Computational Statistics & Data Analysis 18 (1994) 3–13
North-Holland

An introduction to multiway data and thei ınalysis

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Abstract: This paper provides a presentation of the main types of multiway data and the most known methods proposed in the literature. General guidelines are provided concerning the various aspects of statistical information conveyed by different data arrays or sets and the methods of data analysis enabling the researcher to extract this information. The description of the techniques focuses on the different methodological approaches in order to enable the reader to find out links among the methods. Hopefully, this introduction may act as a reference system when utilising a multiway approach to the analysis of statistical data.

Keywords: Multiway analysis; Multilinear models; Three-way arrays.

Multiway data: definitions and notation

In traditional multivariate analysis the "data matrix" is usually defined as a set of "elementary data" x_{ij} $(i = 1, I;\ j = 1, J)$ concerning the values taken by J variables X_j on I statistical units (individuals, areas, etc.). In this case, we are dealing with "two-way data", since each element of the data set is characterised by a pair of indices: i for the mode "units" and j for the mode "variables".

When the "elementary datum" is referred to three or more indices (or ways, or criteria of classification), we get "multiway data". A common example of this type of data is provided by the "three-way array"

$$X = \{x_{ijk}\}, \qquad i = 1, I;\ j = 1, J;\ k = 1, K,$$

where i denotes the "units", j denotes the "variables" and k denotes the "occasions" (different times of observation, different locations, different experi-

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SSDI 0167-9473(94)00003-2

mental conditions, and so on). In this case, the three ways are fully crossed, namely on each occasion the same I units are observed with respect to the same J variables. Moreover, each "way" corresponds to a different "mode" (respectively: units, variables, occasions). We get a "three-way, three-mode array".

Another example of three-way array is given by data concerning proximity measures between all pairs of individuals in a set of I individuals, as assessed by K independent "judges" (occasions):

$$P = \{p_{ii'k}\}, \qquad i, i' = 1, I;\ k = 1, K,$$

where $p_{ii'k}$ stands for the proximity (similarity, distance, etc.) between individuals i and i', as measured by "judge" k. Also in this case, the three ways (i, i', k) are fully crossed, since on each occasion the same set of pairs of individuals is observed. However, differently from the previous example, we are now coping with a "three-way, two-mode array", because the same mode "units" is repeated twice in the data array. It is worth noting that the array P might also be a "derived" array, namely an array obtained by means of computations made on an original set of data concerning the values taken by the same group of variables, or even by different groups of variables, on the same individuals, on different occasions. In this case, the proximity $p_{ii \Cup 7k}$ is calculated on the basis of the values taken by the group of variables observed on occasion k, on individuals i and i' (e.g. an Euclidean distance, if the variables are quantitative). When the ways, or criteria of classification of the data, are not fully crossed, we use the denomination: "multiway data set", as opposed to "multiway data array" (see, also, Kiers, 1991, for a similar distinction). A common instance of a "three-way data set" is provided by the values taken by different groups of variables, say, $(X_1^1, \ldots, X_{J_1}^1), \ldots, (X_1^k, \ldots, X_{J_k}^k), \ldots, (X_1^K, \ldots, X_{J_K}^K)$, on I units at K different occasions. This "three-way, three-mode data set" is the usual object which can be studied by means of generalised canonical analysis (see, for instance, the paper devoted to OVERALS, in this volume).

A similar three-way data set could be obtained when considering the same group of variables as observed on different groups of individuals at different occasions.

The basic distinction between "arrays" and "sets", in the framework of multiway data, is further detailed by referring to the more traditional classification into "quantitative" and "categorical" data. In the latter case, various types of multiway data might be considered. When the same set of categorical variables, say $A_1, \ldots, A_J$ with, respectively, $m_1, \ldots, m_J$ categories, is observed on K different groups of individuals with, respectively, $I_1, \ldots, I_K$ units, we may set up K J-way contingency tables:

$$(C_1, \ldots, C_k, \ldots, C_K) = C,$$

where $C_k = \{n_{j_1 j_2 \ldots j_J}^k\}$, $j_1 = 1, m_1$, $j_2 = 1, m_2, \ldots, j_J = 1, m_J$ and $n_{j_1 j_2 \ldots j_J}^k$ denotes the number of units, out of I_k, presenting the combination of category j_1 of A_1, category j_2 of $A_2, \ldots,$ category j_J of A_J.

Although the original data might be classified as a "three-way, three-mode data set", the "derived" data C can be considered a "$(J+1)$-way data array", since it refers to the full crossing of J ways with the K "occasions" (groups of individuals). This example witnesses a certain degree of ambiguity in the systematic classification of different types of multiway data. Nevertheless, the reference to the above mentioned distinctions reveals very useful when devising and presenting different types of data analysis techniques, as it will be illustrated in the course of this volume. In this connection, the ambiguity related to the definition of the appropriate type of multiway data can actually add more flexibility in the methodological treatment of statistical information.

For instance, as we shall see in other papers of this volume, the data array C can also be usefully presented in a different form. If we attach to each category of a variable A_j an indicator variable taking value 1 or 0 on individual i according to whether this individual presents or does not present that category of A_j, we get the following four-way, four-mode data set:

	A_1	...	A_J	
Group 1	D_{11}	...	D_{1J}	
⋮	⋮		⋮	$= D$,
Group K	D_{K1}	...	D_{KJ}	

where, for instance, D_{11} denotes the indicator matrix referring to the categories of A_1 as observed on the I_1 individuals belonging to group 1. Each element of the above data set (either 0 or 1) is characterised by four indices concerning, respectively, the group of units, the individual within the group, the categorical variable, the category within the variable.

Therefore, the same complex statistical information can be represented in two different ways, either C or D, giving rise to different types of multiway data. Different techniques of analysis may be utilised for studying the two forms of data. Of course, one can expect that different features of the same information are extracted, according to the way the data are presented. This is but one example of the freedom of choice the researcher has when dealing with multiway data.

Another, more technical, aspect of this freedom is provided by the preliminary manipulation of the data, such as, for instance, centering and/or standardising the rows, columns or layers of a three-way array (see paper on PARAFAC, in this volume, for a detailed treatment).

2. The analysis of multiway data: a general framework

As it was underlined in section 1, different types of multiway data may represent different information and require appropriate techniques of analysis.

It is, perhaps, impossible to classify in a systematic manner the various aspects of statistical information conveyed by the different data arrays or sets, and the methods of data analysis enabling the researcher to extract this information. However, some general guidelines can be provided in this connection, which may act as a reference system when utilising a multiway approach to the analysis of statistical data.

We shall first refer to the type of information one may wish to extract from multiway data. We shall limit ourselves to considering the most common (at the present stage of research) type of data, in this framework, namely the three-way array X, related to the same set of quantitative variables observed on the same set of units on different occasions. In what follows we denote the occasions, units and variables respectively by O, U and V. The main information we would like to draw concerns the following aspects:

(1) Comparison of the occasions, on the basis of the overall structure of the "units $\times$ variables" matrix characterising each occasion.
(2) Evaluation of units and, separately, of variables, on the average (i.e. independently of each particular occasion), on the basis of the overall association structure among units (with respect to the values taken by the variables), and of the overall association structure among variables (with respect to the values taken on the units).
(3) Evaluation of units and, separately, of variables, on the different occasions, in order to ascertain whether and how each particular unit (or variable) modifies its "behaviour", with respect to the variables (or units), across the various occasions.
(4) Joint evaluation of units and variables, in order to determine the "interaction" between them. This, in turn, can be done either "on the average" or with reference to the various occasions.

Generally speaking most methods of analysis deal with the above types of information by assigning, in various ways, appropriate "scorings" to the involved elements.

Thus, scores O_k, U_i, V_j are attached to the occasions, units and variables as to aspects (1) and (2). For aspect (3) the scores of U and V should be specified for each occasion k, thus providing values U_i^k and V_j^k. Finally, with respect to aspect (4), joint scores $(UV)_{ij}$ and $(UV)_{ij}^k$ might be used for evaluating the interactions between units and variables. We should notice that, in the factor analytic approach, the above mentioned scores can be specified according to various latent dimensions, so that, instead of having just one evaluation, e.g. O_k, for each information element, we can consider several scores, one for each latent dimension, say $O_{k1}, O_{k2}, \dots, O_{kt}, \dots,$ etc.

It should be added that these scores allow us to get graphical displays of the respective elements, usually as points on Cartesian planes. This kind of visualisation may be very useful in interpreting the results of the analysis, as it will be thoroughly illustrated in the course of this volume.

It is impossible, in the framework of this introduction, to deal in detail with the various aspects of information conveyed by the different multiway data arrays and sets.

The above hints concerning the three-way array "units × variables × occasions" may, however, provide a general indication of the type of questions one can formulate when analysing this kind of data. Moreover, the "translation" of these questions into appropriate "scores" to be attached to the different elements in the analysis and the derived graphical displays, are quite typical of the various approaches to the analysis of the different types of multiway data. The scores might be considered as "parameters" to be estimated, irrespectively of whether a probability model is assumed for the data generation process or, instead, a pure descriptive-exploratory approach is adopted.

In fact, coping with the second problem to be dealt with in this section (namely the analysis of multiway data), we may introduce several types of distinctions among different methods of multiway analysis.

A traditional distinction is between "factor analytic" techniques and "scaling" techniques (see, for instance, Law et al., 1984, chapter 1). This distinction is deeply rooted in the psychometric area of studies, but it seems to be rather restrictive, if we take into account the increasing number of contributions to the field of multiway analysis, stemming from other traditions of research (social and economical areas, mathematical disciplines, etc.).

A more general distinction is the one referring to the use of probability models. This is connected with the sampling or non sampling nature of the data. In the former case the data generation process may or may not be modelled according to some probability distribution. If a probability model is adopted, this is generally parametrized in such a way that either the parameters themselves or suitable reparametrizations represent the basic information we wish to draw from the data. Techniques related to the use of the likelihood function (e.g. maximum likelihood estimation and likelihood ratio testing, in the classical "repeated sampling" framework of statistical inference) are most often devised in this connection. An illustration of this approach is provided by De Sarbo et al. (this volume) with CATSCALE methodology for studying three-way sorting data (see also, for instance, Ramsay, 1982, for contributions to the analysis of multiway data in a likelihood framework). However, even in the sampling setups, it is not strictly necessary to adopt a probabilistic approach. In fact, the stochastic component of a statistical model may constitute, in many situations, a minor factor in the determination of the overall variation in the data. In this case the "structural" part of the model, expressed in terms of "parameters" related to the basic information to be extracted, is assumed to account for most of the variation. Following Kruskal (1984), we might formalise our data (e.g. of the type "units × variables × occasions") by means of the general model:

$$\begin{cases} x_{ijk} = m_{ijk} + \epsilon_{ijk} \\ m_{ijk} = f_{ijk}(\boldsymbol{\beta}) \end{cases} \qquad i = 1, I;\ j = 1, J;\ k = 1, K, \tag{1}$$

where m_{ijk} represents the structural part of the model, depending on a vector of unknown parameters $\boldsymbol{\beta}$ according to a given function f_{ijk}, and ϵ_{ijk} stands for an erratic additive component whose importance is relatively small as compared to the structural component, so that it is not necessary to model it further. In this case, the analysis is limited to m_{ijk}. Usually techniques based on "least squares" are utilised for estimating the $\boldsymbol{\beta}$ parameters of the structural model. Suitable illustrations of this approach are provided by Kroonenberg (the TUCKALS line) and Harshman and Lundy (PARAFAC), in this volume. In these instances, the structural model is formulated, in a rather standard way, as a multilinear function of appropriate parameters (see section 3 for more details). Interpreting with more flexibility model (1) enables us to include also, within this framework, other approaches to the analysis of multiway data, such as OVERALS (see van der Burg et al., in this volume). In this case, the structural component is expressed in terms of two sets of parameters. One set refers to the data: parameters expressing the quantification of categorical or ordinal variables or the re-quantification of quantitative variables (for example, through splines). Another set refers directly to the type of statistical model adopted in the specific situation (e.g. the coefficients of the canonical variates in OVERALS, which is specifically tuned for generalised canonical analysis of mixed data). Also in this case, a least squares approach is utilised for estimating the parameters.

It should be remarked that a "partial" probabilization of the analysis may be introduced at some stage, as it is underlined in the mentioned paper by van der Burg et al., with reference to some intermediate outputs of the procedure. This does not modify the "non probabilistic" nature of the approach, as witnessed by the lack of an overall probability model whose parameters or appropriate reparametrizations should coincide with those appearing in the above mentioned structural model.

When probability models do not play the basic role in the analysis, as illustrated before, we act in a descriptive-exploratory framework, still allowing us to draw the essential information in the data. Possible disturbing effects, caused by the stochastic component in sampling setups, might be faced by adopting alternative procedures, such as bootstrap and jackknife, which do not require the use of a probabilistic formalization (see, for instance, van der Burg et al. in this volume).

Not all the descriptive-exploratory techniques are based on model (1). An important part of the procedures of analysis of multiway data is inspired to a geometrical approach. In particular, but not only, the French scholars have made contributions from this point of view. In this case, the basic elements in the data array or set (e.g. individuals, variables, etc.) are represented as vectors or tensors in appropriate Euclidean spaces, and the procedures of analysis generally consist in trying to find "optimal" low-dimensional representations of these elements, retaining the maximum information with respect to the original data. Obviously, the coordinates of the represented elements constitute, in this case, the "scores" we referred to before. Moreover, the geometry involved in the procedure, adds further pieces of information, in particular related to the quality of the analysis along with the natural visualisation of the results. Illustrations of this approach are provided in this volume by Escofier and Pages (AFMULT) and Lavit et al. (ACT). Generally, an eigenvalue-eigenvector technique of analysis is associated to these procedures.

3. Methodological approaches to the analysis of multiway data

As we have already underlined in section 2, it is practically impossible to provide an exhaustive and systematic framework for the description of the numerous techniques which are, nowadays, available for analysing multiway data. Nevertheless, it might be opportune to sketch a few pathways which have so far guided the scholars in this field in their search for sound procedures of multiway analysis. While enabling the reader to find out links among different methods, this effort may turn out to be useful in suggesting new techniques or appropriate modifications of old ones.

A first line of research is based on *multilinear models.*

This is particularly suited to the analysis of multiway arrays, whose main instance is provided by the "units × variables × occasions" array.

Referring to model (1), we may write the following quadrilinear expression for the structural part:

$$m_{ijk} = \sum_{p=1}^{s} \sum_{q=1}^{t} \sum_{r=1}^{u} g_{ip} h_{jq} l_{kr} c_{pqr}, \tag{2}$$

where g, h, l are, respectively, the loadings of the units, variables and occasions related to their respective "ideal" components (s for the units, t for the variables and u for the occasions), and c_{pqr} represents the generic element of the so called "core matrix" describing a kind of three-way "interaction" among the ideal components of each mode. This is the Tucker3 model (Tucker, 1964, 1966).

Usually an approximation of (2) is looked for, involving a low dimensional solution for the latent dimensions (small values of s, t, u) still retaining a good fit to the original data. An alternating least squares procedure has been suggested by Kroonenberg and de Leeuw (1980) for the estimation of the parameters of Tucker3 model (see Kroonenberg, in this volume). If in (2) we drop the parameters l_{kr} and let the latent dimensions for the occasions coincide with the occasions themselves, we get the Tucker2 model:

$$m_{ijk} = \sum_{p=1}^{s} \sum_{q=1}^{t} g_{ip} h_{jq} c_{pqk}. \tag{3}$$

Model (3) is a less restricted version of Tucker3, allowing a full analysis of the occasions' mode, not filtered by the "ideal" (latent) components related to it. Also in this case, an alternating least squares solution has been devised (see Kroonenberg, in this volume). It is interesting to note that Tucker2 model can usefully be adopted for analysing a set of scalar product matrices referring either to the units or the variables, examined across the occasions. For instance, let us consider the set of K matrices:

$$V_k = X_k' X_k, \qquad k = 1, K,$$

where X_k is the generic 2-way "units $\times$ variables" array corresponding to occasion k (a "slice" of the 3-way array). If we assume that the columns of X_k (the "variables") are centered with respect to the column mean, then V_k is a covariance matrix, and the derived array $\{V_k\}_{k=1,K}$ can be analysed by means of Tucker2 model:

$$m^*_{jj'k} = \sum_{q=1}^{t} \sum_{q'=1}^{t} h_{jq} h_{j'q'} c_{qq'k}, \tag{4}$$

where $v_{jj'k} = m^*_{jj'k} + \epsilon_{jj'k}$, $v_{jj'k}$ being the generic element (covariance) of V_k. It should be noticed that, in this case, there is only one type of latent dimension (related to the variables' mode), represented by scores h_{jq}. This model was first proposed, in a different framework, by Carroll and Chang (1970, 1972) under the name IDIOSCAL.

If the core matrix of Tucker2 is diagonal ($c_{pqk} = 0$ if $p \neq q$), then we get the "parallel factors" model (PARAFAC):

$$m_{ijk} = \sum_{p=1}^{s} g_{ip} h_{jp} c_{kp}. \tag{5}$$

This model has very attractive interpretative properties, such as the "intrinsic-axis" one (see Harshman and Lundy, in this volume, for a detailed treatment), related to the essential unicity of the parameters of (5), as opposed to the indeterminacy connected with the analogous 2-way factorial model.

Moreover, if the PARAFAC model is applied to the scalar product matrices, as in (4), then the INDSCAL model (Carroll and Chang, 1970) is obtained.

Multilinear models constitute a powerful tool for analysing multiway data. They are enough flexible for fitting different types of arrays and sets. Moreover, the interpretation of their parameters is made clear by the algebraic formulation of the model. In particular, referring to what has been said in section 2, these parameters represent an appropriate system of scorings for the elements of the array or set of data, enabling the researcher to analyse them both separately and jointly (see Kroonenberg, in this volume).

An alternative approach to the analysis of multiway data consists of devising an adequate *strategy of analysis*, taking into account the complex nature of the data. A central role, in this respect, is played by the STATIS method (see Lavit et al., in this volume) for 3-way data. The strategy underlying this method might be denominated "Interstructure-Compromise-Intrastructure" (ICI). In fact, if we refer to an array or set of data concerning units, variables and occasions, we may, first of all, put the emphasis on the "occasions". Then the 3-way array or set X, can be considered as a set of K "vectorized" matrices:

$$X = (vecX_1 \mid vecX_2 \mid \dots \mid vecX_K), \tag{6}$$

where X_k ($k = 1, K$) is the "units $\times$ variables" matrix on occasion k. A principal component analysis of matrix (6), or of the corresponding "vectorized" matrices of scalar products, may provide the overall structure of the occasions, allowing us to carry out a global comparative evaluation of them. This constitutes the "interstructure" stage of the strategy (scores O_k are computed as coordinates of the occasions on the principal axes).

A second stage of the analysis consists in looking for a good "compromise" matrix, summarising in some sense the K matrices X_k. STATIS suggests to take a weighted scalar product matrix, using as weights the components of the first eigenvector of the PCA performed at the interstructure stage. Other types of compromise matrices could be devised. Then, a second principal component analysis can be applied to the compromise matrix. This provides detailed information on units and variables, both on the average (compromise scorings) and as function of the occasions ("trajectories").

The idea of the ICI strategy underlies also other procedures of analysis, as we shall see later on. Its strength relies on its logical foundations, which make a clear distinction between the different types of information conveyed by 3-way data that can be considered as a set of 2-way matrices. This, in turn, is a limitation to the use of this approach for other types of multiway data.

A third kind of methodological approach is linked to the idea of "*collapsing*" the multiway data to a lesser number of dimensions, before analysing them. A typical illustration is provided by generalised canonical analysis. Referring to a three-way data set concerning K different groups of variables observed on the same units, we may represent this set as a 2-way matrix:

$$X = (X_1 \mid X_2 \mid \dots \mid X_K), \tag{7}$$

where X_k ($k = 1, K$) denotes the matrix related to the k-th group of variables, and X is seen as the "juxtaposition" of these matrices. The 3-way data are, therefore, collapsed to two ways, providing a matrix which can undergo various kinds of analysis. Multiple factor analysis (see Escofier and Pages, this volume) suggests, for instance, to perform a weighted principal components analysis of (7). Weights inversely proportional to the eigenvalues determined by the principal component analysis of each group of variables are proposed by Escofier and Pages (this volume). Interesting geometrical properties characterise this method, in connection with the Euclidean representation of units, variables and groups of variables (see the mentioned paper by Escofier and Pages).

A similar arrangement of the data is utilised by OVERALS (see van der Burg, this volume), with some more generality due to the possibility of simultaneously analysing qualitative and quantitative variables. The methodological framework, in this case, is provided by generalised canonical analysis as applied to the K groups of variables. The interpretation is enriched by the use of transformations (splines for quantitative variables, appropriate sets of scorings for ordered and categorical variables), casting light on possible non-linear relationships among the variables.

Collapsing the data is a useful device, though by this operation we may loose information related to the interactions between the collapsed mode and the remaining ones. Therefore, also in this case (as for the ICI strategy), the utilisation is to be limited to appropriate data sets, like (7).

Another class of methods may be classified with the general label of "*Analysis of Relation Matrices*" (see, e.g., Coppi, 1986, 1988, in particular for multiway data concerning categorical variables). Let us, first, consider a three-way array or set of the type "units × variables × occasions". We may construct, in several ways, pairwise relation matrices among the elements of one mode based on the elements of a second mode, for each element of the third mode. Immediate examples are the set of covariance matrices (pairwise relations among variables, with respect to the units) for each occasion, or the set of scalar product matrices between units (with respect to the variables) for each occasion. It is also possible to consider pairwise relations between occasions with respect to the units (variables) for each variable (unit). In any of these cases, we shall get a three-way two-mode array which can be analysed by means of appropriate techniques. One of these techniques is the already quoted INDSCAL method, which provides scores for both modes of the array, in a multidimensional framework. From a factor-analytic viewpoint, the set of relation matrices may be studied by means of principal component analysis or principal coordinate analysis, provided that the matrices are symmetric and positive definite. In fact, the above mentioned STATIS method can also be interpreted in this way, if we refer to the relation matrices (or "operators") concerning the pairs of units or the pairs of variables for each occasion (see Lavit et al., this volume).

Relation matrices are not necessarily two-way one-mode matrices. We may also think of defining pairwise relations between elements of two different modes (e.g. between units and variables) according to some criterion (e.g. "degree of proximity" or "affinity": for instance a given unit may be "characterised" by a given variable, if this variable takes an "extreme" value, above or below the mean, on that unit). Again, this set of relation matrices can be analysed by means of suitable techniques. In this case, in a scaling framework, the Unfolding methods may be usefully applied (see, for instance, Heiser 1981).

Another kind of multiway data that can be studied by the relation matrices' approach is the set of multidimensional contingency tables introduced in section 1:

$$C_k = \left\{ n^k_{j_1 j_2 \dots j_J} \right\}, \qquad j_1 = 1, m_1,\ j_2 = 1, m_2, \dots, j_J = 1, m_J. \tag{8}$$

On each occasion, we may define appropriate measures of pairwise relationship between categories pertaining to different variables (and also, in a conventional manner, between categories of the same variable). Coppi (1988) suggests a few measures of this type. On this basis a pairwise relation matrix among the categories of all variables can be set up, for each occasion. This set of matrices might then be analysed by means of principal coordinate analysis followed by the PCA of a compromise matrix related to the average scores of pairs of categories. Otherwise an INDSCAL approach may be used. As an output of these analyses, we get different types of scores: for the occasions globally considered, for the single categories on the average, for the single categories on each occasion, for pairs of categories on the average and on each occasion.

The various methodological approaches to the analysis of multiway data, so far briefly described in this section, are far from including all the techniques already available in this field. In fact many useful methods of multiway analysis cannot be easily classified in a more general group presenting a specific methodological characterisation (see Bove and Di Ciaccio, this volume, for more detailed indications concerning other methods). By the same token, it does not seem possible to find systematic links among all different types of techniques, though we have already underlined a few interesting links among some of the mentioned methods of analysis (see, e. g., Kiers 1988, 1991 for a detailed study of the hierarchical relations among some techniques dealt with in this section).

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