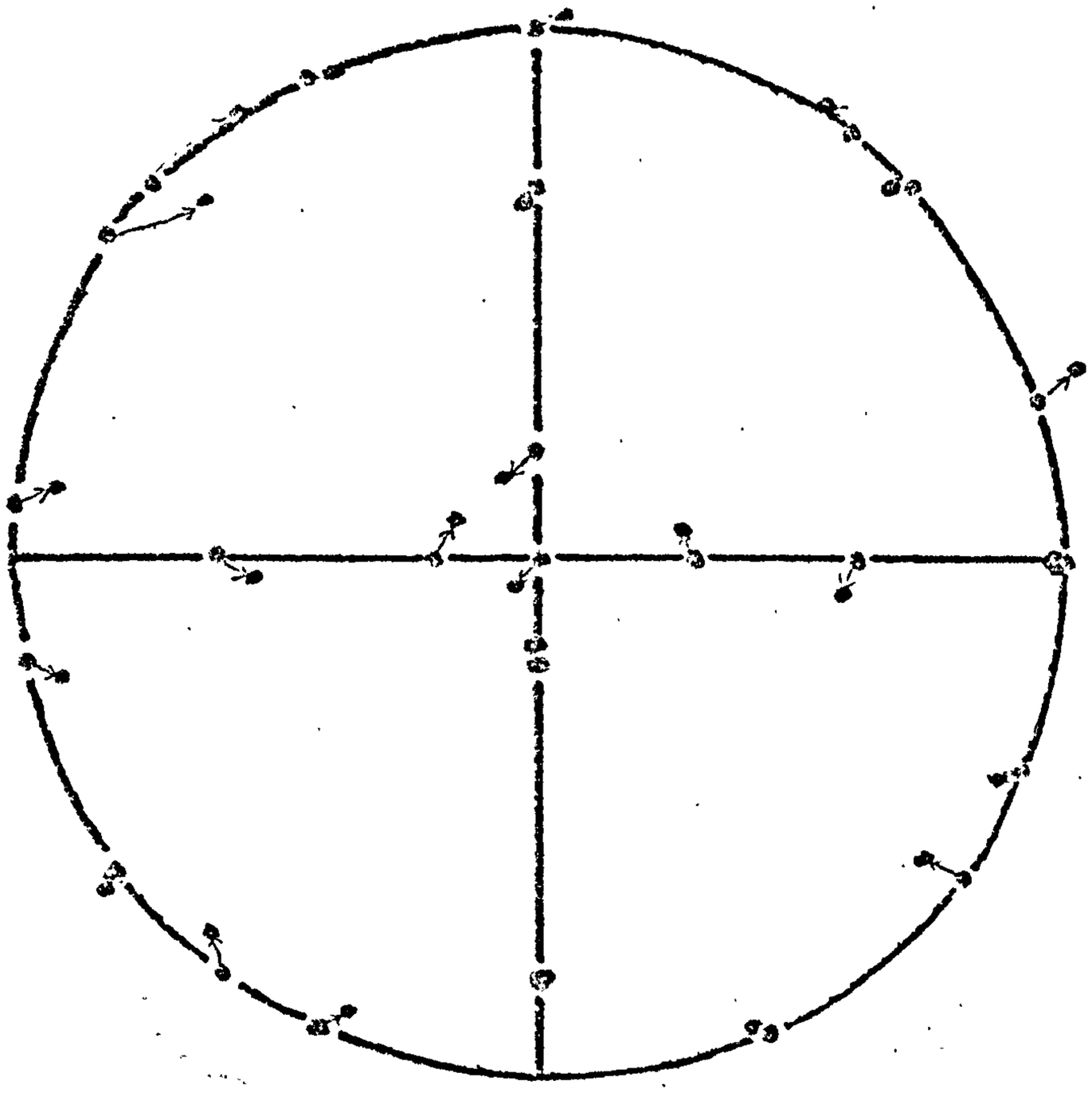
BRAY + CURTIS' ORDINATION

FIGURE 32



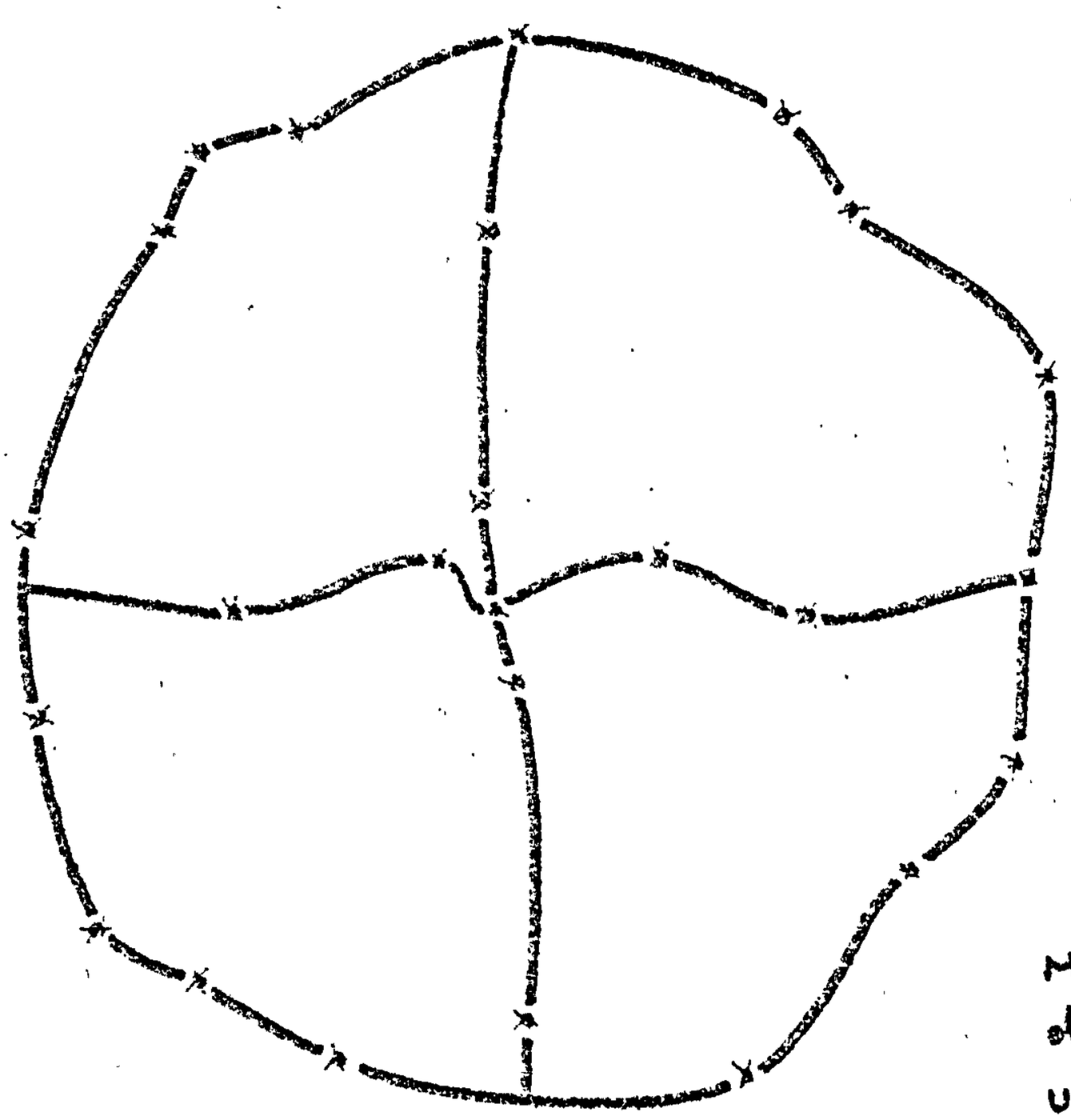
MINIMIZATION OF $\Sigma(D-d)^2$

FIGURE 33



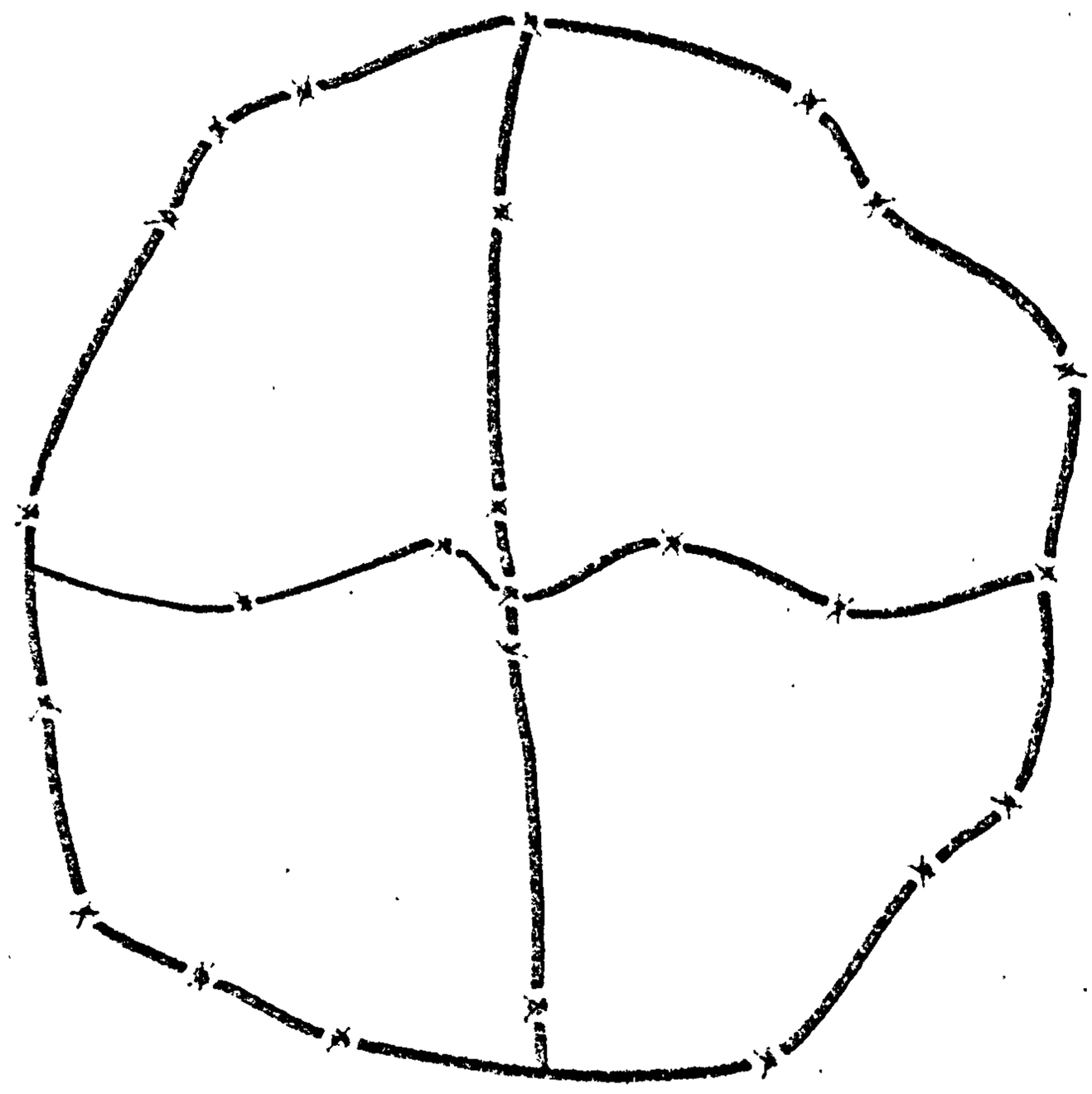
'TRUE' CONFIGURATION AND ERROR OF FIRST TWO DIMENSIONS

FIGURE 34



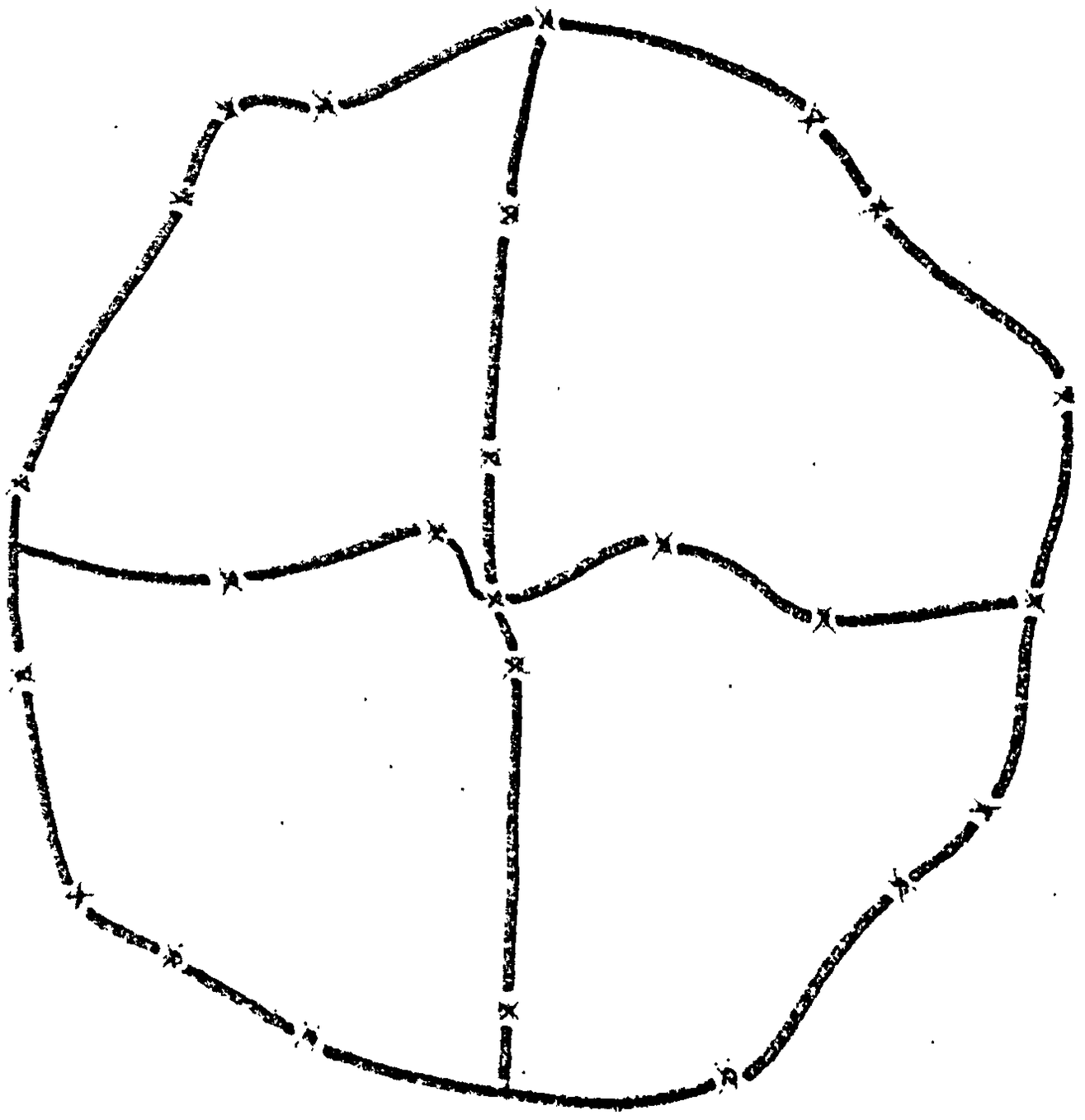
Minimization of data + transform using $\Sigma(D-d)^2$

FIGURE 35



Minimization using
$\sum \left(\frac{D-d}{D}\right)^2$

FIGURE 36



BRAY + CURTIS
ORDINATION

FIGURE 37

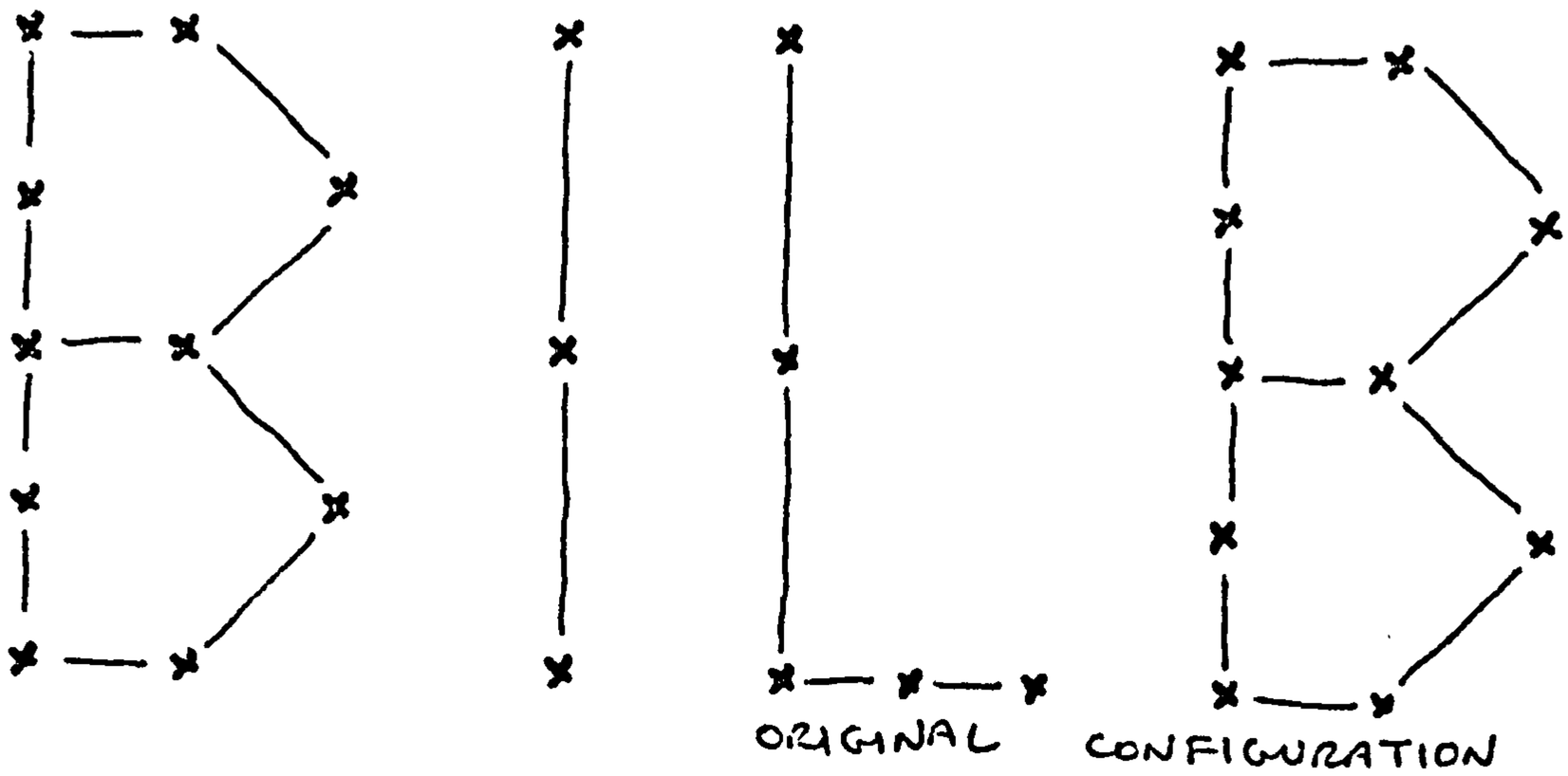
similar result - although many programs for p.c.a. normalize the data initially, which, in this case, grossly exaggerates the error in the third dimension.

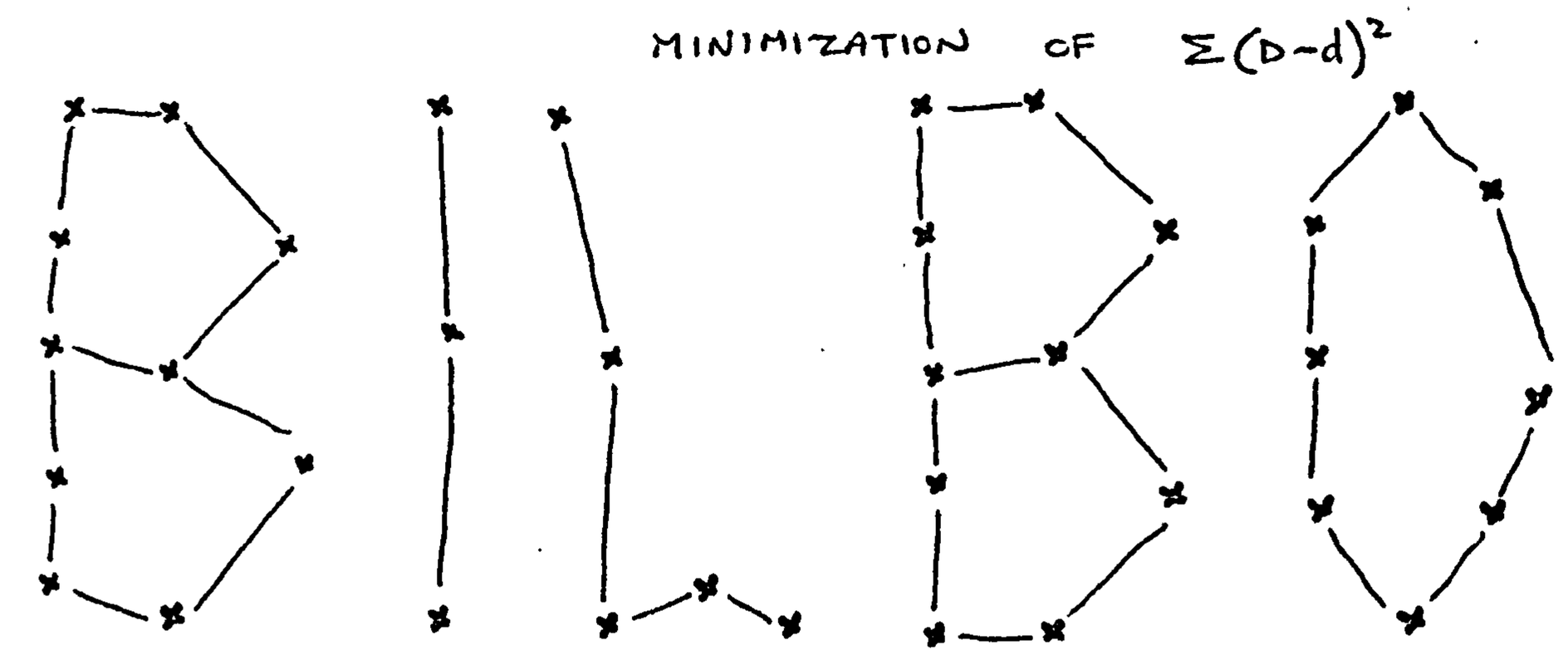
Next we took a two-dimensional data set and calculated the distance matrix, and we added a random error term to each distance. The error terms were independent of the magnitude of the distances, but had a mean value of .2 of the mean inter-point distance. The results are shown in Figure 38 along with the original configuration. The two loss function methods performed better than our version of Bray and Curtis' method, and the loss function $\sum (D - d)^2$ achieves almost perfect results.

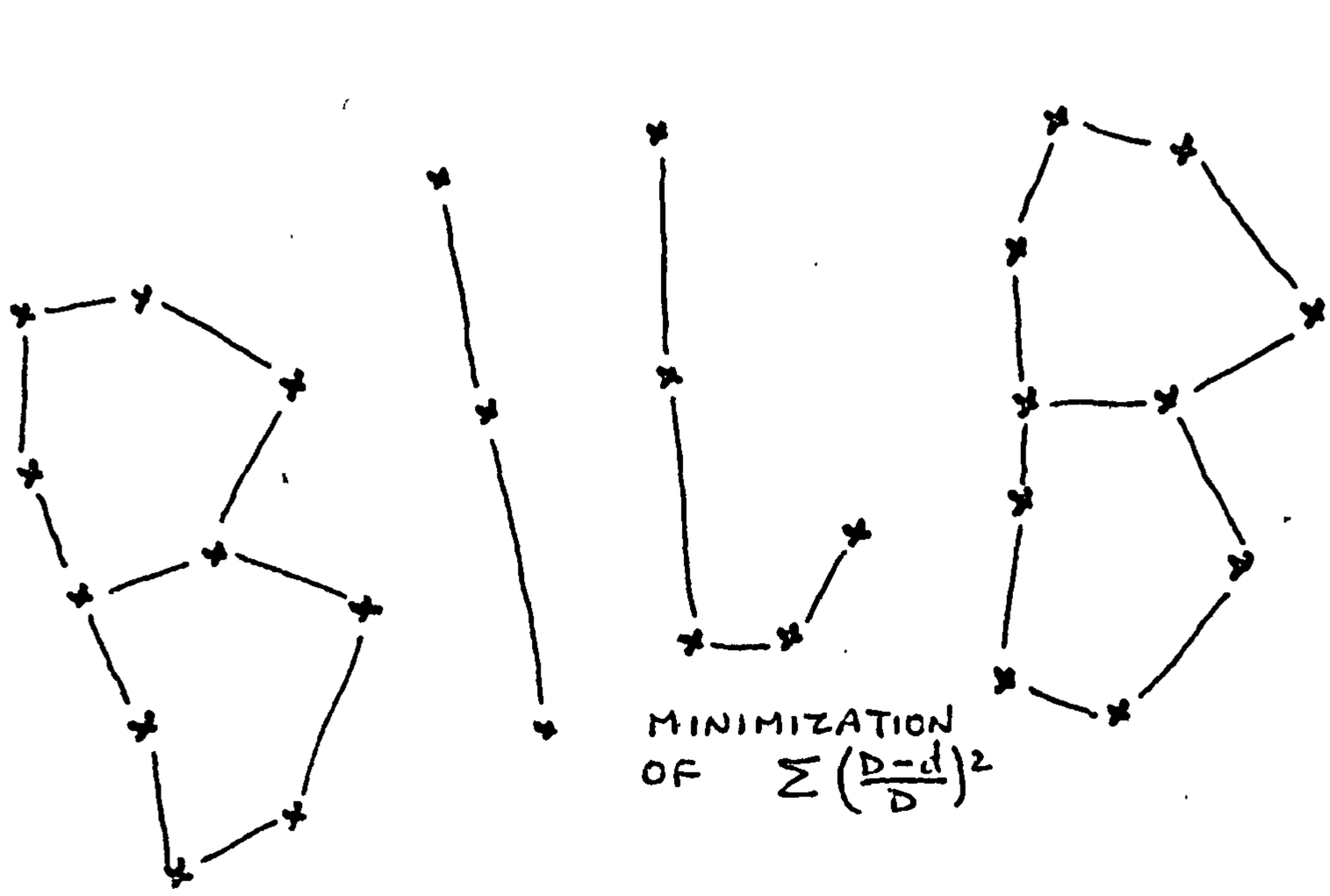
We also transformed the data with an error term dependent on the inter-point distances (the transformation $D' = D(1 + \epsilon)$, with the mean magnitude of ϵ equal to .2). The results in this case were not so accurate. The two loss functions gave recognizable results, with the function $\sum (\frac{D - d}{D})^2$ giving the best configuration. Bray and Curtis' method failed to reproduce the shape of the original data, but distances were not greatly distorted. The results are given in Figure 39.

The comparative tests have shown the possibilities of loss-function methods, and the disadvantages of Bray and Curtis type ordinations (apart from speed and convenience). The use of the function $\sum (D - d)^2$ is recommended, as it has given good results in all our tests. Loss functions can

FIGURE 38


ORIGINAL CONFIGURATION


MINIMIZATION OF $\Sigma(D-d)^2$

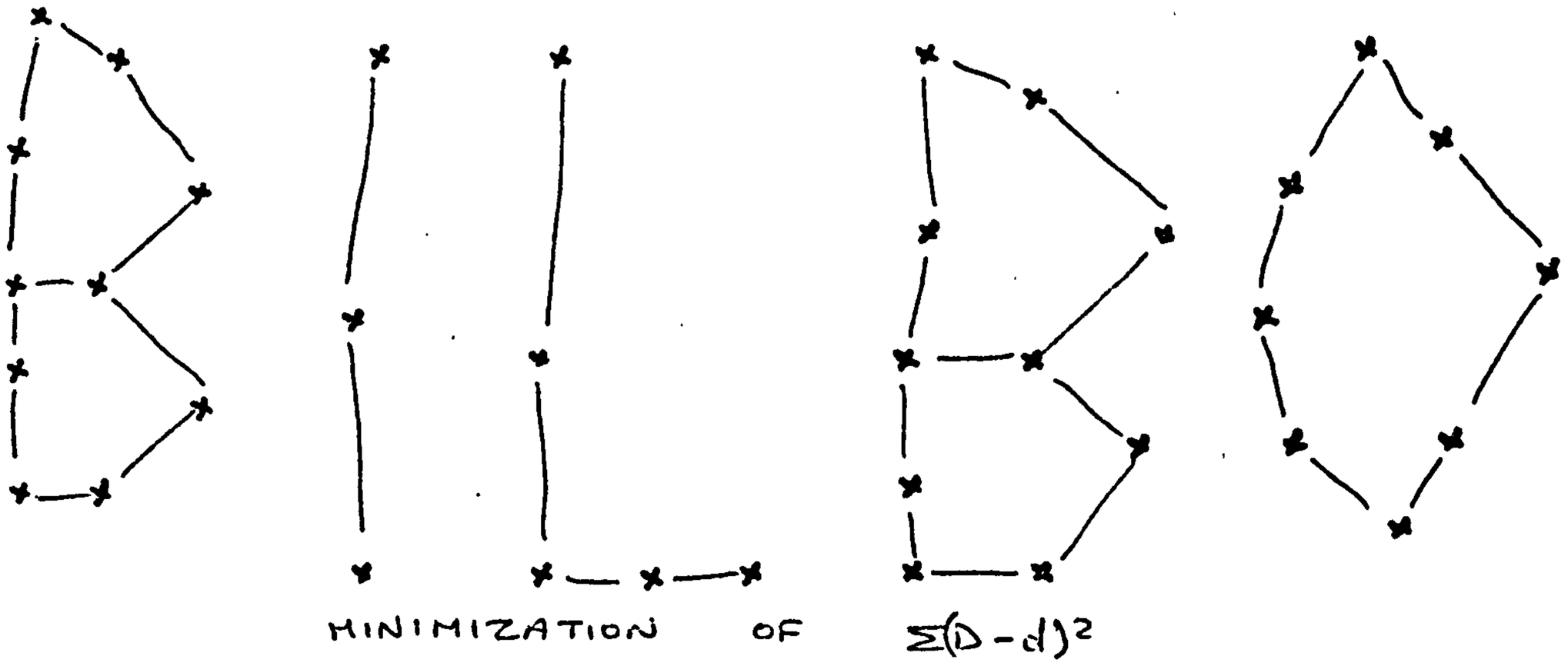

MINIMIZATION OF $\Sigma\left(\frac{D-d}{D}\right)^2$

BRAY + CURTIS'

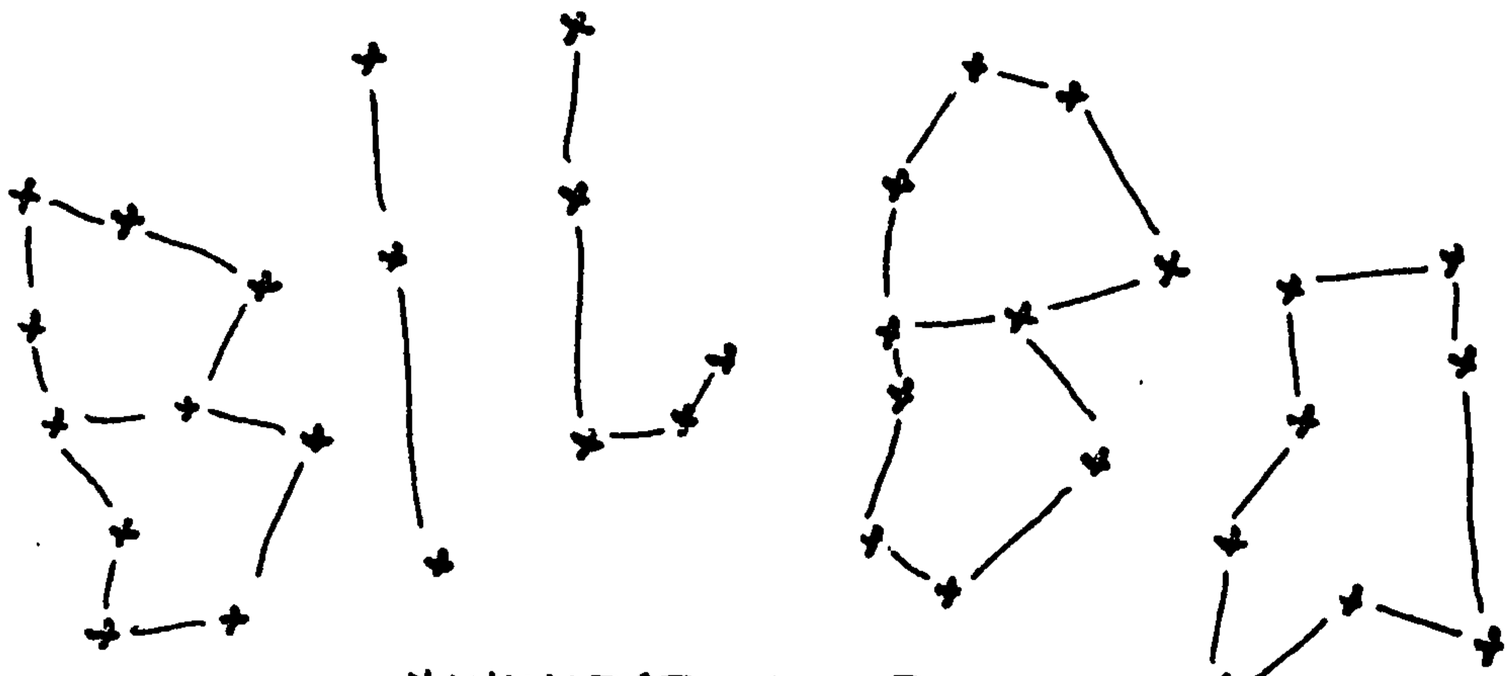
FIGURE 39

ORIGINAL CONFIGURATION AND % ADDED ERROR

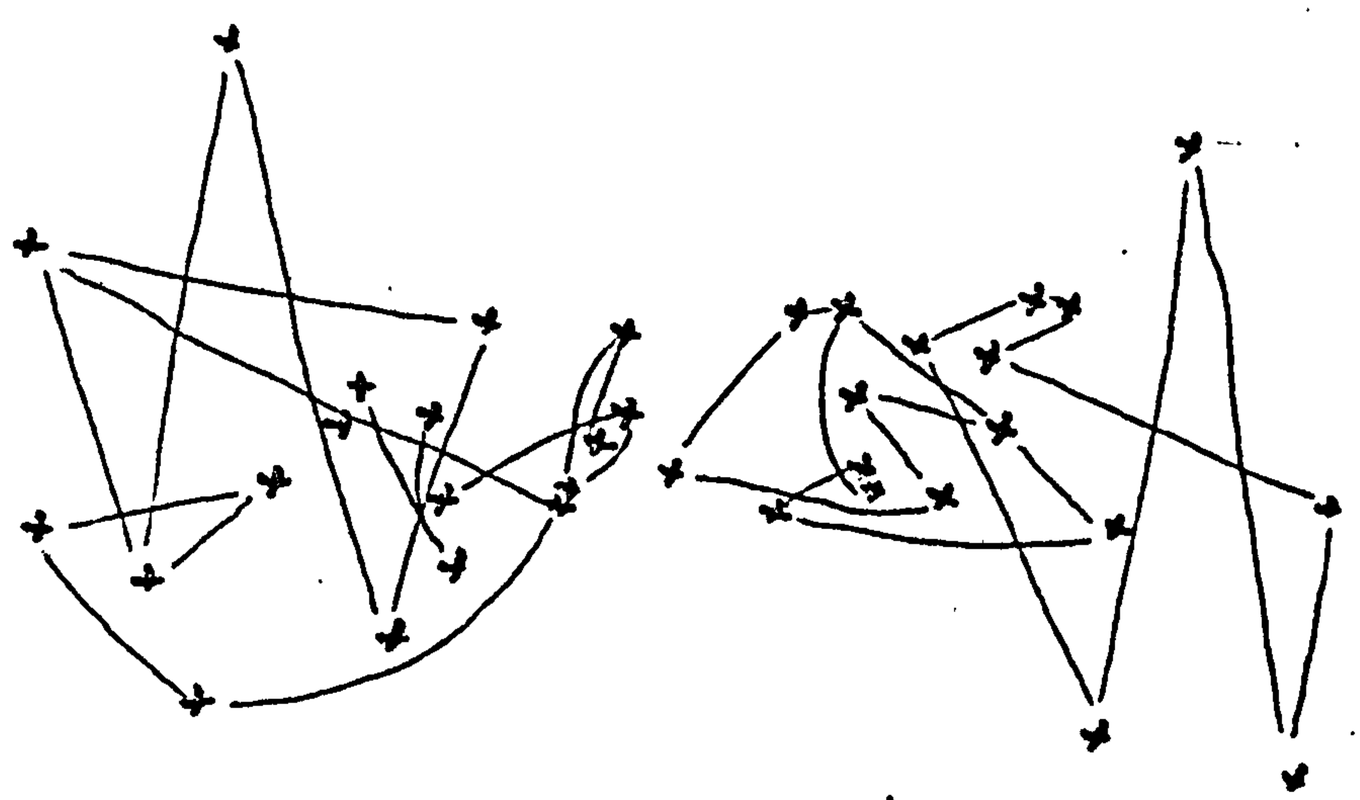
(NOT TO SAME SCALE)



MINIMIZATION OF $\Sigma(D-d)^2$



MINIMIZATION OF $\Sigma\left(\frac{D-d}{D}\right)^2$



BRAY + CURTIS'

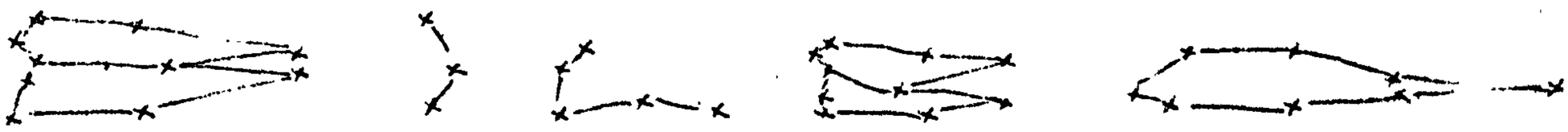
have difficulty in cases where the original data is strongly non-Euclidean. As an example we have used the loss function $\sum(D - d)^2$ on the previous data set, but using the squared distances between the configuration points. This gives non-Euclidean input data. The resultant configuration and the Shepard diagram (the graph of input distances against recovered distances) are given in Figure 40. Whilst the shape of the curve in the Shepard diagram represents the transformation fairly accurately, the smaller distances in the recovered configuration have been considerably reduced and the ordination distorted.

However if we replace the values in the distance matrix by their rank order values (note that the rank order of a set of distances is the same as the rank order of the squared distances), then we obtain the results shown in Figure 41. Here the Shepard diagram gives only a slightly curved line and the ordination is very good.

We therefore recommend, in situations where a curved line is obtained in the Shepard diagram using the given distance matrix, that one should then use the rank order of the distances.

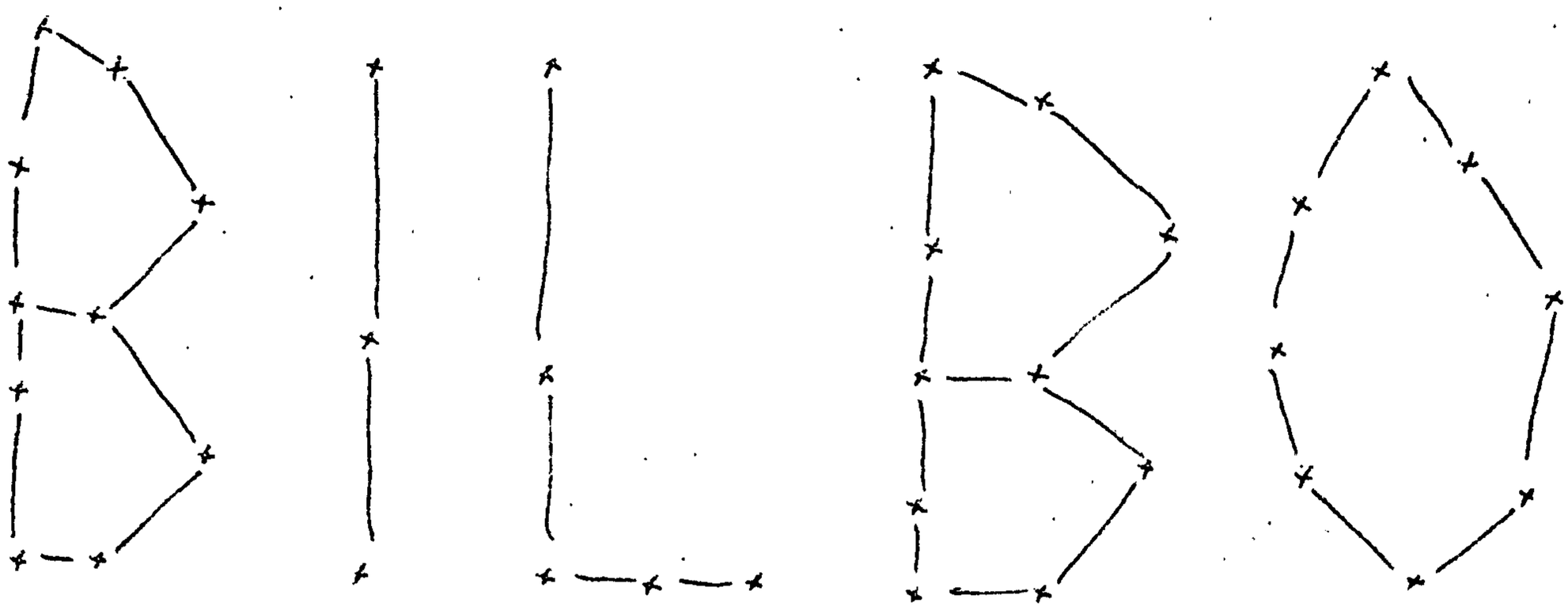
The use of a particular loss function in any particular case depends to some extent on the type of error which is expected in any experiment. For example, in the case where we examined error dependent on the magnitude of the distances, the function $\sum(\frac{D - d}{d})^2$ performed best, but with error independent of the size of the distances, $\sum(D - d)^2$ gave the best results.

FIGURE 40



ORIGINAL DISTANCE
SHEPARD DIAGRAM
(EACH DIGIT REPRESENTS THAT NUMBER OF POINTS. * INDICATES OVER 9)
RECOVERED DISTANCE

FIGURE 41



```
I                                                                    1573 32
I                                                                     24564
I                                                                   1 3*6
I                                                                  35742
I                                                                13475
I                                                               48441
I                                                            114564
I                                                             6771
I                                                           2963
I                                                         4917
I                                                     1 1   2*5
I                                                   1 21476
I                                                   223751
I                                                1113375
I                                              2524251
I                                              433641
I                                            126434
I                                        1 132473
I                                              1151571
I                                             1 65621
I                                           143642
I                                           366411
I                                        125742
I                                         23493
I                                        6456
I                                    12773
I                                    17472
I                                  133*3
I                                 1*73
I                               29621
I                               25
I++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

We have yet to examine the problem of recovery of dimensionality in metric methods. We took an example of 30 points normally distributed in six dimensions and reduced to each lower dimension for both the unranked and ranked distances using $\Sigma(D-d)^2$. We obtained the stress vs. dimension graph for each case. These are shown in Figure 42. The difficulty of selecting the appropriate dimension which we discussed in the non-metric case still exists although in neither case does a misleading 'elbow' exist.

The horse-shoe effect is still possible with non-ranked data, but is less likely to occur with the ranked case unless large numbers of ties are present.

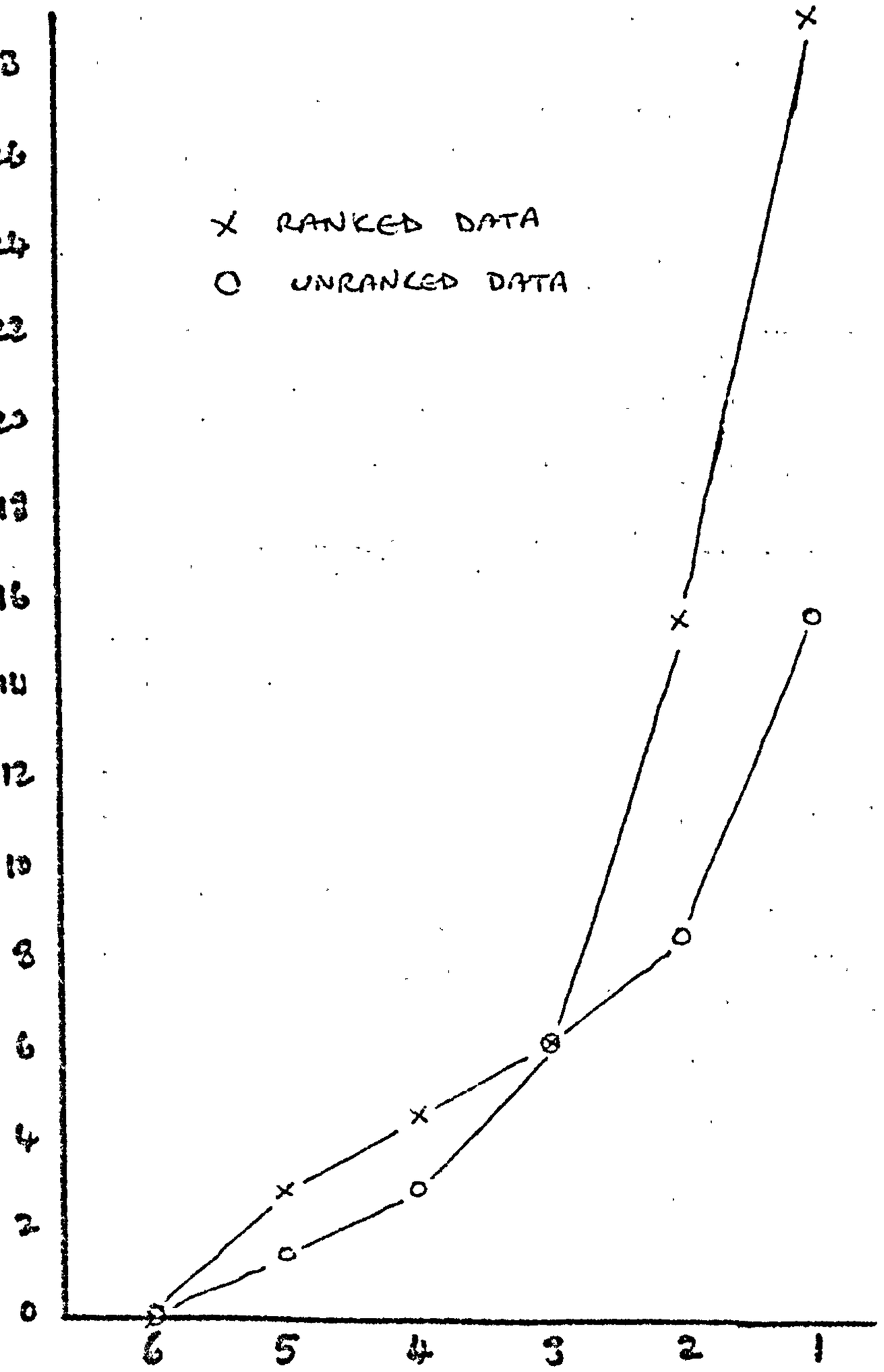
The metric methods have been fairly successful in recovering configurations under error and under transformations. In fact, failure of the metric methods may be indicative of the non-Euclidean nature of data, or an attempt to over-reduce the dimension of the result.

Non-Metric vs. Metric

We have now considered aspects of the behaviour of both metric and non-metric scaling and have shown that metric methods can produce good results even with non-metric data. We begin by giving two examples where metric scaling is better than non-metric on purely theoretical grounds.

Our first is an ordination of 34 towns on the basis of the shortest road distance between them. Here non-metric

FIGURE 42


X RANKED DATA
O UNRANKED DATA
24
22
20
18
16
14
12
10
8
6
4
2
0
6
5
4
3
2
1

methods reduce the input data unnecessarily - the distance which we wish to represent is exact in the input matrix. We show the geographical location and the recovered road distance map in Figures 43 and 44. The coastline in Figure 44 is simply drawn to show the way the geographical configuration has been changed, and has no real meaning of its own. The method used was the minimization of $\sum(\frac{D-d}{d})^2$. The main differences in the maps are the turning down of Cornwall and Devon due to the Severn and the stretching of the middle of Wales due to the Welsh Mountains. One can envisage that such a map could be useful in transportation-type problems.

Our second example is similar - the input data is a matrix of distances by London Underground. We define the distance between two stations as the minimum number of stations passed through in travelling from one to the other, counting a change of train as one more station. The tube stations in central London were used, with the approximate boundary of the circle line - 57 stations (the matrix is given in Appendix 2). In this instance non-metric methods would involve a large number of tied values which cause difficulties. The result, using minimization of $\sum(\frac{D-d}{d})^2$, is given in Figure 45. One interesting feature of the diagram is the way in which the main-line railway stations (Victoria, Waterloo, Kings Cross, etc.) have been 'drawn in' to the centre of the configuration, with the notable exception of Paddington.

Carlisle
Newcastle
Kendal
Middlesbrough
Leeds
Hull
Holyhead
Manchester
Liverpool
Sheffield
Colwyn Bay
Stoke
Nottingham
Shrewsbury
Norwich
Peterborough
Aberystwyth
Birmingham
Cambridge
Fishguard
Gloucester
Oxford
Harwich
Swansea
Cardiff
London
Bristol
Dover
Southampton
Brighton
Exeter
Bournemouth
Plymouth
Penzance

FIGURE 43

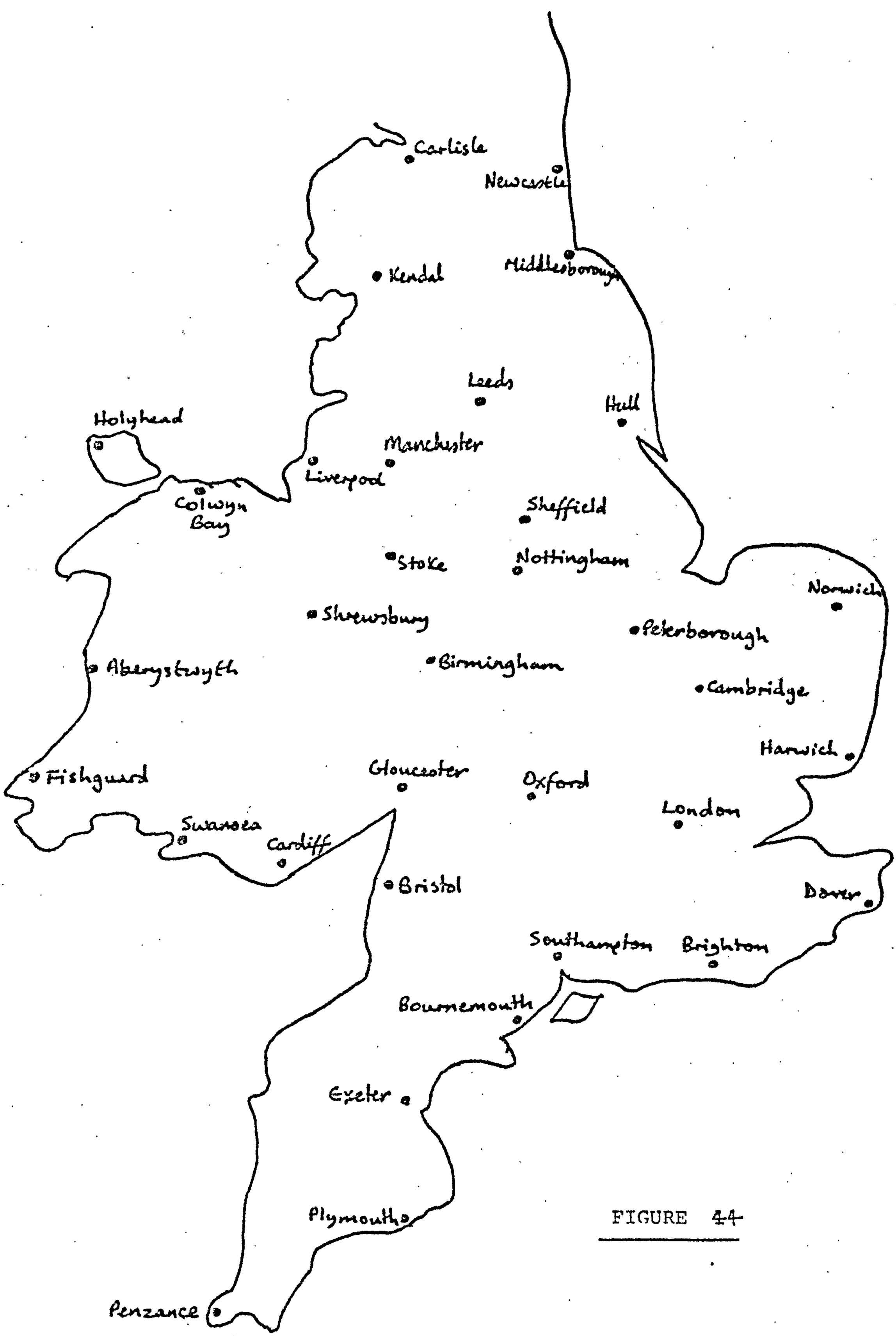

Carlisle
Newcastle
Middlesbrough
Kendal
Leeds
Hull
Holyhead
Manchester
Liverpool
Colwyn Bay
Sheffield
Stoke
Nottingham
Norwich
Shrewsbury
Peterborough
Aberystwyth
Birmingham
Cambridge
Harwich
Fishguard
Gloucester
Oxford
London
Swansea
Cardiff
Bristol
Dover
Southampton
Brighton
Bournemouth
Exeter
Plymouth
Penzance

FIGURE 44

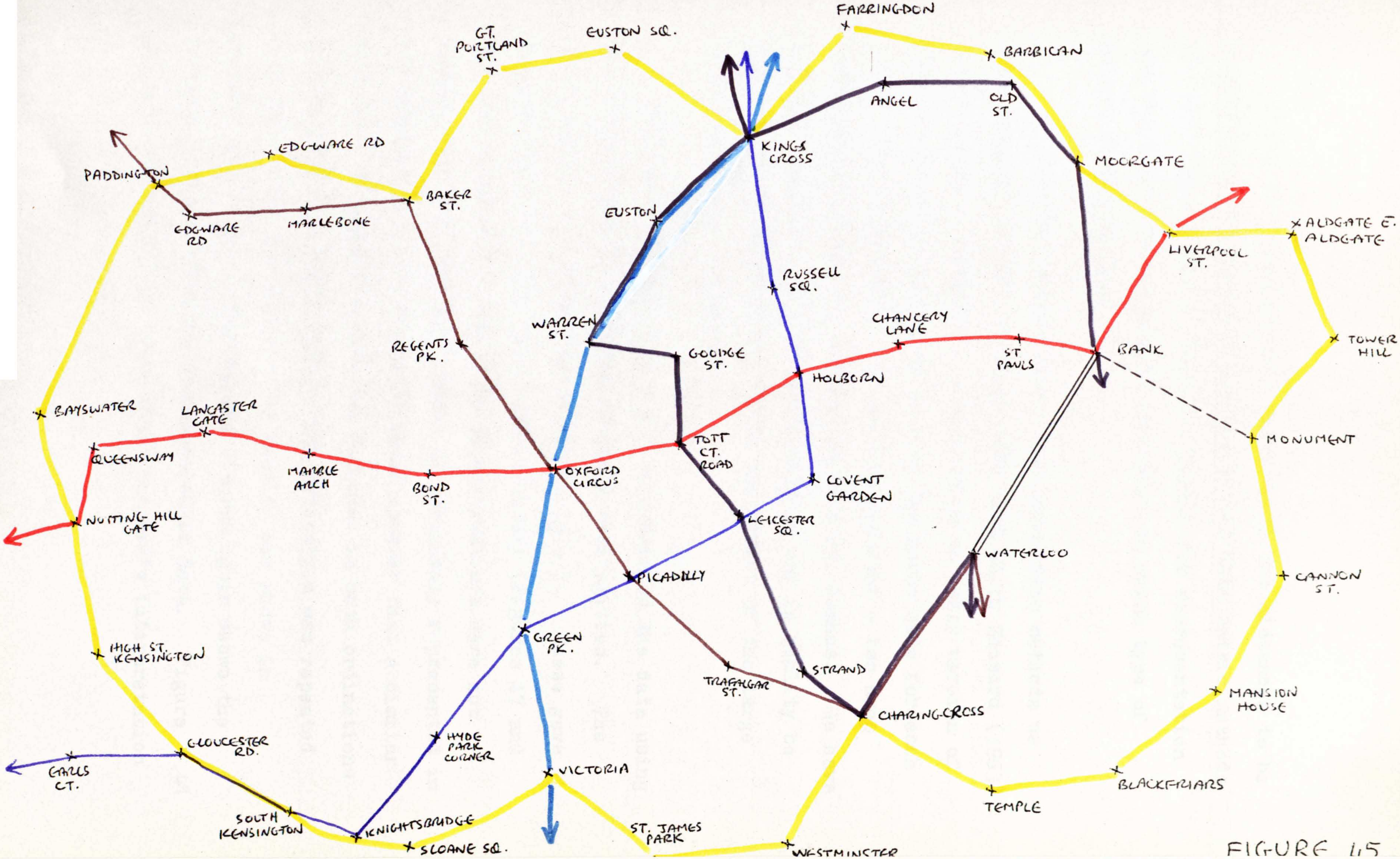

FARRINGDON
BARBICAN
G.T. PORTLAND ST.
EUSTON SQ.
ANGEL
OLD ST.
KINGS CROSS
MOORGATE
EDGWARE RD
PADDINGTON
BAKER ST.
EUSTON
EDGWARE RD
MARLEBONE
LIVERPOOL ST.
ALDGATE E.
ALDGATE
RUSSELL SQ.
WARREN ST.
CHANCERY LANE
REGENTS PK.
GOODGE ST.
ST PAULS
BANK
TOWER HILL
HOLBORN
BAYSWATER
LANCASTER GATE
TOTT CT. ROAD
MONUMENT
QUEENSWAY
MARBLE ARCH
BOND ST.
OXFORD CIRCUS
COVENT GARDEN
NOTTING HILL GATE
LEICESTER SQ.
WATERLOO
PICADILLY
CANNON ST.
GREEN PK.
HIGH ST. KENSINGTON
TRAFFALGAR ST.
STRAND
MANSION HOUSE
CHARING-CROSS
GLOUCESTER RD.
HYDE PARK CORNER
EARLS CT.
VICTORIA
BLACKFRIARS
SOUTH KENSINGTON
KNIGHTSBRIDGE
ST. JAMES PARK
TEMPLE
SLOANE SQ.
WESTMINSTER

FIGURE 1.5

These two examples show cases where the distances to be represented have interval properties and thus metric methods are more appropriate. Thus the reason for representation and the data matrix can give an answer to which type of method should be used.

In order to compare metric and non-metric methods we have analysed the set of Morse Code data which Shepard (1963) investigated. Shepard's result (using an early version of MD-SCAL) is shown in Figure 46 with the Morse code for each item. The structure of the data is apparent - two axes representing number of symbols and dots vs. dashes. We have already suggested that the configuration may in reality be curved in more dimensions, due to the effect of the large number of small similarities.

With the function $\Sigma(D - d)^2$ we ordinated the data using two transformations from the original similarities. The first was $D = 1 - S$ and the second $D = \frac{1}{S} - 1$. These gave Shepard diagrams which were unsatisfactory (Figures 47 and 48) indicating that either the transformations were not suitable or that the data cannot be adequately represented in two dimensions. It should be noted however that a similar structure to Shepard's could be detected in both ordinations (although not so clear-cut). The ordination was repeated with rank order distances - the results are shown in Figures 49 and 50. The Shepard diagram again shows the success of metric methods with non-metric data. Figure 49 gives a representation which shows Shepard's interpretation

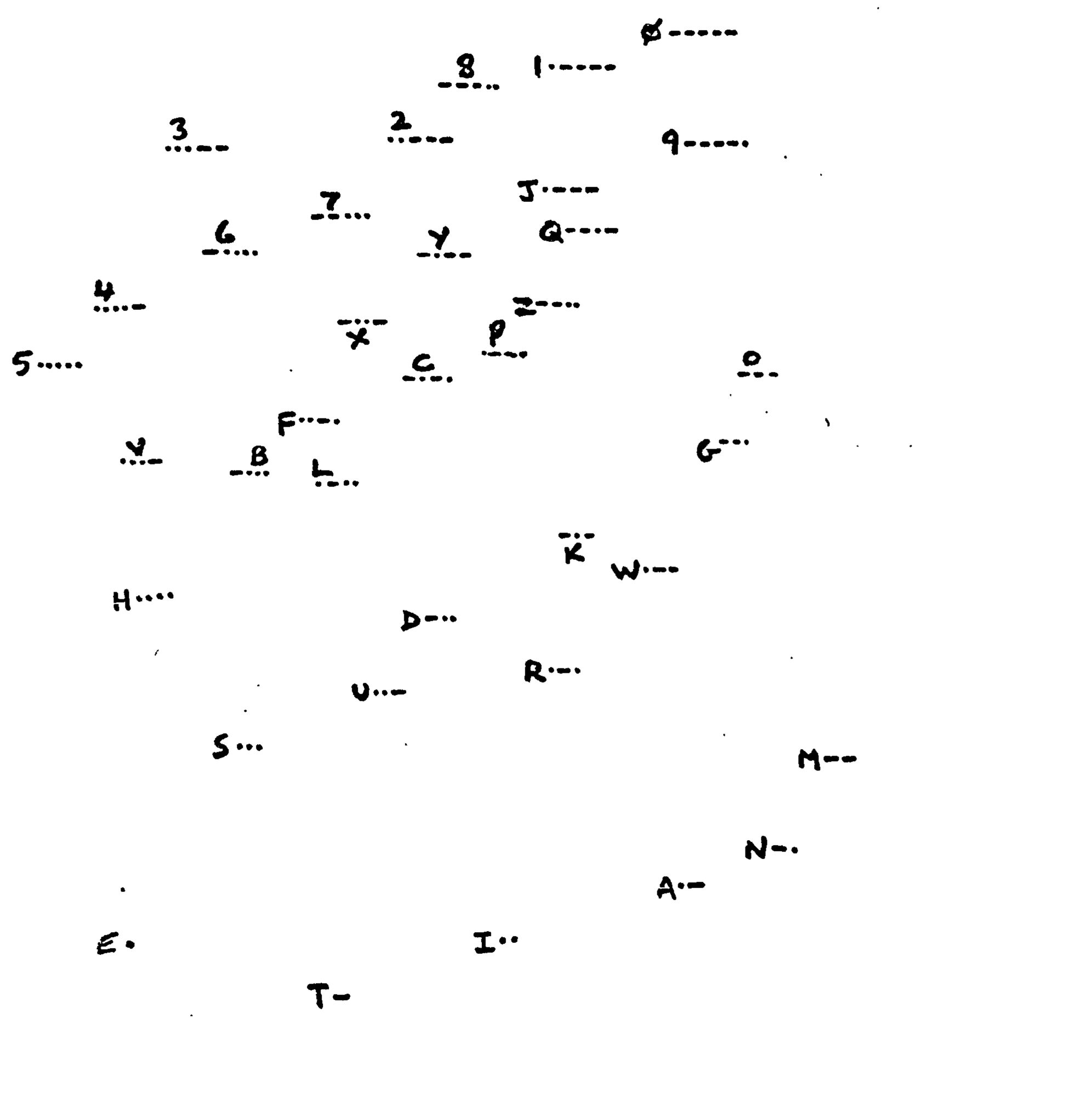
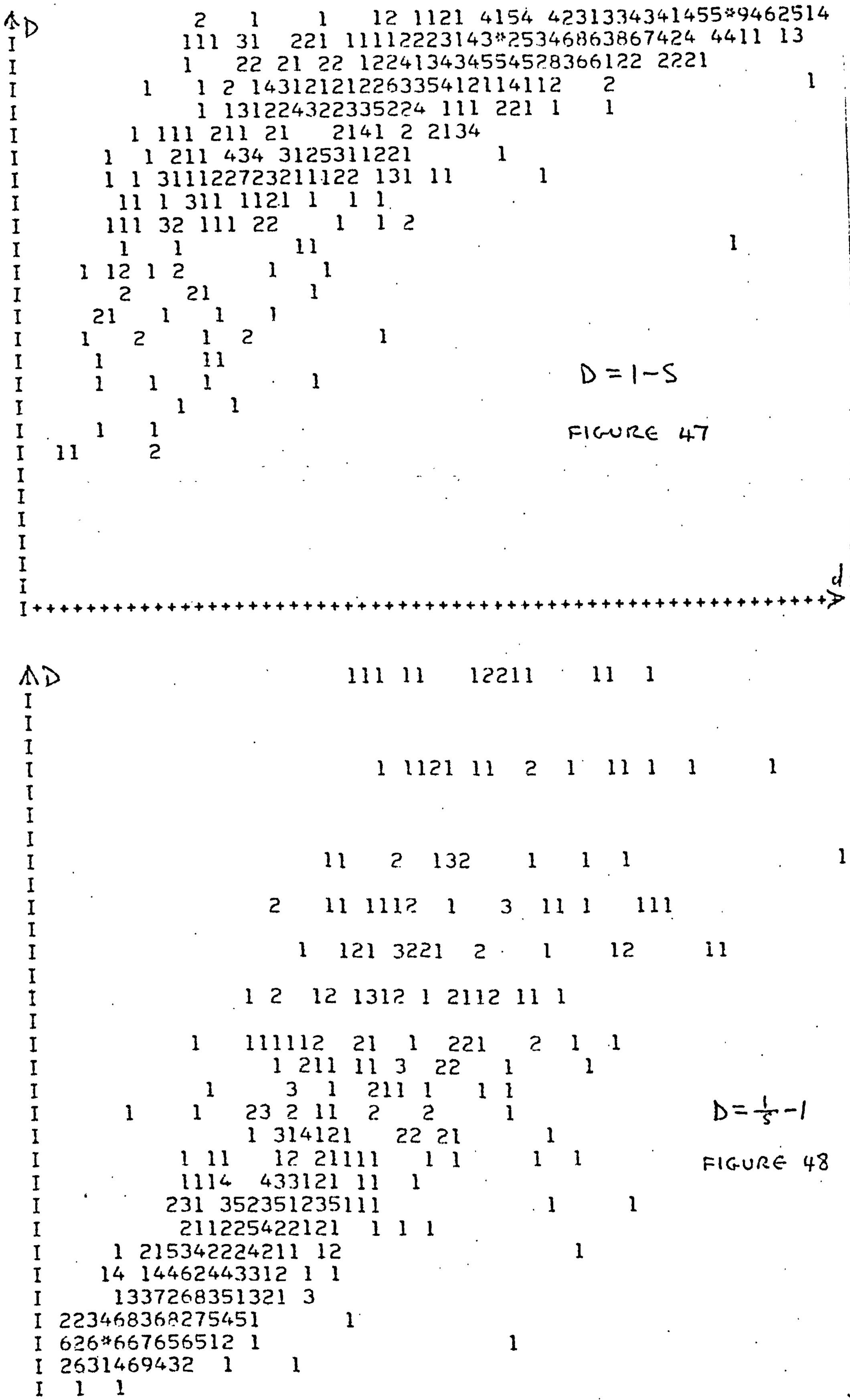


FIGURE 46


2 1 1 12 1121 4154 42313343414555*9462514
111 31 221 11112223143*2534686386742 4411 13
1 22 21 22 122413434554528366122 2221
1 1 2 1431212122633541211411 2 1
1 13122432233522 111 221 1 1
1 111 211 21 2141 2 2134
1 1 211 434 3125311221 1
1 1 311122723211122 131 11 1
11 1 311 1121 1 1 1
111 32 111 22 1 1 2
1 1 11 1
1 12 1 2 1 1
2 21 1
21 1 1 1
1 2 1 2 1
1 11
1 1 1 1
1 1
1 1
11 2
D = 1-S
FIGURE 47
111 11 12211 11 1
1 1121 11 2 1 11 1 1 1
11 2 132 1 1 1 1
2 11 1112 1 3 11 1 111
1 121 3221 2 1 12 11
1 2 12 1312 1 2112 11 1
1 111112 21 1 221 2 1 1
1 211 11 3 22 1 1
1 3 1 211 1 1 1
1 1 23 2 11 2 2 1
1 314121 22 21 1
1 11 12 21111 1 1 1 1
1114 433121 11 1
231 352351235111 1 1
211225422121 1 1 1
1 215342224211 12 1
14 14462443312 1 1
1337268351321 3
223468368275451 1
626*667656512 1 1
2631469432 1 1
1 1
D = 1/5 - 1
FIGURE 48

Ø-----
9----·
O ---
M --
1·----
G---·
N -·
8---··
J·---
Q--·-
2·---- Z----
P·---
T -
Y----
K W·--
C----
7 -----
E·
A·-
X---·
R·--
L·---
D---
3·---- 6----- B----
F···-
I··
U···
4 Y···-
····-
H····
5·····
S···

FIGURE 49

FIGURE 50

of the data clearer than his own result. The over-reduction of the data caused by the use of rank order can be shown by the three-dimensional result represented in Figure 51. It can be seen that the data is roughly coplanar with the exception of the two symbol letters (M, N, A, I). This clearly shows the low similarities between the one and two symbol groups from each other and the other groups. In an attempt to remove the horse-shoe effect, we tried the distance measure, similar to that suggested by Kendall, of

$$d_{ij} = \sum_{k} (S_{ik} - S_{jk})^2$$

this gave the result as in Figures 52 and 53. The Shepard diagram shows a clear linear relationship but the result is not as clear to interpret as the earlier solutions we found. This indicates some danger in the use of such similarity measures.

This completes the experimental section of our investigation into ordination methods. Our conclusions will be reiterated in the next section.

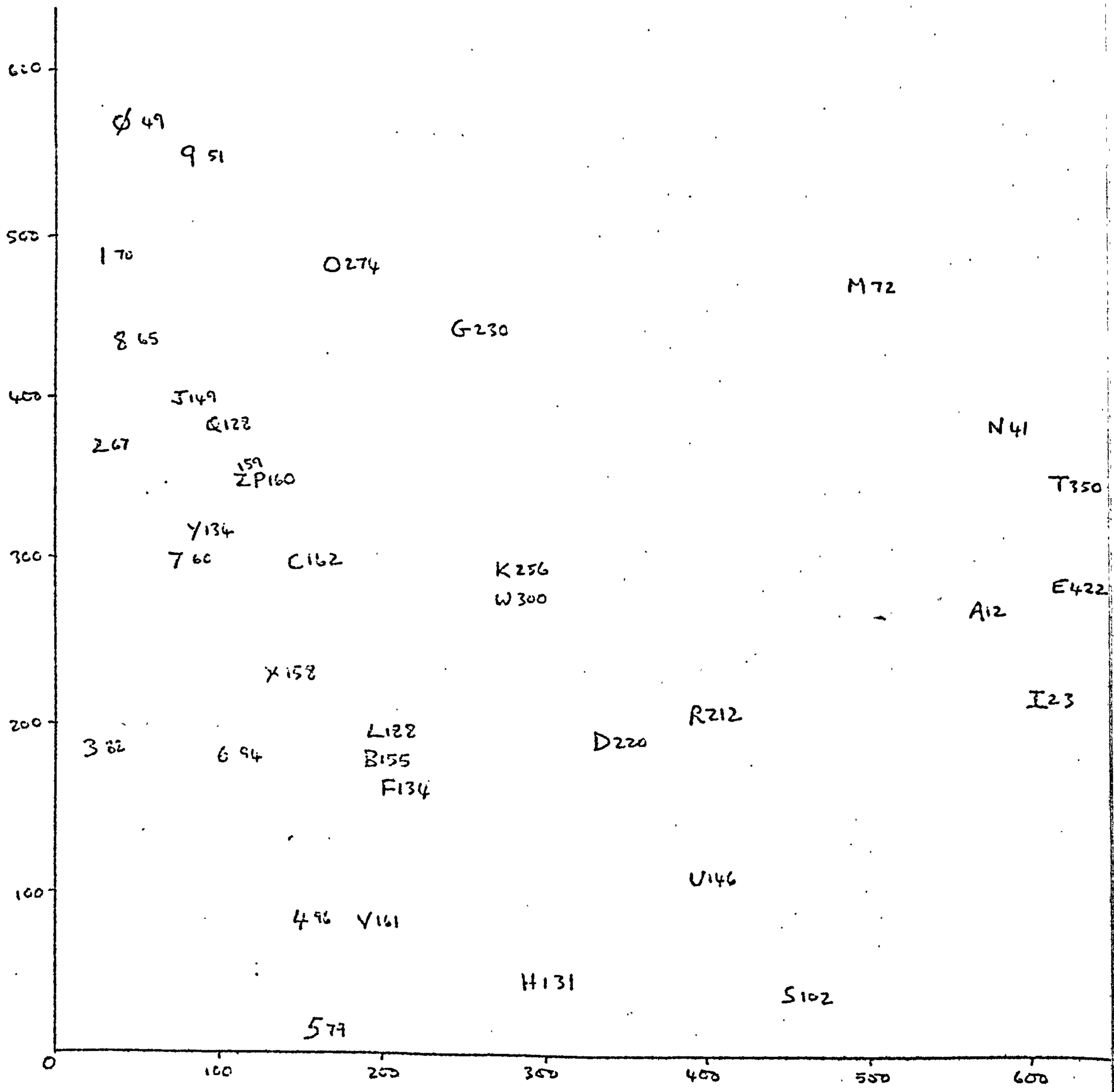


FIGURE 51

FIGURES AFTER LETTERS REFER TO THE THIRD CO-ORDINATE VALUE

FIGURE 52

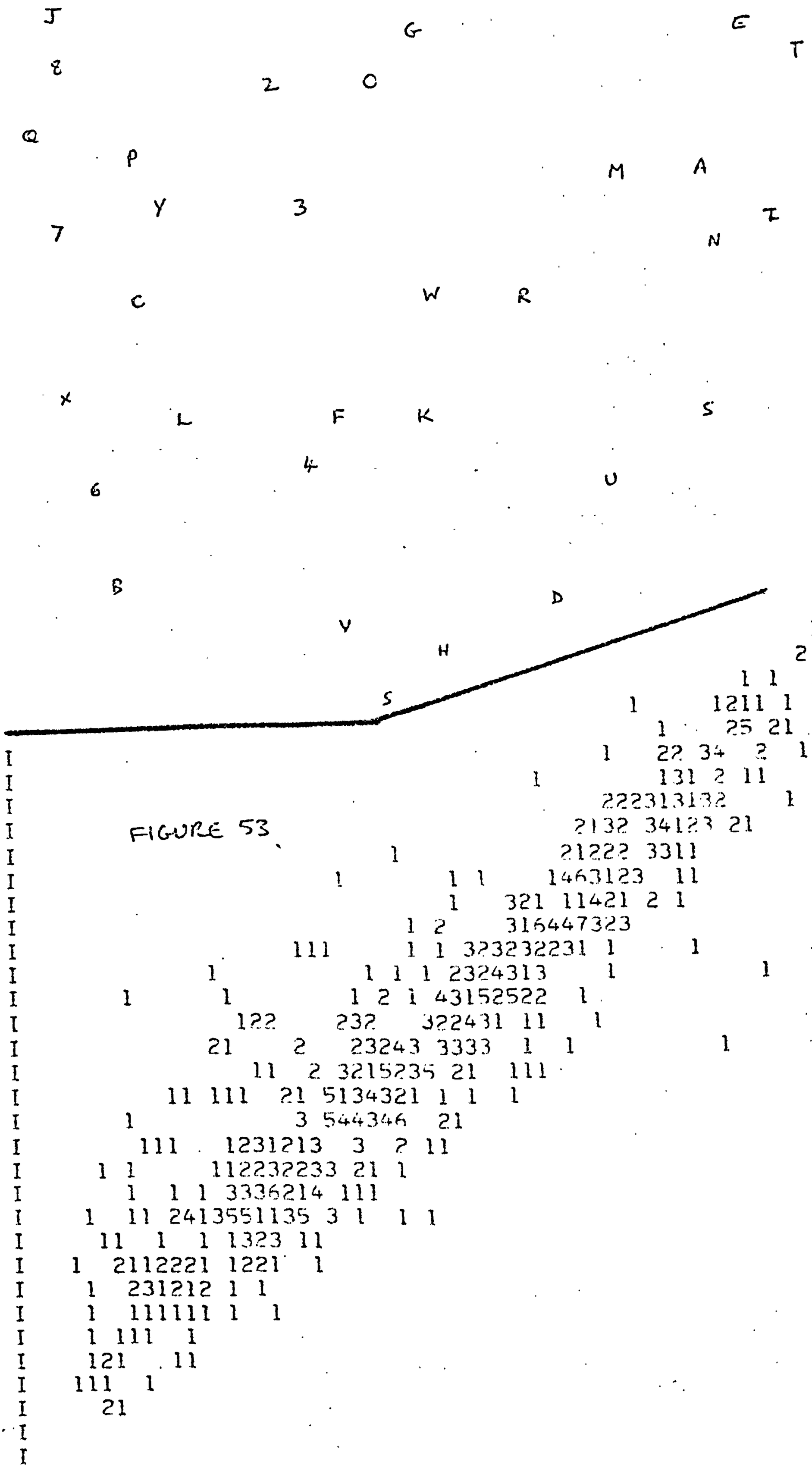


FIGURE 53

D.4 CONCLUSIONS

We have only managed to discuss the subject of ordination in general terms, but have given some important groundwork as a basis for future researches.

Both metric and non-metric methods have been shown to give representations of data which aid the interpretation of the data set, and give information not readily obtainable by other methods. Both types of method give good recoveries of monotonically transformed data, and error in the distance matrix can be largely eliminated, but not error terms connected with the original data, and in the same plane.

Difficulties have been discussed with stress measures that have been employed, and the fact that the 'elbow' effect is not often obtained in practice. These and other possibilities lead to a difficulty in the recovery of dimensionality, which has not been pointed out in the literature. There is a greater tendency to over-reduce the data in non-metric methods, but this effect is common to some extent with all such methods. Over-reduction has been shown to lead to possible twisting or elimination of dimensions which can cause difficulties in dimension labelling and interpretation of results. The resultant ordination may also be less good at representing inter-point distances than inter-group distances.

One difficult problem raised by the scaling methods is whether the data can be meaningfully represented in any

Euclidean space. This is an open question, but may be partially resolved if a metric ordination gives a good low-dimensional result which is easily interpretable.

Our results have indicated that the answer to the horse-shoe problem may not, in all cases, be as straight-forward as in Kendall's works. We have also given an instance of a published example where a two-dimensional horse-shoe has occurred, apparently unnoticed by the author.

As yet there is little evidence on which to differentiate between particular non-metric methods. With the loss functions, $\sum(D-d)^2$ was shown to be generally preferable to $\sum(\frac{D-d}{d})^2$ although in this case, as with non-metric, the choice of method is strongly dependent on the type of error which is expected with the particular data set. Bray and Curtis' method has been shown to be of little value. Metric methods have been demonstrated to be as good as and better than non-metric in some cases. They also give good results with non-metric data.

Our general conclusions are that the methods can give very useful results, but that they need very careful consideration, and need to be executed by someone with experience with the methods and knowledge of the data. Metric methods have been shown to be of equal importance to non-metric, and have been too neglected by other workers, considering that they have some useful and unique properties. The main problem with the methods under discussion is in

over-reducing dimensionality, and the difficult problem of whether a Euclidean representation is valid. We suggest that the methods are more useful for examining inter-group relationships than for identifying dimensions or investigating the relative positioning of single points. Two practical improvements which we have put forward, and which involve only marginal extra computation, are the printing out of the residual matrix, and the calculation of a stress value for each object.

The data has an important bearing on the choice of method. For instance it may be metric, approximately metric, or non-metric. A measure of 'how non-metric' the data is, can be given by the number of sets of three points which do not satisfy the triangle inequality. The data may contain a large number of tied values which may give problems. The error structure to be expected may also give a useful clue to the method to be employed. It is also important to consider if one has reason to expect or require a low-dimensioned Euclidean ordination. The possible use of other methods such as principal components analysis should also be considered at this stage, bearing in mind what is hoped to be obtained from the ordination. For example if dimensions are required, then p.c.a. will be more appropriate.

Clustering and ordination are similar types of technique - both are approaches which look for structure in, or impose structure on, the result. Ordination is a somewhat more exploratory technique since the nature of the

structure is less well defined. Ordination can be used to find overlapping clusters, or clusters which are so close as to be difficult to separate by clustering techniques, in situations where a certain grouping is under examination. We have used ordination as such a technique in two of the case studies given in Section E.2.

The whole area of ordination is one where further research is necessary and desirable. It may be possible to overcome problems in dimension recovery by better methods of stress measurements, or by better similarity measures. The properties of the different non-metric methods have not been determined as yet to such an extent that one may choose between them. The field of applications is also one where research is needed as it is in real situations where the greatest advancements and practical improvements may be made in ordination. The stress-type methods can easily incorporate side-conditions, as these can be included in most optimization procedures. The extension to large data sets may be simpler with ordination than clustering by simply fitting points gradually into the ordination, after suitable choice of the initial points to fit in as the first reference points.

E

USES IN OPERATIONAL RESEARCH

The multivariate methods discussed in the preceding sections have wide application in the business and scientific spheres and can thus be important weapons in the hands of operational research workers. However the use of these methods in O.R. has not been at all extensive, and indeed many operational research departments are unfamiliar (if not ignorant) of these techniques. This may be due to the lack of training which O.R. scientists receive in this area. It may also be because of lack of confidence in the methods due to the shortage of evaluations of the methods. This has been the object of the preceding sections of this work. The small amount of usage of multivariate methods can also be due to the lack of known implementation areas - this is the object of this section.

Operational research, when it began during the Second World War, possessed a technique called search theory (see Morse and Kimball 1951, Engel 1957, Paloheimo 1971), which was concerned with the location of enemy positions. The two-stage search problem (Houlden 1962) involves a general search followed by a more intensive (and expensive) search of areas thought worth investigating on the information gained from the general survey. The use of search theory has diminished in peace time, although Houlden gives the example of an aircraft with a magnetometer searching for anomalies in the earth's magnetic field which might be associated with

mineral deposits. The concept can be extended to the example of an auditor looking through a company's accounts where an investigation of a random sample of transactions is made and any errors are further investigated; however, since errors are often found, not all of them are worth following up. The procedure of search theory assumes knowledge of (in the terminology of this example) the expected number of accidental errors, and the expected number of other errors, etc. The problem becomes straightforward if cluster analysis is used, the results from the first survey may be clustered to show areas worth investigating fully in the second stage.

The problem of inverted search referred to by Ackoff and Sasieni (1968) is that of maximizing the chance of something being found, for example goods in a large store, or information in retrieval. This is also a clustering or ordination problem for if the items are grouped or laid out so that similar objects are near each other, then the search procedure of the searcher will be assisted by the minimization of false trails.

Unfortunately, because of the reduction in search theory usage, the base that could have been the foundation of clustering in operational research was lost.

Another connection between operational research methods and clustering is through graph theory - the nearest neighbour method and the minimum spanning tree contain identical information.

One of the problems in a discussion of applications in operational research is to decide where it ends and other sciences begin. The methods discussed here are all approaches to problems, thus if we took operational research in its widest sense, then any use of the methods would be, by definition, operational research. However, in this section, we will concentrate on those areas which are more connected with managerial decisions.

Management situations and problems are very apt areas for the application of multivariate methods since in many situations data is plentiful but information sparse. The mere presence of large blocks of data does not necessarily imply that the information which is within this data is apparent, and the reduction to a smaller and more usable set can yield facts which were hidden in the original volume of numbers. All the methods discussed are designed for the examination of data structure, thus as simple exploratory tools, they have wide applicability. Examples of this type of investigation are given later.

There are also areas of application with management where the structure of the problem is such that a particular multivariate method will yield a solution, for instance where the desired output is in group form. These will also be discussed later.

A third type of application is where classification is an end in itself, for example in libraries, part numbers, etc., where cluster analysis is of direct use.

The use of cluster analysis and ordination methods can be widened by the introduction of side conditions and weightings of objects. It is a simple process to include in a cluster method constraints which limit cluster size, shape, or dispersion. Weighting of objects can also be incorporated to allow for differing importances between them. The only areas where side conditions have been used to any extent are geographical regionalization and political districting. Geographical regions are normally required to be contiguous and political districts are also required to be compact in some sense.

We begin by surveying some of the operational research applications which have been published.

Marketing

This is the business area in which there has been the greatest use of multivariate methods. Some of the papers published have been of the data investigation type, but the following have been specific areas of investigation:

Market Segmentation - Cluster analysis has been used in several studies to group people who buy a certain product into types to enable brands to be aimed at particular types. This idea is suggested in Christopher (1969). An example using AID is given by Assael (1970) - the advantage in using monothetic methods in this instance is that new individuals may be assigned to existing groups very easily. Lessig and Tollefson (1971) used a polythetic method and experimented with alternate weightings of variables to test the stability of the clusters produced. One of

the best examples of this type of study is Boggis and Held's (1971) analysis of electricity users. They used the Friedman and Rubin method to group consumers according to their demand curves, and proceeded to use discriminant functions to determine which group users were in, on the basis of several easily measured variables such as size of family, etc.

Doyle (1972) uses market segmentation rather differently as the way in which customers see the products. He produces a two-dimensional ordination of beverages by factor analysis to investigate the relative positions of types and to suggest the important dimensions.
R.M. Johnson (1971) in a similar study using multiple discriminant analysis introduced ideal points into the product space. Studies by Klahr (1970) and Rao (1972) are of this type.

Green and Carmone (1968) segment the computer market on size, performance, etc., to produce market segments, from which one could investigate how well spread each company is within the market. Gibson et al (1972) also group according to physical characteristics and also produce a 3D ordination - they used complete link and TORSCA.

Gap Analysis - Obtaining low dimensioned ordinations of points representing different brands of a particular product, such that the more similar two brands are, the closer they are in the ordination. This can be used to investigate 'gaps' in the market where new products could be 'inserted' (see Morgan and Purnell 1969), their characteristics being obtained from the dimensions of the configuration. This concept is examined in more depth later. The idea is somewhat opposed to the market segmentation point of view which supposes different groups of people buying different brands.

This idea suggests a continuum of buyers who will select the brand nearest to their ideal.

Readership Analysis - Certain newspapers, magazines tend to overlap in readership. By taking a sample of the public the similarity between papers can be assessed by the number of people that read both. Thus newspapers may be grouped. This grouping can be used as a basis for advertizing - if one wishes to reach a broad public then one can choose one paper from each group (on the basis of ad price and circulation), or one can try for segment saturation and advertize in all papers of one group. This basic idea is discussed in Joyce and Channon (1966) and Frank and Green (1968), and an example is given using Lorr's method in Bass et al (1969). This could be extended to clustering commercial television or radio programmes. Television programmes have been considered from the market segmentation view by Green et al (1969) - here they produced a three-dimensional ordination of programmes according to their similarity and attempt to fit ideal points within this ordination. This is a misuse of the concept of ideal points, since programmes which are alike can be a long way apart in preference - for example a good western and an incredibly bad western are very <u>similar</u> but will be distant in <u>preference</u> from one another. An example given by Massey (1971) divided people into groups according to the radio stations they listened to.

Test Marketing - If one could group towns according to population characteristics, or stores on customer characteristics, then for a stratified sample for test marketing purposes one could be selected from each group. Alternatively, in test marketing for different price levels, then stores which were most similar would be required, and thus stores from one particular group would be chosen. A pilot study of this type is given

in Green et al (1967a) who grouped American cities. The method used a side condition so that groups contained the same number of cities, the reason for this is not given; this of course forces outliers into groups, which seems undesirable. (The paper has been further discussed by Morrison (1967), Scuchman (1967) and Green et al (1967b).) A similar study using Rubin's hill climbing method and complete link on several stores is given in Day and Heeler (1971). An MD-SCAL orientation is used as a check.

Other areas of marketing have also been subjected to this form of data analysis. Sethi (1971) used the BC-TRY system to cluster countries, in order that a similar marketing policy could be used for each group, saving the expense of formulating a different plan for each. Heald (1972) uses AID to group stores into various physical factors to determine which influence turnover. Other examples of marketing applications are given in Joyce and Channon (1966), Frank and Green (1968) and Green and Carmone (1972).

Personnel

This area of management is one where data is plentiful and thus it is one of the areas in which data methods have been applied.

Ford and Borgatta (1970) have used factor analysis to analyse work satisfaction into five types of satisfaction - interest, not wasteful of effort, freedom in planning, say in how job is done, opportunities. Schutz and Siegal (1964) examined the dimensions of the job of Naval aviation technicians by multidimensional scaling to determine four

basic dimensions. Thomas (1952) in a very early application of cluster analysis (BCTRY) grouped office operations, using a list of 139 basic clerical tasks - they analysed a sample of office workers and obtained eight basic operations - typing, filing, calculation, etc. Brown (1967) investigated the dimensions of interpersonal relations in jobs to find seven basic dimensions. Gardner (1972) has produced a grouping of the interests of naval officer candidates which gives a clear division into introvert and extrovert interests.

Other Topics

The grouping of land (especially urban) areas for planning is one which has recently been analysed by cluster analysis. This approach to planning is related to geography by the science of land use analysis. Examples are Kelly (1969) and Goddard (1968, 1970).

The investigation of stock market share price movements can give valuable information for the diversification of investment portfolios. See King (1966) and discussion later in the Addenda. Companies have also been analysed for their similarity in financial performance (see Gupta and Huefner 1973, Jensen 1971). Other work on grouping firms (Goronzy 1969a, b, Pinto and Pinder 1972) simply find types of company from performance and size characteristics. This type of analysis could be useful for defining industries and competitors, or for identifying possible fields of diversification.

Klahr (1969) has examined the decision-making processes of college admission officers and found strong evidence to support the idea of ideal points. Kernan (1968) analysed decisions to determine whether such concepts as maximizing minimum gain (the minimax criterion) were actually applied.

The Local Government Operational Research Unit (1971, 1972) have undertaken work in social services planning. By grouping a representative sample of elderly persons they arrive at a set of 'typical' old people from which they can determine the type of service required by each, and hence use this data for planning purposes.

From Kruskal and Hart (1966) can be seen an interesting application in the analysis of computer malfunctions. By grouping the circuits of the computer which were mal-functioning (the data is supplied by the computers own fault diagnosis mechanism) in each breakdown, they were able to find groups of 'symptoms' which lead them to diagnose various 'ailments'. This could be of advantage in the location and early rectification of faults which is of importance with such costly machines.

The relationship between cluster analysis and the problem of warehouse (hospital, bank, etc.) location has been noted by Scott (1969) and an example is given in Cooper (1973). The problem is simply to group demand and evaluate the cost for several numbers of groups. The groups would of course be non-overlapping and iterative relocation would be a good method since it ensures a type of optimum at each stage.

A solution to the travelling salesman problem has been suggested, by the use of seriation (Wilkinson 1971) and by clustering (Jardine 1970). Seriation (and of course one-dimensional ordination) gives a linear arrangement of the objects. To ensure that the tour begins and ends at a given point, the first and last elements of the matrix can be fixed and equal. With scaling methods two objects would be included which are the same except they have dissimilarity M (where M is some very large number). Since dissimilarity between two towns can be turned directly into the cost of travel between them, then we can use costs in our matrix and use metric scaling methods. The clustering approach entails finding points which are very close and hence need to be close in the tour.

In the following discussion, we will consider possible applications of the methods which we have analysed. These will be partially speculative, but in the Addenda we will give several case studies of our methods in action.

Data Investigation Applications

We have already divided the uses of multivariate methods into two main classes - data investigation and specific applications. The examination of data has two main uses:

1. To reduce the size of data set with the minimum loss of information.

2. To gain information from the data.

Areas of application are difficult to discuss since these methods may be applied to any sizeable data set, and the actual approach will differ according to the reason for studying the data, and the type of data itself. However, we will outline typical investigation areas here and give examples in the next section.

For the past ten years exploratory studies have been carried out on stock market prices, to investigate the way in which they move, in order to obtain information which could be of possible advantage to investors. Personnel data is normally readily available (in depersonalized form), and could yield information as to whether departments tended to employ certain types of person, whether other factors were correlated with success, etc. Data from market research questionnaires could be clustered instead of immediately aggregated to see if respondents were homogenous, and if not what factors separated groups. The examination of data on production line failures or work accidents, over a period of time, could yield possible underlying causes. For any sort of planning purposes one must generalize to groups, normally these are dissections and not clusterings - the use of cluster analysis would obviously give more meaningful groups, and less sweeping generalizations. Examination of demand curves of items of stock could yield 'types' of demand which would mean different stock levels. Analysis of accidents, fires, etc., could yield more meaningful classifications of risks for assessing insurance premiums.

Specific Applications

The problem of store layout was considered earlier as an inverted search problem. Supermarket layout differs in that many purchases are made in the same shop. In order to encourage customer traffic flow (and also to ensure each shopper visits as much as possible of the store), certain 'demand' lines, such as butter, bacon, sugar and tea must be placed as far away as possible from each other. The concept of 'making one line sell another' implies that one should arrange items next to the ones shoppers associate with them. This produces a similarity matrix of associations, with demand items having little similarity. From this items can be clustered to shelves (with approximately equal sized clusters) or by ordination a two-dimensional layout can be found directly. The matrix of associations can be built up to include any other items which are associated with certain products. Thus one might sell teapots near tea and rubber gloves near washing powder.

These principles can be extended to shopping centre, housing, library and factory layout (which is considered in Section E.3). Here similarities are assessed somewhat differently, but all measure the importance of having items close. Here ordination would normally be used, but possibly preceded by a cluster analysis to divide the data into smaller groups because of physical constraints.

This leads to the division of organizations between buildings (or floors of a building). Here the similarities are provided by the importance of contact between people,

departments, and physical movements of parts, information, etc. This can be of particular importance when reorganizations or takeovers take place. A good example is the recent local government reorganization which increased the size of many council areas and hence they had several sets of buildings between which staff had to be reallocated. The splitting of organizations into units with the least connection between them can readily be applied in situations where effective communication is of some importance such as in government or the armed forces. The idea is related to that suggested by Jardine (1970) where large electronic machines are divided into sections which have the least number of connections with the rest of the machine, for easy removal and replacement.

Several network problems can be approached by clustering - the travelling salesman problem has already been considered. The vehicle routing or clover leaf problem is also one which is amenable to a cluster-type approach. The Fletcher, Clarke, Wright algorithm (Clarke and Wright 1964, Fletcher and Clarke 1964), which is normally applied to this problem (see NCC 1969), is a simple type of agglomerative hierarchical linkage clustering. This will be discussed more fully later. School bus scheduling is of course a very similar problem.

Another network problem is that of supply networks, where for example houses must be supplied with water. This will be considered later.

Warehouse location has been suggested as a cluster problem already, and this can be extended to the problem of location of new factories and warehouses by subtracting the demand which can be supplied by existing warehouses (using the transportation algorithm) and proceeding as in the simple case.

Similar problems such as the location of hospitals (c.f. Abernathy and Hershey 1972) can also be approached in this way, also sales regions and administrative regions (such as local government areas), where possibly constraints such as equal size or compactness would be introduced. The data for use in these regionalizations (especially sales regions) can be obtained from market research bureaus, who have the whole country analysed by street.

The use of clustering for stratifying samples is an obvious application for market research and other investigations., This cannot of course be used in all cases since one is often in the position where one does not know until after the data has been collected what clustering exists. The use of cluster stratified samples reduces the error by ensuring a correct balance between certain factors.

Another (oversimplified) problem for clustering is the prediction of regions, for example in the case of oil-drilling in the North Sea, one has known points where this has been successful and a measure of that success, and also known failure points, often with measures of failure. These weightings can be used in cluster methods to suggest new

areas where drilling might be successful. It might be possible to use ordination, using the difference in success between strikes as distance, to obtain a two or three dimensional map of strikes where distance was a measure of yield. By beginning with the geographical configuration, points with the same success measure that were far apart would be 'kept apart' by the dissimilar oil finds between these points.

An application, which will be considered later, which is allied to the cluster problem is that of making teams, sales regions, samples, etc., to be as similar in make up as possible to each other - i.e. ensuring the groups themselves are similar, rather than the elements within groups.

Ordination could be used in an extension to the gap analysis idea to find a two-dimensional layout of the distance people travel to their nearest shop, bank, post office, etc., as a basis for the siting of new branches, or the closing of branches.

It can be noted that if each person in an organization could be measured on various criteria measuring his particular function within that company, and if a dendrogram were produced from this by clustering, then the output would be an organizational hierarchy. Thus if an organization were analysed in this way various information could be obtained which could help with company structure. This could be extended to include intended expansions and their impact on the hierarchical structure could be assessed.

Clustering is also a useful concept in model generation. For example the so-called 'gravity' model of shopping (see Reilly 1931, Heald 1972) assumes that shopping centres have an associated 'mass' which attracts customers according to their distance from that mass. Another idea is that of empty taxi flows. This model is that a cab driver knows of certain areas where he is more likely to pick up a fare, thus when he puts down a fare he will travel directly to the nearest cluster centre, tour there for a while, and then move directly to the next nearest cluster centre, and so on until he picks up a fare.

Conclusions

Several wide ranging problems have been suggested and the exploration of each of these topics could be of value to operational research. The methods have widespread applicability and hence deserve a place among operational research techniques. In order to show their usefulness further we proceed in the next two sections to examine a few of the applications mentioned here, in more depth.

ADDENDA

OPERATIONAL RESEARCH CASE STUDIES

1. Data Investigation
   - (a) Input-Output Analysis
   - (b) Stock Market Data
   - (c) A Manpower Study

2. Specific Applications
   - (a) Vehicle Routing
   - (b) Sewer Pipes Problem
   - (c) Team Organizing Problem
   - (d) Gap Analysis
   - (e) Factory Layout

ADDENDA

1. Data Investigation

We have considered, in Section E, the way in which cluster and ordination methods may be used for data reduction and exploration, and concluded that this is best shown by example. In this section we shall give three examples of the use of cluster methods and ordination methods on data sets, in which one of the aims is simple investigation. Some of these analyses were carried out before the final conclusions had been arrived at from the cluster comparison, and thus the actual methods used on the examples may not have been optimal, but in these cases, a discussion of which method to use is included, in the light of our comparison results.

The first example is the investigation of the input-output matrix for British industry. The purpose was to see if further aggregation of the table is possible, and also to investigate the interrelations of industries, and their behaviour over time.

The other two examples are on much larger data sets. The second case study concerns the returns on stock market shares in the 1960's obtained from the City University Data Bank. The investigation was to examine co-movements of shares, the information from this being of particular importance for portfolio selection. This study included the use of ordination as a technique for finding overlapping clusters.

The last data set consisted of manpower statistics from 584 companies - this was a commissioned study for the Printing and Publishing Industry Training Board. The study was into the comparative manpower structure of the companies. This involved a cluster analysis of 438 firms, and it is in this section that our method for analysing large data sets by clustering is explained.

(a) INPUT-OUTPUT ANALYSIS

In economics, cluster analysis can be used to aggregate large sets of data into smaller sets which are more suitable for planning purposes. For example one divides a country into regions when discussing unemployment and areas for development, and companies are grouped into industries for research and training purposes. This type of agglomeration of data is necessary in macro-economics in order for plans to be workable, and because of large errors in the system any further division into more classes may not achieve much greater sophistication.

Cluster analysis has not been used to any great extent for the purposes of aggregation, although it is of obvious use in this application. The normal methods which are employed are heuristic, largely based on experience, and traditional or historical grounds.

One particular area in which aggregation can play an important role is in input-output tables, and here the use of cluster analysis is of some interest, because of the relationship between the observations and the variables. In input-output tables the information which is displayed is data which would not be immediately apparent from the full matrix of which it is a summary. A similar type of aggregation problem has been examined by Fisher (1969) using cluster analysis.

The tables we have chosen to investigate are the input-output matrices of inter-industry transactions for Great Britain and Northern Ireland. As an example of

cluster analysis in action we will investigate the possibility of a reduction of the size of the table without reducing the information it conveys appreciably, and we will also consider the relationships amongst the industries, and over time. It might also be possible to reduce to a rectangular matrix if two industries were only similar in their suppliers or in the industries they supplied (this would also have to continue with time).

Our data sets are the two most recent tables to be published - the 1963 and 1968 industrial input-output tables. We consider only inter-industry dealings, and exclude final buyers. In 1963 there were 27 industries, and in 1968 there were 34, the main changes, as far as can be judged, are set out below:

1963	1968
Leather and Clothing	Leather, etc. Clothing and Footwear
Road Transport Rail Transport Other Transport	Transport
Metal Manufacture	Iron and Steel Non-ferrous Metal
Other Engineering	Mechanical Engineering Instrument Engineering Electrical Engineering Other Metal Goods
Other Manufacturing	Paper and Printing Timber and Furniture Bricks, etc. Other Manufacturing

In order to examine temporal relationships we will analyse each data set separately. The other two relationships could possibly be analysed in a single data set. We have an unusual type of matrix where the observations and variables are the same set of objects, and the rows and columns of the matrix represent different quantities. We could analyse the data for each year by taking the row values and column values for each industry as a single set of variables, and hence use an n by 2n matrix. However this would involve scaling difficulties between the row and column values, and this would preclude the possibility of reduction of the matrix to a rectangular set. This can be overcome by considering each matrix as two sets of data - by rows and columns, and by using judgment to relate the results.

If we were to cluster the data as they stand, with all values in monetary terms, then the size factor would determine the groupings. In the matrix of outputs we could eliminate this by using, for each industry, the percentage of output consumed by each other industry (and in the input data set we convert to the percentage of input from the other industries). This however would mean that in the output matrix, industries with high consumption would dominate the matrix, and in the input matrix large suppliers would determine the clustering through overweighting. We therefore normalize our variables in each case. Our data is now in a suitable form for analysis.

In view of our favourable results in other studies we used Euclidean distance squared for our distance measure. The data sets were very small and thus could be clustered quickly with any method. We thus chose to evaluate them by more than one technique. We chose Centroid, Beale's and the Neighbourhood method as representing different types of cluster method, and also Nearest Neighbour as an outlier test.

(In the light of our cluster method comparison in Part C we may have done better to include a method which was better at investigating the presence of less rounded clusters, such as MODE 2 for example. However, nearest neighbour was included in the methods used, and produced a close enough dendrogram to the centroid result for conclusions to be drawn.)

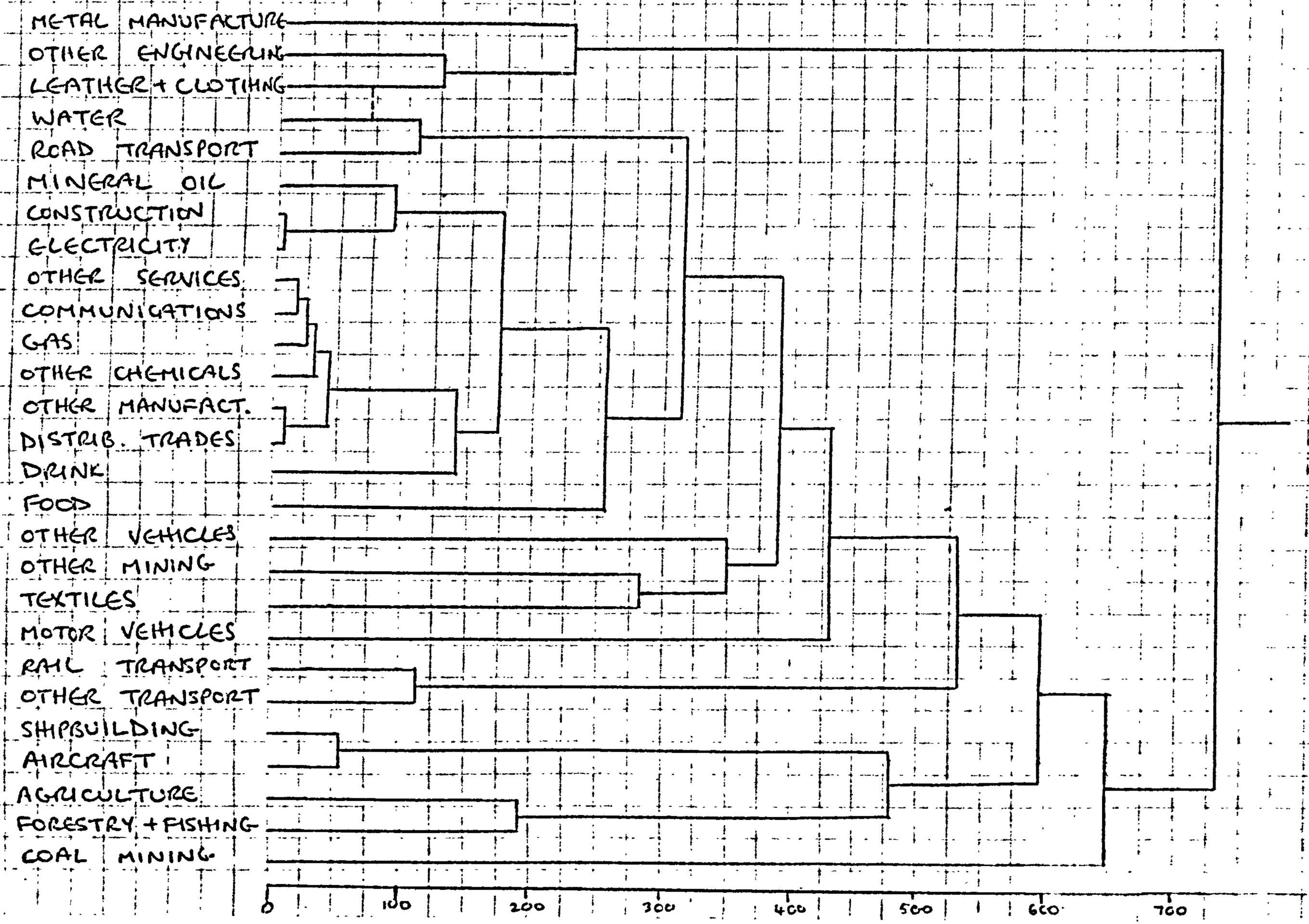
We first examine the results for each of the two years separately.

1963 Data

We first considered the results with the output matrix. From the nearest neighbour output there was no evidence of the existence of outliers. The Centroid and Neighbourhood methods gave almost identical results. They both contained a large amount of chaining, and were very similar to the nearest neighbour output - indicating an almost perfectly unimodal group. Beale's method showed a less chained result, which had only one relocation, as shown in Figure 54, which was the splitting of Water from Leather and Clothing.

FIGURE 54

1963 OUTPUT MATRIX — BEALES METHOD



The grouping is not very marked, this lack of distinct clustering is shown by the split of Water and Leather, which had joined very early, and which end up one in each of the final two clusters. From these results the only consistent grouping which could be detected was as follows:

GROUP 1: Distributive Trades, Other Manufacturing, Other Services, Communications, Gas, Other Chemicals

GROUP 2: Construction, Electricity

GROUP 3: Shipbuilding, Aircraft

The first group supply nearly all industries to an equal extent and form a General Services group. The second group also supply most of the industries, but a disproportionately high amount of the Water industry's input. The third group give almost all their output to Other Transport indicating that perhaps this group should be divided into Air and Sea Transport.

The data was also ordinated using the matric stress minimization of

$$\sum \left(\frac{D_{ij} - d_{ij}}{D_{ij}} \right)^2$$

The result is shown in Figure 55. The lack of distinct groups is evident. The groups we have tentatively identified and the dendrogram we have given, can be clearly related to the ordination result.

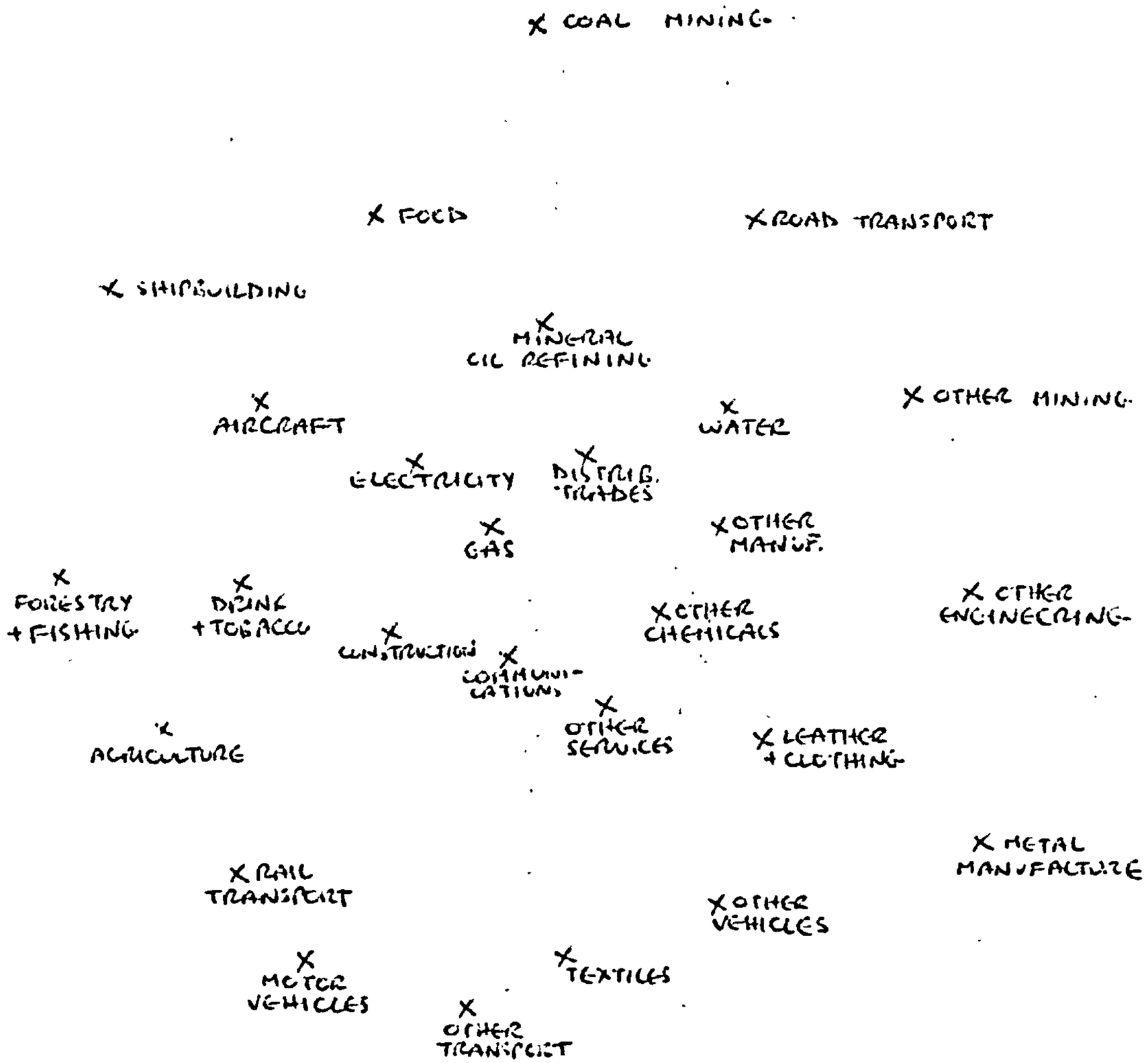

COAL MINING
FOOD
ROAD TRANSPORT
SHIPBUILDING
MINERAL OIL REFINING
AIRCRAFT
WATER
OTHER MINING
ELECTRICITY
DISTRIB. TRADES
GAS
OTHER MANUF.
FORESTRY + FISHING
DRINK + TOBACCO
CONSTRUCTION
COMMUNI-CATIONS
OTHER CHEMICALS
OTHER ENGINEERING
AGRICULTURE
OTHER SERVICES
LEATHER + CLOTHING
METAL MANUFACTURE
RAIL TRANSPORT
OTHER VEHICLES
MOTOR VEHICLES
TEXTILES
OTHER TRANSPORT

FIGURE 55

The input matrix also gave no outliers. The Centroid and Neighbourhood methods gave similar results, and again the data chained but for two or three early groups - the Neighbourhood clustering is shown in Figure 56.

The Beale's method result included a very large number of relocations, and the objective function did not increase very much at the higher levels of clustering. This also indicated the lack of distinct groups, but that the points were possibly more evenly spaced than in the previous data set. From the results the following groups were extracted:

GROUP 1: Shipbuilding, Aircraft, Motor Vehicles, Other Vehicles, Other Engineering

GROUP 2: Gas, Electricity

GROUP 3: Metal Manufacturing, Other Manufacturing

Group 1 is mainly a transport manufacturing group which has one main supplier - Metal Manufacturers. Gas and Electricity receive half their inputs from coal mining. Group 3 has two main suppliers - other chemicals and other engineering.

The only similarity in the groupings of the input and output matrices is that of shipbuilding and aircraft, who have similar suppliers and who both are inputs for Other Transport.

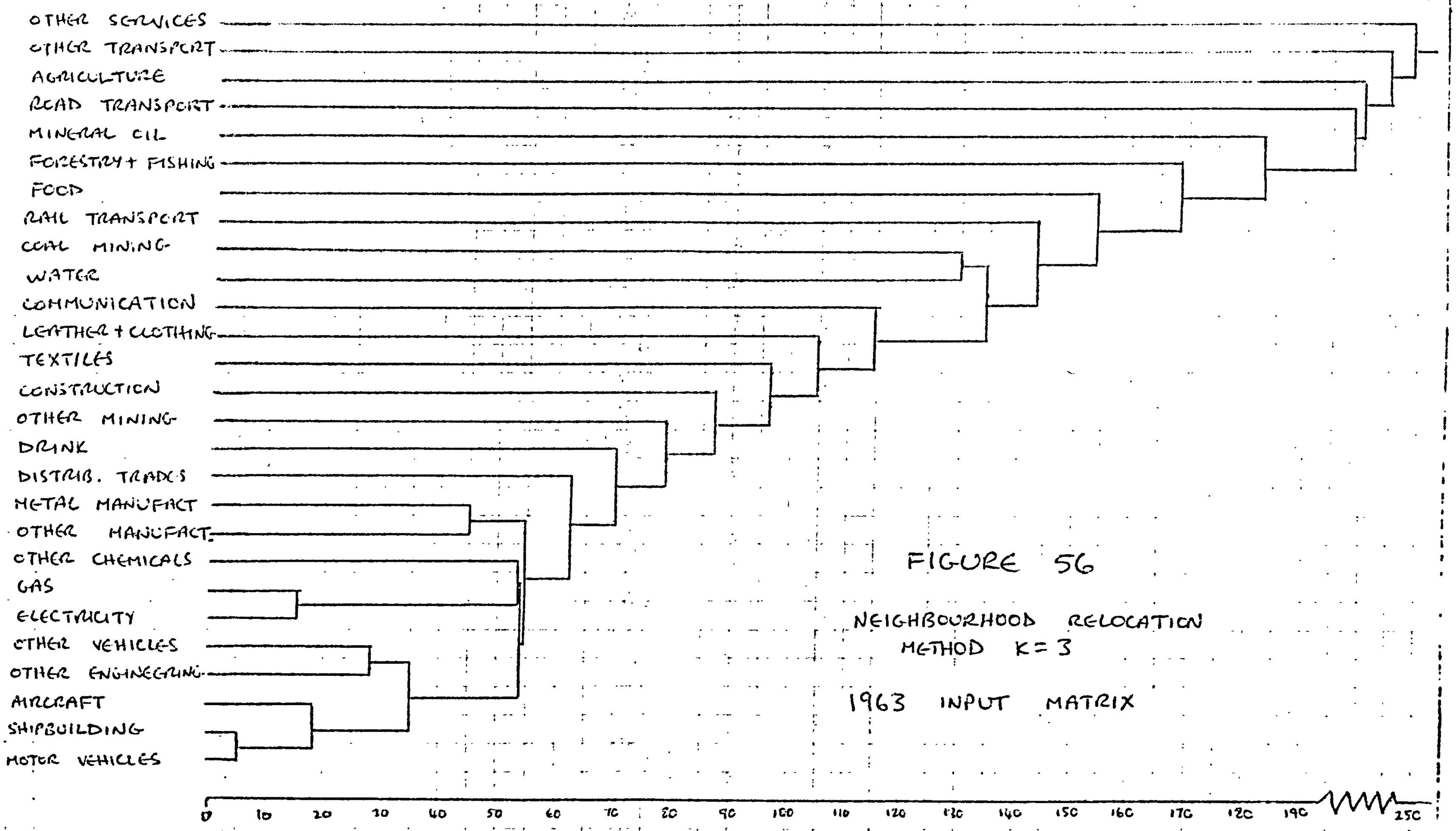


FIGURE 56

NEIGHBOURHOOD RELOCATION METHOD K = 3

1963 INPUT MATRIX

1968 Data

With the output data no outliers were found. As with the 1963 data a large amount of chaining was present in the Centroid and Neighbourhood methods. The dendrogram for Centroid is given in Figure 57. Beale's method again showed a large number of relocations. The only groupings in the Centroid and Neighbourhood methods which were borne out by Beale's were:

GROUP 1: Mineral Oil, Construction, Water, Distributive Trades, Misc. Services

GROUP 2: Motor Vehicles, Aerospace, Other Vehicles, Gas

GROUP 3: Textiles, Leather

GROUP 4: Bricks, Timber and Furniture

GROUP 5: Iron and Steel, Non-ferrous Metals

The first two groups supply most other industries, but a particular difference is that the first group are suppliers of the chemical industry. Group 3 are suppliers of Clothing and Footwear, Group 4 of the Construction industry and Group 5 the Vehicle manufacturers and other engineering sectors. It is interesting that the last three groups had in the 1963 table been combined to Leather and Clothing, Other Manufacturing and Metal Manufacturing respectively. The first two groups do not bear any resemblance to those found in the earlier table, but the first group again appears to be a type of General Services group.

The input data yielded one outlier - Transport, which has most of its input from the vehicle industries. The results followed a similar pattern to the previous ones, but

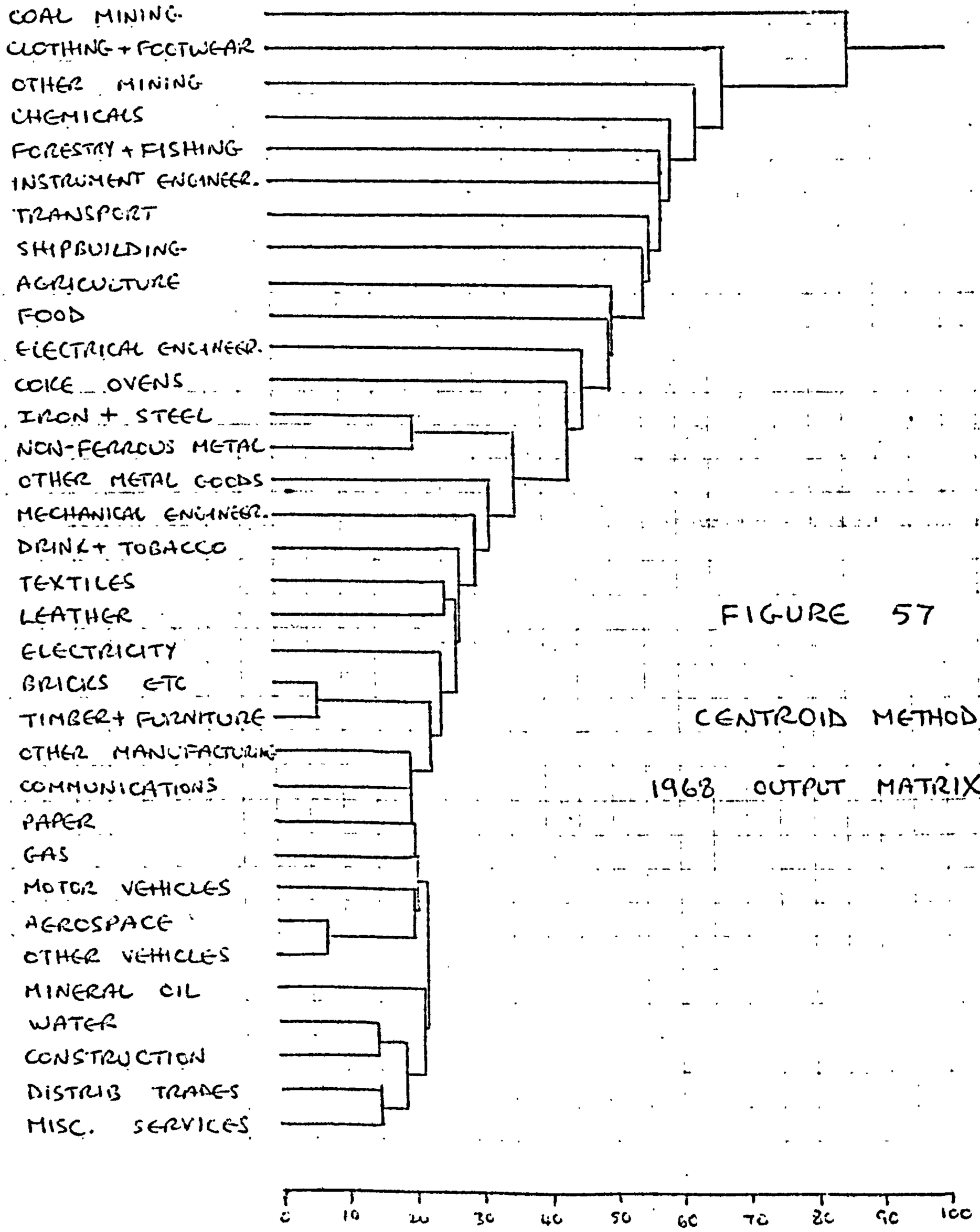


FIGURE 57

CENTROID METHOD

1968 OUTPUT MATRIX

with more small groupings. The resultant groupings were as follows:

GROUP 1: Coke Ovens, Electricity

GROUP 2: Bricks, Non-ferrous Metal

GROUP 3: Aerospace, Electrical Engineering

GROUP 4: Shipbuilding, Motor Vehicles, Mechanical Engineering

GROUP 5: Other Mining, Mineral Oil

GROUP 6: Drink and Tobacco, Chemicals

GROUP 7: Other Manufacturing, Leather, Paper, Textiles

Group 1 are heavy coal consumers, Group 2 have common inputs from Other Mining and Quarrying, Group 3 have high inputs from Other Metal Goods and most of the engineering sectors, Group 4 is similar to Group 3, but uses proportionately more Iron and Steel, Group 5 have high usage of Transport and Misc. Services, the inputs of Group 6, which might seem an unlikely pairing, are dominated by Misc. Services, and Group 7 have high Chemical inputs.

There is only one similarity with the output groupings - the combining of Leather and Textiles, which are similar products both used for Clothing and Footwear. None of the input groups bears any relation to the changes in classification between 1963 and 1968.

The only grouping similar to that of the 1963 input groups is the pairing of shipbuilding with motor vehicles.

Of particular interest is the ordination of the 1968 input data. This is shown in Figure 58. The lack of

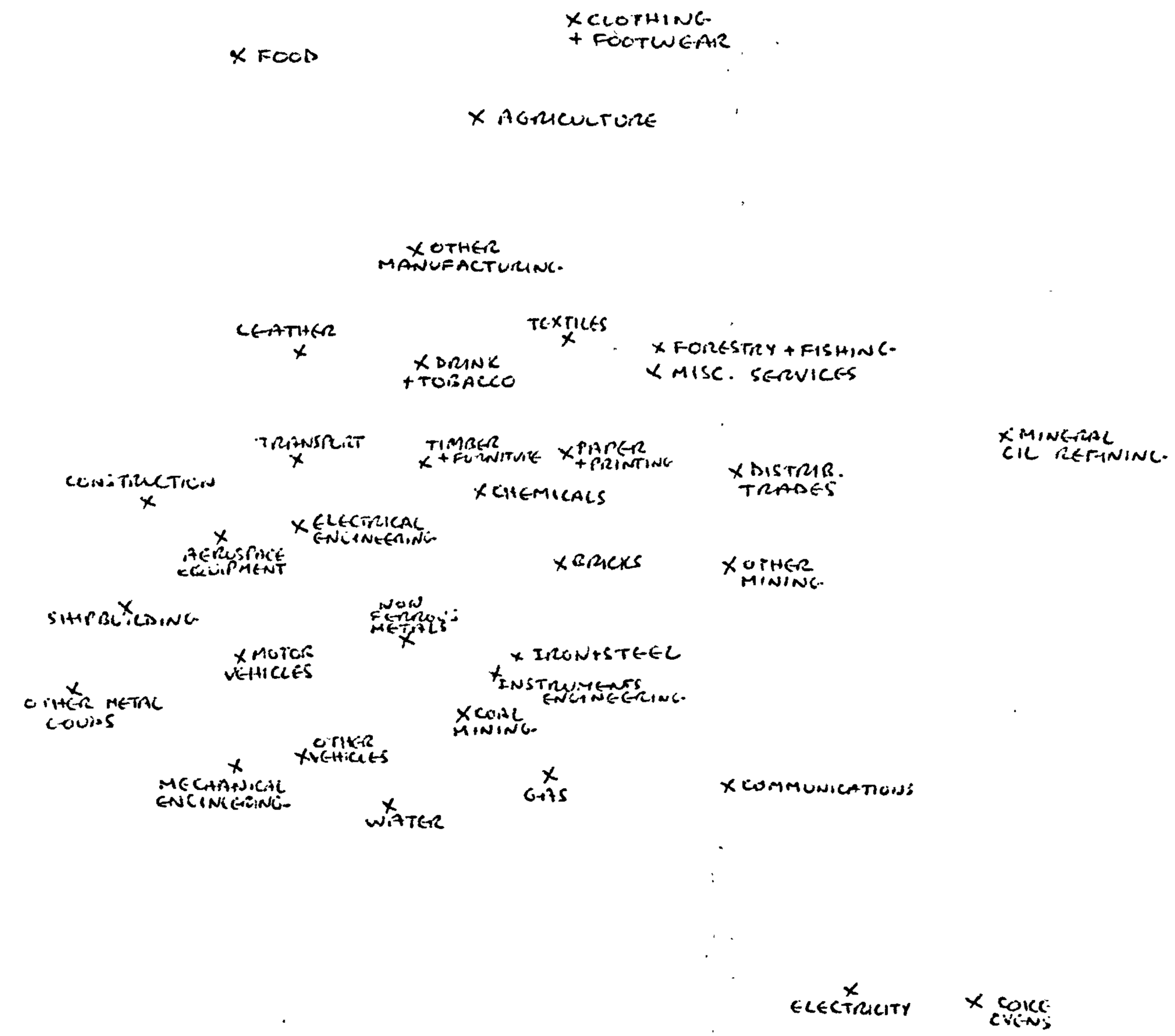

CLOTHING + FOOTWEAR
FOOD
AGRICULTURE
OTHER MANUFACTURING
LEATHER
TEXTILES
DRINK + TOBACCO
FORESTRY + FISHING
MISC. SERVICES
TRANSPORT
TIMBER + FURNITURE
PAPER + PRINTING
MINERAL OIL REFINING
CONSTRUCTION
CHEMICALS
DISTRIB. TRADES
ELECTRICAL ENGINEERING
AEROSPACE EQUIPMENT
BRICKS
OTHER MINING
SHIPBUILDING
NON FERROUS METALS
MOTOR VEHICLES
IRON + STEEL
INSTRUMENTS ENGINEERING
OTHER METAL GOODS
COAL MINING
OTHER VEHICLES
MECHANICAL ENGINEERING
GAS
COMMUNICATIONS
WATER
ELECTRICITY
COKE OVENS

FIGURE 58

grouping is apparent, but if one considers the type of industry in particular regions of the diagram then an interpretation becomes easier. Consumer goods are at the top of the diagram, engineering and other heavy industry are at the lower left, and services are found at the lower right. This vague grouping was also present in the 1963 input ordination. No such simple interpretation could be placed on the output ordinations. This shows the possible use of ordination as a visual aid when one has knowledge of relationships which may exist in the data.

Discussion

There appears to be no consistent results which would lead to the combining of industries into a smaller square matrix. From the groups found there is some evidence of transport industries such as Motor Vehicles, Aircraft and Shipbuilding forming a weak group.

Some of the groupings suggested enlargement of the table rather than reduction - for example Other Mining and Quarrying was the main input for both the Bricks and Non-ferrous Metal, and suggested that quarrying might be separated from mining.

The ordination results suggested that overlapping groups might be present, and there was some evidence that industries could be divided into consumer goods, services and engineering on the basis of their suppliers, although this grouping did not appear with the output ordinations.

The case study has shown the way that the results from clusterings and ordinations are used in data investigation, as complementary techniques. The cluster analysis showed the lack of distinct groups, and the ordination result was able to suggest overlapping classes which might be a possible interpretation of the data.

(b) STOCK MARKET DATA

A major factor in the movement of stock market prices is the information which is received by investors. Information such as a new dividend, a takeover bid, etc., can affect the shares of a single company; more general information such as new trade figures or tax changes may affect a large number of share prices; this is normally called the market effect. One can also envisage specific subsets of shares which may be affected by particular types of information and hence show a tendency to vary together. For example, the existence of industry indices shows some belief in an industry effect. Other groupings can be hypothesized, for example ICI may be more similar to BP than to a small chemicals company.

The importance of the existence of correlated groups is in portfolio selection. Two main factors characterize a portfolio from the investors' viewpoint - the expected return and the risk. If one has shares of two companies which have correlated stock prices, then if one company's shares fall, the shares of the other are likely to fall also; whereas if one has shares of two independently moving companies then one can have the same expected return but with reduced risk.

Models

Markovitz' pioneering work on portfolio investment (1952, 1959) considers the movement of each share individually and implies that an investment analyst should estimate and examine a full n by n matrix of covariances between the n shares under consideration. Sharpe (1963) has

simplified this task by introducing the market factor and assuming that all shares are related to this factor and that no other interrelationships exist. Thus only the covariance of each share with a market index need be assessed. This model is sometimes called the diagonal model because only the diagonal elements of the covariance matrix need be assessed. It can be formulated:

$$r_{it} = \alpha_i + \beta_i I_t + \varepsilon_{it}$$

with $\text{cov}(\varepsilon_{it}, I_t) = \text{cov}(\varepsilon_{it}, \varepsilon_{jt}) = \text{cov}(\varepsilon_{it1}, \varepsilon_{it2}) = 0$, where the return r_{it} of stock i after time t is linearly related to an index number I_t at time t with an error term ε_{it}.

Wallingford (1967) has demonstrated by simulation that a two index will out-perform the single index model (the opposite result has been demonstrated by Cohen and Pogue (1967) however) and suggests the use of a multi-index model:

$$r_{it} = \alpha_i + \beta_{ik} I_{kt} + \varepsilon_{it}$$

where stock i is related to index k and no other.

King (1964, 1966) was investigating industry effects and suggested the model:

$$r_{it} = \alpha_i + \beta_i I_t + \lambda_{ik} I_{kt} + \varepsilon_{it}$$

where stock i belongs to industry k.

The model suggested here, based on the preceding argument, is similar:

$$r_{it} = \alpha_i + \beta_i I_t + \sum_k \lambda_{ik} F_{kt} + \varepsilon_{it}$$

where $\lambda_{ik} = 0$ if stock i does not belong to group k. Stock i may belong to several groups, or none.

The importance of secondary factors to the market factor is of growing importance. King (1964, 1966) and Meyers (1973) both show a decrease in the effect of the New York market from about 60% forty years ago to 30% ten years ago. The size of the London market effect may be even lower (see later). King states that the industry effect (although varying from industry to industry) is about 11%, and does not vary significantly over time. However Meyers finds the effect to be somewhat smaller, and reports a slight decline over time. This study is concerned with evidence of group factors in the British market, and is an exploratory work to determine if, and what type of, factors F_{kt} exist.

Previous Related Work

The earliest investigation of grouping effects appears to be that of Farrar (1962) who grouped 47 American monthly index prices for the period January 1946 to September 1956 by principal components and rotation to oblique axes by Quartimax. Three groups were obtained, the group corresponding to the first component (which accounted for 70% of the variance) being very large. None of the three groups could be interpreted. The main criticism of Farrar's work is the high autocorrelation of prices, which is accentuated by using industry indices.

King (1964, 1966) analysed 63 American stocks for the period June 1927 to December 1960, dividing this period into four sub-periods. He extracted the market factor by factor analysis and proceeded to use cluster analysis on the

residual covariance matrix. King worked with monthly returns rather than prices, and demonstrated the low level of autocorrelation present in his data. He found market industry groups which persisted over time, and found evidence of the existence of sub-industry groups.

Feeney and Hester (1967) considered 30 American stocks on their quarterly returns over the period December 1950 to December 1961 and find support for industry groups, but mention the fact that for investors orthogonal groups would be of more interest. One of the few reports of investigations on British data has been that of Russell and Taylor (1968) which grouped 50 industry indices according to their half-yearly returns over the period June 1952 to June 1967. The groups were extracted by inspection of the correlation matrix. They found one large group, three smaller ones, and four outliers. The groups were difficult to interpret. This study has the failing of using indices instead of individual stocks, coupled with the fact that only 10 values are used for each variable.

Elton and Gruber (1971) analysed 180 American companies' shares on their annual growth for the years 1948 to 1963. They used cluster analysis after first scaling the data by using principal components. They test their 'pseudo-industries' which they find against recognized industry groupings and show that the pseudo industries give better forecasts of earnings. The groupings are not discussed but are presented. Ten groups are found, two of which comprise

mainly drugs and a few chemicals companies, one appears to be an oil and industrial machinery group, another appears to be a speciality machinery group, and two seem to be related to steels.

Sarnat (1972) using British industry indices constructs diversified efficient portfolios, and finds some strong negative relationships between them, the highest being -0.67 between coppers and rubbers. The data used was annual returns from 1963 to 1970, which means only eight values are obtained for each index.

Brown and Ball (1967) investigated earnings of companies for industry effects for yearly data from 1947 to 1965. They found a 35-40% market effect and a 10-15% industry effect.

A related study by Gupta and Huefner (1973) attempts to cluster industry indices of fixed asset turnover, inventory turnover, etc., taken separately by furthest neighbour clustering. The clusters found corresponded well with expected groups.

Meyers (1973) is a reply to King's investigation, and King's data is re-examined. Meyers says King overstates the industry effect by use of slightly inappropriate techniques. Meyers extracts the first factor by principal components and then uses the group average method of cluster analysis rather than weighted average. The argument for not using weighted average is that if a single stock joins a group, then the single stock is given the same weight as the group, and Meyers suggests all items should be weighted equally.

However the opposing argument is that if a group of stocks are very similar and a more dissimilar stock joins this group then the new group centre should lie half way between the point and group, because we have two sub-groups, one of which just happens to be more fully represented. The groups Meyers finds are certainly less distinct, but unfortunately it is not shown whether this is due mainly to the method of market extraction or the method of cluster analysis. Meyers also analyses King's stocks for the period 1961 to 1967 and finds the same pattern continues. He also analyses another 60 stocks from 12 industries over the full 40-year period, and finds even less distinct groups, suggesting King's choice of industries was fortuitous.

King, Meyers and others have attempted to extract the market factor before proceeding to search for other factors. This procedure uses the assumption that other factors will be orthogonal. The procedure used in the following study is to examine the full correlation matrix for group factors, and hence no implicit assumptions of orthogonality are introduced.

Data

The City University Stock Market Data Bank consists of weekly prices of around 700 British securities for the period June 1960 to September 1968 (425 weeks), of these slightly less than 500 securities are present throughout the period. The week's price is the closing price on the Wednesday of that week. Normal adjustments are made for

stock splits, etc. An account of the data bank, the way it was set up, and some preliminary investigations can be found in Russell (1972).

Returns were calculated from the prices by taking the differences in log prices, i.e:

$$r_{it} = \log\left(\frac{\text{price}_{it}}{\text{price}_{it-1}}\right)$$

Of the related papers mentioned above, only Farrar discusses the choice of time interval; he suggests that daily data may be too subject to fluctuation, whilst yearly data would be too insensitive. In the present study we do not make such assumptions. We are limited to at least weekly data by our data bank. Quarterly data would give 32 values for each stock, and as we wish to consider the grouping effect over time, and split the data in two halves, this would give too small a set of values. We thus choose to analyse both weekly and monthly (4-weekly) data, and investigate the effect of time periodson groups. Thus two sets of data were analysed for the half periods,

June 1960 - August 1964 (212 weeks, 53 months)
August 1964 - September 1968 (212 weeks, 53 months)

and for the whole period, making six analyses in all.

The number of stocks used in this study was limited to sixty. These were selected from the six largest industry groups in the data bank. The stocks are shown in Table 20.

TABLE 20

HEAVY ENGINEERING - MECH.

1 Allen (Edgar)
2 Babcock & Wilcox
3 Brit. Rollmakers
4 Butterley
5 Chubb
6 Chubb 'A'
7 Cohen, Geo.
8 Davy-Ashmore
9 GKN
10 Head Wrightson

LIGHT ENGINEERING - MECH.

11 A.P.V.
12 Amal. Dental
13 Averys
14 Baker Perkins
15 Braby, Fredk.
16 Brit. Ropes
17 Brit. United Shoe
18 Brockhouse, J.
19 Broom & Wade
20 Carrier Engineering

FOOD AND CATERING

21 Allied Suppliers
22 Assoc. Biscuits
23 Assoc. Biscuits 'A'
24 Assoc. Brit. Food
25 Berisford, S.W.
26 Bovril
27 Brit. Sugar
28 Brooke Bond 'A'
29 Brooke Bond 'B'
30 Express Dairy

BREWERIES AND DISTILLERS

31 Assoc. Brit. Maltsters
32 Bass
33 Brickwoods
34 Brown, Matthew
35 Cameron, J.W.
36 City London Brewery
37 Courage
38 Distillers
39 Gilbeys
40 Greenall Whitley

MULTIPLE STORES

41 Brit. Home Stores
42 Burton, Montague
43 Burton, Montague 'A'
44 Currys
45 Great Univ. Stores
46 Great Univ. Stores 'A'
47 Hepworth, J. 'A'
48 Hepworth, J. 'B'
49 Johnson Group Cleaners
50 Marks & Spencer

INVESTMENT TRUSTS

51 Brown Shipley
52 Hambros Bank (£10)
53 Hambros Bank (£1)
54 Schroders
55 Singer & Friedlander
56) Other Trusts
57)
58)
59)
60)

In several instances two stocks from the same company have been included. These were included as they were expected to be very similar, and they would give an indication of the density of the resultant groups.

Method

As a preliminary investigation the weekly prices for the whole period were subjected to principal components analysis. All stocks were positively correlated with the first component, which is equivalent to the market return. This component accounted for 20.7% of the total variance. This figure is somewhat lower than that found by Kind and Meyer in a similar time period on American data, and accentuates the need for investigation of group effects. For components 2 to 7 which accounted for a further 17.2% of the variance the eight stocks which scored highest are shown in Table 21.

It can be seen that component 2 is highly loaded on financial trusts, component 3 has two food firms weighted highest, component 4 has two stores highest, and component 5 is weighted on breweries. Beyond this, no evidence exists of industry groupings, and no other connecting factors are apparent. Thus we have some evidence of the existence of industry groups.

This leads us to the cluster analysis stage. Correlation is the obvious choice for a similarity measure since it is the co-movement over time which we are investigating. The data was not normalized in any way save that already implied in using returns. A first analysis

TABLE 21: PRINCIPAL COMPONENTS 2-7

2 (3.4%)		3 (3.3%)		4 (2.8%)	
⁂ Singer & Fried	-0.31	O Assoc. Biscuit	0.46	Δ Burton 'A'	-0.28
⁂ (8406)	-0.31	O Assoc. Bisc. 'A'	0.42	Δ Gt. Univ. St. 'A'	-0.27
⁂ Hambros £10	-0.28	O Brooke Bond 'A'	0.23	Δ Gt. Univ. St.	-0.26
⁂ (8411)	-0.26	Δ Johnson Cleaners	0.20	Δ Burton	-0.23
⁂ Brown Shipley	-0.21	I Chubb	0.17	O Assoc. Bisc. 'A'	-0.23
O Assoc. Bisc. 'A'	-0.19	x A.P.V.	0.17		
				I Head Wrightson	0.24
Δ Burton	0.19	⋈ Courage	-0.19	x Carrier Eng.	0.24
Δ Gt. Univ. Stores 'A'	0.20	⋈ Distillers	-0.24	x A.P.V.	0.26

5 (2.8%)		6 (2.5%)		7 (2.4%)	
⋈ Brickwoods	-0.37	I Cohen	-0.31	O Brooke Bond 'A'	-0.35
⋈ Cameron	-0.27	Δ Hepworth 'A'	-0.28	O British Sugar	-0.32
⋈ Bass	-0.25	I Butterley	-0.26	⋈ Brown	-0.21
O Assoc. Bisc.	-0.25	Δ Hepworth 'B'	-0.24		
O Assoc. Bisc. 'A'	-0.24			I Brockhouse	0.19
⋈ Courage	-0.22	x Braby	0.23	O Assoc. Bisc.	0.20
⋈ Greenall Whitley	-0.19	x British Ropes	0.23	O Assoc. Bisc. 'A'	0.22
		O Brooke Bond 'B'	0.26	I Chubb 'A'	0.25
O Assoc. Brit. Food	0.23	O Brooke Bond 'A'	0.28	x Amal. Dental	0.26

⁂ Investment Trusts Δ Multiple Stores I Heavy Engineering - Mechanical

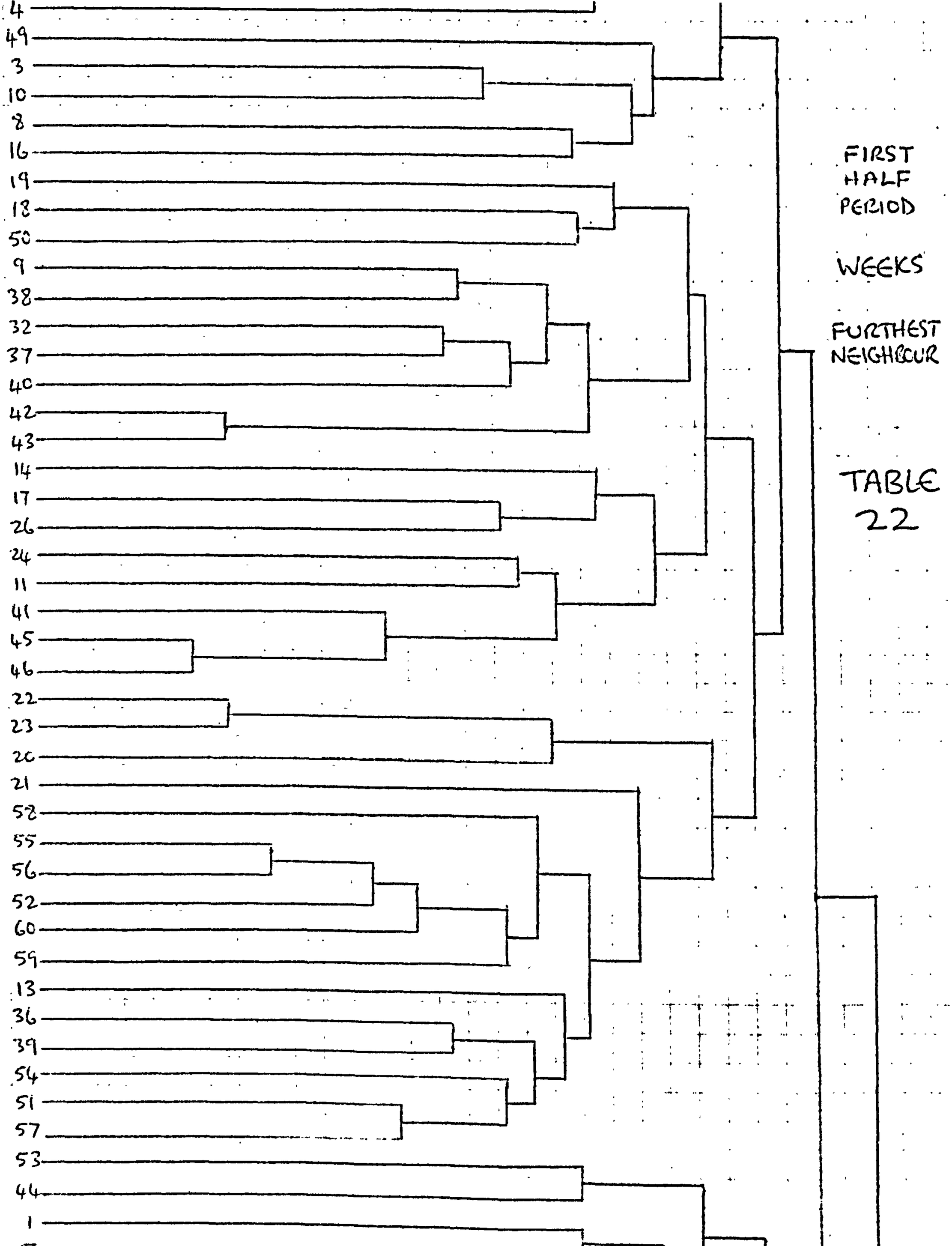
O Food & Caterers ⋈ Breweries & Distillers x Light Engineering - Mechanical

using nearest neighbour clustering was performed for two reasons - firstly an optimistic search for clear-cut groups, and secondly to look for outliers, to ensure that no stocks were especially different to the others, which could have been caused by takeover bids, etc. No outliers were found, and no clear-cut groups, in fact there appeared to be an excessive amount of chaining in all six data sets. The methods used in the full cluster analysis were somewhat crude but the results were very similar; these methods were furthest neighbour and centroid. Strictly speaking, the centroid method should not be applied directly to correlations because the notion of an average correlation is an unhappy one. But we can gain some peace of mind by simply considering the correlation matrix as a matrix of similarities, and take consolation in the closeness of results with the furthest neighbour analysis.

Weekly Data

The two dendrograms for the first half period are shown in Tables 22 and 23. There is no natural clustering present. By comparing the two tables, the stocks that keep together are:

1 7	2 4	3 8 10 16	5 6	11 24
15 30	18 50	22 23	25 29	42 43
9 32 37 38 40	33 34 35	41 45 46		
47 48	44 53	13 51 52 55 56 57 58 60		


4
49
3
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8
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42
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14
17
26
24
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41
45
46
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21
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1
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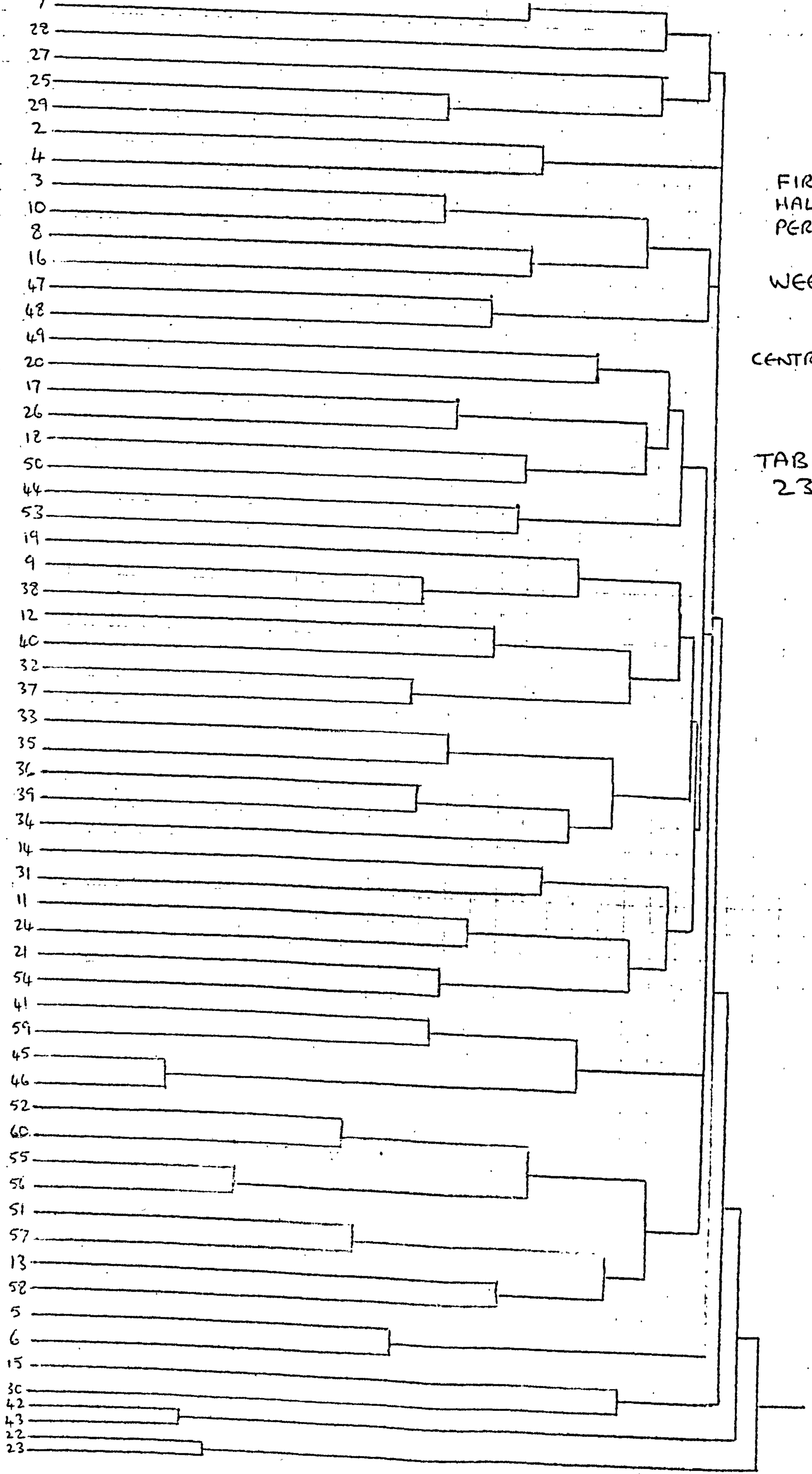
15
30
FIRST HALF PERIOD
WEEKS
FURTHEST NEIGHBOUR
TABLE 22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60
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51
57
13
58
5
6
15
30
42
43
22
23
FIRST HALF PERIOD
WEEKS
CENTROID
TABLE 23

The grouping again appears to be industrial with a large investment trust group, and two brewery groups. Also there are, as expected, pairs of shares from the same company which link together.

The dendrograms for the second half period were obtained. Again no obvious natural groups can be postulated. The groups which correspond in the two diagrams are:

2 8 10 | 3 21 | 4 34 | 5 6 | 11 16 19 53

7 17 | 14 39 | 12 24 | 22 23 | 27 28 29

32 33 35 37 40 | 47 48 | 30 59

41 42 43 45 46 50

51 52 54 55 56 57 58 60

Again industry groups are the easiest to interpret. The investment group persists, a brewery group is present and a stores group has appeared. Notice how the membership of these industry groups change slightly. Over the whole period (see Tables 24 and 25), the following groups appear:

2 8 10 16 | 5 6 | 17 53 | 7 19 | 13 50

14 31 | 11 24 | 22 23 | 35 39 | 28 29

32 33 35 37 40 | 42 43 | 41 45 46

47 48 | 51 52 54 55 56 57 58 60

34
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1
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42
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41
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46
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36
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56
52
60
22
23
15
28
29
30
59

ALL WEEKS

FURTHEST NEIGHBOUR

TABLE .24

7
24
11
1
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37
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33
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10
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16
41
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13
50
15
4
34
47
48
28
29
5
6
52
60
55
56
51
57
54
58
59
30
42
43
22
23

ALL WEEKS

CENTROID

TABLE 25

The picture is very similar to the sub-periods. From consideration of the above groupings and the six dendrograms, the groups which seem to continue over time are shown below:

GROUP 1

11 A.P.V.
24 Assoc. Brit. Food

GROUP 2

32 Bass
33 Brickwoods
35 Cameron, J.W.
37 Courage
40 Greenall Whitley

GROUP 3

41 British Home Stores
42 Burton
43 Burton 'A'
45 Great Univ. Stores
46 Great Univ. Stores 'A'

GROUP 4

51 Brown Shipley
52 Hambros Bank (£10)
54 Schroders
55 Singer & Friedlander
56 } Other Trusts
57 }
58 }
60 }

GROUP 5

2 Babcock & Wilcox
8 Davy-Ashmore
10 Head Wrightson
16 British Ropes

Also the 2 stocks of Chubb pair together and also those of Associated Biscuits, Brooke Bond and Hepworths.

The groups that exist are nearly all industry groupings. The only cross industry groupings are that a light engineering company combines with three heavy engineering which does not seem too surprising, and a light engineering company that is together with a food company, this seems more difficult to interpret.

Monthly Data

The dendrograms from the analysis of the first half-period of monthly data were calculated. Grouping is slightly more marked but still not very distinct. The stable groups are:

1 7 25 | 3 10 16 | 5 6 | 11 27 | 12 18

9 13 59 | 14 17 | 15 28 30 34 | 19 42 43

20 22 23 | 26 36 | 31 33 | 24 50 | 45 46

2 32 35 39 40 | 38 54 60 | 47 48 | 56 58

29 37 51 52 57

Industry groups are less apparent and the groups are smaller. For the second half-period we have:

1 3 | 2 20 | 5 12 | 10 17 | 6 13

4 28 | 11 29 | 14 53 | 16 39 | 22 23

18 25 30 49 | 24 38 44 | 45 46 | 47 48

52 54 55 56 57 58 59 60

32 33 34 35 37 40 42 43

The investment and breweries groups are strong, but a lot of the smaller groups have not continued over time. For all the period (Tables 26 and 27) we have groups:

6 13 | 5 12 | 8 9 | 11 4 | 3 14

15 34 | 21 31 | 25 49 | 22 23 | 38 44

42 43 | 50 53 | 47 48 | 41 45 46

16 36 51 52 54 55 56 57 58 59 60

32 33 35 37 40

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17
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25
50
53
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ALL MONTHS

FURTHEST NEIGHBOUR

TABLE 26

13
22
23
5
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35
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30
25
49
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47
48
19
3
14
20
31
21
34
15
7
2
10
27
29
28
45
46
41
17
1
24
50
53

ALL MONTHS

CENTROID

TABLE 27

Again there is a profusion of small groups which seem not to last with time. The groups below seem to be those which continue from period to period, with monthly data.

GROUP 1

32 Bass
33 Brickwoods
35 Cameron, J.W.
37 Courage
40 Greenall Whitley

GROUP 2

15 Braby, Fredk.
34 Brown, Matthew

GROUP 3

5 Chubb
12 Amal. Dental

GROUP 4

6 Chubb 'A'
13 Averys

GROUP 5

51 Brown Shipley
52 Hambros Bank (£10)
54 Schroders
55 Singer & Friedlander
56)
57)
58) Other Trusts
59)
60)

GROUP 6

38 Gilbeys
44 Currys

GROUP 7

25 Berisford, S.W.
49 Johnson Group

Also the stocks of Associated Biscuits, Burtons, Great Universal Stores and Hepworths stay together.

This confirms the strong brewery and investment groups. More weak evidence of an unnatural division between light and heavy engineering, with each Chubb stock pairing with a light engineering firm which is engaged upon specialist engineering work - Amalgamated Dental make dental equipment and Averys manufacture weighing machines. Chubb make locks, safes, etc. The three other pair groupings are difficult to interpret, and the occurrence of many unusual pair groups in the monthly analysis seems to indicate that these may be spurious groups. The groups in general are not as strong as

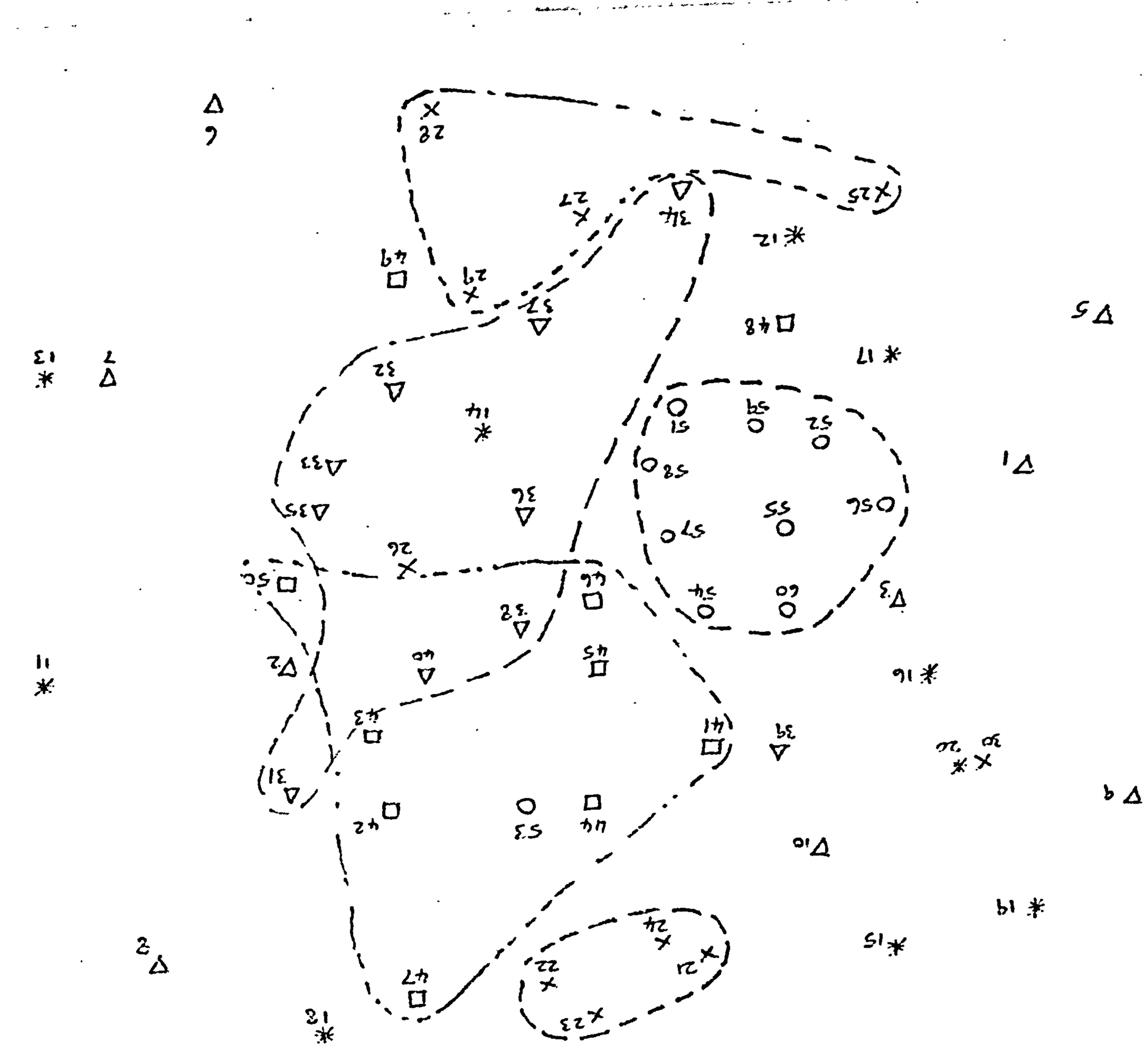
with the weekly data, the stores group is missing entirely, and engineering much weaker.

As an attempt to look for overlapping groups, an ordination using the minimization of $\sum(\frac{D-d}{D})^2$ was performed on the full monthly data. This result is shown in Figure 59. The industry groupings can be seen to be well represented as overlapping groups, with the engineering groups perhaps less tightly grouped as the other industries. Ordination is thus seen to have advantages over cluster analysis when one is looking for certain groups. The configuration also gives more information than discriminant analysis, because of the large overlaps between groups.

Conclusions

Although no markedly distinct groups exist, there is some evidence for shares moving together in industries, although the strength of this seems to depend on the particular industry. No evidence of other groupings has been found. We had looked at the size, products and location of each company in our attempts to find alternate groupings but found none. Investment trusts form a very strong group, all except Hambros £1 show evidence of being in one group. Breweries also seem to move together, in fact the companies which have grouped are those which particularly specialize in beer making. With the weekly data, three stores - B.H.S., Burtons and Great Universal Stores formed a group. The food and caterers group have shown no evidence of homogeneity. There was slight evidence of some engineering companies moving together, with no division

FIGURE 59



between light and heavy, but this seems weak over time. In fact, this industry is one of the most interesting, if we look at the groups found for the whole period analysed by months we find five pairs of engineering firms (four of which comprise one heavy and one light engineering company). On examination of the groupings for the other analyses these small engineering groups are quite common, but the same groups do not often repeat themselves in the analyses of the other data sets. This phenomenon can be seen in the other industry groups, where some stocks will only appear with the parent group on one or two occasions. One possible explanation of this joining and separating of reasonable group members is that of overlapping industry groups with stocks moving about within the group boundary over time. The ordination with the monthly data tended to confirm the overlapping group idea. It is suggested that ordination may be the best technique for further investigation.

One important result is that the analysis on the weekly data seems to show up the industry effects more than the monthly which appears to introduce many small 'accidental' groups. However it can be dangerous to assume that groups which have no apparent reason to form are spurious - on investigating each company we found that the full name of company 36 was the City of London Brewery and Investment Trust, and only then did we notice from the dendrograms a tendency for company 36 to be grouped with the investment trusts.

The implications of our results from the investment analysts viewpoint are that some inter-industry diversification is of value, but that some industries are tightly grouped, and others may exhibit little evidence of clustering. A model incorporating a market index and industry indices from those close-knit groups may be a useful practical compromise to our full investment model given earlier.

(c) A MANPOWER STUDY

Data

This consisted of manpower statistics from 584 companies, in the area of business covered by the Printing and Publishing Industry Training Board. The data was in three sets - 63 companies in Periodicals Publishing, 83 companies in Book Publishing, and 438 from the rest of the industry. The statistics for each company consisted of a matrix breakdown of the number of employees of each sex, in each particular occupation, against 6 age bands. There were 15 occupations in the Books sector, 19 in Periodicals and 25 in the main section. These were not directly comparable since they overlapped to some extent, and also the smaller data sets were much larger samples of their sub-industry than the main block, and thus the data was analysed in three sets. An example of one of the data sheets is shown in Table 28.

	Companies	Occupations	Sex	Ages
MAIN SET	438	25	2	6
BOOKS	83	15	2	6
PERIODICALS	63	19	2	6

Approach

As the data stood it was difficult to digest because of its volume. Cluster analysis was employed with two main objectives:

(a) In order to investigate the data;

(b) And more specifically, to see if any 'natural' sectoring of the companies was possible since sectoring

Main Categories of Employment		Numbers at 31st July 1972 Men/Women					
		16-20	21-25	26-35	36-55	56-65	66+
1. Directors and managers:							
(a) Editorial	M						
	W						
(b) Marketing/ sales	M						
	W						
(c) Production	M						
	W						
(d) Finance/ administration	M						
	W						
(e) General	M						
	W						
2. Sub-editors	M						
	W						
3. Designers/ artists	M						
	W						
4. Production staff	M						
	W						
5. Computer staff	M						
	W						
6. Secretarial staff	M						
	W						
7. Clerical staff requiring mechanical skills	M						
	W						
8. Other clerical staff	M						
	W						
9. Sales and promotion staff	M						
	W						
10. Training staff	M						
	W						
11. Others	M						
	W						

TABLE 28

was required for administrative purposes. The existing sectoring was by type of work, geographical area and size.

Two main difficulties were immediately apparent:

(a) The companies under study were three dimensional data sets;

(b) The size of the main data set.

Difficulty (a) was of course present with all three data sets, and here the two smaller sets could be used for pilot studies, thus the two problems could be considered independently. Since all three variables (age, sex, occupation) were considered to be of possible value, none of them could be simply ignored. The sex variable was eliminated by considering each occupation by male and by female as separate jobs. This was because jobs tended to be sex-dominated, for example managerial and craft jobs contained nearly all males and secretarial and clerical jobs nearly all females. Also a job description such as 'sales staff' tended to be different according to sex - i.e. male sales staff were more concerned with travelling and administration, whereas female sales staff often worked by telephone, or were clerical workers. Some occupations such as computer staff and journalists were of course the same whichever sex performed them, but these were in a very small minority. This gives a two-dimensional matrix for each firm. Each matrix consisted of many zero entries - most comprising over 70% zeros. Thus any similarity matrix which used the matrix values would yield very low values and be

subject to error, thus some aggregation was necessary. Matrices we summed by age and also by occupation - yielding a set of variables which can be considered one-dimensional and hence be analysed by clustering. This assumes to some extent that the age structure of each occupation is similar for each company, and also occupational structure for each age is similar for each company. This was investigated by inspection of the smaller data sets, and in general was found to be true. Exceptions were some of the female clerical and secretarial jobs where workers tended to be either young or old, and the ratio of these in companies did tend to vary somewhat. However the benefits in simplification were considered to be greater than the disadvantages of these assumptions.

All companies were scaled to 1,000 employees, since size was not to be considered. Scaling of the data had thus been achieved because both the sets (age and occupation variables) summed to 1,000, and age variables were fewer but carried proportionately more weight.

Thus our data set was now:

	COMPANIES	VARIABLES
MAIN SET	438	56
BOOKS	83	36
PERIODICALS	63	44

The data was now in a suitable form for analysis. We had eliminated the size factor and thus ordinary Euclidean

distance was used. Euclidean distance squared was not used because age differences would be weighted too strongly. The method to be used was next to be decided. We chose to use a method for finding round groups for the following reasons:

(a) For sectoring purposes we wished to be able to use the centroid of the cluster as a 'typical' profile;

(b) Greater speed of calculation;

(c) Greater accuracy of cluster finding.

It was however noted that further information could be gained from the use of a 'straggly' method, and this was partially resolved by deciding that if resultant clusters did not seem to have 'natural' groupings we would re-analyse using Mode Analysis. By 'natural' groupings we mean an obvious interpretation. We thus used our most accurate method - the extended flexible method with $\alpha = 0.6$ and $\beta = -0.7$ and used $\alpha = 0.5$ and $\beta = -0.6$ as a check.

Periodicals Sector

This was the smallest set of data, the analysis of the set being carried out in less than 100 seconds (on the City University 32K ICL 1905) and resulted in one outlier and two groups - one of ten companies and the other of fifty-two companies. The outlier company was certainly atypical - comprising only 8 employees, all of whom were in the 3 youngest age bands, and 5 of whom were classified as woman 'other clerical' workers. The profiles of the 3 groups are given in Table 29, the smaller group is typified by having older workers, more managers and directors, and more production staff, whilst having less editorial staff,

PERIODICALS SECTOR

TABLE 29

			1	2	3
OCCUPATIONAL PROFILES	CLUSTER				
	NO OF FIRMS		1	10	52
	D+M (A)	M	250	73	58
		W	0	14	8
	D+M (B)	M	0	68	54
		W	0	15	6
	D+M (C)	M	0	6	5
		W	0	4	0
	D+M (D)	M	0	21	14
		W	0	7	5
	D+M (E)	M	0	28	12
		W	0	0	1
	D+M (F)	M	125	45	41
		W	0	17	7
	D+M (G)	M	0	7	11
		W	0	4	6
	ED. STAFF	M	0	90	114
		W	0	40	62
	PRODUCTION	M	0	38	25
		W	0	56	20
	DESIGNERS	M	0	6	24
		W	0	3	14
	COMPUTER STAFF	M	0	0	3
		W	0	4	10
	SECRETARIAL	M	0	4	8
		W	0	82	119
	CLERICAL	M	0	8	7
		W	0	44	51
	OTHER CLERICAL	M	0	11	38
		W	625	151	108
	DISPLAY STAFF	M	0	42	50
		W	0	12	19
	CLASSIFIED	M	0	0	6
		W	0	5	17
	CIRCULATION	M	0	0	28
		W	0	0	1
	TRAINING	M	0	0	0
		W	0	0	1
	OTHERS	M	0	53	24
		W	0	40	27
AGE PROFILES	16 - 20		167	151	224
	21 - 25		500	147	375
	26 - 35		333	151	214
	36 - 55		0	228	100
	56 - 65		0	204	68
	66+		0	120	14
			2000	2000	2000

designers, classified and circulation workers. The PPITB interpreted this distinction from their knowledge of the particular companies as the difference between periodicals which were for mass circulation and hence were more concerned with sales and editing and the technical periodicals which required less production but more administration. The difference in age structure was considered to be mainly due to the tendency of managerial workers to be older.

The implications from the Training Board view was that there was a distinction not previously recognized between the two types of publishing and hence the training and manpower requirements were different.

Books Sector

This group was slightly larger than the periodicals section but still proposed no problems from the computational view. The result was 5 outliers and 4 groups of sizes - 35 companies, 28, 10, 5. Of the 5 outliers, 3 were owned by the same parent company - one consisted of 2 managers, 2 sub-editors and a secretary, another had 8 of its 12 employees being managers and the other had 5 managers and 3 secretaries among its 12 members. These three appeared to have a special function in regards their parent company. One of the other outliers had over two-thirds of its work force in the age range 36-55, and the fifth outlier had half its 82 workers under the heading male training staff, which indicates a training rather than a producing company.

The group of 5 companies were typified by a large number of female 'other clerical' workers. These were identified by the PPITB as book distributors rather than actual publishers (i.e. book clubs). The group of 10 were difficult to label, but they had a high number of 'other' workers (about 30%) suggesting perhaps that they had more diverse interests. The two main groups differed in occupational structure - in particular the ratio of managers to back-up staff. This was again the difference between general publishing and the smaller technical book publishing. Also included in this second group were offices of overseas publishers which had proportionately more managers. See Table 30.

Main Data Set

The special difficulty here was size. The data set consisted of 438 companies each measured on 56 variables - over 24,000 numbers, and if the lower off-diagonal distance matrix were stored this would mean 4 times as many as this.

A first stage in the analysis was to perform a nearest neighbour clustering. This can be executed without storage of the full data or distance matrices. From this hierarchy outliers were found and also near-identical pairs. The outliers were removed from the analysis and one of each of the identical pairs; this eliminated 43 companies.

The second stage was based on progressive analysis of subsets of companies, analysing the 'densest regions' (i.e. those which had joined early in the nearest neighbour run)

	CLUSTER		1	2	3	4	5	6	7	8	9
	NO OF FIRMS		35	23	10	5	1	1	1	1	1
OCCUPATIONAL PROFILES	D + M (A)	M	37	63	26	36	83	83	400	0	122
		W	10	7	3	2	0	0	0	20	12
	D + M (B)	M	35	53	21	19	167	0	0	40	24
		W	3	3	0	0	167	83	0	0	0
	D + M (C)	M	19	30	10	3	83	0	0	40	12
		W	2	1	2	0	0	0	0	0	0
	D + M (D)	M	28	35	29	41	0	0	0	40	0
		W	5	9	2	22	0	0	0	0	0
	D + M (E)	M	24	36	23	6	167	333	0	40	0
		W	3	4	2	0	0	0	0	0	0
	SUB-EDITORS	M	35	29	8	11	83	0	0	0	12
		W	66	60	29	23	0	0	400	40	12
	DESIGNERS	M	24	20	4	10	0	0	0	0	12
		W	17	10	1	0	0	0	0	0	0
	PRODUCTION	M	24	23	17	9	0	0	0	40	0
		W	15	40	20	15	0	83	0	0	0
	COMPUTER	M	6	0	5	9	0	0	0	0	0
		W	10	0	24	32	0	0	0	0	0
	SECRETARIAL	M	0	17	0	0	0	0	200	0	0
		W	134	124	73	43	83	250	0	0	171
	CLERICAL	M	2	7	3	0	0	0	0	0	0
		W	34	77	55	62	0	0	0	360	0
	OTHER CLERICAL	M	50	34	53	21	0	0	0	0	0
		W	121	45	205	501	83	83	0	0	24
	SALES	M	93	86	43	0	0	0	0	80	98
		W	34	50	32	12	83	0	0	160	0
	TRAINING	M	1	1	3	0	0	0	0	0	500
		W	4	0	1	0	0	0	0	0	0
	OTHERS	M	101	70	217	54	0	83	0	0	0
		W	62	59	87	63	0	0	0	80	0
AGE PROFILES	16-20		171	102	208	243	167	250	0	80	0
	21-25		388	422	244	371	83	167	400	40	342
	26-35		217	301	175	177	0	0	200	80	219
	36-55		128	95	221	161	667	333	200	680	439
	56-65		82	73	128	44	83	167	200	120	0
	66+		14	8	24	3	0	83	0	0	0
			2000	2000	2000	2000	2000	2000	2000	2000	2000

BOOKS SECTOR

TABLE 30

first, and replacing them by representative elements and then including some more of the companies from less dense areas.

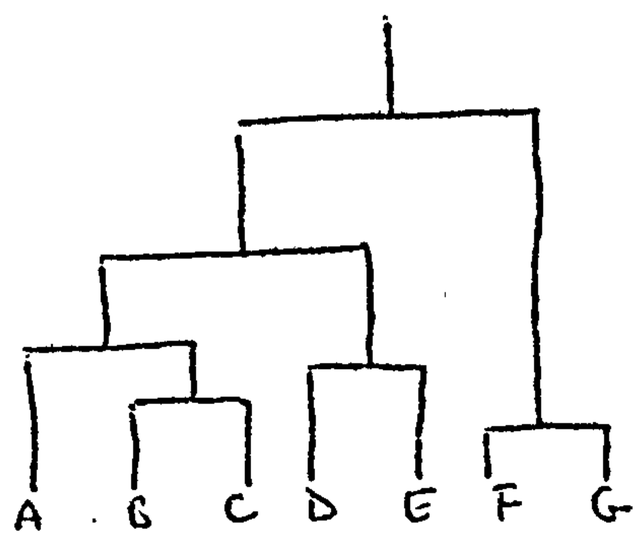
The 90 firms which linked first in the nearest neighbour analysis (apart from the near-identical items which had been eliminated), were subjected to the extended flexible method with parameters as before. This formed three main groups. However, as a precaution the four group solution was used. From these a roughly 25% sample was taken (more from smaller groups) as representatives of the original groups for subsequent runs.

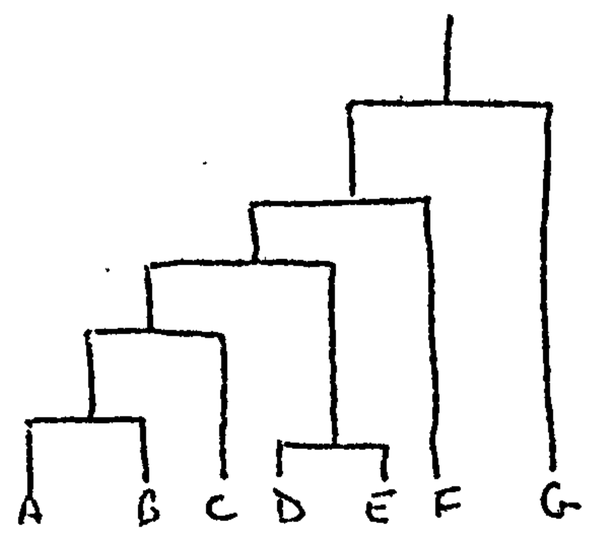
This sampling was performed with reference to the way in which the cluster was built up. The dendrogram of each cluster was inspected and the points are sampled with regard to:

(a) A fair distribution across sub-clusters; and

(b) A fair distribution central, middle-distance and outlying members.

For example in the following examples:





if we had to take a sample of three from the seven items, in the first case a representative cross-section would be

B, D and F, and in the second example A, D and F. (This problem is allied to what we have called the team organizing problem - see later.)

This procedure resulted in 23 representatives which were combined with the next 67 companies to be linked in the nearest neighbour analysis, in another cluster run. This resulted in four groups - one entirely new one, a pair of the previous groups having combined. All of the 23 representatives had stayed with their 'brother' representatives from the original groupings. As before one more group than required was taken, to be sampled in the same manner as before, but by reducing the number of original representatives according to the number of points they represent, and sampling from the sub-dendrograms as before.

This produced 23 points for the next run, and this was executed and analysed as before, giving a new sample of 24. The next run, with these representatives and 66 others, produced the unfortunate break-up of the representatives of one group, which had split and joined with two other clusters. This was thought to be possibly due to an unfortunate choice of sample, and the procedure was re-run with the 3 groups (the split group and the two it joined to) more fully represented and with only members of those groups present. The three group solution came out nearly intact, with only one or two changes in classification - these were eliminated from being chosen as representatives in further runs.

In order to improve the samples, for the last two runs 35 and 40 representatives were chosen. No further problems arose and this completed the second phase of the method. Nine clusters were produced.

The third phase of the method was to output the distance of each point from the centroid of each cluster, and from the nearest point in every cluster. This produced the final information from which companies whose cluster membership was in doubt, could be allocated to groups, by inspection.

This process yielded 9 groups of sizes 8, 9, 12, 21, 22, 25, 36, 65 and 211 companies, and 29 outliers. Half of the outliers had a disproportionate number of workers in a particular age band, most of these had a workforce of under 50 employees, but some had many more, indicating an atypical age distribution and possible manpower problems - for example one firm had 117 of its 126 workers aged over 35 years, as against an industry average of 51%. The other outliers had a large number of employees in a specific function, and tended not to be small, indicating a specialist type of firm. Six of these had over 40% of their employees in the category 'other', indicating that they were possibly engaged in work outside the industry, or that they were diversifying in different ways or to a different extent.

The profiles of the 9 groups are set out in Table 31. The groups tend to be typified by a few occupations, rather than by age distribution. Differences in age structure are due largely to the difference in occupational structure - for

MAIN DATA SET

TABLE 31

	CLUSTER		1	2	3	4	5	6	7	8	9
	NO OF FIRMS		8	9	12	21	22	25	36	65	211
OCCUPATIONAL PROFILES	D+M (A)	M	20	8	24	12	10	25	17	18	15
		W	0	0	6	1	0	0	1	1	1
	D+M (B)	M	63	34	47	34	61	61	40	27	46
		W	0	4	16	7	13	0	3	0	4
	D+M (C)	M	0	0	8	0	1	0	2	20	2
		W	0	0	0	0	0	0	0	0	0
	D+M (D)	M	17	14	12	18	13	12	13	13	16
		W	2	2	0	2	3	3	3	1	2
	D+M (E)	M	18	14	10	8	5	13	8	7	10
		W	3	0	0	0	0	0	0	0	1
	SUB-EDITORS	M	0	0	9	0	1	0	1	34	3
		W	0	0	3	0	0	0	1	3	0
	JOURNALISTS	M	0	0	5	0	0	0	2	85	7
		W	0	0	3	0	0	0	0	23	0
	DESIGNERS	M	14	0	6	3	6	39	11	6	4
		W	6	0	1	2	1	2	0	1	1
	TECHNICAL	M	18	7	7	17	17	23	37	12	26
		W	5	2	1	1	2	1	4	3	4
	COMPUTER	M	0	0	0	0	0	0	2	2	0
		W	0	4	2	0	0	0	7	1	1
	SECRETARIAL	M	0	0	0	0	2	0	1	0	0
		W	6	6	18	10	8	18	18	16	14
	CLERICAL/MECHANIC.	M	13	14	15	0	1	1	3	4	5
		W	20	36	35	19	17	17	25	20	25
	OTHER CLERICAL	M	7	21	4	10	13	9	8	21	14
		W	14	7	20	29	13	17	23	63	32
	COMPOSITORS	M	301	61	516	67	178	14	56	200	173
		W	12	0	1	0	1	2	3	7	2
	PLATE MAKERS	M	169	126	9	4	13	535	40	44	18
		W	6	0	0	0	6	0	1	0	1
	LETTERPRESSERS	M	9	3	45	50	173	3	47	51	117
		W	0	0	0	32	11	0	0	0	6
	LITHOGRAPHERS	M	30	7	0	22	21	8	152	15	49
		W	3	0	0	4	1	0	2	0	3
	MACHNE OPGAT.	M	11	11	0	1	3	39	9	11	5
		W	0	0	0	0	6	0	3	1	5
	BINDERS	M	50	247	51	115	210	6	104	14	76
		W	55	194	29	427	94	7	201	9	178
	SALES	M	32	24	18	19	9	40	31	70	25
		W	0	0	7	0	0	1	1	60	3
	PRESS PHOTOGR.	M	0	0	0	0	0	0	0	19	1
		W	0	0	0	0	0	0	0	0	0
	OTHER PHOTOGR	M	2	0	0	0	0	4	1	4	1
		W	0	0	0	0	0	0	0	0	0
	LABORATORY	M	3	0	11	0	0	4	1	3	3
		W	3	0	0	0	0	2	2	1	0
	TRAINING	M	6	0	0	1	0	2	2	3	1
		W	0	0	0	2	0	0	1	1	0
	OTHERS	M	70	125	45	67	70	82	91	77	77
		W	9	27	2	11	16	9	23	24	19
AGE PROFILES	16-20		34	78	94	218	55	76	97	100	149
	21-25		107	82	112	145	95	127	130	122	148
	26-35		227	216	244	206	242	268	209	231	205
	36-55		403	373	398	318	396	365	403	335	331
	56-65		143	208	140	99	197	136	149	134	151

example the large number of people under 20 in group 4 is probably due to the large number of female binders who tend to be young, and the large number of older workers in groups 2 and 5 are probably due to the large numbers of male binders who tend to be older. The groups can be typified by the high number of the following occupations:

GROUP 1: Male Compositors and Plate Makers

GROUP 2: Binders

GROUP 3: Male Compositors

GROUP 4: Female Binders

GROUP 5: Male Compositors, Letterpressers and Binders

GROUP 6: Male Plate Makers (and Hardly any Binders)

GROUP 7: Binders and Male Lithographers

GROUP 8: Journalists, Sales and Male Compositors

GROUP 9: Male Compositors and Female Binders

The interpretation of some of the groups by the PPITB was fairly easy. Group 8 which was virtually the only sector to employ Sub-Editors, Journalists and Press Photographers were mainly newspaper companies. The largest group (Group 9) consisted of diversified companies and smaller general printers. Group 6 had over 50% of their workers male platemakers, and hardly any of the binders typical of the industry, these were simply specialist plate-makers. Group 7 was also specialist firms - lithographic printers. Group 5 was very similar to Group 9, but employed male rather than female binders. The four smallest groups proved difficult to interpret, but they certainly appeared to exist as separate groups.

Conclusions

From the PPITB point of view the analysis brought out clearly several points:

1. The distinction between technical and general publishing.

2. The division between types of printers being determined by the percentage of people in certain key occupations - binders, compositors, lithographers and platemakers.

3. The large number of similar 'general' printers.

4. Several firms whose age structure needed careful inspection.

5. The need to examine companies who listed a large number of workers in the 'other' occupation.

From a cluster analysis point of view the exercise was considered successful (especially the difficult task of clustering the main data set), and because of the ease of interpretation of the groups, and the pinpointing of clear outliers, it was thought that meaningful groups had been found.

2. Specific Applications

In this section we shall discuss five particular problems which can be considered as cluster analysis and/or ordination type problems. Methods of solution are also given from this viewpoint. Although examples are given in most cases, it is the approach to the problem which is largely under examination - the case studies are intended to show cluster analysis and ordination in action. These studies have been chosen to show the variety of problems on which the methods we have discussed may be brought to bear, and the different ways in which the methods are applied, to emphasize the way in which these methods form an angle of attack to problems, rather than a bag of techniques.

The relationship between some network problems and cluster analysis is demonstrated in our first two case studies. The first - vehicle routing - is an instance where the current algorithms for solution are, in fact, clustering methods, although this does not appear to have been discussed in the literature. We consider the problem from a cluster analysis stand-point, and improvements are suggested. The second network problem is one which occurs in large distribution networks, and the current methods of solution are also related to classification procedures. The problem is also shown to be related to the vehicle routing problem, and a new solution procedure is proposed.

The third study is called the team organizing problem. Here cluster analysis seems an obvious approach since the problem is to find 'equal' groups of people, but the solution is not a straightforward application of clustering.

The fourth example is based upon ordination, unfolding theory and some clustering. It is an application similar to gap analysis, but which has advantages over previous methods. The last example is in factory layout, and this is also based on ordination. Here an entirely new method is introduced with an example.

(a) VEHICLE ROUTING

The problem of vehicle routing can be simply stated as that of dispatching goods from a single warehouse to a group of delivery points by more than one vehicle or trip. The problem with one vehicle becomes that of the travelling salesman. The vehicle routing problem, which is sometimes referred to as the clover leaf problem, is basically a type of cluster analysis - delivery points must be grouped to vehicles in an optimal way.

In its full form the problem can have side constraints, such as the volume or maximum load of vehicle, or the mileage that a vehicle may cover, the time taken at each stop, etc. Also other complications such as a minimum mileage or two sizes of vehicle, can be envisaged.

The criterion to be optimized is not as clear as in the travelling salesman problem - the traditional approach has been to minimize total mileage, but some have taken the number of vehicles as the criterion. The best one to use in a given instance obviously depends on the particular problem.

Vehicle routing was originally formulated by Dantzig and Ramser (1959) as the 'truck dispatching problem'. Their approach was to use linear programming and attempted to minimize mileage. The method proposed by Clarke and Wright in 1964 (also Fletcher and Clarke 1964) has gained widespread acceptance, and generally leads to a better solution. It is simple in operation - it is assumed initially that each delivery point is served by one vehicle, and a 'savings matrix' is built up, in which each element S_{ij} is the saving

in distance if one vehicle supplies both delivery points i and j. This matrix is examined and the largest element is found, say S_{kl}, and if no constraints are violated then both k and l are formed into one route. Then the next highest element is found and further links are formed as long as they do not violate side conditions. If a route of three or more delivery points is formed, then only the first and last points on the route may link to further points - thus the savings in linkages to intermediate points are ignored. This procedure may be carried out sequentially, considering one vehicle at a time until it reaches mileage or capacity constraints. The approach outlined above is called the multiple approach. The method is very fast (Yellow 1970 suggests using polar co-ordinates, which speeds up the program further), but does not guarantee an optimum. This is basically an application of nearest neighbour clustering - the largest element is selected from a matrix to gradually build up clusters. From the clustering point of view there are two differences in the Clarke-Wright method - the use of a special similarity measure, and only enabling certain cluster members to link with other points.

The savings in the Clarke-Wright algorithm, as it is called, are simply given from the distance matrix by the expression:

$$S_{ij} = d_{oi} + d_{oj} - d_{ij}$$

where d_{ok} is the distance from the depot to delivery point k.

Others have experimented with variations on this equation. Gaskell (1967) has used the variations:

$$\lambda_{ij} = S_{ij}(\bar{d} + d_{oi} - d_{oj} - d_{ij})$$

where $\bar{d}$ = average of the d_{oi}

$$\pi_{ij} = d_{oi} + d_{oj} - 2d_{ij}$$

and he also experimented with the multiple and sequential versions of Clarke-Wright's algorithm. He found the multiple approach to be preferential to the sequential, and found neither of his variations above to be consistently better than Clarke-Wright, but suggested that the expression:

$$S_{ij} = d_{oi} + d_{oj} - (1+\sigma)d_{ij}$$

would be worth further investigation.

Unwin (1968) defended the use of the sequential approach in cases where vehicle utilization was the objective, although it does probably give increased mileage. It is theoretically possible, with the multiple approach, to end up with many routes each filling a vehicle to just over half capacity, and thus none of them can be combined. Unwin and Weatherby (1969) give a manual method building routes sequentially that appears to outperform the multiple Clarke-Wright approach in terms of vehicles used.

McDonald (1972) has analysed variations of the savings factor (σ) in Gaskell's expression from 0 to 1, and his results show a low value of σ to be possibly optimal, in the range $\sigma = 0 - 0.2$. Webb (1972) has completed a similar

study with random delivery points and found values of $\alpha = 0.2$, 0.4, 0.7 and 1.0 to be inferior to $\alpha = 0$.

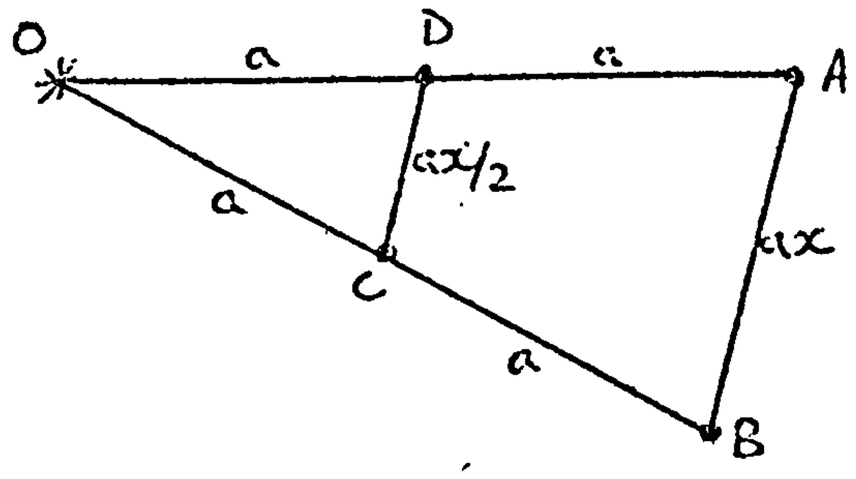
A paper by the National Computing Centre (1969) shows that the method employed by the majority of people using computers for vehicle routing is the Clarke-Wright algorithm. They also refer to an ICL package which uses:

$$S_{ij} = \alpha(d_{oi} + d_{oj}) - d_{ij}$$

where is selected by the user on the basis of local geography. Other approaches have included that by Christophides and Eilon (1969) which is based on a method of solution to the travelling salesman problem, and generally outperforms the savings approach, but takes much longer to calculate (computer times are given by Yellow (1970)). Eilon et al (1971) discuss this and other approaches. Wren (1971) and Wren and Holliday (1972) suggest a method which is basically an iterative relocation procedure, and has an obvious cluster analysis parallel.

Our Approach

The variation of the savings approach which we have investigated arises from the fact that the Clarke-Wright method has a tendency to make trips circumferential rather than radial. This can be seen from the following example of four delivery points each requiring half a vehicle load from the depot O:



The savings matrix is:

A	X			
B	4a-ax	X		
C	2a	2a	X	
D	2a	2a	$2a-\frac{ax}{2}$	X
	A	B	C	D

It can be seen that if $x < 2$ then the result will be the two routes - ODCO and OABO which have total length $6a + \frac{3ax}{2}$.

The routes ODAO and OCBO have combined length 8a and so if

$$6a + \frac{3ax}{2} \leq 8a$$

then the optimum will have been found. And if $2 > x > \frac{4}{3}$ then the wrong solution will be given.

We thus use a correction factor based on the angular separation of points from the depot. We use the model

$$S_{ij} = (1-\mu)(D_{oi}+D_{oj}) - D_{ij}$$

and have experimented with $\mu = \frac{\phi}{40}$, where ϕ is the angle of separation in radians.

Results

We have used the six examples given in Gaskell's paper in order to test our results against the Clarke-Wright and

savings factor approaches. Some of these examples have also been tackled by Christophides and Eilon by their method. The results are as follows:

	1	2	3	4	5	6
Our method	923	1423 (1417)	840 (839)	598	963 +964	949
Clarke-Wright method	923	1427	839	598	963	955
Sequential Clarke-Wright	947	1427	850	648	1017	949
Christophides' method	-	1414	810	585	875	949

In cases 2 and 3 the tour within the resultant groups was not optimal, and if these were improved then the mileages shown in brackets could be obtained. In case 5 there was a tie in the matrix which led to two different solutions - in practice a computer method would often select one of these values, without the other solution being considered. Case 2 is from Clarke and Wright's original paper. Gaskell points out an error in the distance between customers 1 and 17 which should be 5 not 45, and there are other errors where several sets of towns do not obey the triangle inequality. These were ironed out (since the angular separation cannot be calculated otherwise) and the resultant matrix was re-analysed by the Clarke-Wright method, which gave the same result as in their paper. Case 6 of Gaskell's also included an error - the second co-ordinate of point 13 should be 255 not 265.

In cases 1 and 4 the resultant tours were exactly the same as in the Clarke-Wright solution, and the result in case 3 after one tour had been optimized was also the same as

the Clarke-Wright result. The result in case 6 was the same as in the sequential version of the Clarke-Wright method. The result in case 2 and case 5 solutions are given below:

CASE 2

		Miles	Load
1.	0-6-5-9-15-16-11-7-13-29-0	216 (215)	617
2.	1-17-12-14-23-22-0	194	601
3.	0-27-26-0	199	519
4.	0-30-21-0	138	612
5.	0-18-8-10-19-0	179 (176)	612
6.	0-28-4-3-24-0	188 (186)	606
7.	0-2-1-25-20-0	145	613
8.	0-19-0	164	700
		1423(1417)	

CASE 5

		Miles		Load
1.	0-29-27-25-24-1-5-0	237		2900
2.	0-21-14-8-12-11-10-23-18-0	186		3725
3.	0-15-16-13-7-17-9-0	185		1400
4.	0-22-2-4-6-3-20-0	199		3875
5.	0-19-26-28-0	156		850
4'.	0-22-2-4-6-3-20-19-0		212	4275
5'.	0-26-28-0		144	450
		963	964	

The results are generally slightly better than with the Clarke-Wright method. The Christophides method does better in all cases than these methods but is lengthier computationally. We believe that our results show that the expression given earlier containing an angular correction in the saving equation is worthy of further investigation.

Discussion

The vehicle routing problem is structured in such a way that an approach by cluster analysis is immediately apparent. The side constraints which are typical of real problems can be easily dealt with by clustering methods. The problem has been usually approached by the savings type methods we have referred to, which are themselves a form of nearest neighbour clustering, and attention has been so far focused largely on the calculation of suitable similarity functions.

The use of nearest neighbour as an appropriate technique can be seen to be due to the way in which, as routes are built up, the delivery points which are connected to the source are the most appropriate ones to join to other delivery points, and so only the similarity to these need be considered.

A possible improvement to the savings type method is by examination of those links to points which are already connected to two other delivery points, which are supressed. The saving in allowing these points to 'break into' the route can be calculated by:

$$S_{ijk} = D_{ik} + D_{jk} - D_{ij} - 2D_{ok}$$

$$= S_{ij} - S_{ik} - S_{jk}$$

(where S_{ijk} is the saving by inserting k into the existing link of point i to point j, and S_{ij} etc. are as in the Clarke-Wright savings expression). This would lead to higher computation time, but not storage, and may well lead to a better solution.

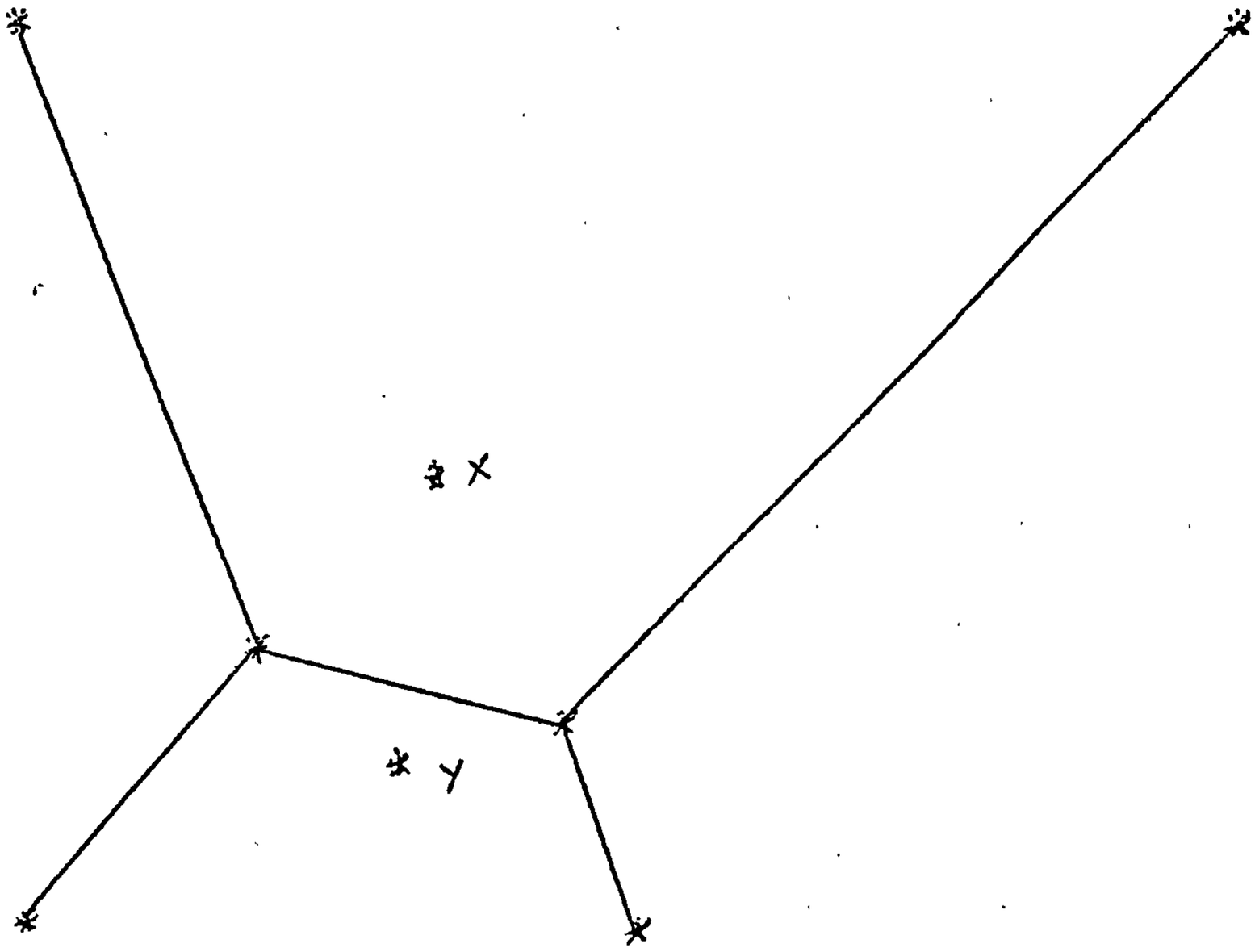
The viewing of the problem from a cluster analytic standpoint can be of value, and could lead to better methods of solution - for example as in the use of iterative relocation by Wren and Holliday. The consideration of this problem is also of value to clustering itself - particularly in the way similarity is assessed and side conditions used. It is also of interest to see an example where a method which is of less value in ordinary clustering, is particularly apt for a very real problem.

(b) THE SEWER PIPES PROBLEM

A problem which occurs in large distribution networks, like those for sewer pipes for example, is that of forming a minimum cost network from a number of sources to a single sink. In these cases the cost of an arc depends on the flow through it, whilst total cost increases with flow, as flow increases the cost per unit flow decreases. This kind of problem also occurs in the layout of electricity, gas, water and road networks. Another instance of the problem is in the positioning of fuel lines in aircraft, where weight must be minimized (which is a function of pipe length and diameter).

This has some similarities to the vehicle routing problem, since each sink must be connected to the source by a single sequence of arcs, but this particular problem has two main differences - firstly 'routes' do not have to be circular, and, more importantly, arcs do not only join to sources, but link to junction points, the positions of which are unknown. Thus there are an infinite number of possible solutions.

One of the few published works on this problem is Miehle (1958). He uses a mechanical analogy with pulleys and weights which finds an optimum (assuming no friction in the system), but is of course complicated to set up. He also describes another analogy with soap films, but which cannot incorporate moveable junction points, varying weights to sources, etc. He also gives an iterative numerical method which he claims has 'high precision'. He gives the following example of the minimum link length between four points:



Whereas if the junction points X and Y are used the total link length is 1.5% better.

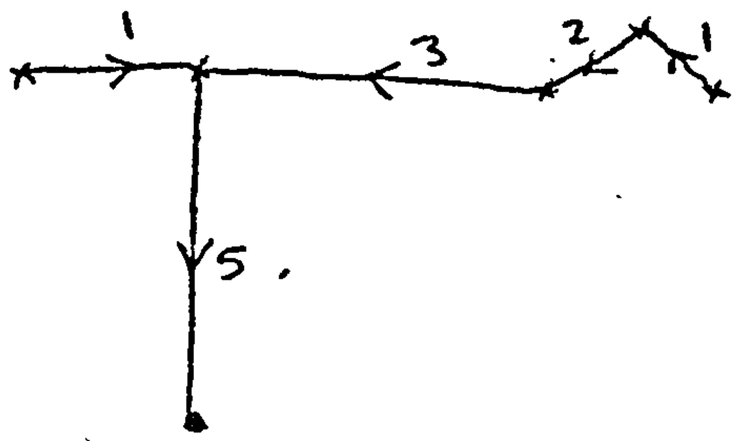
Some unpublished work has been carried out on the problem at the Local Government Operational Research Unit (personal communication from Dr. John Green of the LGORU) in the distribution networks of sewer pipes. Their approach is to begin with the minimum spanning tree, and attempt to find various heuristic improvements on this solution. They claim to be able to achieve networks of up to 10% saving on the minimum spanning tree solution.

The problem becomes increasingly difficult with a large number of nodes to be linked, and because of the limitations of computer time, the solution found to large problems will normally be further from the optimal than with smaller problems. A useful approach could be to divide the nodes

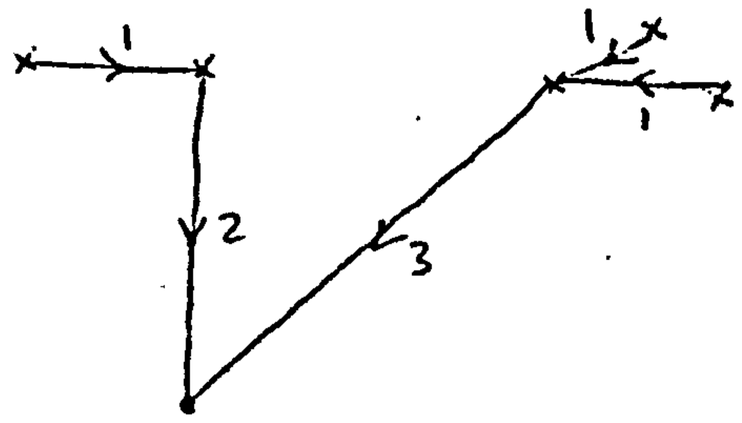
into groups by cluster analysis and perform this algorithm on each cluster. Certainly if clearly separated groups were present then one would expect, intuitively, that this would yield a similar result. The problem of connecting the groups together would entail a final application of the algorithm.

There are two simple networks which are worth enlarging upon, as they can form useful initial solutions to the problem:

1. The minimum spanning tree - this forms a network with the least total length of arcs with no junctions, and would be the solution if cost was independent of flow and no junction points were allowed. The defect of this network can be shown by a simple example.



Minimum spanning tree



A better solution

The defect can be seen to be in that the relative position of the nodes with respect to the source is not considered, and also junction points are not included.

2. <u>The fan</u> - this is the network which connects each node to the source by a single straight line (c.f. the starting position in the Clarke-Wright vehicle routing algorithm). This would be the solution if cost increased proportionately with flow. A typical example is the telephone wires from telegraph poles to houses. The fan normally includes a lot of duplication of arcs in nearly parallel lines, but has the advantage of flexibility in that a sink may join or leave the network without affecting the remaining arcs.

Our interest in the problem arose from the fact that the use of the minimum spanning tree is equivalent to the nearest neighbour clustering method, and the possibility that a better solution could be obtained by considering the problem from a cluster analysis viewpoint. An early breakthrough was the realization that the network formed by any solution is a tree diagram equivalent to a dendrogram. Thus if the sources are clustered and a dendrogram formed, then we have the basis of a solution to the problem. We have the order in which pipes will link together in the network, but not the location of the junction points.

From the above development we can explain our suggested approach more fully, as follows:

Each source i has a weight w_i related to its 'output'. We consider the network as 'beginning' at the sources and 'ending' at the sink, thus when we speak of points which are 'early' in the network we refer to those parts where arcs carry flows which are directed from only a few sources.

1. If two sources are relatively far apart then the flow from each will be unlikely to pass along a high number of common arcs, whereas if two sources are geographically close then the flow from each will pass through common arcs from early in the network. Thus we suggest that the closer two sources are, then the earlier their flows will join in the network.

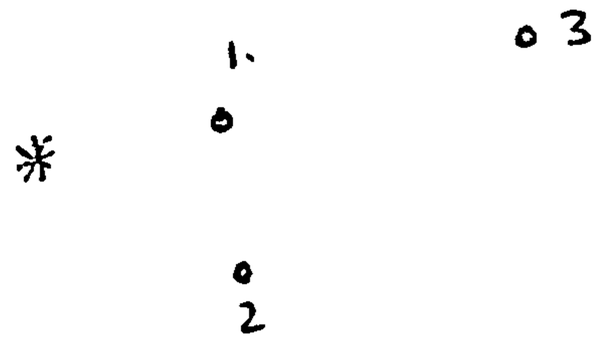
2. If the sources are clustered using an appropriate measure of proximity and a dendrogram tree is formed linking the points, then the network will be in accordance with the supposition above.

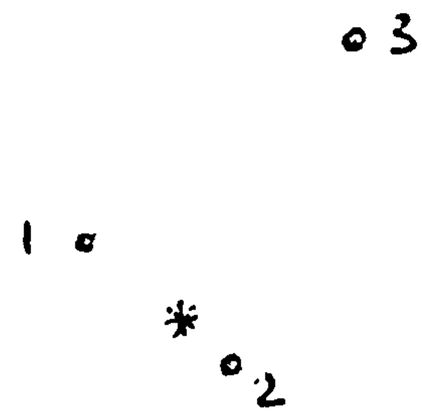
3. Given the tree, we can now optimize the position of the junction points mathematically. If the cost of an arc is proportional to its length, and related to the flow through it, then we have to minimize

$$\sum_{\substack{\text{each arc} \\ k}} d_k f(W_k)$$

where d_k is the length of arc k, and W_k is the flow in arc k, which can be calculated from the sum of the weights w_i' of the sources from which the arc is directed. The minimization can be performed by hill-climbing methods such as steepest descent (although faster converging methods exist).

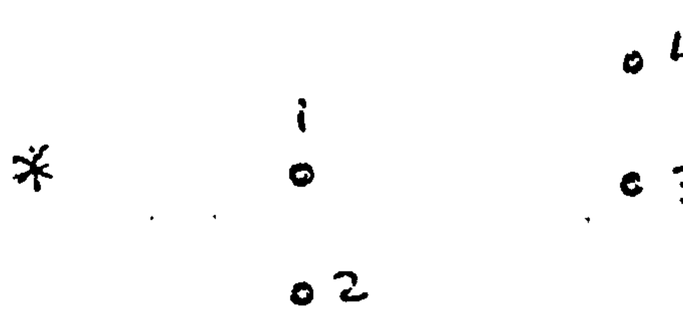
This type of approach leads to the important consideration of the similarity measure to employ. If we use some form of Euclidean distance, then in the following cases:



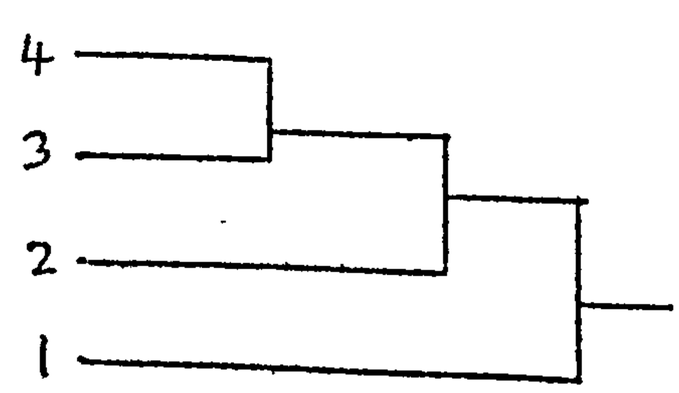


we will obtain non-optimal hierarchies, since points 1 and 2 will join first.

Clearly we must use the notion of angular separation from the sink. The use of angular separation as the sole criterion would solve the two cases above, but consider:



A wrong result would be obtained, since points 1 and 3 would combine before 4 joined 3. Also most distance measures would give the wrong result. The optimal dendrogram in the case above, would be:



Thus we also wish our measure to depend on the distance from the sink. We wish to use a function which increases with angular separation and also with the inter-source

distance (d_{ij}), and which decreases with the distances from the (d_{oi}, d_{oj}). A function which has these properties is $d_{ij} - d_{oi} - d_{oj}$, which is the same expressed as the Clarke-Wright savings expression. This is in fact always negative, and is not a proper distance function, but a negative similarity measure. The analogy of 'savings' breaks down because the actual saving is dependent on the particular function between size of pipe and cost.

We have examined the dendrogram found, using this measure, and with several cluster methods, on one example. The example is of 21 sources scattered around a sink (the data is actually taken from Gaskell's case study 4 in his vehicle routing paper).

The methods tested were: nearest neighbour, furthest neighbour, group average, weighted average and Ward's method. Of these furthest neighbour was the best and weighted average was probably next. The furthest neighbour solution is shown in Figure 60. The junction points have been fitted by eye and their position in practice will depend on the cost function. This can be compared with the minimum spanning tree in Figure 61. The differences in pipe length for each volume of flow is given in the following table:

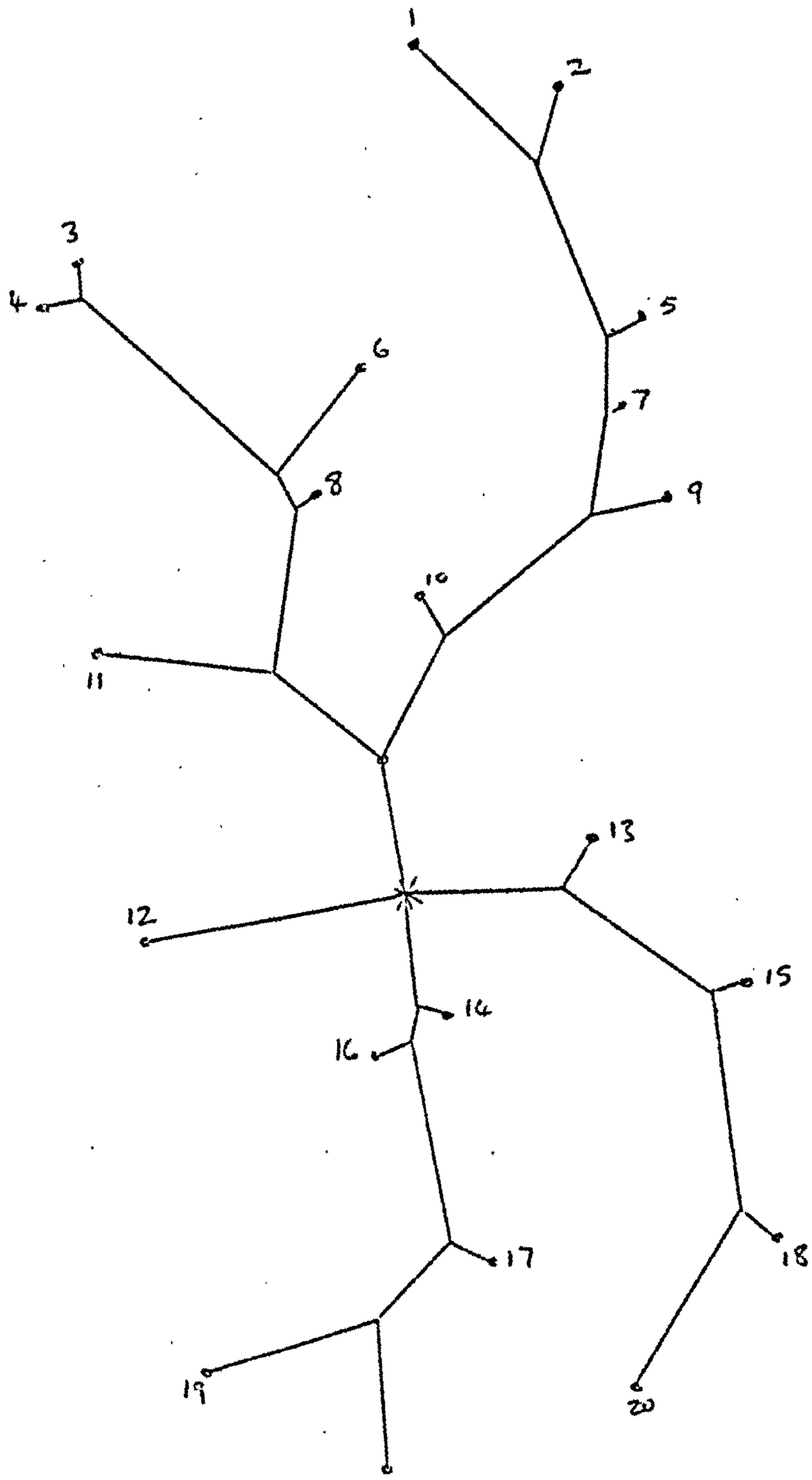


FIGURE 60 – FURTHEST NEIGHBOUR

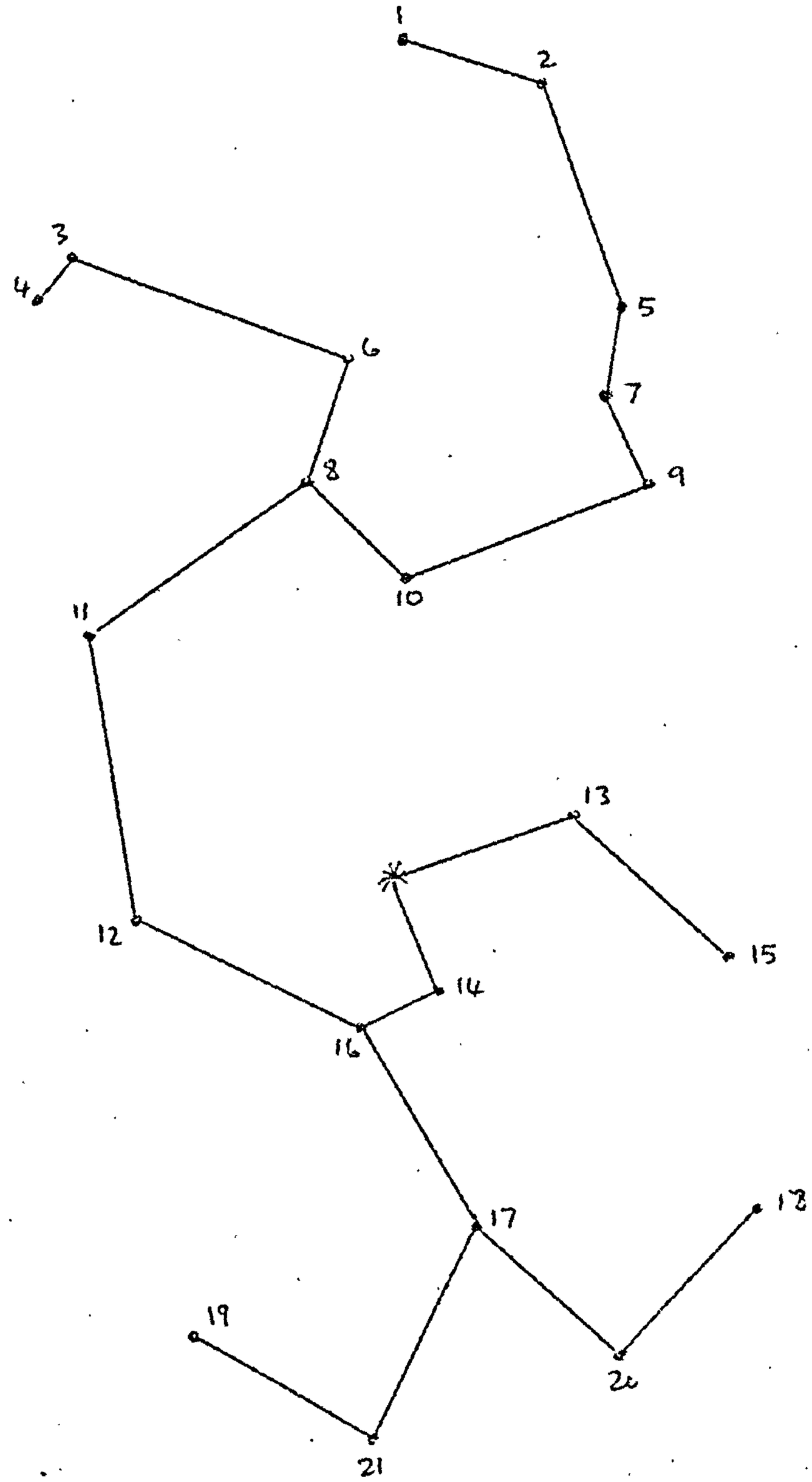


FIGURE 61 – MINIMUM SPANNING TREE

No. of Units of Flow	Furthest Neighbour	Minimum Spanning Tree
1	22.7	9.8
2	9.2	13.7
3	6.0	2.7
4	5.6	1.3
5	5.2	6.1
6	1.7	1.8
10	-	3.2
11	1.6	3.5
12	-	3.0
18	-	1.0
19	-	1.5
TOTAL	52.0	47.6

Thus the total pipe length is only 9% longer using the cluster method. Supposing we had a cost function such that the cost varied with the square root of the flow, then the furthest neighbour solution we have drawn would have value 78.3 (the full method would find a lower value) and the minimum spanning tree would give 97.2. This represents a saving of 19%.

Our method is thus shown to have value in this application. It is possible that using the levels of the objective function in the clustering dendrogram, that a fairly accurate result could be obtained, without recourse to optimization phase of the method explained.

(c) THE TEAM ORGANIZING PROBLEM

A related problem to that of cluster analysis is that of selecting equally balanced teams. The problem in its pure form is to select n groups from m people such that each group is as similar to the others as possible in respect of aggregate attributes of team members, each of whom carries a vector of attributes, and such that within each group there is as wide a spread as possible of team members' attributes. The problem occurred at the Graduate Business Centre, where each year 80-90 M.Sc. students are placed into 15 groups for management exercises. For fairness, and effectiveness as teams, the groups must be balanced in various factors, such as number of natural English-speaking people, amount of industrial experience, etc.

Other instances of the problem:

(a) Eliminating bias from experiments and ensuring control samples are as similar as possible to an experimental sample.

(b) Selecting varied special diets from a list of admissible foods and ensuring calcium, protein contents, etc., are similar.

This problem concerns maximizing within group heterogeneity and between group homogeneity, the opposite to cluster analysis.

Formulation

Suppose we have m criteria in which we wish the K groups to be similar, and these are weighted according to their importance by w_j (j=1,...m). Then we wish each group to have its correct proportion of these, i.e., if C(I,J) is the amount to which objects I (I=1,...n) possesses criterion J (j=1,...m) and object i belongs to group G_i, then, assuming a least squares cost function, we wish to maximize:

$$\sum_j w_j \sum_{G_i} \left\{ \left(\frac{1}{K} \sum C(I,J)\right) - \sum_{i \in G_i} C(I,J) \right\}^2$$

This assumes that criteria are independent - that one would not prefer a group to have quality B if quality A were not present.

Approach

The problem was considered in the light of experience gained in cluster analysis, but the only technique that seemed to bear any light on the possible solution was iterative relocation. The approach taken was to consider all possible interchangings between any 2 students, and if a possible improvement is noticed then the improvement is made. One complete pass, in this example, was enough to achieve an optimal solution, even with a bad initial grouping.

Results

In our specific problem the lecturer in charge of the management exercises was interviewed to find the criteria by which he normally tried to equate groups. These were:

people with English as a first language, sex, accountancy qualifications, class of degree, Oxbridge students, polytechnic students, industrial experience, and the 8 different management specializations which the students had opted to take. This resulted in 15 variables, 13 of which were binary. The remaining 2 variables, class of degree and industrial experience, were also converted to binary because of other uncertainties in the data, e.g., difference in degree classes from one country to another, and lack of comparability information on foreign students, and also to simplify the problem. All weights were initially set to unity. Two sets of data were analysed - 85 1971/72 students and 83 1972/73 students, a (non-optimum) manual solution to which had been found (each taking 2 man-evenings). Beginning from a random grouping optimal solutions were found (in about 200 seconds) but the actual groups bore no relation to those found by trial and error, and so the analysis was retried with the hand solution as the initial groups; this also produced an optimum after 11 exchanges in each case, and was faster than starting with the random grouping. The manual and computer results are given in Tables 32 and 33. The method was used to group 62 1973/74 students with the same criteria and the result was Table 34, after 16 exchanges.

Discussion

Weighting was not used in these examples because it was possible to 'distribute' each property equally with unit weights and thus weighting changes would not change the

1971/2 STUDENTS — ORIGINAL DATA — OBJECTIVE FUNCTION = 1·590

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	TOTAL
LANGUAGE	1	1	1	1	2	1	1	1	1	1	1	0	1	1	1	1	15
SEX	2	1	0	0	0	1	0	1	0	0	0	0	0	0	0	0	3
ACCOUNTANT	3	1	0	1	0	0	1	0	0	1	0	1	0	0	1	1	7
DEGREE	4	2	2	2	0	2	2	1	2	1	4	0	2	1	2	1	24
OXBRIDGE	5	0	2	0	0	0	0	0	0	1	1	0	1	0	1	1	7
POLYTECH	6	1	1	1	0	2	0	0	1	1	2	0	1	2	1	1	14
OVER 30	7	1	1	2	1	1	0	1	0	2	2	0	1	0	1	1	14
FINANCE	8	1	1	1	1	1	1	1	0	1	1	1	1	0	1	1	13
ENGINEERING	9	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	15
MARKETING	10	1	1	1	0	1	1	1	1	1	1	1	1	0	0	1	12
IND. RELATIONS	11	1	1	1	2	1	1	1	1	1	1	1	1	1	1	1	16
ECONOMICS	12	1	1	1	1	1	1	1	2	1	1	0	1	2	1	1	16
INVESTMENT	13	1	1	1	1	1	1	1	1	1	1	1	0	1	1	0	13

NEW GROUPINGS — OBJECTIVE FUNCTION = 0·781

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	TOTAL
LANGUAGE	1	1	1	1	2	1	1	1	1	1	1	0	1	1	1	1	15
SEX	2	1	0	0	0	1	0	1	0	0	0	0	0	0	0	0	3
ACCOUNTANT	3	1	0	1	0	0	1	0	1	1	0	0	0	0	1	1	7
DEGREE	4	2	1	2	2	1	2	2	1	1	2	2	2	1	2	1	24
OXBRIDGE	5	0	1	0	0	0	0	0	0	1	1	0	1	1	1	1	7
POLYTECH	6	1	1	1	1	1	0	1	1	1	1	1	1	1	1	1	14
OVER 30	7	1	1	1	1	1	0	1	1	1	1	1	1	1	1	1	14
FINANCE	8	1	1	1	1	1	1	1	1	1	1	0	1	0	1	1	13
ENGINEERING	9	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	15
MARKETING	10	1	1	1	0	1	1	1	1	1	1	1	1	0	0	1	12
IND. RELATIONS	11	1	1	1	2	1	1	1	1	1	1	1	1	1	1	1	16
ECONOMICS	12	1	1	1	1	1	1	1	1	1	1	1	1	2	1	1	16
INVESTMENT	13	1	1	1	1	1	1	1	1	1	1	1	0	1	1	0	13

1972/3 STUDENTS — ORIGINAL DATA — OBJECTIVE FUNCTION = 2·251

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	TOTAL
LANGUAGE	1	3	1	1	1	1	1	2	1	1	2	1	1	1	1	1	19
SEX	2	1	1	0	0	1	0	1	1	0	0	1	0	1	0	0	7
ACCOUNTANT	3	0	0	0	1	1	1	2	0	1	1	0	1	0	1	2	11
DEGREE	4	1	2	3	2	1	2	1	1	2	1	2	1	2	1	1	23
OXBRIDGE	5	0	0	0	0	1	0	0	1	0	0	1	0	1	0	0	4
POLYTECH	6	2	1	1	3	0	1	2	2	2	1	1	1	0	2	1	20
OVER 30	7	1	1	0	1	0	1	1	0	2	1	0	1	0	1	1	11
FINANCE	8	0	1	0	1	0	1	1	0	0	1	1	1	0	1	1	9
ENGINEER	9	2	2	2	0	0	1	2	2	1	1	1	1	2	0	0	17
MARKETING	10	1	1	1	1	2	2	1	1	2	1	1	1	1	1	1	18
IND. RELATIONS	11	1	1	1	1	1	1	1	1	0	1	1	0	1	1	0	12
ECONOMICS	12	1	1	1	1	1	1	0	1	1	1	0	1	0	1	1	12
INVESTMENT	13	0	0	1	0	1	0	0	1	0	0	1	1	1	0	0	6
INSURANCE	14	0	0	0	1	1	0	1	0	1	0	0	0	0	0	1	5
OPER. RESEARCH	15	1	0	0	1	0	0	0	0	0	0	0	0	0	1	1	4

NEW GROUPINGS — OBJECTIVE FUNCTION = 1·468

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	TOTAL
LANGUAGE	1	2	1	2	2	1	1	1	1	1	2	1	1	1	1	1	19
SEX	2	1	1	0	0	1	0	1	1	0	0	1	0	1	0	0	7
ACCOUNTANT	3	1	0	0	1	1	1	1	1	1	1	0	1	0	1	1	11
DEGREE	4	2	2	2	2	1	2	2	1	2	1	2	1	1	1	1	23
OXBRIDGE	5	1	0	0	0	1	0	0	1	0	0	1	0	0	0	0	4
POLYTECH	6	1	1	2	2	2	1	1	1	1	1	1	1	1	2	2	20
OVER 30	7	1	1	0	1	0	1	1	0	1	1	0	1	1	1	1	11
FINANCE	8	1	1	0	1	0	1	0	1	0	1	1	1	0	1	0	9
ENGINEER	9	1	2	1	1	1	1	1	1	1	1	1	1	2	1	1	17
MARKETING	10	1	1	2	1	1	2	2	1	1	1	1	1	1	1	1	18
IND. RELATIONS	11	1	1	1	1	1	1	1	1	1	1	1	0	0	1	0	12
ECONOMICS	12	1	1	1	0	1	1	0	1	1	1	0	1	1	1	1	12
INVESTMENT	13	0	0	1	0	1	0	0	1	0	0	1	1	1	0	0	6
INSURANCE	14	0	0	0	1	1	0	1	0	1	0	0	0	0	0	1	5
OPER. RESEARCH	15	1	0	0	1	0	0	0	0	0	0	0	0	0	1	1	4

1973/4 STUDENTS NEW GROUPINGS OBJECTIVE FUNCTION = 2·568

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	TOTAL
LANGUAGE	1	2	2	1	1	2	1	1	1	2	1	2	1	2	1	1	21
SEX	2	0	1	1	0	0	0	1	0	0	0	1	0	0	0	1	5
ACCOUNTANT	3	1	1	1	1	1	1	1	1	0	1	1	1	0	1	1	13
DEGREE	4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	15
OXBRIDGE	5	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	2
POLYTECH	6	1	1	0	1	1	0	1	0	1	1	1	1	1	1	1	12
OVER 30	7	1	1	1	0	1	1	0	1	1	1	0	1	1	1	0	11
FINANCE	8	1	1	1	1	0	0	0	0	0	0	1	1	0	1	1	8
ENGINEER	9	1	0	0	0	0	1	0	1	1	1	0	1	1	0	0	7
MARKETING	10	0	1	1	0	0	1	0	1	1	1	1	1	1	1	1	11
IND. RELATIONS	11	1	1	1	1	1	1	1	0	0	0	1	0	1	0	1	10
ECONOMICS	12	1	1	1	1	1	0	1	0	0	0	0	0	0	0	1	7
INVESTMENT	13	0	0	0	0	1	0	1	1	1	1	0	1	1	1	0	8
INSURANCE	14	0	0	0	0	0	1	1	0	1	1	0	0	0	1	0	5
OPER. RESEARCH	15	1	1	0	1	1	0	0	1	0	0	1	0	0	0	0	6

result. If a solution could not be obtained which distributed the properties evenly then weights would normally be employed. Other criteria could easily be incorporated by extending the program to incorporate other properties, for example in our problem people with the same surname could be placed in separate groups, each nationality could be divided between groups, etc.

The above formulation did not allow for second best alternatives. For example the inclusion of an accountant in each group was considered important and as an alternative (as there were more groups than accountants) an economist was considered next best. This can easily be incorporated by the inclusion of a dummy variable Accountant + Economist which has value 1 if a student is one or both of these, and 0 otherwise. By use of a weighted sum third, fourth, etc., alternatives may be included.

With the present formulation properties are spread as evenly as possible between groups, but this could mean a particular group lacks most or all of the properties. If this was considered to bias the groups then other dummy variables could be introduced to even out the advantages of certain properties, for example -

ADVANTAGE = DEGREE + OVER 30 + OP.RSCH - LANGUAGE

and again a weighted sum could be used.

In order to test the method's ability to find a global optimum, we tried 10 different random starts with the 1971/72 data. Four found optimum results, all the runs had

about 35 exchanges between students. Of the six non-optimal results four failed to 'distribute' only one criterion and this property was possessed by 15 students, two failed to distribute two criteria, in one case the properties were possessed by 14 and 16 students respectively and in the other case 15 and 16. This shows that difficulties can arise when the number of people possessing a property is similar to the number of groups. This type of error can be reduced by an initial allocation which sorts students on the basis of a few criteria such as these, as an input to the optimization routine. This procedure produced an optimum on the 1971/72 data, beginning with a manual grouping based on three criteria. Thus given a fairly good starting position, either manually or by a computerized program based on the above, the relocation technique is a useful method in this type of problem.

(d) GAP ANALYSIS

Several marketing papers have tackled the problem of producing an orientation of different brands of the same product (called a product-space) and hence determining possible specifications for new brands. Morgan and Purnell (1969) have used factor analysis to produce an orientation of products and then by an interesting combination of linear programming and cluster analysis find the largest 'gap' between existing products. The American group of researchers Green, Carmone and others (see for example Green, Carmone and Fox 1969, and Green and Carmone 1970) have concentrated on non-metric multidimensional scaling to obtain product spaces and also to place individual 'ideal points' in the same space, using the method of Carroll and Chang (1970).

The present article is an attempt to produce product spaces and individual ideal points on the same two-dimensional representation, by a simpler procedure which is not as time-consuming or as costly as the non-metric multi-dimensional scaling method of Carroll and Chang, whilst having theoretical advantages over the Morgan and Purnell method.

The procedure is in two stages, the first stage produces the product space and the second stage places the ideal points in this space.

Stage I: The Product Space

The first step is to choose the brands for study, ideally they should include all the major brands of the chosen product. Once the brands have been chosen, then data must be collected, normally from market research questionnaires. The aim of the product space is to represent the similarity between each pair of brands by their nearness on the diagram; thus the data collected must be such that the similarity between brands can be quantified. This can be done by several methods including:

1. Measuring the brands of chosen criteria (e.g. measuring the milk content, sugar content, softness at different temperatures, etc., of chocolate);

2. Rating the brands subjectively on chosen criteria (e.g. rating cars on a 0-5 scale on criteria such as luxuriousness, ease of handling, shape, etc.);

3. Assessing similarities between brands directly (e.g. respondents are asked to rank pairs of washing powders in order of similarity).

Of these three methods the first two have the difficulty that the criteria may not be the whole set of criteria by which consumers differentiate between brands, and they will not be weighted in the way consumers weight them. The third method overcomes this difficulty to a great extent, but the task of ranking all pairs of products in order of descending similarity is not easy, and thus data obtained in this way may be subject to large errors. This problem increases as the number of brands increases, for example if ten brands are

to be assessed then the respondent must rank forty-five pairs, and if there are fifteen brands, then one hundred and five pairs must be ranked.

Assuming that the similarities data has been obtained the next step is to attempt to use cluster analysis on the set of similarities to determine whether the respondents all 'see' the brands in approximately the same way, or in psychological terms whether they all have roughly the same perceptual space. If clusters are present in the data, then the analysis should be carried out separately on each cluster.

After we have collected the similarities data into one or more homogenous groups then we have to decide which method to employ in order to obtain the product space from this data. Several methods exist which are capable of producing such a geometrical model from similarities data, most of which fall under the general heading of ordination.

Once the ordination technique has been chosen and applied to the data then a two-dimensional configuration is obtained (this technique can be applied in one dimension but will contain less information; an extension to three dimensions can be visualized but the complexity would increase markedly). The problem of dimensionality is a difficult one.

At this stage the plausibility of the configuration should be checked by inspection, and if possible meaningful axes constructed. The selection and naming of axes is a difficulty with all methods of multidimensional scaling and

this problem is perhaps best solved only by experience with such configurations coupled with knowledge of the particular brands in the study. Once this check for plausibility has been successfully completed, then we move on to Stage II.

Stage II: Ideal Points

The input data for this stage is each respondent's ranking, in order of preference, of the brands chosen for analysis. The method of finding the ideal points is linked to psychological scaling (see Coombs 1964). It is based on the assumption that if a respondent prefers brand A to brand B then his ideal point will be nearer the point representing brand A than that representing B, thus if we construct the perpendicular bisector of the line joining point A to point B, then the respondent's ideal point will lie on the same side of the line as the point representing brand A. On the product space the perpendicular bisector of each pair of brands is drawn; if there are n brands then there will be $\frac{1}{2}n(n-1)$ lines. This will define, in general $1 + \frac{1}{24}n(n-1)(3n^2 - 7n + 14)$ regions each corresponding to a particular preference ordering of the brands. Since there are n! ways of ordering n objects, then for $n > 3$ there will be orderings for which there is no corresponding region.

BRANDS	LINES	REGIONS	POSSIBLE ORDERINGS
5	10	46	120
6	15	101	720
7	21	197	5,040
8	28	351	40,320
10	45	916	3,618,800

If a respondent's ideal point lies in one of these regions then his expected ordering will be that associated with that region. Each of the regions is labelled according to its associate order. By inspection of the respondent's preference orderings, all those which correspond to a particular region are allocated to that region and scattered uniformly throughout it. The error in this assumption is not normally large, since within the group of brands the regions are normally small, and the exact position of ideal points in regions outside the group of brands is not of great importance (see later). This procedure is continued until no remaining respondents preference orderings correspond to regions.

The next step is to allocate the remaining respondents to their 'best' position in the product space. This is best explained by example (see later) but in principle one finds in each case the region which has an ordering most like the particular respondent's ordering. Within this region the ideal point is placed nearest feasibility, i.e. if the

respondent's preference order is ACDEB and the 'best' region that exists is ACEDB then the ideal point is placed within the region ACEDB at the point nearest to the perpendicular bisector of the line between D and E. Thus an ideal point may be found for all remaining respondents.

At this stage the diagram can be redrawn showing only the points representing the brands and the ideal points. The 'best position' for a new brand is the point on the diagram which is nearer than any other brand point to the most ideal points. This position can be found fairly easily by trial and error. In practice several near-optimal points are found and the strategic advantages of each are considered, for example one may wish to maximize the lead in sales over the next highest selling brand, in which case sales would be taken mainly from the present market leaders, or one may wish to take sales mainly from the smaller selling brands in order to avoid upsetting the market leaders. Similarly one could consider the repositioning necessary for existing brands in order to increase sales. Once a position for the new brand, or a new position for the old brand has been found, its characteristics can be determined from the axes of the product space.

Example

The following six brands of a particular product were used because of the wide knowledge of their characteristics:

Edward Heath
Roy Jenkins
Reginald Maudling
Jeremy Thorpe
Enoch Powell
Harold Wilson

They were selected as representative of other brands and as having major market shares. The respondents were 39 post-graduate management students of the Graduate Business Centre, who completed a questionnaire in June 1972. They were asked to rank the politicians in the order in which they agreed with the politicians' views. Secondly they were required to order each pair of politicians according to their similarity of views. The questionnaires were completed anonymously. Each individual's questionnaire was scrutinized to eliminate wrongly completed forms, and practical jokers. If a respondent listed the brands in the order of preference HJMTPW, then they would be expected to put J as the person most similar to H in views. This eliminated 5 of the questionnaires leaving 34. Any other 'spoilt' papers not picked out by this simple method would probably show up as outliers in the cluster analysis, which was the next part of the procedure.

In order to test that all individuals had the same perception of the six brands and 34 dissimilarity matrices produced by the respondents were subjected to cluster

analysis by an iterative relocation method similar to that of Beale (1969). The method showed that no clusters were present. The existence of identical orderings ruled out the possibility that n clusters and not 1 cluster existed.

To obtain the product space the dissimilarity matrices were summed for all respondents, and this matrix was subjected to metric multidimensional scaling. The method used was to minimize the loss function:

$$\sum_{i<j} \frac{(D_{ij} - d_{ij})^2}{D_{ij}^2}$$

(where D_{ij} is the dissimilarity between brands i and j, and d_{ij} is the Euclidean distance between brands i and j in a two-dimensional space). This method produces a best fit of the data in two dimensions. The resultant product space is shown in Figure 62.

The axes of the configuration were then considered, the horizontal axis can be confidently labelled as a radical-conservative dimension, whilst the other axis, possibly oblique seems to be a 'toughness' dimension. These axes agree to a large extent with those found by Eysenck (1970). (Also see Brittan 1973.)

The fifteen perpendicular bisectors were drawn and the orderings for each region labelled on the diagram. Figure 63 shows the bisectors and some of the orderings for the regions. Of the 34 respondents, 18 had orderings for which regions existed, these were scattered uniformly

POWELL

WILSON

JENKINS

HEATH

THORPE

HAUSLING

FIGURE 62

FIGURE G3

Powell Division

T7MHWF

T7MHWF

T7MHWF

T7MHWF

T7MHWF

T7MHWF

T7MHWF

MAYBURG

THORPE

HEATH

JENKINS

WILSON

POWELL

throughout their respective regions. Note that Carroll and Chang's method would normally allocate these points to the perimeter of this area. In order to illustrate the method by which the other orderings were allocated to points, consider respondent 25 whose ordering of the brands was JTMHPW. Since he placed J first his ideal point must lie in the dotted region marked on Figure 63. As he placed T second in his ordering his ideal point must lie in the quadrilateral region marked by the wavy line. Similarly his choice of M as a third preference restricts the position of his ideal point to the region JTMHWP. The only contradiction in his ideal point lying in this region is that of his preference for P over W, thus within the region JTMHWP his ideal point is placed as near to the perpendicular bisector of the points representing W and P as possible, i.e. in the top right-hand corner of the triangle. Similarly all the remaining ideal points were placed on the diagram, resulting in Figure 64. The diagram shows the ideal points concentrated in the centre and centre-left, with some tailing off in both directions along the radical-conservative axis.

The implications for launching a new brand in order to try and capture this specialized market of post-graduate business students can now be considered. The most niticeable concentration of ideal points is around Jenkins, and thus the best position for a new brand will be near his point on the diagram. By successive trial and error the optimum position can be quickly found. This is shown in Figure 65 together with the first-preference areas, and the

POWELL

WILSON

JENKINS

HEATH

THORPE

MAUDLING

o BRAND
x IDEAL POINT

FIGURE 64

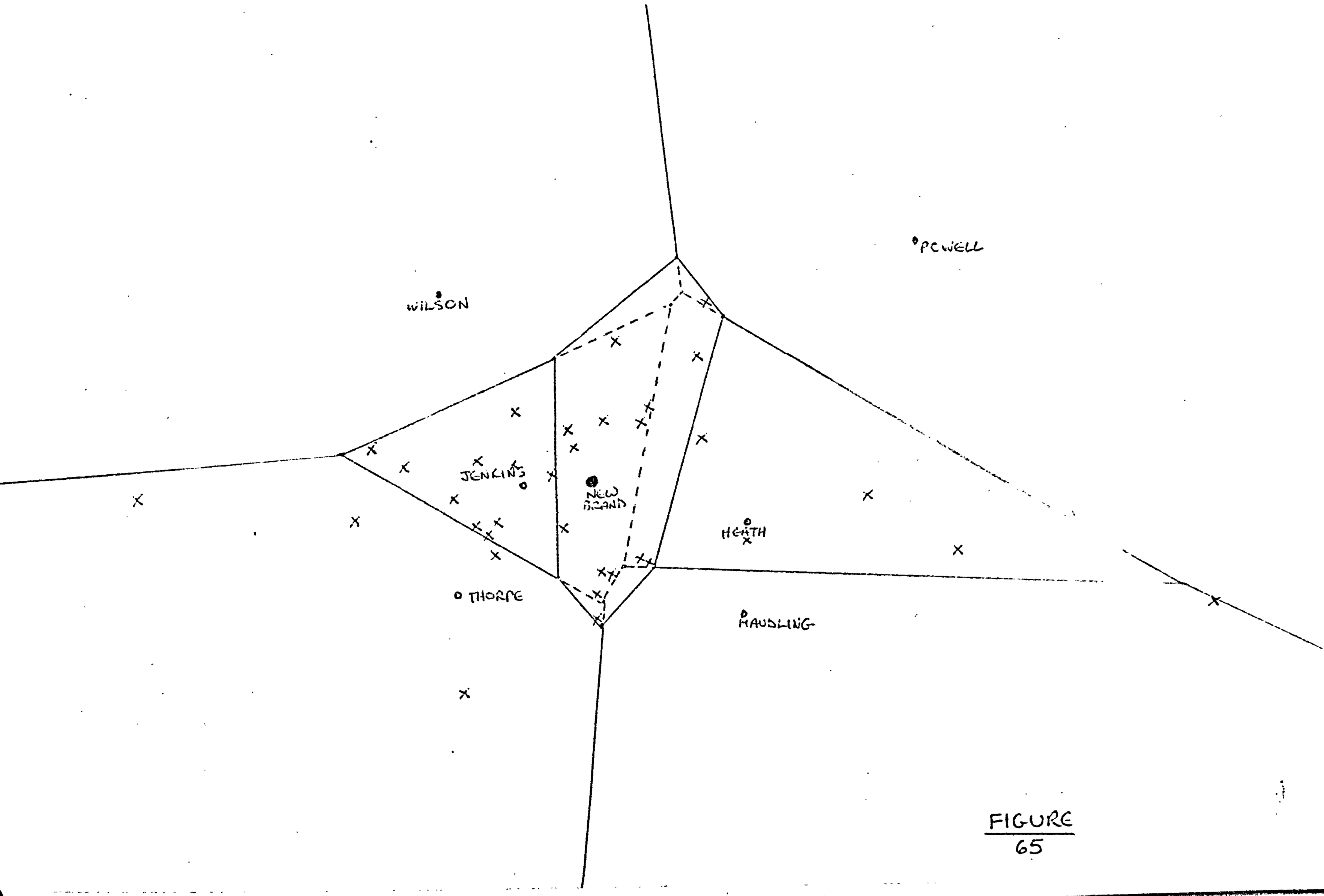


FIGURE
65

previous first-preference areas are shown by dotted lines. Thus the characteristics of the new brand to maximize sales can be determined from the axes of the diagram - the new brand would be similar to Jenkins but more to the right politically.

It has been mentioned earlier in this article that if an ideal point lies outside the group of points representing the brands, then its exact position is not of great importance; this statement can best be explained with reference to the present example. If a new brand was marketed which was slightly to the right of Heath then this brand would be preferred to Heath by all the people whose ideal points are out to the right of Heath, no matter how far they are away. Thus if a new brand is to be marketed outside the present group of brands, it need only be just outside in order to 'capture' the most ideal points, and so the exact position of exterior points is not critical.

Figure 64 has implications for the existing brands, because if a number of ideal points are just outside the region of first preference of a particular brand, then it may be of advantage for that brand to be changed (or to change its brand image) so that it lies nearer these ideal points. It can be seen that with respect to this particular specialized market Jenkins is in a near optimal position and other brands would have to move nearer to him to obtain more support. An important consideration is that a movement in position cannot be too great as it would cause loss of credibility and so only small changes in position can be made.

It can be seen from Figure 65 that Thorpe and Heath have the most to gain from a movement towards the position occupied by Jenkins, i.e., a small move by Heath to the political left and a 'toughening' of Thorpe's image. Whilst some gain can be obtained by Wilson and Maudling in moving towards the centre, Powell would need too great a shift in views to increase his support, that his following cannot be increased at all.

Conclusions

The method explained above has advantages over the Morgan and Purnell method which proceeds from the product space by finding the largest space between existing brands. This relies on the supposition that ideal points are spread uniformly through the space, which as shown by the above example is an oversimplification of the true situation. The Carroll and Chang method has the advantage that it allows for respondents who have different conceptual spaces to be mapped on the same diagram, but it is more complex and time consuming, whereas the current method proceeds rapidly from the product space by manual methods.

(e) FACTORY LAYOUT

One of the most important considerations in factory layouts is to ensure that movements between work centres are kept to a minimum - this becomes especially important with heavy equipment movements, or in production which requires speed; it also saves space as gangways can be smaller, and can reduce accidents. Normal approaches are very heuristic, and consist of either manually attempting to form a network of work centres with all movements being between adjacent centres (see Buffa 1955, 1969), or by computer algorithms which attempt similar arrangements, such as CORELAP (Lee and Moore 1967) and CRAFT (Armour, Buffa and Vollman 1964) (also ALDEP - IBM 1967 and RMA - Muther et al 1970).

The problem can be approached by the use of ordination, which, we suggest can lead to a better solution than the above procedures. The approach in most of these methods is to begin by obtaining a matrix of intermovements between centres, normally in units such as weight or volume to be transported. This matrix is a similarity matrix, and if an ordination is attempted then the pairs of centres with the most intermovement will be placed closest, which is the required solution to the problem. The previous type of solution to ordination have been two-dimensional, but the ordination approach can be easily applied in higher dimensions, and can give an indication of whether a 3, 2 or 1 dimensional solution is best.

The simplest problem of factory layout is when the overall shape of the work centres and the layout space is not specified. Complicating factors which affect real life problems, and can be incorporated in most solution procedures, are the shape or exact dimensions of the layout space being defined, the splitting of the layout into several rooms or buildings, and work centres that cannot be placed adjacently, etc.

The method of network shuffling as performed by Buffa is fairly simple if few interactions exist, but can soon become too complex with a large number of work centres or intermovements. The Buffa example has 11 nodes and 19 interactions and the final layout is still not optimal in the improved 1969 version of his solution (see Figures 66 and 67). The solution is normally in two parts - shuffling the network, and the fitting of this into a pre-defined or regular shape. With ordination a good solution to the first part of the problem can be found by the computer. The measurement of optimality is difficult. A possible criterion is to minimize the total centre to centre cost (perhaps in terms of distance x flow), or alternatively one could count costs between contiguous work centres as zero.

The choice of ordination method is a fairly simple question. Since we are trying to 'force' a solution in a certain dimensionality, and are searching for a solution in which objects of high similarity are closest, then stress minimization would seem appropriate. The choice between matric and non-metric depends on our data - if we can say

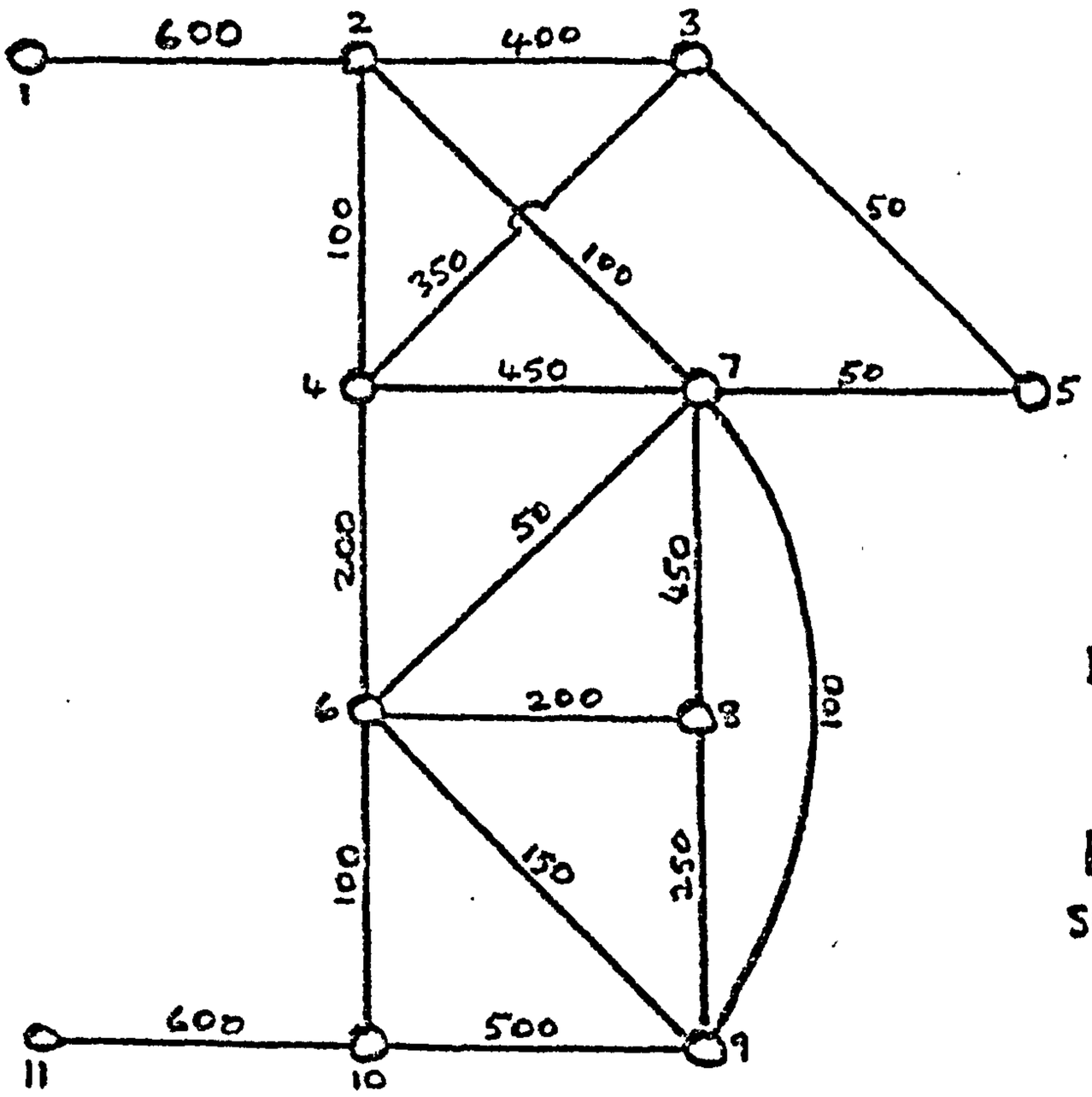


FIGURE 66

BUFFA'S SOLUTION

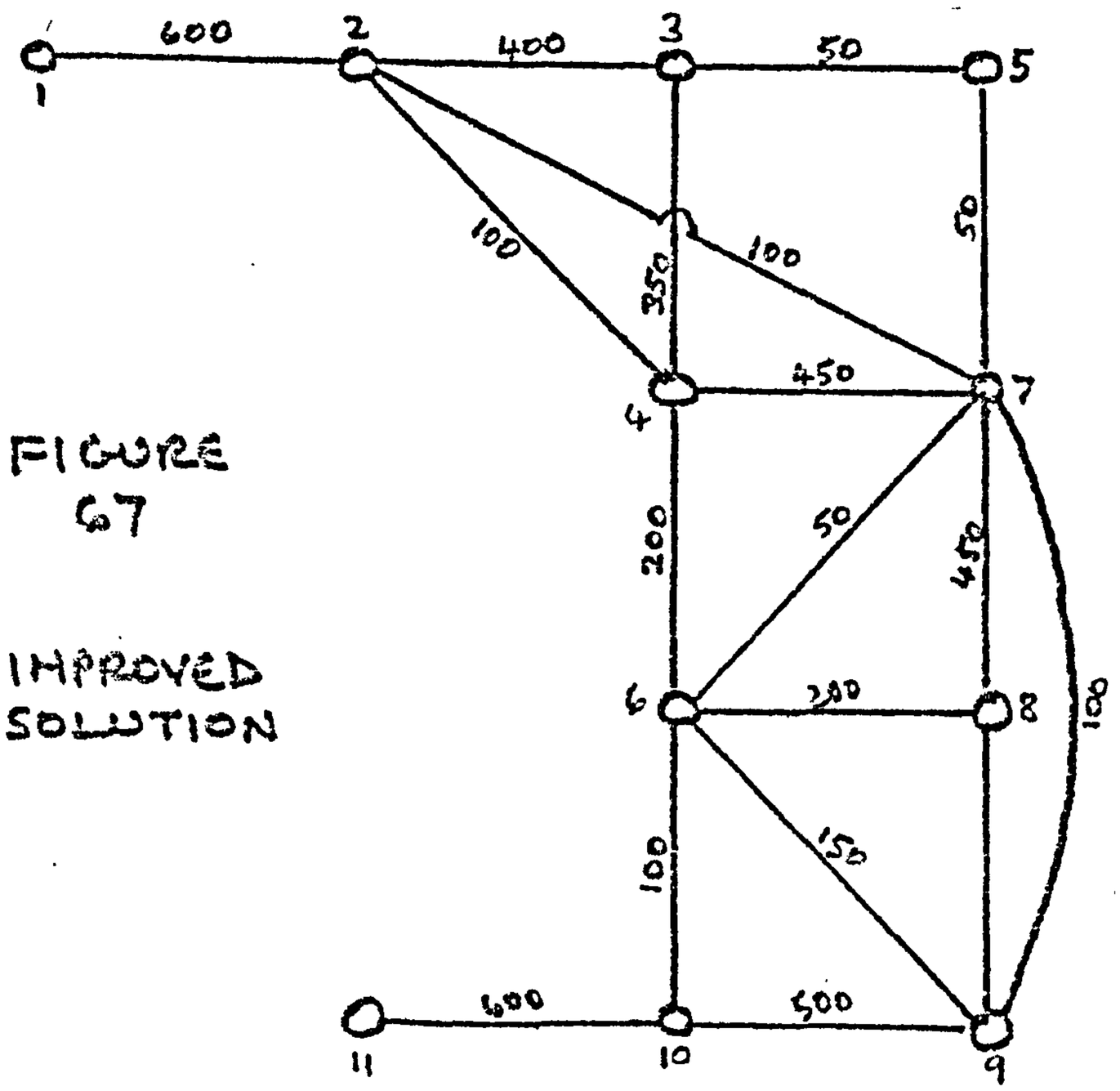


FIGURE 67

IMPROVED SOLUTION

that the cost is proportional to the distance travelled then we may use metric stress minimization. One difficulty is that there may be a large number of zeros in the matrix, one would have the occurrence of a two-dimensional horseshoe effect which would make the configuration more circular, and with more points near the perimeter - this may be overcome by eliminating these values from the minimization, or by a method of changing the distance function, such as employed by D. Kendall (1971). The ordination technique can be used to form a one-dimensional solution, which would be equivalent to line production. Since a one-dimensional solution is to be forced on the problem in this case, one could perhaps use seriation.

It may be that work centres are forcibly constrained to several buildings or rooms, or it may be considered desirable to split the work centres into groups for a Group Technology approach (see Drurie 1970 and Gallaher et al 1973). Group Technology calls for the grouping of machines on a product and not process basis. The similarity between two machines is determined by the number of types of components in which both machines are used. The obvious procedure is to use cluster analysis to divide the similarity matrix into the required number of groups, possibly using side conditions, limiting the size of groups in terms of area, for example. This kind of approach (without constraints) is considered by McAuley (1972) and Carrie (1973). McAuley's paper was criticized by Crook and Kirkpatrick (1972) as unpractical, and mentioned a case of

200 machines manufacturing 12,000 components - as had been shown earlier in this work this is within the capabilities of cluster methods. Carrie's (1973) is more detailed than McAuley's paper, but the methods in both papers use single link clustering which is perhaps not the best method to use for small (250 machines) problems.

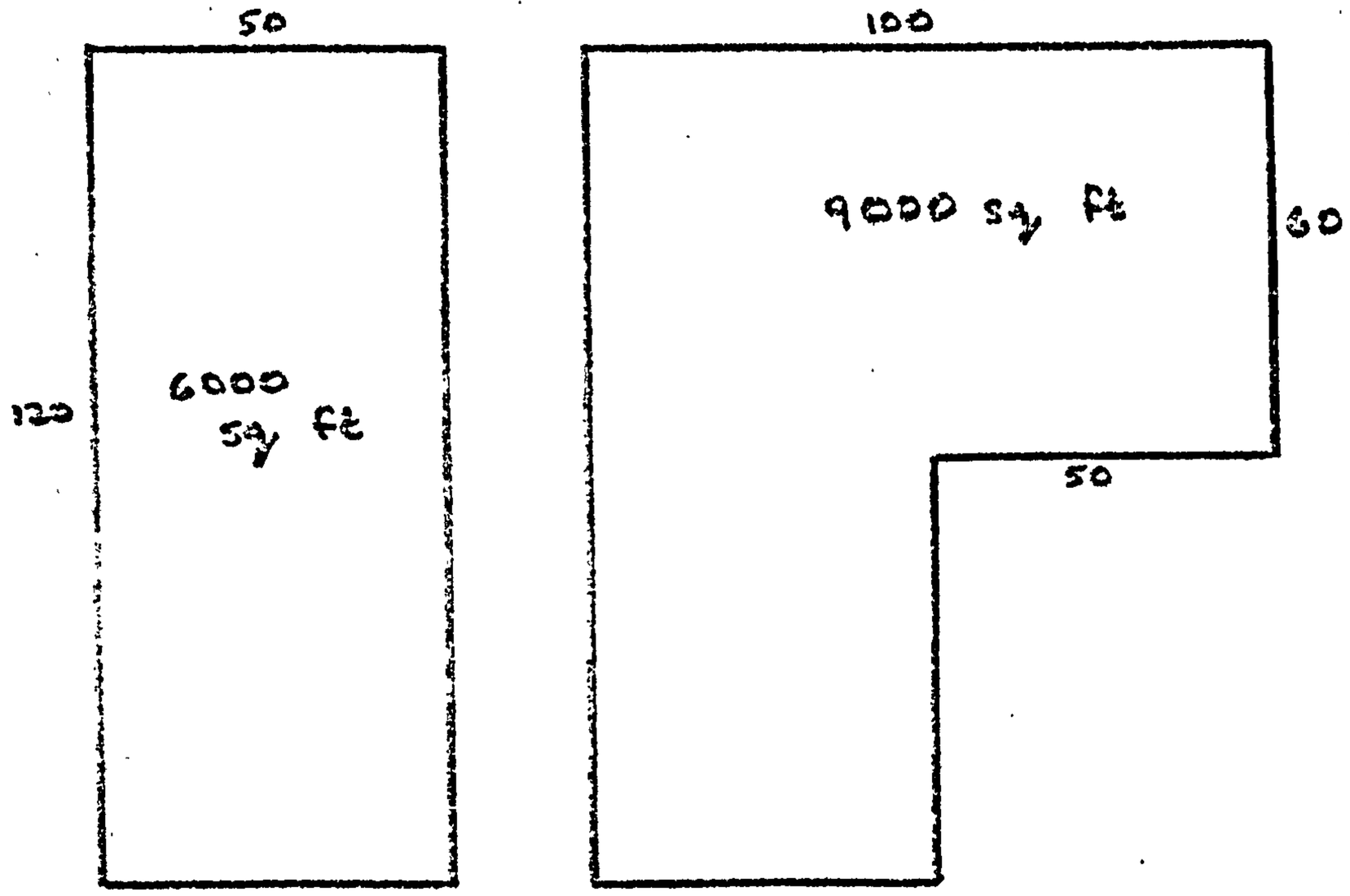
Method and Example

In order to justify our faith in the above procedure, and to explain the process, we shall give our method in detail, as applied to an example. The following matrix shows the weight of parts which flow between 20 processes, and the area taken by each.

FROM \ TO	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	SIZE
1	X	20					190														400
2	50	X	10		100																600
3			X		200			100							20						900
4	100			X	500	100	20														500
5				200	X	50		100	400												200
6	200			200		X	400				50				70		40				400
7		100	100				X			50	100	25					100		50	200	1200
8						100		X	400		100				60						900
9				400		200	150	120	X			30	50	110	100	130				20	2000
10										X		75	20								450
11						300					X	20		60			60				150
12									200	50	50	X		100	70						1000
13			40				150				20	X	40	90	100					75	700
14					50								X							200	100
15														X	30	20	20			200	700
16															X	20	200	20			200
17						50				100	200			60	X	30	60				500
18													30	50	50	X	40	20			550
19																100	X	60			150
20																		X			1500

13100

We will consider two cases in detail, one where the layout must be in two buildings of the dimensions below, and one where one building is to be used, being the combined shape of the two given below, forming an L-shape of overall dimensions 120 by 150 feet.



We consider first the one building layout. The ordination method used was a metric stress minimization procedure with no modifications. This produced a final configuration in less than 100 seconds. Next the perpendicular bisectors of adjacent pairs of points were drawn on the diagram - this gives convex polygonal regions each enclosing one ordinate point. These define neighbourhood regions - all other positions within the region enclosing a particular ordinate point will be nearer to that point than any other. Thus these regions are regions of 'least interference' with other points.

Next a rough scale is introduced by consideration of the total layout area needed, and the present area which covers most of the ordinate points. The whole area is then divided into unit squares (about 20n of them, where n is the number of work centres). The orientation of the squares is decided by the final shape required for the layout, but is not crucial at this stage. In our example we are now at Figure 66.

The next stage is to introduce the area of each work centre. Using the scaled squares, mark in the correct number of squares required for each work centre, beginning with those which have the smallest neighbourhood regions, and of these the ones with the largest required area. These areas are drawn around the corresponding ordinate point, and as much as possible within its neighbourhood region. We are now at the stage of Figure 67.

The layouts are then moved together as compactly as possible, whilst still covering the corresponding ordinate point, and being as much as possible within the neighbourhood region. At this stage the orientation of the building shape is fitted onto the layout as best as possible. The lattice is then rotated to be more in line with the building shape. In our example this rotation was unnecessary, and we are now at Figure 68. The precise scaling of the original points is not critical since we are only trying to orientate the shapes in the same way as the orientation of points, and not fit each shape round its related point.

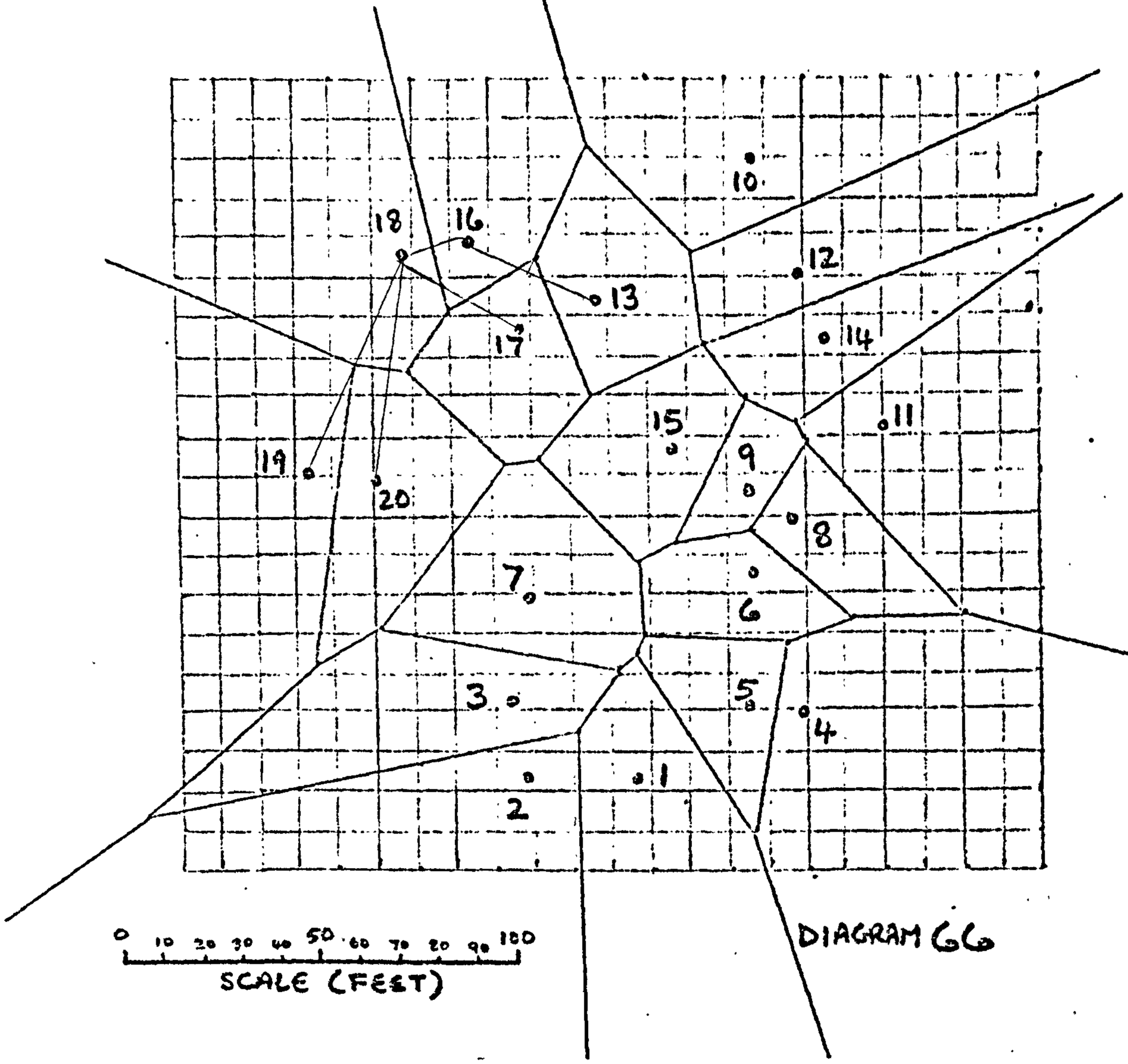


DIAGRAM 66

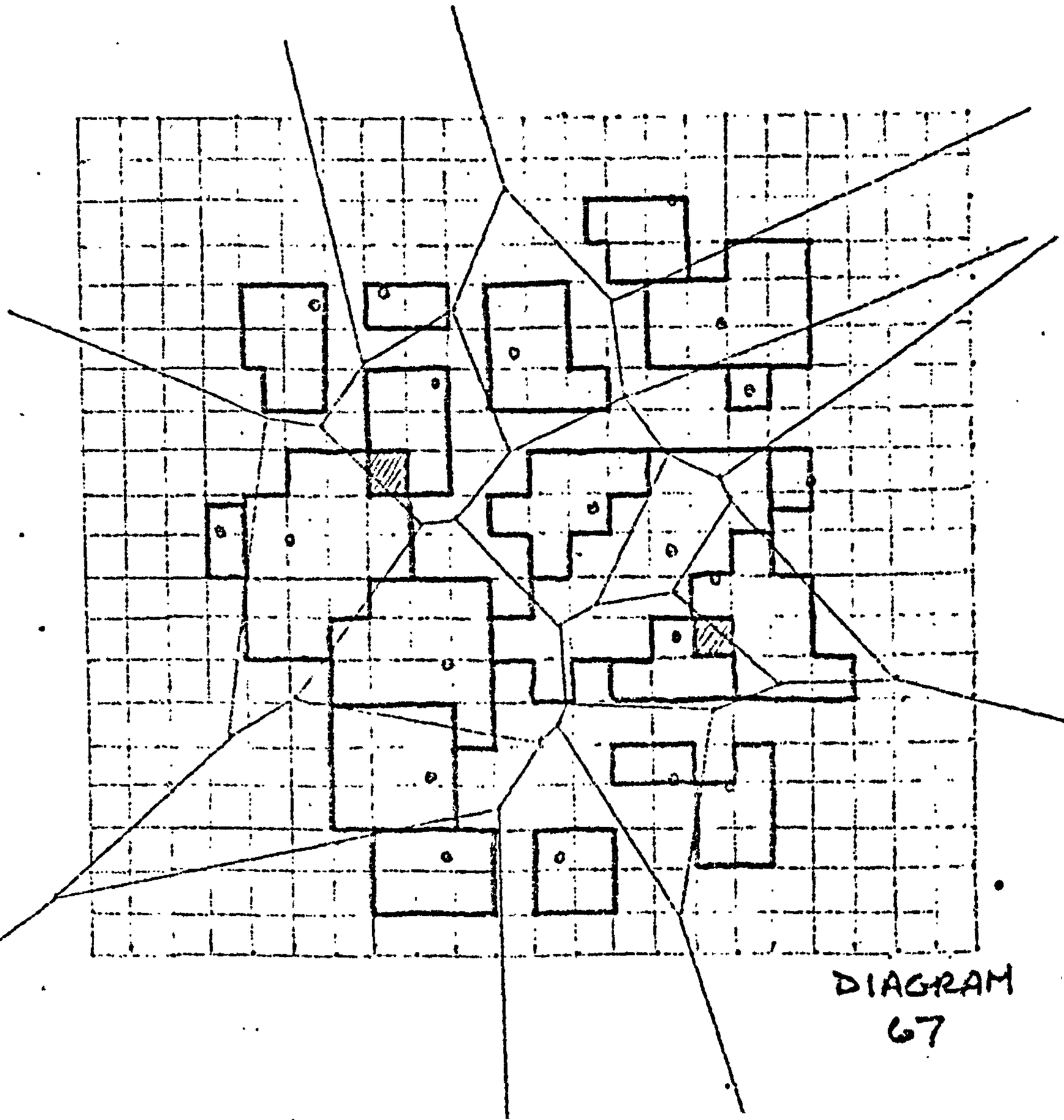


DIAGRAM 67

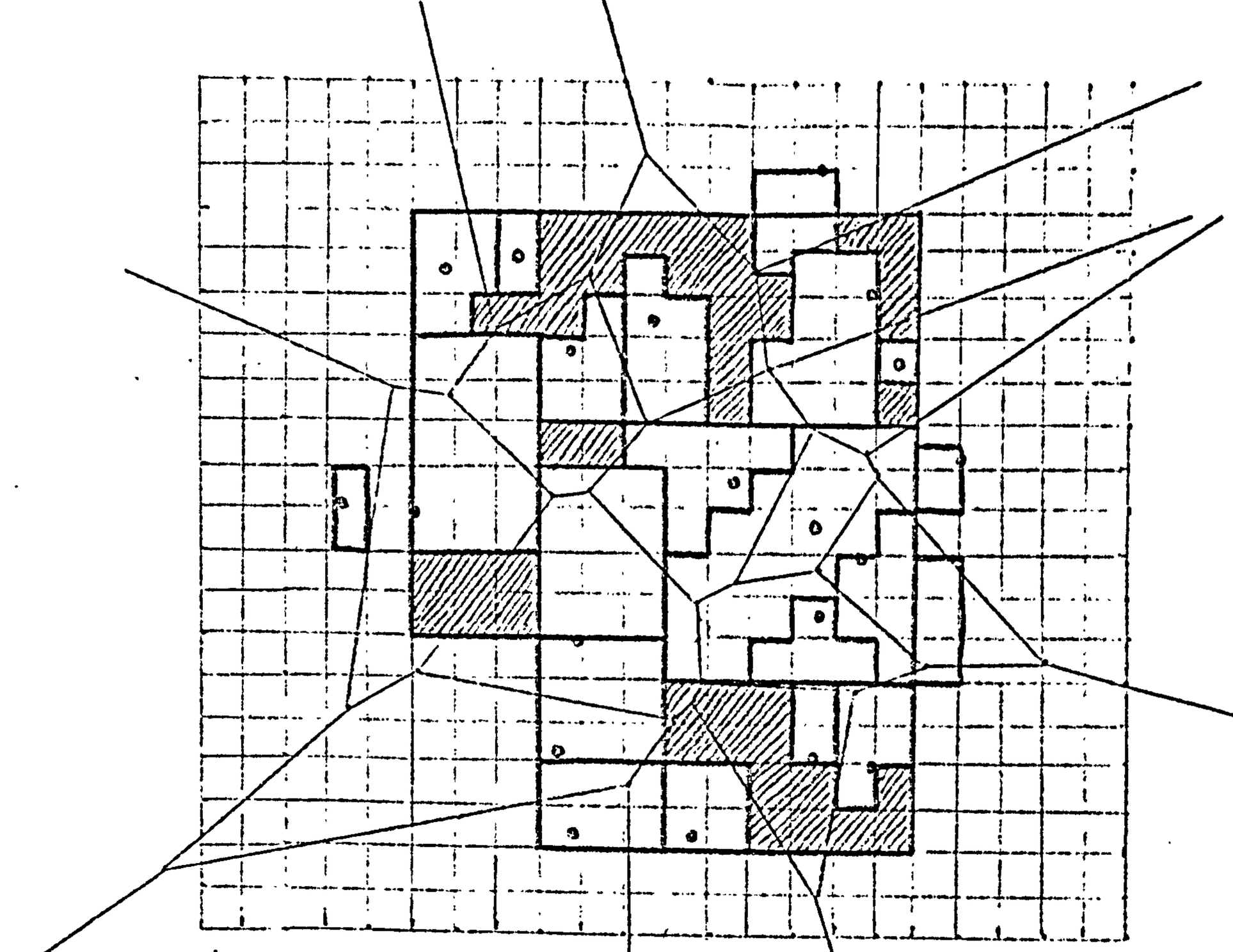


DIAGRAM
68

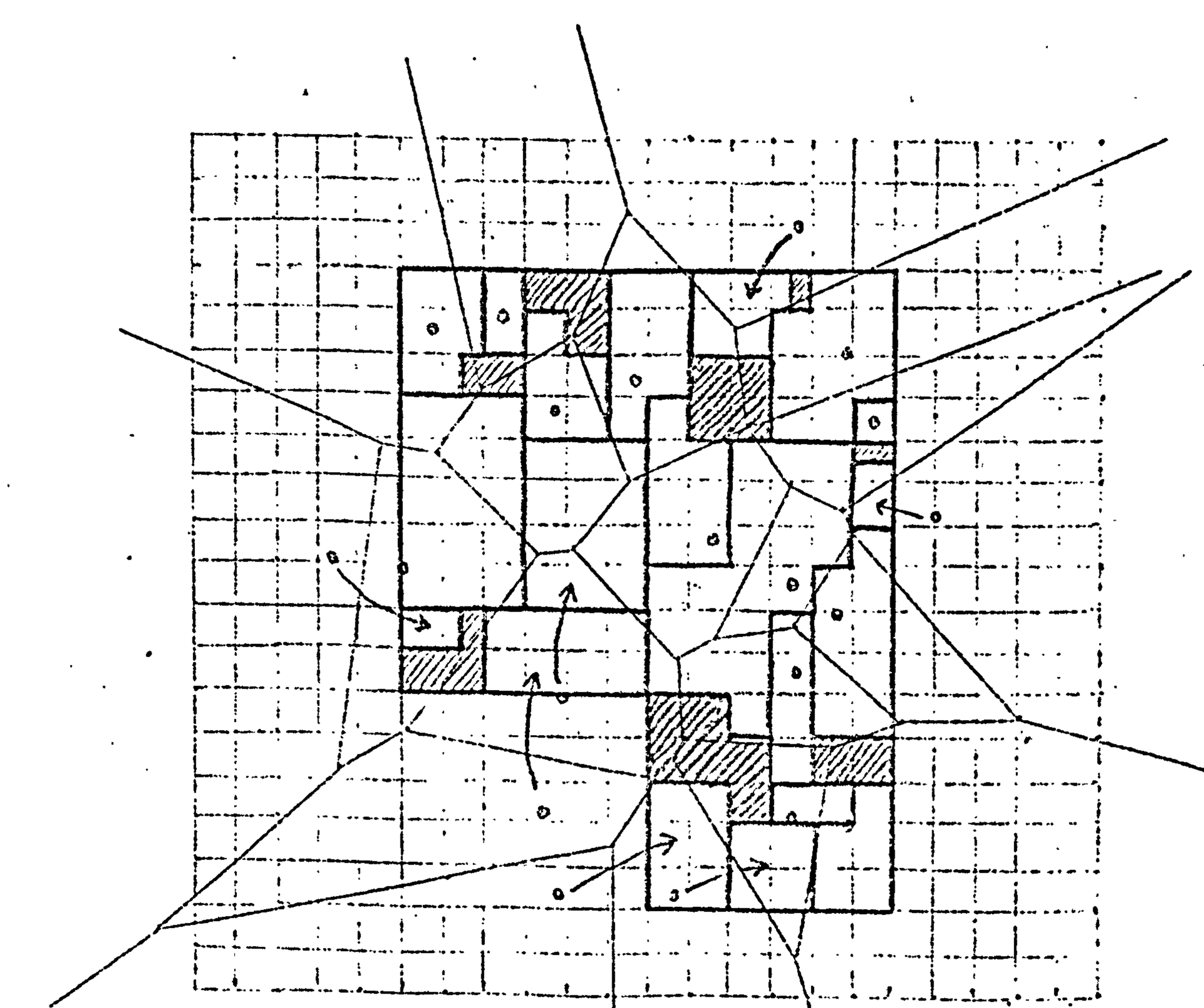


DIAGRAM
69

Next the layouts are then fitted into the building shape (this may take more than one fitting stage - during which the orientation of the building may be altered). Decisions on position are based on the original points and their associate regions, but now the ordinate point need not necessarily be enclosed by the layout shape. This gives Figure 69, which would give an approximate solution if work centres could be any continuous shape.

The work centres are then made into the required shape or class of shapes (in this case rectangles), by a similar process (this again may take more than one fitting). Our example is now shown at this stage in Figure 70, which is nearly our solution. Further slight rearrangements give our final result given in Figure 71. Further possible considerations, such as the positions of pillars, etc., would be resolved by further similar movements of work centres.

Our second problem - that of a split workplace involves cluster analysis. The similarity matrix was clustered using the extended flexible method with $\alpha=0.6$ and $\beta=-0.7$ and took 15 seconds. The resultant grouping is shown schematically (since the method does not produce a scaled dendrogram) below.

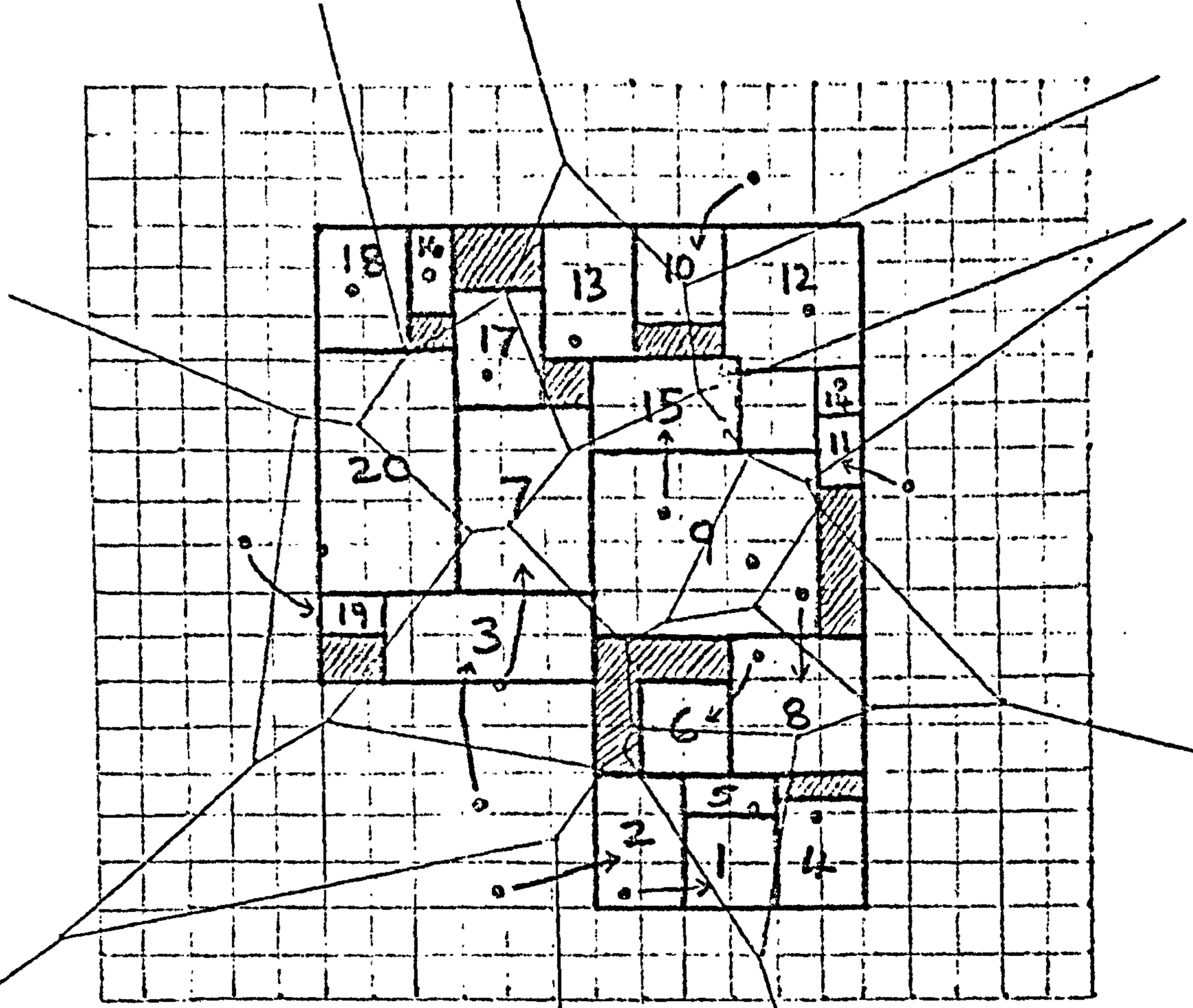
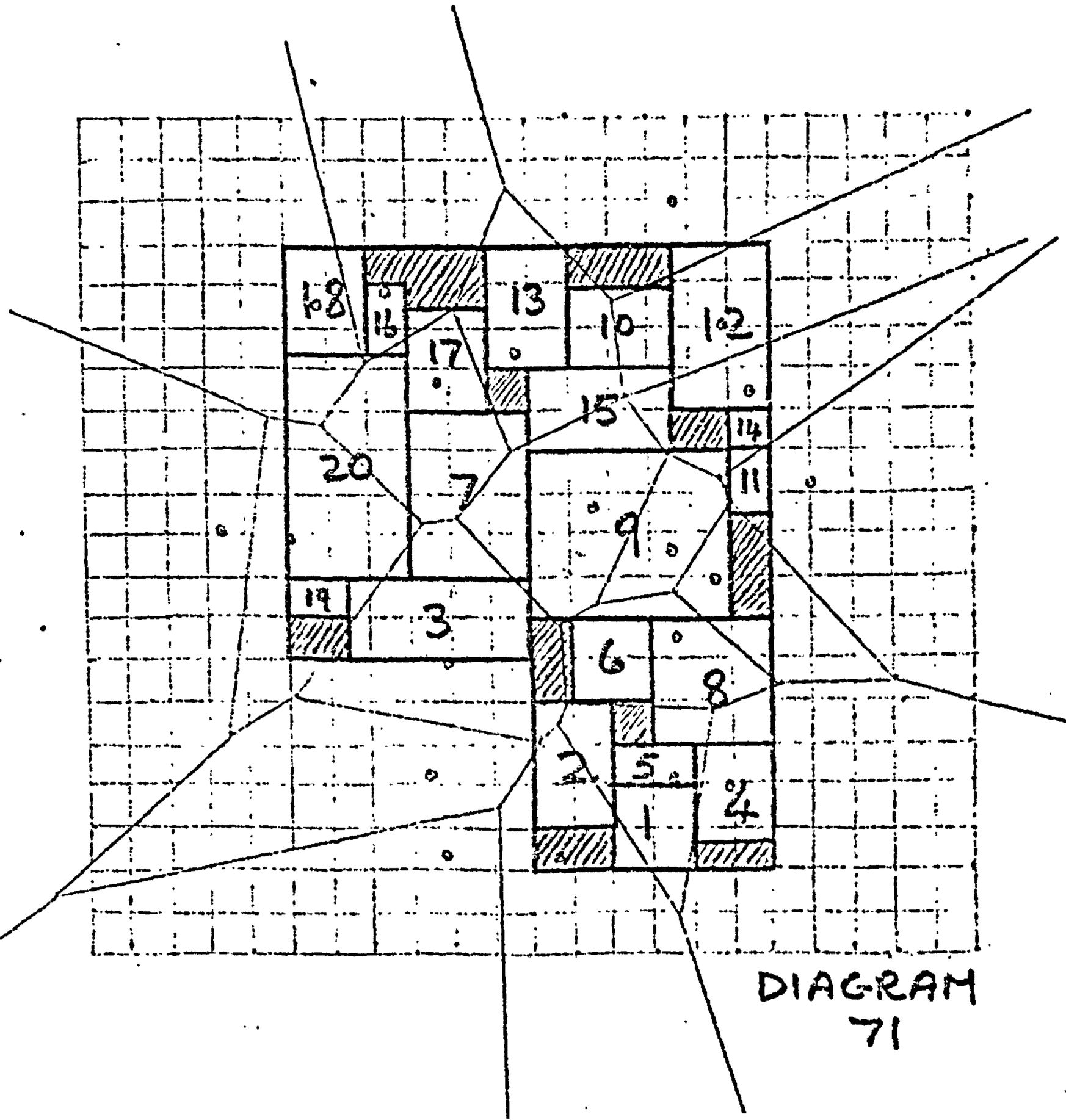


DIAGRAM
70



DIAGRAM
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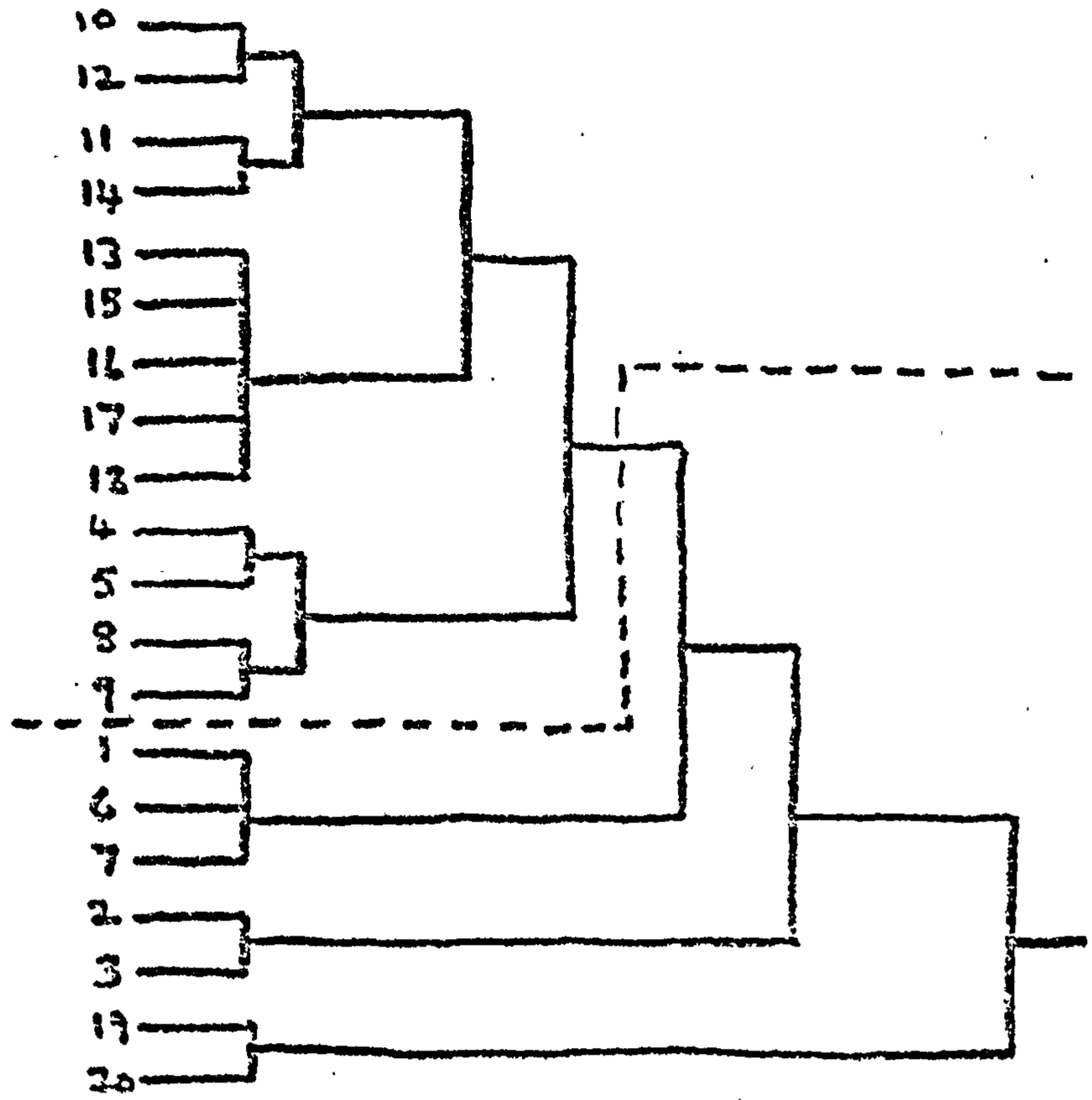

Constraints could have been introduced into the program, but we attempted first to see if an unrestricted run could produce a good result. The two group clustering was not suitable for splitting into the required sizes and so by consideration of the clusters and the ordination of the 20 points, the division shown on the cluster diagram was made which gave two total areas of 5150 and 7950 square feet (an alternative arrangement could give areas of 8750 and 4350, but this would give hardly any slack in the larger building.

Each subset of points was then ordinated. The initial plans for each case and the final solutions are shown in Figures 72-75. It is interesting to note the reproduction of our clustering result in the final layouts.

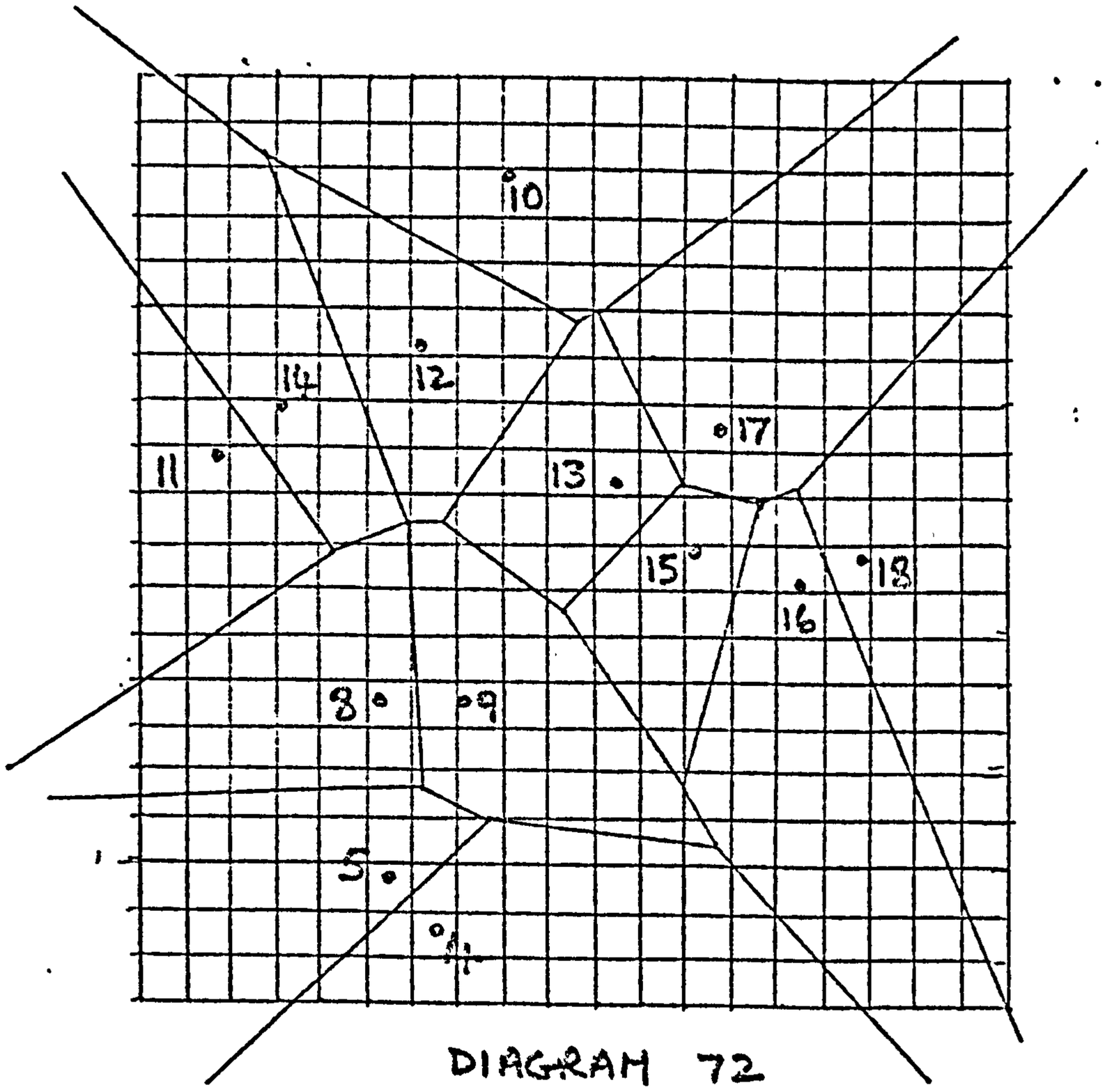

DIAGRAM 72

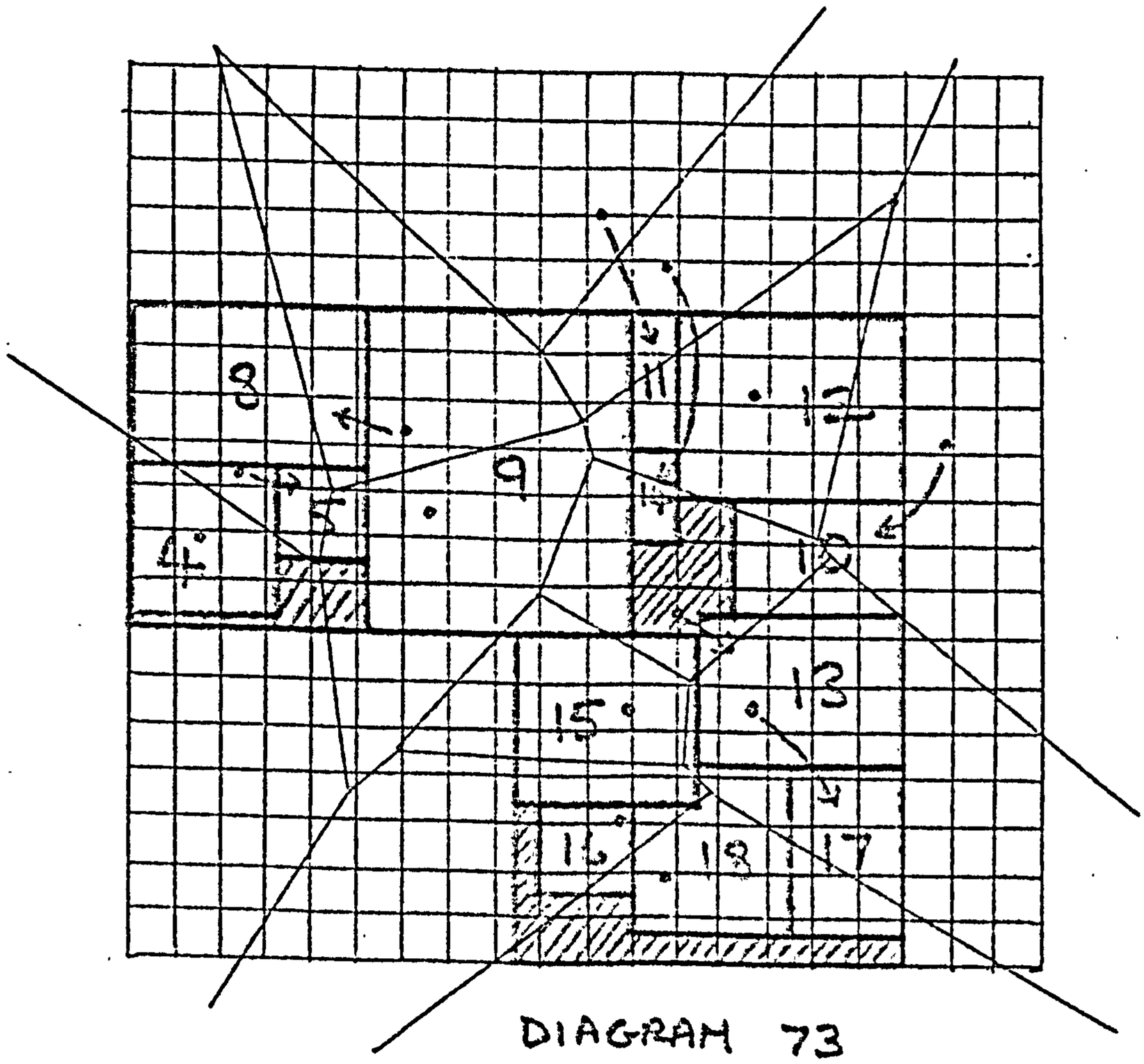

DIAGRAM 73

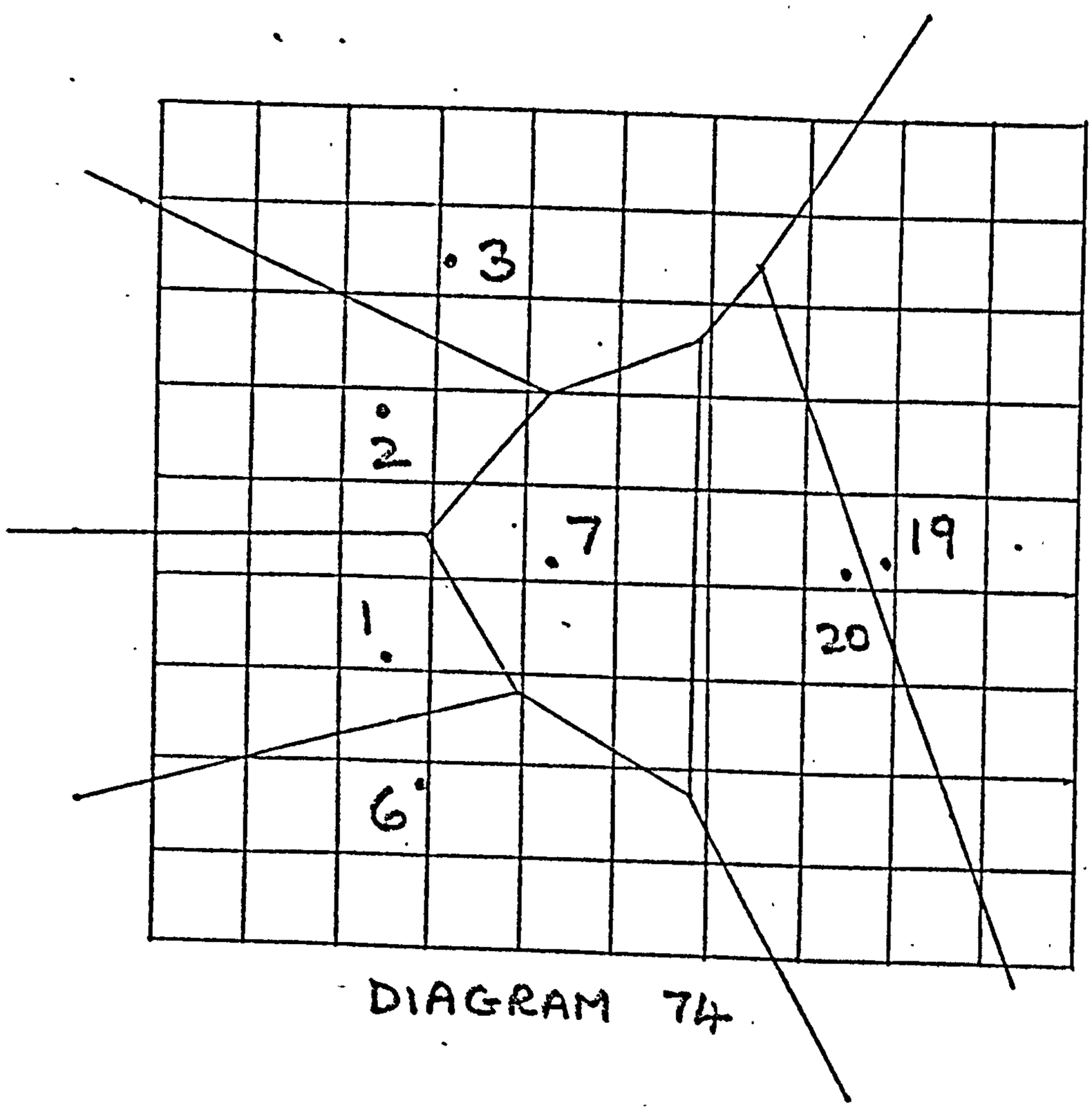

DIAGRAM 74

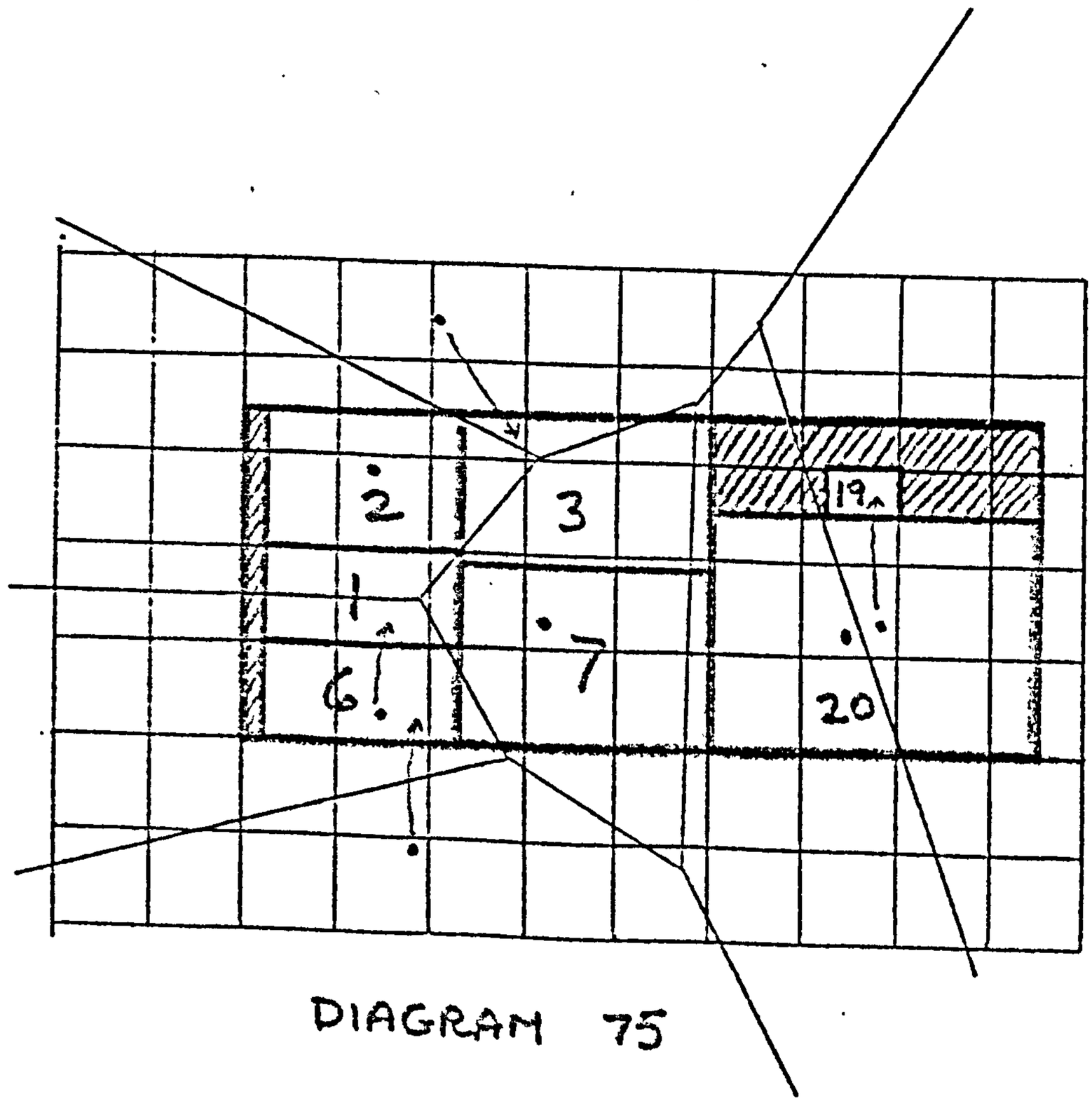

DIAGRAM 75

Conclusion

An ordination method of arranging factory layouts in order to minimize movements between work places has been described. The method is believed to have advantages over other techniques in terms of solution, at slightly higher computational cost. The use of cluster analysis in grouping work centres has also been illustrated, which is fairly rapid in calculation. The cluster result could be used as a basis for a heuristic manual layout method, by placing work centres into a full layout in the order in which they cluster in an agglomerative routine.

APPENDIX I

Fortran program to perform hierarchical methods outlined on pages 133-164.

```
      DIMENSION  D(34,34),A(34,34),K(34),C(34),TI(10)
      INTEGER  P,Q,X,C,A3
      INTEGER PP(33), QQ(33)
      DIMENSION DD(33)
      READ(1,898) (TI(I), I = 1, 10)
      WRITE(2,899) (TI(I), I = 1, 10)
      WRITE(2,904)
      READ(1,901)  N,M
      DO 120 I = 1, N
      READ(1,4704)  (A(I,J), J=1,M)
120   WRITE(2,905)  (A(I,J), J = 1, M)
320   READ(1,52) X
      IF(X .LT. 0)  GO TO 1200
      IF (X .NE. 0) GO TO  340
      READ(1,53)  A1
      A2 = A1
      B1 = 1.0 - 2.0*A1
      C1 = 0.0
      WRITE(2,40)  A1,A2,B1
      GO TO 551
340   IF (X .NE. 1) GO TO 380
      WRITE(2,41)
      C1 = -0.5
      B1 = 0.0
      GO TO 550
380   IF (X .NE. 2)  GO TO 420
      WRITE(2,42)
      C1 = 0.5
      B1 = 0.0
      GO TO 550
420   IF (X .NE. 3)  GO TO 480
      WRITE(2,43)
      B1 = -0.25
      GO TO 540
480   IF (X .EQ. 7)  WRITE(2,47)
      IF (X .EQ. 4)  WRITE(2,44)
      IF (X .EQ. 5)  WRITE(2,45)
      IF (X .EQ. 6)  WRITE(2,46)
540   C1 = 0.0
550   A1 = 0.5
      A2 = 0.5
551   DO 564  I=2,N
      I1 = I - 1
      DO 564 J = 1, I1
      D(I,J) = 0.0
      DO 556  K1 = 1, M
556   D(I,J) = (A(J,K1) -A(I,K1))**2 + D(I,J)
564   D(I,J) = SQRT(D(I,J))
      DO 574  I=1,N
      K(I) = 1
574   C(I) = I
      K3 = 1
580   D3 = 100000.0
      DO 660  I = 2,N
      I1 = I - 1
      DO 660 J = 1, I1
      IF ( D(I,J) .GE. D3)  GO TO 660
      IF ( K(I) .LE. 0)  GO TO 660
      IF ( K(J) .LE. 0)  GO TO 660
      D3 = D(I,J)
      P = I
      Q = J
660   CONTINUE
      IF (X .LT. 4) GO TO 770
      A3 = (K(P)+K(Q))
```

```
      IF (X .EQ. 6) GO TO 770
      IF (X .EQ. 7) GO TO 736
      A1 = FLOAT(K(P)) /A3
      A2 = FLOAT(K(Q)) /A3
      IF (X .EQ. 5) GO TO 760
      GO TO 740
736   C1 = 0.0
740   B1 = 0.0
      GO TO  770
760   B1 =  -A1*A2
770   DO 900  I=1,N
      IF (K(I) .LE. 0) GO TO 900
      IF (I .EQ. P) GO TO 900
      IF (I .EQ. Q) GO TO 900
      IF (X .NE. 6) GO TO 850
      A1 = FLOAT(K(I) + K(P))/(K(I)+A3)
      A2 = FLOAT(K(I) + K(Q))/(K(I)+A3)
      B1 = -FLOAT(K(I))/(K(I) + K(P) + K(Q))
850   IF (I .LT. P) GO TO 880
      D(I,P) = A1*D(I,P)+A2*D(I,Q) + B1*D(P,Q) + C1*ABS(D(I,P)-D(I,Q
      GO TO 900
880   IF (I .GT. Q) GO TO 894
      D(P,I) = A1*D(P,I)+A2*D(Q,I) + B1*D(P,Q) + C1*ABS(D(P,I)-D(Q,I
      GO TO 900
894   D(P,I) = A1*D(P,I)+A2*D(I,Q) + B1*D(P,Q) + C1*ABS(D(P,I)-D(I,Q
900   CONTINUE
      K(P) = K(P) + K(Q)
      K(Q) = 0
      PP(K3) = P
      QQ(K3) = Q
      DD(K3) = D3
      DO 940 I = 1, N
940   IF (C(I) .EQ. Q)  C(I) = P
      WRITE(2,990)  D3
      IF ( K3 .EQ. N-1 ) GOTO 1
      WRITE(2,1011)
      WRITE(2,1010)  (I,  I = 1, N)
      WRITE(2,1012)
      WRITE(2,1010)  (C(I),  I = 1,N)
      WRITE(2,1013)
      K3 =K3 + 1
      GO TO 580
    1 CALL DENDRAW(PP,QQ,DD,N)
      GOTO 320
1200  STOP
40    FORMAT(1H1,20HFLEXIBLE METHOD A1=,F6.3,3HA2=,F6.3,3HB1=,F6.3)
41    FORMAT(1H1,17HNEAREST NEIGHBOUR)
42    FORMAT(1H1,18HFURTHEST NEIGHBOUR)
43    FORMAT(1H1,6HMEDIAN)
44    FORMAT(1H1,13HGROUP AVERAGE)
45    FORMAT(1H1,8HCENTROID)
46    FORMAT(1H1,12HWARDS METHOD)
47    FORMAT(1H1,16HWEIGHTED AVERAGE)
52    FORMAT(I2)
53    FORMAT(F8.4)
898   FORMAT(10A8)
899   FORMAT(1H1,10A8)
901   FORMAT(2I3)
904   FORMAT(1H ,8HRAW DATA)
905   FORMAT(1H ,12F6.2)
906   FORMAT(I2)
907   FORMAT(1H1,15HNORMALISED DATA )
990   FORMAT(1H ,29HRISE IN OBJECTIVE FUNCTION = , F8.3)
1010  FORMAT(1H ,40I3)
1011  FORMAT(1H ,11HOBSERVATION)
1012  FORMAT(1H ,7HCLUSTER)
1013  FORMAT(1H ,50H**********************************************
4704  FORMAT(2F4.0)
      END
```

```
      SUBROUTINE DENDRAW(PP,QQ,DD,N)
      DIMENSION DD(1), L(34), LP(121), ID(34), LI(34), DX(34), DY(10
      INTEGER PP(1), QQ(1), C(34), P, Q
      DO 1 I = 1, N
      L(I) = I
      C(I) = I
    1 CONTINUE
      DO 17 I = 1, 121
   17 LP(I) = 1H
      N1 = N - 1
      DO 8 I = 1, N1
      P = PP(I)
      Q = QQ(I)
      M2 = 0
      DO 2 J = 1, N
      IF ( C(J) .NE. P ) GOTO 2
      M1 = L(J)
      IF ( M1 .GT. M2 ) M2 = M1
    2 CONTINUE
    3 M3 = 0
      DO 4 J = 1, N
      IF ( C(J) .NE. Q ) GOTO 4
      M1 = L(J)
      IF ( M1 .LE. M3 ) GOTO 4
      M3 = M1
      K = J
    4 CONTINUE
      IF ( M3 .EQ. 0 ) GOTO 8
      C(K) = P
      DO 7 J = 1, N
      IF ( L(J) .GT. M2 ) GOTO 7
      IF ( L(J)-M3 ) 7, 5, 6
    5 L(J) = M2
      GOTO 7
    6 L(J) = L(J) - 1
    7 CONTINUE
      GOTO 3
    8 CONTINUE
      READ 100, ( ID(I), I=1,N )
      PRINT 101
      DO 9 I = 1, N
    9 LI(L(I)) = I
      DO 10 I = 1, N
      DX(I) = 0.0
   10 C(I) = I
      DO 16 I = 1, N1
      P = PP(I)
      Q = QQ(I)
      DO 12 J = 1, N
   12 IF ( C(J) .EQ. Q ) C(J) = P
```

```
      DO 16 J = 1, N1
      K = LI(J)
      IF ( DX(J) .NE. 0.0 ) GOTO 16
      IF ( C(K) .NE. P ) GOTO 16
      M2 = J + 1
      DO 11 M1 = M2, N
      IF ( C(LI(M1)) .NE. P ) GOTO 11
      DX(J) = DD(I)
      GOTO 16
   11 CONTINUE
   16 CONTINUE
      DX(N) = DD(N1)
      SCALE = DX(N) / 120.0
      DO 15 I = 1, N
      J = INT(DX(I)/SCALE) + 1
      DO 13 K = 1, J
   13 LP(K) = 1H-
      PRINT 104, ID(LI(I)), LP
      DO 14 K = 1, J
   14 LP(K) = 1H
      LP(J) = 1H1
      IF ( I .NE. N ) PRINT 105, LP
   15 CONTINUE
      DY(1) = SCALE * 12.0
      DO 18 I = 2, 10
   18 DY(I) = DY(I-1) + DY(1)
      PRINT 102, DY
      RETURN
  100 FORMAT(40A2)
  101 FORMAT(*1*)
  102 FORMAT(8X,10(6X,F6.1))
  104 FORMAT(3X,A2,* 1*121A1)
  105 FORMAT(6X*1*121A1)
      END
```

Fast program for the extended flexible method. See pages 157-164.

```
      DIMENSION D(5000),A(100,6),K(100),C(100),TI(10)
      INTEGER  P, Q, C
      READ(3,898) (TI(I), I = 1, 10)
      WRITE(4,899) (TI(I), I = 1, 10)
      N = 100
      M = 6
      DO 100  I = 1, N
      READ(3,2004)  (A(I,J), J = 1, M)
100   WRITE(4,997)  (A(I,J), J = 1, M)
320   READ(3,53)  A1, B1
      WRITE(4,40)  A1,A1,B1
      IJK = 1
      DO 564  I=2,N
      DO 564  J=1,I-1
      D(IJK) = 0.0
      DO 563  K1 = 1, M
563   D(IJK) = (A(J,K1) -A(I,K1))**2 + D(IJK)
564   IJK = IJK + 1
      DO 574  I=1,N
      K(I) = 1
574   C(I) = I
      K3 = 1
580   D3 = 100000.0
      IJK = 1
      DO 660  I = 2,N
      DO 660  J = 1,I-1
      IF ( K(I) .LE. 0)  GO TO 660
      IF ( D(IJK) .GE. D3)  GO TO 660
      IF ( K(J) .LE. 0)  GO TO 660
      D3 = D(IJK)
      P = I
      Q = J
660   IJK = IJK + 1
      MAP = ((P-1)*(P-2) + 0.5)/2.0
      MAQ = ((Q-1)*(Q-2) + 0.5)/2.0
      IPQ = MAP + Q
      DO 900  I=1,N
      IF (K(I) .LE. 0) GO TO 900
      IF (I .EQ. Q) GO TO 900
      MAI = ((I-1)*(I-2) + 0.5)/2.0
      IF (I-P) 880,900,850
850   IJP = MAI + P
      IJQ = MAI + Q
      D(IJP) = A1*D(IJP)+A1*D(IJQ) + B1*D(IPQ)
      GO TO 900
880   IF (I .GT. Q) GO TO 894
      IPJ = MAP + I
      IQJ = MAQ + I
      D(IPJ) = A1*D(IPJ)+A1*D(IQJ) + B1*D(IPQ)
      GO TO  900
894   IPJ = MAP + I
      IJQ = MAI + Q
      D(IPJ) = A1*D(IPJ)+A1*D(IJQ) + B1*D(IPQ)
900   CONTINUE
```

```
      K(Q) = 0
      DO 940  I=1, N
940   IF (C(I) .EQ. Q)  C(I) = P
      WRITE(4,990)  D3
      IF (K3 .EQ.  N-1)  GO TO 1200
      WRITE(4,1011)
      WRITE(4,1010)  (I,  I = 1, N)
      WRITE(4,1012)
      WRITE(4,1010)  (C(I),  I = 1,N)
      WRITE(4,1013)
      K3 =K3 + 1
      GOTO 580
1200  STOP
40    FORMAT(1H1,20HFLEXIBLE METHOD  A1=,F6.3,3HA2=,F6.3,3HB1=,F6.3
53    FORMAT(2F7.3)
898   FORMAT(10A8)
899   FORMAT(1H1,10A8)
990   FORMAT(1H ,29HRISE IN OBJECTIVE FUNCTION = , F8.3)
997   FORMAT(1H ,10F9.3)
1010  FORMAT(1H ,40I3)
1011  FORMAT(1H ,11HOBSERVATION)
1012  FORMAT(1H ,7HCLUSTER)
1013  FORMAT(1H ,50H**********
2004  FORMAT(6X,6F5.2)
      END
```

Program for the condensation method explained on pages 196-201.

```
      DIMENSION  A(100,6),B(100,6),D(100,100),NC(100),TI(10)
C=============================================================
C====READ IN DATA
      WRITE(2,1010)
      READ(1,1020)  (TI(I), I = 1, 10)
      WRITE(2,1030)  (TI(I),  I = 1,10)
      READ(1,1040)  N,M
      DO 100  I = 1, N
      READ(1,1050)  (A(I,J), J = 1, M)
100   WRITE(2,1060)  (A(I,J), J = 1, M)
      READ(1,1090)  SMALL, SPEED, BOT
1090  FORMAT(3F6.3)
      WRITE(2,1070) SMALL, SPEED, BOT
C=============================================================
C====NORMALIZE DATA BY AVERAGE INTERPOINT DISTANCE /
      DSO = 0.0
      N1 = N - 1
      DO 260 I = 1, N1
      I1 = I + 1
      DO 260  J = I1, N
      D(I,J) = 0.0
      DO 250 K = 1, M
250   D(I,J) = (A(I,K)-A(J,K))**2 + D(I,J)
      D(I,J) = SQRT(D(I,J))
260   DSO = D(I,J) + DSO
      DSO = 2*DSO/(N*(N-1))
      DO 270 I = 1, N
      NC(I) = 0
      DO 270 J = 1, M
270   A(I,J) = A(I,J)/DSO
      NTZ = 0
      NIX = 1
280   NTZ = NTZ + 1
C=============================================================
C====ARE  ANY  POINTS SO CLOSE AS THEY CAN BE AMALGAMATED
      DO 305  I = 1, N1
      IF (NC(I) .EQ. 1)  GO TO 305
      I1 = I + 1
      DO 300  J = I1, N
      IF (NC(J) .EQ. 1)  GO TO  300
      D(I,J) = 0.0
      DO 290  K = 1, M
290   D(I,J) = (A(I,K) - A(J,K))**2 + D(I,J)
      D(I,J) = SQRT(D(I,J))
      IF (D(I,J) .GT. SMALL)  GO TO 300
      NC(J) = 1
      NIX = NIX + 1
      WRITE(2,1080)  I,J,NTZ
300   CONTINUE
305   CONTINUE
      IF (NIX .EQ. N)  GOTO 1000
C=============================================================
C====FIND THE FORCE IN EACH DIRECTION AND MOVE EACH POINT
      DO 340  I = 1, N
      IF (NC(I) .EQ. 1)  GO TO 340
      DO 335  J = 1, M
```

```
      Z = 0.0
      DO 330  K = 1, N
      IF (NC(K) .EQ. 1)  GO TO 330
      IF (I - K)  310,330,320
310   Z = (A(I,J)-A(K,J))/((D(I,K)+BOT)**3)   +  Z
      GO TO 330
320   Z = (A(I,J)-A(K,J))/((D(K,I)+BOT)**3)   +  Z
330   CONTINUE
335   B(I,J) = A(I,J) - SPEED*Z
340   CONTINUE
      DO 350  I = 1, N
      DO 350  J = 1, M
350   A(I,J) = B(I,J)
      GO TO 280
1000  STOP
C=============================================================
1010  FORMAT(1H1,23HTHE CONDENSATION METHOD/)
1020  FORMAT(10A8)
1030  FORMAT(1H ,10A8)
1040  FORMAT(2I3)
1050  FORMAT(6X,6F5.2)
1060  FORMAT(1H ,12F6.2)
1070  FORMAT(1H1,6HSMALL=,F6.3,9H  SPEED =,F6.3,7H  BOT =,F6.3/)
1080  FORMAT(1H ,I3,4H AND,I3,19H JOIN AT ITERATION ,I4)
      END
```

Program to perform the neighbourhood relocation method.

See pages 186-187.

```
      DIMENSION A(34,34),B(34,34),C(34),ND(34),U(34),TI(10),Z2(34),
     1 DA(34)
      INTEGER U,C,P1,P2,Z2
C=====================================================================
C====READ IN DATA
      WRITE(2,119)  KIP
      READ(1,898)  (TI(I), I = 1, 10)
      WRITE(2,899)  (TI(I),  I = 1,10)
      READ(1,101)  N, M
      WRITE(2,904)
      DO 120  I = 1, N
      READ(1,102)  (A(I,J), J = 1,M)
120   WRITE(2,905)  (A(I,J), J = 1, M)
      KIP = 3
      DO 190  I = 1,N
      U(I) = 1
      C(I) =I
      DO 190  J = 1,M
190   B(I,J) = A(I,J)
      N3 = N

C=====================================================================
C====JOIN NEAREST TWO CLUSTERS
400   SM1 = 1000000.0
      DO 550  I = 1, N-1
      IF (U(I))  550,550,430
430   DO 550  K = I+1,  N
      IF (U(K)) 550,550,450
450   S3 = 0.0
      DO 470  J = 1, M
470   S3 = (B(I,J) - B(K,J))**2 + S3
      IF (S3 - SM1)  510,550,550
510   P1 = I
      P2 = K
      SM1 = S3
550   CONTINUE
      WRITE(2,116) P1, P2
      U(P2) = 0
      N3 = N3 -1
      NZ1 = C(P1)
      NZ2 = C(P2)
      DO  810  I = 1, N
810   IF (C(I) .EQ. NZ2) C(I) = NZ1
C=====================================================================
      NCOD = 1
1000  NP = 0
      TWIT = 0.0
      SUMAV = 0.0
      DO 1405  I4 = 1, N
      DO 1200  I = 1, N
      IF  (I .EQ. I4)  GO TO 1200
      IF (C(I) .EQ. C(I4))  GO TO 1210
1200  CONTINUE
      GO TO 1405
1210  DO 1290   I = 1, N
1290  Z2(I) = 0
      COST = 0
      DAB = 1000000.0
      DAX = 1000000.0
      DO 1400  I = 1, N
      IF  (I4 .EQ. I)  GO TO 1400
    0 IF  (Z2(I) .EQ. 1)GO TO 1400
```

```
      DAV = 0.0
      NUMB = 0
      DO 1320 K = 1, N
      IF (I4 .EQ. K )  GO TO 1320
      IF (C(I) .NE. C(K))  GO TO 1320
      NUMB = NUMB + 1
      Z2(K) = 2
1320  CONTINUE
      IF (NUMB .GT. KIP)  GO TO 1350
C=====================================================
      DO 1340  K = 1, N
      IF (Z2(K) .NE. 2)  GO TO 1340
      Z2(K) = 1
      DAW =0.0
      DO 1330  J1 = 1, M
1330  DAW = (A(I4,J1) - A(K,J1))**2 + DAW
      DAV = SQRT(DAW) + DAV
1340  CONTINUE
      DAV = DAV/NUMB
C=====================================================
      GO TO 1392
1350  NL = 1
      DO 1370  K = 1, N
      IF (Z2(K) .NE. 2)  GO TO 1370
      Z2(K) = 1
      DA(NL) = 0.0
      DO 1360  J1 = 1, M
1360  DA(NL) = (A(I4,J1)-A(K,J1))**2 + DA(NL)
      NL = NL + 1
1370  CONTINUE
1373  NSOX = 0
      DO 1375  J3 = 1, NL-2
      IF (DA(J3) .LE. DA(J3+1))  GO TO 1375
      NSOX = 1
      TEM = DA(J3)
      DA(J3) = DA(J3+1)
      DA(J3+1) = TEM
1375  CONTINUE
      IF (NSOX .EQ. 1)  GO TO 1373
      DO 1380  J3 = 1, KIP
1380  DAV = SQRT(DA(J3)) + DAV
      DAV = DAV/KIP
1392  TWIT = TWIT + DAV
      IF  (C(I) .EQ. C(I4))  GO TO 1394
      IF (DAV .LT. DAX)  DAX = DAV
1394  IF (DAV - DAB)  1395,1400,1400
1395  DAB = DAV
      NCOST = C(I)
1400  CONTINUE
      IF (NCOST .EQ. C(I4))  GO TO 1403
      C(I4) = NCOST
      NP = 1
1403  SUMAV = DAX + SUMAV
1405  CONTINUE
      NCOD = NCOD + 1
      IF (NCOD .EQ.  8)  GO TO 1410
      IF (NP .EQ. 1)  GO TO 1000
```

```
C==========================================================
C====CALCULATE CLUSTER CENTRES
1410  DO 1420  I = 1,  N
      ND(I) = 0
      U(I) = 0
      DO 1420  J = 1,M
1420  B(I,J) = 0.0
      SUMP = 0.0
      DO 1600 I = 1, N
      NQ7 = 0
      IF (ND(I) .EQ. 1)  GO TO 1600
      DO 1550  K = 1, N
      IF (ND(K) .EQ. 1)  GO TO 1550
      IF (C(I) .NE. C(K))  GO TO 1550
      NQ7 = NQ7 + 1
      DO 1530  J = 1, M
1530  B(I,J) = A(K,J) + B(I,J)
      ND(K) = 1
1550  CONTINUE
      DO 1580  J = 1,M
1580  B(I,J) = B(I,J)/NQ7
      U(I) = NQ7
1600  CONTINUE
C==========================================================
C====OUTPUT RESULTS
      WRITE(2,103)  N3, SUMAV
      WRITE(2,104)
      WRITE(2,115) (I,  I = 1, N)
      WRITE(2,106)
      WRITE(2,115)  (C(I),  I = 1, N)
      WRITE(2,112)
      IF (N3-1)  1760,1760,400
C==========================================================
1760  STOP
101   FORMAT(2I3)
102   FORMAT(8F5.2)
103   FORMAT(1H ,I5,15H CLUSTER RESULT,8X,23HRESIDUAL SUM OF SQUARES,
     14)
104   FORMAT(1H ,11HOBSERVATION)
106   FORMAT(1H ,7HCLUSTER)
112   FORMAT(1H ,100H**********************************************************
     1**********************************  )
115   FORMAT(1H ,30I4)
116   FORMAT(1H ,I3,3HAND,I3,11HHAVE JOINED)
119   FORMAT(1H1,25HNEWPORTS METHOD  WITH K =, I2)
898   FORMAT(10A8)
899   FORMAT(1H ,10A8)
904   FORMAT(1H ,8HRAW DATA)
905   FORMAT(1H ,12F6.2)
906   FORMAT(I2)
      END
```

Program to minimize the loss function $\sum (\frac{D - d}{D})^2$ referred to on page 353.

```
      DIMENSION D(36,36),E(36,36),G(2,36),X(2,36),Y(2,36),TI(10)
C*****************************************************************
C     READ  IN  DATA
      READ(1,1000)  (TI(I),  I = 1,10)
      WRITE(2,1001)  (TI(I),  I = 1,10)
      NDIM = 2
      09 = 0.1
      MOUNT = 0
      READ(1,40) N,M
131   DO 110  I = 1, N
      READ(1,904)  (E(I,J), J = 1, M)
110   WRITE(2,940)  (E(I,J),  J = 1,M)
C*****************************************************************
C     CALCULATE DISTANCE MATRIX
      DO 152  I = 1, N-1
      DO 152  J = I+1, N
      D(I,J) = 0.0
      DO 151  K = 1, M
151   D(I,J) = (E(I,K) - E(J,K))**2 + D(I,J)
152   D(I,J) = SQRT(D(I,J))
      DO 160  I = 1, N
160   WRITE(2,940)  (D(I,J), J = 1,N)
      DO 172 K = 1, NDIM
172   READ(1,42)  (X(K,I),  I = 1, N)
C*****************************************************************
C     CALCULATE DISTANCES IN NEW  DIMENSIONALITY
175   DO 240  I = 1,N-1
      DO 240  J = I+1,N
      E(I,J) = 0.0
      DO 230  K = 1, NDIM
230   E(I,J) = (X(K,I) - X(K,J))**2 + E(I,J)
      E(I,J) = SQRT(E(I,J))
240   E(I,J) = ((D(I,J)/E(I,J))-1)/(D(I,I)**2)
C*****************************************************************
C     CALCULATE THE GRADIENT
      DO 450 NS = 1, NDIM
      T5 = 0.0
      DO 430  K = 1,N
      G(NS,K) = 0.0
      DO 400  I = 1,N
      IF (K .GT. I) GO TO 390
      G(NS,K) = (X(NS,K)-X(NS,I))* E(K,I) + G(NS,K)
      GO TO 400
390   G(NS,K) = (X(NS,K)-X(NS,I))* E(I,K) + G(NS,K)
400   CONTINUE
      G(NS,K) = 2*G(NS,k)- T5
430   T5 = G(NS,1)
450   G(NS,1) = 0.0
      MOUNT = MOUNT + 1
C*****************************************************************
C     CALCULATE  GRADIENT  SUM  OF  SQUARES
      SUMSQ = 0.0
      DO 475 NS = 1, NDIM
      DO 475  K = 1, N
475   SUMSQ = G(NS,K)**2 + SUMSQ
      WRITE(2,476)  SUMSQ
```

```
C*****************************************************************
C     ITERATE TO FIND NEW VALUE OF FUNCTION
      WRITE(2,489) MOUNT
      ITER = 1
      F2 = 1.0E12
      TL = 09
510   DO 560 NS= 1, NDIM
      DO 560  I= 1,N
560   Y(NS,I) = X(NS,I)+TL*G(NS,I)
      F = 0.0
      DO 700 NP= 1,N-1
      DO 700 NQ= NP+1,N
      F8 = 0.0
      DO 699 NS = 1, NDIM
699   F8 = (Y(NS,NP) - Y(NS,NQ))**2 + F8
700   F = ((SQRT(F8)/D(NP,NQ))-1)**2 + F
      IF (F .GT.F2) GO TO 785
      F2 = F
      WRITE(2,760)   TL,   F
      TL = TL+09
      ITER = ITER + 1
      GO TO 510
785   TL = TL - 09
      F7 = 200.0*F/(N*(N-1))
      F7 = SQRT(F7)
      WRITE(2,902)  F7
C*****************************************************************
C     PRINT OUT NEW VECTORS
      DO 890 NS=1, NDIM
      DO 880  I=1,N
880   X(NS,I) = X(NS,I)+TL*G(NS,I)
890   WRITE(2,940)  (X(NS,I),I=1,N)
      IF  (ITER .LT.  4)  09 = 09/10
      IF  (ITER .GT. 30)  09 = 09*5.
      IF (MOUNT .LT.100)  GO TO 175
C*****************************************************************
      STOP
40    FORMAT(2I3)
42    FORMAT(26F3.0)
476   FORMAT(1H ,26HSUM OF SQUARES OF GRADIENT,F11.5)
489   FORMAT(1H0,9HITERATION,I5)
760   FORMAT(1H , 8HLAMDA = ,F7.5,11H       F  = ,F11.4)
902   FORMAT(1H ,8HSTRESS =, F8.4)
904   FORMAT(20F3.0)
940   FORMAT(1H0,10F10.4)
1000  FORMAT(10A8)
1001  FORMAT(1H ,10A8)
      END
```

APPENDIX II

DATA FOR 'R' CONFIGURATION

USED ON PAGES 372/3

1	1.00	10.00
2	1.00	7.90
3	1.00	5.45
4	1.00	3.55
5	1.00	1.89
6	2.19	10.00
7	4.45	10.00
8	2.58	5.40
9	5.13	5.62
10	6.70	9.11
11	5.40	4.93
12	8.16	6.98
13	7.14	5.65
14	6.65	3.36
15	8.13	1.54

DATA FOR CIRCLE CONFIGURATION

ANALYSED ON PAGES 372, 374-376

1	-10.36	0.60	0.49
2	-8.65	5.57	0.02
3	-6.98	6.76	-0.06
4	-3.70	10.34	0.12
5	-9.12	-3.84	-0.25
6	-6.86	-6.19	0.88
7	-8.30	-5.48	0.49
8	0.01	9.73	-0.37
9	4.25	8.76	0.63
10	5.48	7.35	0.26
11	7.11	-6.20	1.00
12	8.54	-3.62	0.12
13	6.12	-8.05	-0.68
14	2.13	-9.00	-0.01
15	-1.46	-9.06	-0.18
16	9.08	4.10	-0.13
17	8.04	-0.03	0.80
18	1.62	0.01	0.45
19	-1.77	-0.48	-0.28
20	-6.68	-0.09	-0.20
21	-0.60	2.90	-0.46
22	0.60	5.81	-0.67
23	0.36	-0.31	-0.15
24	-0.69	-1.36	-0.06
25	0.33	-5.28	0.38

DATA FOR TUBE STATION EXAMPLE

| | | |

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