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MULTIDIMENSIONAL SCALING

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Introduction

The analysis of proximity data by means of multidimensional scaling (MDS) is playing an increasingly important role in several fields of psychology. Nevertheless, as pointed out by Ramsay (1978), there are two factors which still appear to counteract a more extensive use of this technique. One factor is the lack of easily available software packages which can be implemented as computer programs. Another factor is that only a limited number of psychologists so far have been exposed to the basic concepts of MDS. The purpose of this paper is to provide such an exposition.

MDS is for some purposes an important alternative to other multivariate techniques such as factor analysis and cluster analysis. Sometimes MDS should definitely be preferred for reasons related to procedures, mathematical underpinnings, and interpretations of the results (cf. Ramsay, 1978; Schiffman, Reynolds & Young, 1981). In other cases it may be used in conjunction with other techniques.

MDS is basically a method for analyzing proximity data. It can be thought of as a procedure for converting proximity data into multivariate data (Kurskal, 1977, p. 21). Although a proximity refers to any variable for measuring closeness or distance between stimuli (similarities, dissimilarities, correlations, overlap measures, and so forth), we will for simplicity only refer to dissimilarities in the following pages.

In the simplest kind of MDS, an analogy between the psychological concept of dissimilarity and the geometrical concept of distance is assumed. A stimulus is represented by a point x_i in space, and a dissimilarity δ_{ij} by the distance between the points x_i and x_j. Formally,

$$\delta_{ij} = d(x_i, x_j) + \text{error} \qquad (1).$$

Thus, the central thing about MDS is that it takes a matrix of dissimilarities as input and yields a configuration of points as output (Kruskal, 1977, p. 28) so that large dissimilarities between stimuli will be represented by large distances between points and small dissimilarities between stimuli by small distances between points.

When a researcher decides to apply MDS he should consider four main aspects:

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(1) What kind of dissimilarity data to collect?
(2) What model to choose?
(3) What computer program to run?
(4) How to interpret the final configuration?

Below we try to aid a researcher not already familiar with MDS to make decisions in these respects. Some final comments are made on the relationship between MDS and factor analysis and between MDS and cluster analysis.

Theory of data

In order to provide a basis for deciding on which kind of dissimilarity data to collect, we expose in this section some aspects of the theory of data underlying MDS (Coombs, 1964; Carroll & Arabie, 1980). Five major aspects should be considered relative to dissimilarity data:

(1) Shape of the input matrix;
(2) Number of ways;
(3) Number of modes;
(4) Scale of measurement;
(5) Measurement conditionality.

As regard shape, the input matrix can be square or rectangular. In a square matrix both the rows and the columns are stimuli. A cell represents the dissimilarity δ_{ij} between stimuli i and j. In addition, a square matrix can be symetric ($\delta_{ij} = \delta_{ji}$) or asymetric ($\delta_{ij} \neq \delta_{ji}$). In a rectangular matrix most often the rows are stimuli and the columns attributes. Each cell represents the measure v_{ij} obtained for the stimulus i on the attribute j. The attributes may be rating scales and the distances between rows are computed so that they can be interpreted as dissimilarities between stimuli. In Figure 1 both a square and a rectangular matrix are shown.

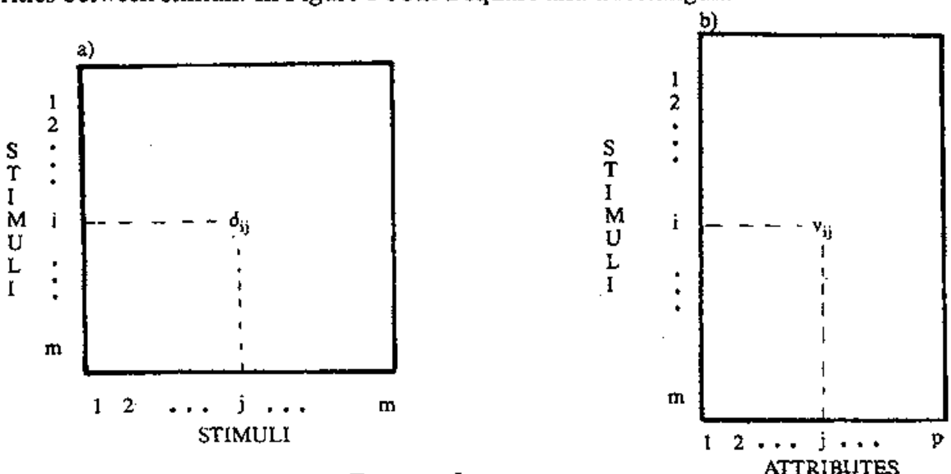

FIGURE 1. INPUT MATRIX.

Regarding number of ways, the input data are usually two-way or three-way, although higher-order ways may also be used. If only one matrix is input, data are referred to as two-way (the ways correspond to the arrangement of the matrix, rows X columns). If more than one matrix is input (for example, one matrix per subject), the data are referred to as three-way, where the third way is subjects. A graphical example is shown in Figure 2, where each one of the dissimilarity matrices of *h* subjects are input. The data source is subjects but it could be any other (experimental conditions, occasions, and so forth).

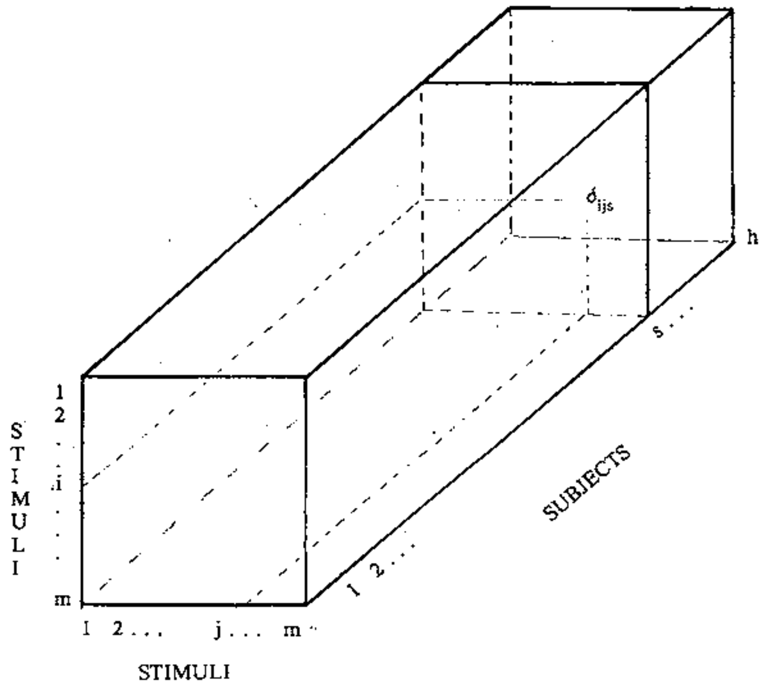

FIGURE 2. TRIDIMENSIONAL REPRESENTATION OF DATA.

The data can also be one-mode, two-mode, three-mode, or higher-order. A mode is defined as a particular class of entities (Carroll & Arabie, 1980, p. 610). In MDS, entities could be stimuli, attributes, subjects, or experimental conditions. A one-mode input data is shown in (a) in Figure 3. Only a class of entity (stimuli) is input. In the same figure, (b) is two-mode because two different classes of entities are input, stimuli and attributes. Finally, a three-mode input data is displayed in (c). The three classes of entities are stimuli, attributes, and subjects.

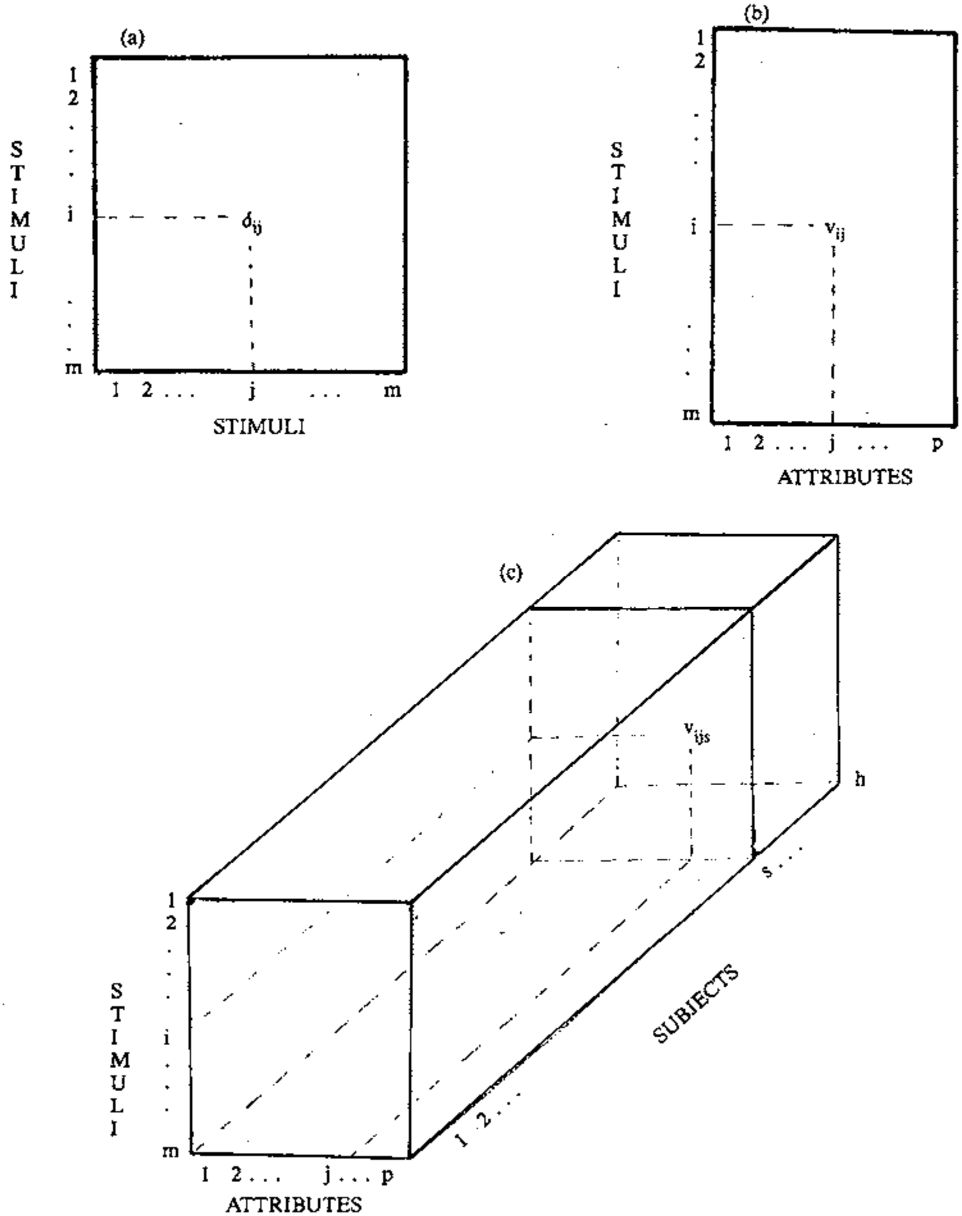

FIGURE 3. DATA INPUT FOR DIFFERENT MODES.

Antoher important question is what scale of measurement is assumed. The four scales which usually are identified are nominal, ordinal, interval, and ratio. If one of the first two is assumed, it is the nonmetric case, whereas if is assumed one of the last two, it is the metric case. The metric case is in general more desirable because the solution is more precise and the computer time is usually less. However the empirical data do not always meet the necessary conditions.

Finally, another measurement aspect is called the conditionality. One can assume that two different subjects use different subjective scales when they judge the dissimilarity within a set of stimuli. If this assumption is made for all subjects, the responses between subjects cannot be compared with each other and the data are referred to as matrix conditional. On the other hand, one could assume the subjective measures can be compared. Under this assumption, data are referred to as unconditional. In addition, it is also possible with asymetric or rectangular matrices to assume that only the elements within a row can be compared. These data would then be referred to as row conditional.

Multidimensional scaling models

Even though the history of MDS is not long, the number of models developed is extensive. Only four basic models of MDS can be chosen to be dealt with here, namely.

(1) Classical metric model (Torgerson, 1958);
(2) Classical nonmetric model (Shepard, 1962; Kruskal, 1964a, 1964b);
(3) INDSCAL model (Carroll & Chang, 1970);
(4) Power metric model (Ramsey, 1977).

All of this models will throughout be evaluated from an application point of view according to six different characteristics: the input, the model itself, the algorithm, the output, the main advantages, and the main limitations. A more extensive treatment of these models is provided by Arce, Seoane, and Varela (1988).

Classical metric model

Input

The input matrix is square and symmetric. The data are one-mode two-way, and the scale of measurement required is interval.

Model

The relationship between dissimilarities and distances is assumed to be linear. Formally,

$$\delta_{ij} = f(d_{ij}) = f\left[[\sum_{k=1}^{n} (x_{ik} - x_{jk})^2]^{1/2}\right] \quad (2),$$

where f is a linear function with positive slope; δ_{ij} and d_{ij} are the dissimilarities and the distances between stimuli i and j, respectively; x_{ik} and x_{jk} are the coordinates of the stimuli i and j on dimension k, respectively, and n is the total number of dimensions.

Algorithm

First, the additive constant is estimated, that is, the dissimilarities (assumed to be at an interval scale) are converted into absolute distances (ratio scale). Secondly, the absolute distances are converted into scalar products. Finally, the coordinates of the stimuli are estimated by principal component analysis (or other factoring techniques).

Output

The output is a rectangular matrix of stimuli coordinates. The rows are stimuli, the columns are dimensions. Each cell x_{ik} is the coordinate of the stimulus i on dimension k (Figure 4). Therefore, from this matrix one can plot a (Euclidean) spatial representation of the data in n dimensions. The dimensions are rotatable, that is, they can be rotated in any arbitrary orientation.

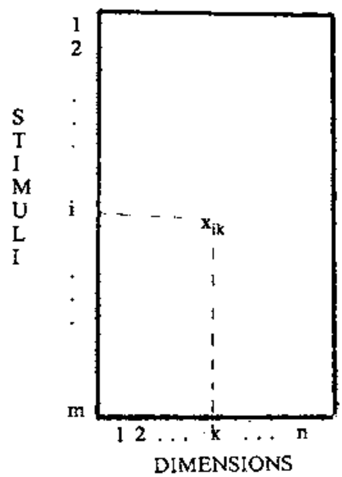

FIGURE 4. TIPICAL OUTPUT OF MULTIDIMENSIONAL SCALING.

Advantages

The main advantages are the relatively precise solution and the very little computer time consumed by the algorithm.

Limitations

The main limitations are (1) that only one symetric matrix is allowed as input, and (2) that the interval scale condition may not always be met in the data.

Classical nonmetric model

Input

The input matrix is square and symmetric. The data are one-mode two-way, and the scale of measurement required is ordinal.

Model

The relationship between dissimilarities and distances is assumed to be monotonic. Formally,

$$\delta_{ij} = f(d_{ij}) = f\Big[[\sum_{k=1}^{n} |x_{ik} - x_{jk}|^{p}]^{1/p}\Big] \quad (3),$$

where f is a monotonic function such that

$$d_{ij} < d_{i'j'} \Rightarrow f(d_{ij}) < f(d_{i'j'}) \text{ for all } i,j,i',j' \quad (4).$$

Algorithm

First, stimuli are randomly represented in a plane or in space. The distances between points are computed and monotonically transformed into disparities (distances which preserve the raw data order). A stress function for measuring the fit between distances and disparities is defined. Then, an iterative process is run until the stress function has been minimized by the method of steepest descent.

Output

The form of the output is the same as in the classical metric model (Figure 4). The dimensions are again rotatable.

Advantages

The main advantages of this model are (1) the high applicability due to the ordinal scale assumption, and (2) that it allows Minkowski-p metric where in equation 3 $p=2$ (ordinary Euclidean space) and $p=1$ (Manhattan or city-block metric) are special cases.

Limitations

The main limitations are (1) that only one symmetric matrix is allowed as input, and (2) that there is a risk of suboptimal solutions, that is, local minima. A local minimun is defined as a minimum of the stress function from which no small movement is an improvement (Kruskal, 1964b, p. 118). But a local minumum may or may not be an overall minimum. If it is not, a suboptimal solution is obtained.

INDSCAL model

Input

The input matrix is square and symmetric. The data are two-mode three-way, matrix conditional, and the scale of measurement is interval.

Model

The relationship between dissimilarities and distances is assumed to be linear, with a different linear function allowed for each subject (or other data sources). Formally,

$$\delta_{ijs} = f(d_{ijs}) = f\Big[\big[\sum_{k=1}^{n} w_{sk}(x_{ik} - x_{jk})^2\big]^{1/2}\Big] \qquad (5),$$

where f is a linear function with positive slope; δ_{ijs} and d_{ijs} are the dissimilarities and the distances between stimuli i and j for subject s, respectively, and w_{sk} is the weight of the dimension k for subject s. Thus, this model can be thought of as a generalization of the classical metric model by substituting a weighted Euclidean metric.

Algorithm

First, dissimilarities are converted into scalar products in a three-way manner (i.e. by applying the additive constant and the transformation for each subject). Then, the INDSCAL model is written in scalar products form and it is considered as a special case of the three-way CANDECOMP (CANonical DECOMPosition) model by imposing some constraints. Finally, a least-squares procedure called NILES (Nonlinear Iterative Least Squares) is iteratively used to arrive at the optimal set of stimulus coordinates and subject space.

Output

The output consists of two rectangular matrices (Figure 5). The first one is called the group stimulus space. The rows are stimuli and the columns are dimensions. Each cell x_{ik} represents the coordinate k for the stimuli i. This space is assumed to be common for all the subjects. The second matrix is called the subject space. The rows are subjects, columns are dimensions. Each cell represents the coordinate k for the subject s.

Advantages

The main advantages of this model could be summarized as follows. First, the model allows systematic differences between subjects and secondly, this model has the dimensional uniqueness property, that is, the solution is unique, unrotatable. As a consequence, the dimensions or coordinate axes play a strong role for the interpretation of the results. They may often be directly interpretable.

Limitations

The main limitations are (1) the symmetry of the input matrices, (2) the interval scale assumption, and (3) the possibility to use only a Euclidean space.

Power metric model

Input

The input matrix is square (symmetric or asymmetric). The data are two-mode three-way (although the model also works as two-way), matrix conditional, and the scale of measurement assumed for the data is ratio (following the terminology suggested by Carrol & Arabie, 1980).

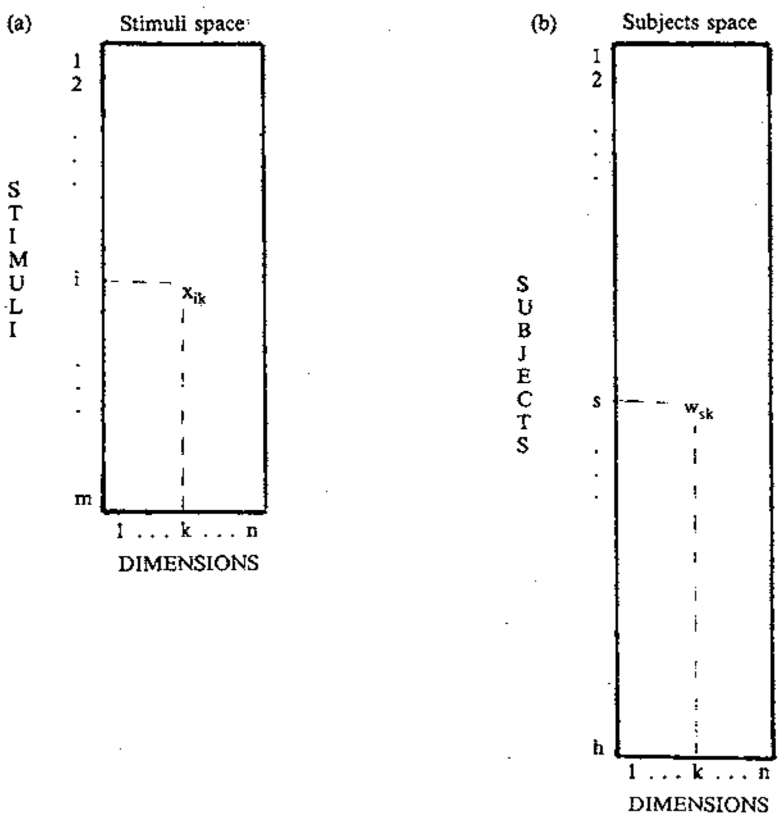

FIGURE 5. INDSCAL MODEL OUTPUT.

Model

The relationship between dissimilarities and distances is assumed to be a power function, with different paramenters for each subject. Formally,

$$\delta_{ijs} = v_s(d_{ijs})^{p_s} = v_s \left[\sum_{k=1}^{n} w_{sk}(x_{ik} - x_{jk})^2\right]^{p_s/2} \quad (6),$$

where v_s and p_s are the regression coefficient (or scaling factor) and the exponent for subject s, respectively.

Algorithm

Several assumptions about the data distribution are made. Then, a log likelihood function is formulated and maximized via an alternating maximun likelihood procedure.

Output

The form of the output is the same as in the INDSCAL model (Figure 5).

Advantages

First, as the main advantage, this model allows confirmatory analysis, in addition to the exploratory analysis allowed by other models. If some asumptions are satisfied, then (a) a test can be applied for comparing different models, groups or dimensionalities, and (b) confidence regions for gauging the relative precision of stimulus coordinates in the spatial representation can be obtained. Secondly, the power function seem to be the most appropiate relationship in certain empirical fields (cf. Gärling, Böök, Lindberg & Arce, 1988).

Limitations

The strong assumptions made such as the independence of the judgments, and the ratio scale dissimilarities are the main limitations of the model.

Some available computer programs for multidimensional scaling

Comparisons between MDS computer programs are provided by Kruskal & Wish (1978), Schiffman et al. (1981) and Arabie, Carrol, & DeSarbo (1987). The name, author and source of some of them is shown in Table 1. All of them have three routines: the initialization routine, the iterative routine, and the termination routine. The main one is the iterative routine, that is, the process of trying over and over again to obtain the best possible solution. The initialization routine provides the way to get the iterations started and the termination routine provides the way to stop the iterations (Schiffman et al., 1981).

TABLE I. SOME AVAILABLE COMPUTER PROGRAMS FOR MULTIDIMENSIONAL SCALING

Name	Author	Source
MINISSA	Lingoes & Roskam	Michigan, Nijmegen
KYST	Kruskal, Young & Seery	Bell Laboratories
POLYCON	Young	Psychometric Laboratory
INDSCAL	Chang & Carroll	Bell Laboratories
SINDSCAL	Pruzansky	Bell Laboratories
MULTISCALE	Ramsey	International Educational Services
ALSCAL	Takane, Young & De Leeuw	Psychometric Laboratories

MINISSA can be considered as the simplest program. The first version was created by Roskam & Lingoes, 1970. Later, Lingoes in Michigan and Roskam in Nijmegen developed two different versions of it. It is capable of carrying out multidimensional scaling by the Shepard-Kruskal nonmetric procedure, although the Guttman's Smallest Space Analysis (SSA) is typically carried out. The major limitation is that it only allows one symmetric matrix as input.

KYST, due to Kruskal, Young, & Seery, and *POLYCON*, due to Young, are very close to each other. Both of them are capable of carrying out either metric or nonmetric procedures. They allow the Minkowski-p metric and more than one (symmetric or asymmetric) matrix as input. However, the matrices are treated as replications, that is, the differences between them are considered as due to random errors. Unlike KYST, POLYCON additionally allows the user: (a) to carry out the power metric model (Ramsey, 1977), (b) to input a target configuration for rotating the final configuration, and (c) to input nominal data.

INDSCAL (Chang & Carroll, 1969), *SINDSCAL* (Pruzansky, 1975), *MULTISCALE* (Ramsey, 1977, 1978) and *ALSCAL* (Takane, Young, & De Leeuw, 1977) are all of them capable of carrying out weighted MDS procedures, that is, procedures where systematic differences between subjects (or other data source) are allowed. INDSCAL, SINDSCAL and MULTISCALE are totally metric. INDSCAL and SINDSCAL were both created for carrying out the INDSCAL model (Carroll & Chang, 1970). SINDSCAL can be thought of as a streamlined version of the INDSCAL program, that is, it was created for reducing the long computer time consumed by INDSCAL. MULTISCALE was created for carrying out the power metric model developed by Ramsay (1977). Unlike INDSCAL and SINDSCAL, it additionaly allows two-way data. A new version called MULTISCALE-II (Ramsey, 1981, 1982, 1983) is now available with new facilities such as the possibility to choose from among several alternatives and distributions (e.g. lognormal, normal and others). Unlike INDSCAL, SINDSCAL, and MULTISCALE, ALSCAL is capable of carrying out both metric and nonmetric procedures. As a major new feature, it provides a nonmetric implementation of the INDSCAL model even with asymmetric matrices as input. Finally, it is important to note that the four programs have a common limitation: they only can yield a Euclidean spatial representation of the data.

Interpretation of the configuration

We will discuss here some ways for interpreting either the final stimulus space or the final subject space.

Without additional information

Sometimes the researcher is not provided with more information than disimilarities. What he or she then could do is mainly as follows.

Stimulus space

First, visual inspection of the configuration looking either for orders of the stimuli along the axes or for meaningful groupings of them. But to elevate subjective groupings to the status of clusters, it is absolutely necessary to apply some clustering technique (Arabie et al., 1987, p. 54). Secondly, if the visual inspection does not lead to a successful interpretation, the researcher still has the possibility to rotate the dimensions. The rotation can be made by hand or by statistical methods (Varimax, Equimax, and so forth). It is known that rotation by hand usually leads to more interpretable axes.

Subject space

Whereas the stimulus space is composed of points, the subject space is composed of vectors. Each subject (or other data source) is represented by a vector. Two different aspects of the vectors should be considered: the length and the direction, the latter being the most important.

The lenght is usually related to the fit of the model. The larger the length the better is the fit for a given subjecte.

The direction is related to the relative salience of the dimensions for a particular subject. The closer the vector is to a given dimension, the more salient it is.

With additional information

Another way of approaching the interpretation problem is to collect additional information about the stimuli and the subjects and then trying to relate it to the solution via some statistical technique.

Stimulus space

Schiffman et al. (1981) summarized three main alternatives:

— Preference analysis (at individual level);

— Property fitting (at group level);

— Canonical correlation analysis (multidimensional properties).

To perform preference analysis it is necessary to have obtained preference ratings of the stimuli from the subjects, in addition to the judged dissimilarities. Then the analysis fits the preference ratings to the stimulus space. As preferences vary widely between individuals, the analysis is mainly interesting at the individual level.

To perform property analysis it is necessary to have measured either objective physical characteristics of the stimuli or subjective judgments of the stimulus characteristics. As it is often reasonable to assume that homogeneous subjects use the same properties, property analysis is usually performed at group level, that is, on ratings averaged over all subjects.

Two different models can also be used to perform both preference and property analysis: (a) the vector model, and (b) the ideal point model. What the vector model does is to find a direction through the stimulus space which corresponds to increasing amounts of the attribute in question (Schiffman et al., 1981).

The statistical tecnique used is multiple regression, thus the multiple correlation coefficient is used to asses how strongly the attribute is related to the stimulus space. On the other hand, the ideal point model finds a point in the stimulus space corresponding to the attribute. In this case, the procedure used to locate the ideal point in the stimulus space is a special kind of multiple regression called optimal multiple regression developed by Carroll (1972), which may be interpreted in the ordinary way with the exception that one should be more conservative in using significance tests.

In addition, both the vector model and the ideal point model can be used in the nonmetric case, that is, when either preferences or properties are measured at ordinal scale (cf. Young, 1984, for references).

There is now available a highly complete program for this purpose, PREFMAP, distributed by Bell Laboratories. The last version is PREFMAP3 and it includes both preference and property analysis, vector and ideal point models, and metric and nonmetric cases.

The statistical techniques already mentioned only fit a single set of preference or property ratings to the stimulus space. However it is not unusual to have many sets. Under such conditions, we could, of course, perform a preference or property analysis separetly for each set but canonical correlation analysis may be a better alternative. Canonical vector analysis is treated in any multivariate statistcs book. A nononmetric version of this type of analysis is also available (cf. Young, 1984, for references). In addition, a first approach to canonical ideal point analysis is made by Schiffman et al. (1981).

Subject space

We assume the researcher has obtained some additional information about the subjects such as, for example, age, sex, and group membership. Then we suppose the resarcher is interesting in knowing if subjects differing in these respects weigh the stimulus space dimensions in a significantly different way. Shiffman et al. (1981) ponted out two main possibilities to investigate the question, ANAVA (Analysis of Angular Variation); and scaling subjects.

ANAVA is a metod for analyzing angular variation and it is part of a new branch of statistics called directional statistics developed mainly by Mardia (1972). As in ANOVA, it is possible to decompose the angular variance into two additive components (within-group and between-group) and under certain conditions the distribution of the ratio of the between to the within mean squares approximates the F distribution.

Scaling subjects is another helpful method for interpreting a subject space. It consists simply of running a classical MDS on a matrix with the distances computed between subject weight vectors, where the intersubject distance d_{ij} is defined as the angle, in radians, between the two vectors. Formally,

$$d_{ij} = \cos^{-1} [\sum_{k=1}^{n} w_{ik} w_{jk}] \tag{7}$$

where d_{ij} is the distance between subjects i and j, and w_{ik} and w_{jk} are the weights of the dimension k for subject i and j, respectively. The output is a configuration of points, but now each point represents a subject. Thus it could be interpreted with using the same methods mentioned for interpreting the stimulus space.

Final comments

The elementary concepts of MDS have been selectively reviewed in the categories (a) the theory of data, (b) basic models, (c) computer programs, and (d) ways of interpreting the results. We hope to have provided some help for investigators to decide on how to apply MDS. Another decision which needs to be made is whether to use MDS instead of some other multivariate technique. Although we cannot cover this issue, in this final section we make some brief comments about the relationship between MDS and factor analysis and between MDS and cluster analysis.

Even though this has not been mentioned above, both MDS and factor analysis can be used to analyze either «direct» dissimilarity data, for instance, dissimilarity ratings (Waern, 1971), or «indirect» dissimilarity data, that is, dissimilarity defined in some way on the basis of attribute measures of the stimuli (Ward & Russell, 1981). In both these applications, the relationship between MDS and factor analysis appears to be competitive. Both techniques uncover an underlying structure in the data and provide a spatial representation, although in different ways. Factor analysis is based on a vector model (i.e. each stimulus is represented by a vector), whereas MDS is based on a distance model (i.e. each stimulus is represented by a point). This may make MDS preferred because it is easier to interpret distances between points than angles between vectors. Several other reasons for preferring MDS over factor analysis have been pointed out. For instance, Schiffman et al. (1981) noted that in MDS, but not in factor analysis, the assumption of linear relationships between the variables needs not be made. The interesting consequence is a solution in fewer dimensions which may be easier to interpret. On the other hand, statistically sounder methods for deciding on number of dimensions have been developed for factor analysis (Jöreskog, 1967, 1981). It should, however, be noted that, under certain circumstances, as Sjöberg (1975) points out, factor analysis has the undesirable property that the number of dimensions may depend on the number of variables included in the analysis. This is not the case with MDS.

Whereas the relationship between MDS and factor analysis has benn thought of as competitive, the relationship between MDS and cluster analysis may be complementary. Holman (1972) has shown the existence of some mathematical incompatibilities between the techniques, but they have nevertheless been empirically employed jointly to uncover complementary aspects of the underlying structure in the data (e.g. Gärling, 1976; Sabucedo & Arce, 1988). This practice was endorsed by Shepard (1972a, 1972b) and Kruskal (1977). Recently, Arabie et al. (1987, p. 53-54) have strongly recommended the conjoint use of MDS and cluster analysis whenever the data permit. Likewise, they strongly advise never to elevate visually detected stimuli groupings to the status of clusters. They feel it is absolutely necessary to apply a clustering technique, taking as input the same dissimilarity matrices as used in MDS. The INDCLUS model and program (Carroll & Arabie, 1983), which can be thought of as the INDSCAL counterpart for cluster analysis, may play an important role for this purpose. It allows more than one matrix as input (e.g. one matrix per subject, one matrix per experimental condition and, so forth), just what three-way MDS models do.

RESUMEN

En la presente investigación se comparan sistemáticamente, y desde un punto de vista aplicado, cuatro modelos centrales para la teoría del escalamiento multidimensional. Además, se consideran algunos aspectos relativos a la teoría de datos, a los programas de ordenador disponibles y a la interpretación formal y no-formal de los resultados. Por último, se discute la relación existente entre escalamiento multidimensional y análisis factorial, y entre escalamiento multidimensional y cluster analysis.

SUMMARY

Four models of multidimensional scaling are compared from an applied point of view. In addition, the underlying theory of data, available computer programs, and formal and informal ways of interpreting the results are discussed. Finally, the relationship between multidimensional scaling and factor analysis and between multidimensional scaling and cluster analysis are examined.

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