Psychological Methods
2001, Vol. 6, No. 1, 84–110

1082-989X/01/$5.00 DOI: 10.1037//1082-989X.6.1.84

Three-Way Component Analysis: Principles and Illustrative Application

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Three-way component analysis techniques are designed for descriptive analysis of 3-way data, for example, when data are collected on individuals, in different settings, and on different measures. Such techniques summarize all information in a 3-way data set by summarizing, for each way of the 3-way data set, the associated entities through a few components and describing the relations between these components. In this article, 3-mode principal components analysis is described at an elementary level. Guidance is given concerning the choices to be made in each step of the process of analyzing 3-way data by this technique. The complete process is illustrated with a detailed description of the analysis of an empirical 3-way data set.

Three-way data refer to data that can be arranged in a three-dimensional array. Such data can emerge in many different contexts. Examples include data pertaining to measurements on various anxiety scales of a number of individuals in various situations; data on the strength of various symptoms observed in various patients by a number of clinicians; data on the importance of various job requirements for various jobs, according to different job analysts; and positron-emission tomography scan data representing different areas of the brain, measured for various individuals performing a number of different mental tasks. The three sets of entities associated with such three-way data sets are called the three *modes* of the array.

One may be tempted to analyze three-way data either after aggregating over one of the three ways or by analyzing all two-way data sets contained in the three-way data set separately. However, it should be noted that such approaches do not offer an explicit description of the three-way interaction in the data; hence, they may lead to conclusions that are incomplete at best.

The strength of three-way component analysis techniques (described further in this article) is that they summarize all information in a large three-way data set (i.e., all main effects and all interactions together) and that they do so in an efficient way. Specifically, three-way methods summarize the entities of each mode through a few components and describe the relations between these components. Thus, in the case of scores of individuals on response variables, measured in different situations, the (most salient) relations among individuals, response variables, and situations are captured by the relations among components summarizing the individuals, response variables, and situations. This is particularly useful in the presence of three-way interaction: Without the use of summarizing components, a full description of a three-way interaction may require as many terms as there are data points, which is not feasible unless the three-way data set is very small.

Another approach is to consider three-way data as multilevel data (with, e.g., responses being nested within persons and situations and with crossing of the latter two). Furthermore, if the primary focus of the research is on detecting the relationship between the three-way data and external predictor variables, multilevel analysis (e.g., Goldstein, 1986) may be called for. However, if the primary focus is on detecting the internal structure of the three-way data, methods of three-way analysis are most appropriate.

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This research was supported in part by University of Leuven Research Fund Grant GOA/2000/02.

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In particular, three-way component analysis techniques are useful for the exploratory analysis of three-way data in which the modes of the data set (or at least some of them) are relatively large and can be summarized through components. Various techniques of this kind have been proposed (for overviews see, e.g., Bro, 1998; Kroonenberg, 1983; Law, Snyder, Hattie, & McDonald, 1984). The most prominent instances are parallel factor analysis (PARAFAC), proposed by Harshman (1970) and Carroll and Chang (1970), and three-mode factor analysis, proposed by Tucker (1963, 1966) and further elaborated by Kroonenberg and De Leeuw (1980), who renamed the method *three-mode principal components analysis* (here abbreviated as 3MPCA). More recently, the latter method has also been called *Tucker3 analysis* (e.g., see Kiers, 2000), but we do not use that name in the present article. Other three-way techniques include those proposed by Bentler and Lee (1978) and McArdle and Cattell (1994). These three-way factor analysis techniques mainly differ from three-way component-analysis techniques in that they are based on distributional assumptions (which is particularly useful in confirmatory analysis) and in that they are modeling covariances rather than the actual data. Then, due to the aggregation over the entities in one mode (usually the participants), information on the entities of that mode is lost (e.g., no component matrix for the participants is given). For a fully exploratory analysis of three-way data, without distributional assumptions, three-way component-analysis techniques appear to be more adequately suited.

Three-way component techniques have not yet been implemented in the major statistical packages, but special-purpose programs for them are available. In these programs (e.g., 3WAYPACK and Tucker3.m; see the Three-Way Component Analysis Techniques section), several choices have to be taken that may require some guidance: for example, the choices of how the data are to be preprocessed (e.g., is standardization called for, and if so, over which of the three modes), how many components are to be used, and which simple structure rotations are to be used. Such problems are analogous to those in principal-components analysis (PCA) but are more complex in the three-way situation.

It is the purpose of the present article to provide some guidance to actually performing a three-way component analysis. We focus on the most versatile method, 3MPCA, and only briefly discuss PARAFAC. Then, the different choices to be made in a three-way analysis are discussed step by step. Finally, the whole process is illustrated with a detailed description of the analysis of an empirical three-way data set with scores of 140 individuals on 14 response scales filled out for 11 different situations, as obtained with a situation–response (S-R) inventory of anxiousness.

Three-Way Component Analysis Techniques

In this section, 3MPCA is described at an elementary level and PARAFAC is discussed briefly. For readers favoring matrix algebraic descriptions, these are given in the text as well, in such a way that they can be ignored by readers not adept at matrix algebra. Because 3MPCA is a generalization of PCA (for the analysis of two-way data), we start with a description of that technique.

PCA

PCA is a popular technique that is often used for the exploratory analysis of a set of variables. The aim of PCA is to find a limited number of *components,* which are unobserved, new variables that are constructed from the observed variables in such a way that they capture most of the information contained in the observed variables. Given an $I \times J$ data matrix $\mathbf{X}$ with standardized scores of I individuals on J variables, PCA comes down to finding an $I \times Q$ component scores matrix $\mathbf{A}$ (with elements a_{iq}, $i=1,\ldots, I$, $q=1,\ldots, Q$) and a $J \times Q$ loading matrix $\mathbf{B}$ (with elements b_{jq}, $j = 1,\ldots, J$, $q = 1,\ldots, Q$), where the number of components, Q, is smaller than I and J (usually much smaller), the component scores are the scores of the I individuals on Q components, and the loadings are the weights applied to the scores on the components so that the weighted sum of component scores optimally reconstructs the standard scores on the original variables. Specifically, PCA finds component scores and loadings such that the standard score of individual i on variable j, x_{ij}, is approximated optimally by

$$\sum_{q=1}^{Q} a_{iq} b_{jq}$$

for all combinations (i, j). Technically, this is achieved by minimizing the sum of squared residuals for this approximation, that is, by minimizing

$$\sum_{i=1}^{I} \sum_{j=1}^{J} \left(x_{ij} - \sum_{q=1}^{Q} a_{iq} b_{jq} \right)^2 \qquad (1)$$

over all possible values for the component scores and the loadings. In matrix algebra, Expression 1 is written as $\|\mathbf{X} - \mathbf{AB}'\|^2$, where $\|.\|^2$ denotes the sum of squares of the elements of the matrix at hand.

The above description of PCA is actually Pearson's (1901) description of PCA as a technique for finding those components that explain the maximum amount of variance in the data, where the total variance is $1/I$ times the sum of squares of the elements of $\mathbf{X}$, and the explained variance is $1/I$ times the sum of squares of its approximations (the elements of $\mathbf{AB}'$). Alternatively, PCA may be defined as finding a $J \times Q$ loading matrix $\mathbf{B}$ such that the correlation between the variables j and j', $r_{jj'}$, is approximated optimally by

$$\sum_{q=1}^{Q} b_{jq} b_{j'q}$$

for all combinations (j, j'), $j = 1, \ldots, J$, $j' = 1, \ldots, J$ (which is achieved by minimizing $\|\mathbf{R} - \mathbf{BB}'\|^2$). Why the latter method, denoted as *Rao PCA,* happens to give a solution to Pearson PCA as well is explained, for instance, by Ten Berge and Kiers (1996).

One solution for the loadings in $\mathbf{B}$ in Expression 1 is obtained by taking the first Q eigenvectors of the correlation matrix $\mathbf{R}$ as the columns of $\mathbf{B}$; the associated Q eigenvalues then give the componentwise-explained variances, and the component scores can be obtained from the loadings straightforwardly (in matrix algebra: $\mathbf{A} = \mathbf{XB}(\mathbf{B}'\mathbf{B})^{-1}$). These components, called the *principal components,* have the additional property that they maximize the explained variance sequentially as well as jointly: The first component explains the maximum amount of variance that can be explained by a single component, the first two give maximal explained variance using two components, and so on. This, however, is not the only solution that minimizes Expression 1 and maximizes the total explained variance. In fact, if we replace each component (i.e., each column in $\mathbf{A}$) by a differently weighted sum of all components, the new components together explain the same amount of variance as do the original components, provided that the loadings in $\mathbf{B}$ are appropriately transformed. Such transformation procedures are called *rotations,* because when one is plotting the variables using the loadings as coordinates with respect to the components (used as axes), such recombinations come down to (possibly oblique) rotations of the axes. In matrix algebra, such rotations are described by a rotation matrix $\mathbf{T}$, and $\mathbf{A}$ is replaced by $\mathbf{A} = \mathbf{AT}$; then, the loading matrix $\mathbf{B}$ is replaced by $\tilde{\mathbf{B}} = \mathbf{BT}'^{-1}$ so as to ensure that $\tilde{\mathbf{A}}\tilde{\mathbf{B}}' = \mathbf{AB}'$, which implies that the same amount of variance is indeed explained by the original as by the rotated components. Such components are denoted as *rotated principal components,* but, as they have the same explanatory power as "unrotated principal components," this distinction is of little practical value.

To interpret the PCA solution, researchers often try to find labels expressing the contents of the components. As the components are not given a priori, this can only be done indirectly, usually by means of the loadings of the variables on the components. If a group of variables has high loadings on the same component, this indicates that the component at hand mainly pertains to what this group of variables has in common. For instance, if variables such as score on arithmetic test, score on calculus test, and score on algebra test have high loadings on one particular component, then this component may be labeled "mathematical skill." Obviously, such labels are subjective and thus debatable. The interpretation will, however, become less debatable as variables are more clearly related to one and only one component. Therefore, it is useful to have simple loadings, that is, loadings that are either high or low (in absolute value) and not in between, and preferably with only one high loading per measured variable (i.e., per row of the loading matrix). In PCA, such a simple structure can be aimed at by using the "rotational freedom" of PCA solutions: Replacing component scores and loadings by rotated versions thereof does not affect the fit, as mentioned above. In practice, the rotational freedom is therefore often used to rotate components such that the loadings become as simple as possible. In this way, PCA followed by simple structure rotation is an important tool for finding groups of variables that measure the same concept, and it is often used as a first step in test construction.

3MPCA

PCA is meant for the analysis of two-way data x_{ij} pertaining to scores of individuals on variables. PCA yields matrices $\mathbf{A}$ and $\mathbf{B}$ that summarize the individuals and the variables, respectively. 3MPCA is meant for the analysis of three-way data x_{ijk} (possibly preprocessed) that give the score of individual i on variable j at measurement occasion k ($i = 1, \ldots, I$, $j = 1, \ldots, J$, $k = 1, \ldots, K$). In 3MPCA, as in PCA, matrices $\mathbf{A}$ and $\mathbf{B}$ are found that summarize the individuals and the variables, respectively, but in addition a matrix **C** is found that summarizes the occasions. Usually, in 3MPCA these matrices are all referred to by the general term *component matrices,* and a distinction between component scores and loadings is not made.

In PCA, each component that summarizes the individuals is uniquely related to a component that summarizes the variables. In 3MPCA, components that summarize the entities in the different modes are not associated uniquely with components for the other modes. Furthermore, the numbers of components used for summarizing the entities of the different modes need not be the same. Thus, in 3MPCA we have an $I \times P$ component matrix **A**, a $J \times Q$ component matrix **B**, and a $K \times R$ component matrix **C**, where P, Q, and R denote the numbers of components used to summarize the entities in the three respective modes (with $P < I$, $Q < J$, $R < K$). In addition, to relate all components of all modes to each other, 3MPCA employs a so-called core array $\underline{\mathbf{G}}$ (of order $P \times Q \times R$). The function of this core array is to give a summary description of the three-way information in the full data table, in terms of the summarizing components for the three different modes. Thus, the core can be considered a strongly reduced version of the full data array, capturing up to three-way interactions between all different modes, but in terms of summarizing entities for all of the modes. The full 3MPCA model reads as follows:

$$x_{ijk} \cong \sum_{p=1}^{P} \sum_{q=1}^{Q} \sum_{r=1}^{B} a_{ip} b_{jq} c_{kr} g_{pqr},$$
$$i = 1, \ldots I; j = 1, \ldots, J, k = 1, \ldots, K, \qquad (2)$$

where $\cong$ refers to optimal approximation in, for instance, the least squares sense; a_{ip}, b_{jq}, and c_{kr} denote the elements of **A**, **B**, and **C**, respectively; and g_{pqr} denotes the elements of core array $\underline{\mathbf{G}}$. The core efficiently describes the main relations in the data, and the component matrices **A**, **B**, and **C** describe how the particular individuals, variables, and occasions relate to their associated components.

To illustrate the 3MPCA model, Table 1 gives a fictitious data set of six individuals with scores on five response variables (indicating to what extent each individual displays an emotional, sensitive, caring, thorough, or accurate behavior) for four different situations. The data were chosen such that they correspond exactly to Expression 2 with $P = Q = R = 2$. The corresponding matrices **A**, **B**, and **C** and the core array $\underline{\mathbf{G}}$ are given in Tables 2–5, respectively.

The interpretation of the person components, response variable components, and situation components is shown in the headings of the corresponding columns in Tables 2–4. The first person component is *femininity,* to which all females are related, although one (Edna) only partly; the second person component is *masculinity,* to which all males are related strongly and to which, in addition, Edna is related partly. Apparently Edna is an androgynous person. The response variable components have been labeled *emotionality* for the component on which emotional and sensitive depend completely and *conscientiousness* for the component on which thorough and accurate depend completely. Caring apparently has features of both components, although a bit more of emotionality than of conscientiousness. The situation components were labeled *performance situations* and *social situations.* It can be seen that doing an exam is a pure performance situation, whereas giving a speech implies performance to a large extent but also implies social aspects. A family picnic on the other hand is entirely social, whereas meeting a new date is to a large extent social but also has performance aspects. It should be noted that, in contrast to what is usually the case in PCA, component and core values in 3MPCA

Table 1
Fictitious Data Set of Scores of Six Individuals on Five Response Variables for Four Situations

	Doing an exam					Giving a speech					Family picnic					Meeting a new date				
Individual	E	S	C	T	A	E	S	C	T	A	E	S	C	T	A	E	S	C	T	A
Anne	0.0	0.0	1.2	3.0	3.0	0.6	0.6	1.3	2.4	2.4	3.0	3.0	1.8	0.0	0.0	3.6	3.6	2.5	0.9	0.9
Bert	0.0	0.0	0.8	2.0	2.0	0.2	0.2	0.8	1.8	1.8	1.0	1.0	1.0	1.0	1.0	1.2	1.2	1.4	1.8	1.8
Claus	0.0	0.0	0.8	2.0	2.0	0.2	0.2	0.8	1.8	1.8	1.0	1.0	1.0	1.0	1.0	1.2	1.2	1.4	1.8	1.8
Dolly	0.0	0.0	1.2	3.0	3.0	0.6	0.6	1.3	2.4	2.4	3.0	3.0	1.8	0.0	0.0	3.6	3.6	2.5	0.9	0.9
Edna	0.0	0.0	1.0	2.5	2.5	0.4	0.4	1.1	2.1	2.1	2.0	2.0	1.4	0.5	0.5	2.4	2.4	2.0	1.3	1.3
Frances	0.0	0.0	1.2	3.0	3.0	0.6	0.6	1.3	2.4	2.4	3.0	3.0	1.8	0.0	0.0	3.6	3.6	2.5	0.9	0.9

Note. E = emotional; S = sensitive; C = caring; T = thorough; A = accurate.

Table 2
Component Values of Individuals (**A**), *Resulting From a 3MPCA That Describes the Data in Table 1 Perfectly*

A: Individual	Femininity	Masculinity
Anne	1.0	0.0
Bert	0.0	1.0
Claus	0.0	1.0
Dolly	1.0	0.0
Edna	0.5	0.5
Frances	1.0	0.0

Note. The components have been labeled by the interpretations given to them on the basis of the component values. 3MPCA = three-mode principal components analysis.

Table 3
Component Values of Response Variables (**B**) *Resulting From a 3MPCA That Describes the Data in Table 1 Perfectly*

B: Response	Emotionality	Conscientiousness
Emotional	1.0	0.0
Sensitive	1.0	0.0
Caring	0.6	0.4
Thorough	0.0	1.0
Accurate	0.0	1.0

Note. The components have been labeled by the interpretations given to them on the basis of the component values. 3MPCA = three-mode principal components analysis.

can exceed 1. In fact, in PCA, loadings do not exceed 1 or −1 because of the common choice to analyze standardized data. In 3MPCA, different procedures of preprocessing are used, as is explained in the *Preprocessing the Data* subsection under The Three-Way Analysis Process.

The core can be used to concisely describe the main information in the data, as follows: In performance situations, feminine and masculine persons behave equally emotionally, whereas feminine persons behave somewhat more conscientiously than masculine persons; in social situations, feminine persons behave considerably more emotionally than masculine persons, whereas in these cases masculine persons behave more conscientiously than feminine persons. This description can be checked with the data, in which it can be seen, for instance, that the feminine individuals indeed tend to respond particularly emotionally to social situations whereas masculine individuals respond relatively conscientiously to social situations. In fact, the core thus gives a summary of all interactions among the three sources of variation present in the three-way data under study, that is, the individuals, behaviors, and situations.

To more completely understand the model, it seems useful to follow how the actual scores are created from the component matrices and the core. For instance, the score of Claus (who is entirely masculine) on sensitive (which is pure emotionality) when at a family picnic (which is an entirely social situation) can be read directly from the core (masculinity, emotionality, social situations), and is 1.0. Similarly, the score of Anne (who is entirely feminine) on sensitive (which is pure emotionality) when meeting a new date (which is a mixture of 0.3 × performance situation and 1.2 × social situation) is 0.3 × 0.0 (score of feminine persons on emotionality in performance situations) + 1.2 × 3.0 (score of feminine persons on emotionality in social situations) = 3.6. All scores can be reconstructed in this way (up to rounding error). These reconstructions illustrate the adequacy of the 3MPCA description, as well as the usefulness of the core to capture the most important information in the data in a conceptually convenient form.

Analogous to what is the case in two-way PCA, in 3MPCA the matrices **A**, **B**, and **C** can be rotated orthogonally or obliquely. In PCA, one usually rotates **B** to simple structure and compensates for this by a related transformation of **A**. In 3MPCA, all matrices **A**, **B**, and **C** can be rotated independently, provided that such rotations are compensated for in the core. This can be exploited by a searching simple structure not only in **B** but also, for instance, in **C**.

One may note, however, that in practice it will not always be possible to find components that meet the principle of simple structure. For the individuals, especially, one may often find several continuous dimensions on which a person may jointly take high values, rather than clearly discrete, nonoverlapping clusters. Even then, however, if one does find useful and well-interpretable components for the response

Table 4
Component Values of Situations (**C**) *Resulting From a 3MPCA That Describes the Data in Table 1 Perfectly*

C: Situation	Performance situations	Social situations
Doing an exam	1.0	0.0
Giving a speech	0.8	0.2
Family picnic	0.0	1.0
Meeting a new date	0.3	1.2

Note. The components have been labeled by the interpretations given to them on the basis of the component values. 3MPCA = three-mode principal components analysis.

Table 5
Core (G) Resulting From a 3MPCA That Describes the Data in Table 1 Perfectly

	Performance situations		Social situations	
G: Core	Emotionality	Conscientiousness	Emotionality	Conscientiousness
Femininity	0.0	3.0	3.0	0.0
Masculinity	0.0	2.0	1.0	1.0

Note. The components have been labeled by the interpretations given to them on the basis of the component values. 3MPCA = three-mode principal components analysis.

variables and the situations, 3MPCA can already lead to interpretable results that give insight in the full three-way data set, as will be illustrated in the section Three-Way Analysis of S-R Inventory Data.

The 3MPCA model is usually fitted in the least squares sense, that is, by minimizing

$$\sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K}\left(x_{ijk}-\sum_{p=1}^{P}\sum_{q=1}^{Q}\sum_{r=1}^{R}a_{ip}b_{jq}c_{kr}g_{pqr}\right)^2 \quad (3)$$

over **A**, **B**, **C**, and **G**. The fit is calculated as the sum of squares of the approximations to the data—i.e., the sum of squares of the values

$$\hat{x}_{ijk}=\sum_{p=1}^{P}\sum_{q=1}^{Q}\sum_{r=1}^{R}a_{ip}b_{jq}c_{kr}g_{pqr}.$$

This sum of squares is often divided by the total sum of squares so as to obtain a *fit proportion*

$$\left(\frac{\sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K}\hat{x}_{ijk}^{2}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K}x_{ijk}^{2}}\right)$$

or *fit percentage* on multiplying the fit proportion by 100. For reasons of simplicity, **A**, **B**, and **C** are usually constrained to be orthogonal, which can be done without loss of generality as it does not affect the optimal fit to be attained. A least squares algorithm for minimizing Expression 3, and hence maximizing the fit, has been proposed by Kroonenberg and De Leeuw (1980). A variant of this algorithm is implemented in the program called Tucker3.m, which runs under MATLAB (MATLAB, 1994) and which is freely available from Henk A.L. Kiers; for commercial software with more refined output possibilities, we refer to 3WAYPACK (see http://www.fsw.leidenuniv.nl/~kroonenb/).

PARAFAC

In 3MPCA, the core can describe any form of interaction between summarized individuals, variables, and occasions. PARAFAC (Carroll & Chang, 1970; Harshman, 1970) can be easily explained as a constrained variant of 3MPCA, in which each person component is related to only one variable component and only one situation component. Specifically, PARAFAC can be seen as 3MPCA with the core array fixed to a unit superdiagonal array, that is, an array with g_{pqr} = 1 if $p = q = r$, and $g_{pqr} = 0$ otherwise. Thus, in PARAFAC all cross-relations between components are eliminated, which makes the model considerably more restrictive than 3MPCA. If this restriction is tenable, however, it does have an important implication: The PARAFAC model has a unique solution, and the components found are to be interpreted without recourse to rotations.

The Three-Way Analysis Process

In the following section seven main steps are discussed: (a) three-way analysis of variance (ANOVA), to assess whether a three-way analysis is indicated; (b) preprocessing the data; (c) balancing fit and parsimony to choose the numbers of components; (d) a detailed study of fit and residuals; (e) choosing a (simple structure) rotation; (f) studying the stability of a solution; and (g) interpreting and reporting the solution. All these steps have been implemented in the program Tucker3.m, guiding the user through each step.

The main steps of a three-way analysis are given in the flowchart in Figure 1. Standard preliminary steps, like inspecting frequency distributions, searching and eliminating outliers, and dealing with missing data, are not discussed here, but we emphasize that in practical data analyses such preliminary steps should not be ignored and may be most revealing.

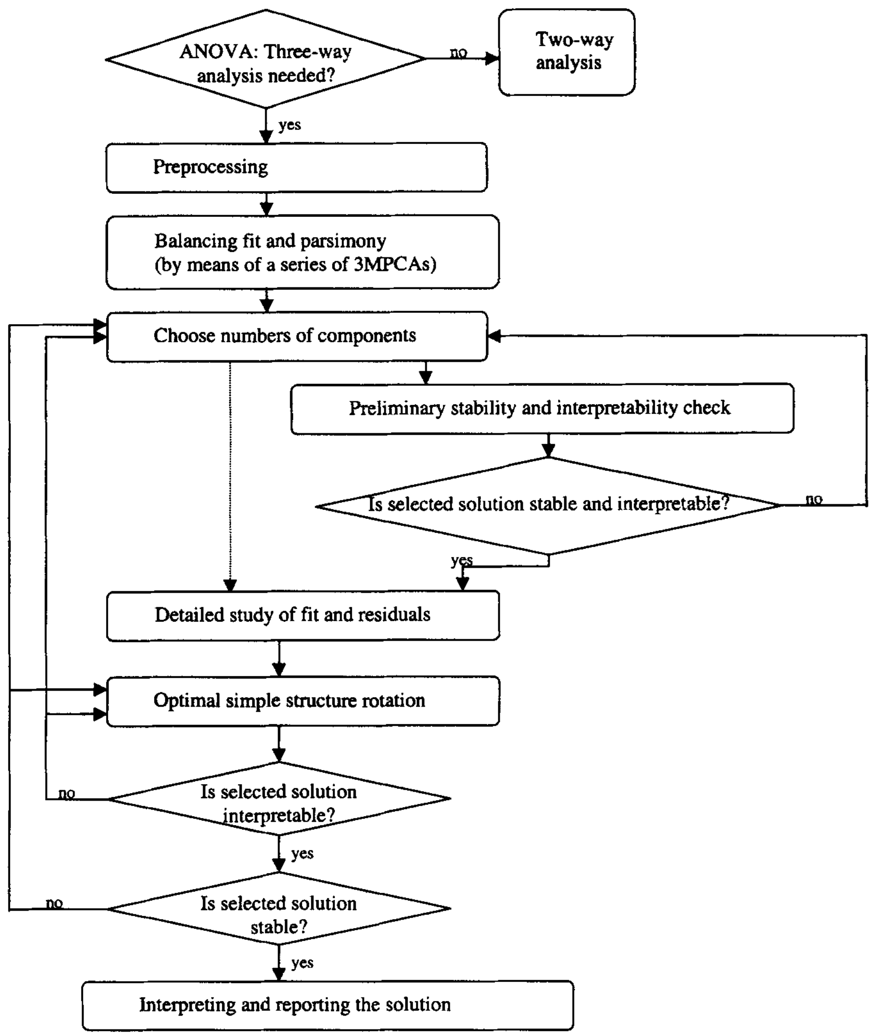

Figure 1. Flowchart for the three-way analysis process. Arrows pointing upward indicate the iterative nature of the analysis process. The dashed arrow indicates that this path will sometimes, but not always, be taken. ANOVA = analysis of variance; 3MPCA = three-mode principal components analysis.

Three-Way ANOVA

As has been mentioned, three-way analysis is indicated in cases in which the data contain a nonnegligible three-way interaction across the three data modes. For example, if all individuals showed roughly the same response patterns with respect to all variables and situations, one could simply take the averages across individuals and analyze the pattern of average responses in all situations with respect to all variables. In general, to inspect whether two-way analysis on data aggregated over one mode would suffice, it is recommended to carry out a simple fixed-effects three-way ANOVA on the three-way data table (using the three different modes as factors), to assess the effect size of all variance components (in which the total variance to be explained is the variance of all data elements with respect to the grand mean). If virtually all information is captured by main effects and at most a single two-way interaction (e.g., between the B and C mode), there is little reason to use a three-way analysis and it suffices to report the main effects and study the interaction (possibly using a two-way PCA on data averaged over the participants [A mode]). However, if two or three substantial two-way interactions are present, one would need two or three different two-way PCAs, whereas a single three-way analysis could be used to represent all these interactions. Furthermore, if substantial three-way interactions are present, these can only be captured by three-way analysis. Hence, as soon as more than one substantial two-way interaction is found, three-way analysis is indicated. The decision as to whether an interaction is "substantial" should be based on effect sizes, not on significance tests, because nonsignificance of an (interaction) effect certainly does not imply that it is absent but only that its presence could not be reliably confirmed given the present sample. Moreover, because there are no replications in this ANOVA design, the three-way interaction is confounded with the error terms, so it is impossible to test the significance of the three-way interaction. Note, however, that in a later stage of three-way component analysis, a stability analysis verifies if the results are reliable or if they are based to a too-large extent on random fluctuations.

Preprocessing the Data

A decision to be made before a three-way analysis is whether to analyze the raw data or some preprocessed version thereof. In two-way PCA, most often the correlation matrix is used, which means that, implicitly, the data are used in their standardized form (centered and normalized to equal sums of squares, per variable, across individuals). In three-way analysis, no such standard rules prevail and it is necessary to carefully decide on any preprocessing steps to be taken. First of all, it should be noted that an analysis without any preprocessing will often be debatable: The 3MPCA model, based on taking triple products of component values, implicitly assumes that the modeled data are treated as ratio-type measurements. Usually, it is more realistic to consider the data as measured on an interval scale or as a ratio scale with an unknown neutral point. For instance, in the case of Likert scales with labels such as *fully disagree* to *fully agree,* measurements take values 1 through 5, with the neutral point perhaps at 3 or at some other value between 1 and 5. If these neutral points are known, one can simply subtract them and analyze the data in deviation from their neutral values. For instance, the midpoints of semantic differential scales could be considered neutral points, and hence one can subtract these from the data to get data at or close to ratio level. Often, however, neutral points are not known. For that reason, in the case of two-way data, data are often analyzed in deviation from their means. This is not only a useful approach in cases in which the mean is considered a good estimate of the neutral point. It is also useful in cases in which the neutral point is unknown but in which there is reason to believe that, with respect to some neutral point, the PCA model holds in a limited number of dimensions (see Harshman & Lundy, 1984). This can be seen as follows.

Suppose the data can be described as $x_{ij} = \Sigma_r a_{ir} b_{jr} + \mu_j$, where μ_j denotes the unknown neutral point for variable j and $\Sigma_r a_{ir} b_{jr}$ gives a PCA model for these data. Then, centering the columns of $\mathbf{X}$ (i.e., by subtracting the means over the individuals) leads to $x_{ij} - x_{.j} = \Sigma_r (a_{ir} - a_{.r}) b_{jr}$, where the subscript "." denotes taking the mean over the individuals; note that μ_j vanishes because the mean of μ_j over the individuals equals μ_j, and hence, these terms cancel upon subtraction. Thus, applying PCA to column-centered data with unknown neutral points gives a PCA solution in which the component scores are centered versions of the original component scores and the loadings are equal to the original loadings. Clearly, centering serves to eliminate the "offset terms" that represent the neutral points.

When using three-way models, a strictly parallel situation holds: Neutral points (which may be unknown) can be eliminated by centering over a single mode while the component matrices are affected only by a mere centering (just as the component scores in $\mathbf{A}$ were centered above). For instance, if $x_{ijk} = \Sigma_p \Sigma_q \Sigma_r a_{ip} b_{jq} c_{kr} g_{pqr} + \mu_{jk}$, then centering over i (i.e., over the individuals), hence subtracting $x_{.jk}$ from the data, eliminates the offset terms. In cases in which neutral points can be expected to differ only across variables (and hence can be written with only one subscript as μ_j), one can eliminate them not only by centering over the individuals (i.e., subtracting $x_{.jk}$) but also by centering over the situations (by subtracting $x_{ij.}$). In practice, variables often have different scale labels and thus can be expected to have different unknown neutral points. Furthermore, it is often assumed that the individuals interpret the scales in (at least roughly) the same way, which could be translated into the assumption that neutral values can be written as μ_{jk} (i.e., the same for all individuals). Whether they are the same for all situations (i.e., whether μ_{jk} can be replaced by μ_j) is no longer important, because simply centering the data over the individuals (i) eliminates the offset terms in either case. If individual differences in response tendencies are deemed too important to ignore, one could consider that the data contain offset terms that differ across individuals (e.g., μ_{ij}). In general, offset terms will be assumed to be equal across at least one of the modes (because otherwise the data x_{ijk} would be indistinguishable from the offset terms μ_{ijk}), and they can be removed by centering over that very mode.

A second type of preprocessing is meant for eliminating artificial scale range differences as well as for equalizing importance of entities (e.g., variables) in an analysis. When entities are conceived to be measured on ratio scales but with considerably differing ranges (e.g., pulse rate, blood pressure, and adrenaline level), the ones with the largest ranges will influence the solution more than those with the small ranges. Such effects are often undesirable and can be eliminated by simply rescaling the variables. In two-way analysis, one often standardizes the variables for this reason. In three-way situations, such normalizations can be applied per entity of a mode by dividing by the square root of the sum of squared elements associated with this entity. For example, one may normalize the (centered) scores on each variable to a unit sum of squares by dividing the scores on this variable by the square root of the sum of squares of the scores of all individuals in all situations $(\Sigma_i\Sigma_k x_{ijk}^2)^{1/2}$ on this variable. Alternatively, one could normalize the scores for all situations or for all individuals to have equal sums of squares (by dividing by $(\Sigma_i\Sigma_j x_{ijk}^2)^{1/2}$ or $(\Sigma_j\Sigma_k x_{ijk}^2)^{1/2}$, respectively). However, one should not normalize combinations of entities of different modes—for instance, variables and situations—because that not only equalizes the influences of the different variables and situations but it also modifies the data in a nontrivial way (see Harshman & Lundy, 1984, for a technical explanation of this), which distorts the underlying three-way structure.

After preprocessing, 3MPCA (or PARAFAC) can be applied to the usually centered and subsequently normalized data. If the data have been centered over the individuals, we then find estimates for $\mathbf{A}_c$ (i.e., the columnwise-centered matrix with elements $a_{ip} - a_{.p}$), **B**, **C**, and $\underline{\mathbf{G}}$. Thus, we do not have estimates for the actual matrix **A**, nor for the offset terms. Procedures for estimating these are currently under investigation but are ignored in the present article, because often the information in the centered version of **A** suffices (e.g., to compute correlations).

Balancing Fit and Parsimony to Choose the Numbers of Components

In choosing how many components to use for describing one's data, three different criteria can be considered: (a) balancing fit and parsimony, (b) interpretability, and (c) stability. In general, one may note that the use of those criteria and the weighting thereof imply, to an important extent, subjective decisions, although these decisions do involve some objective measures (amount of fit, amount of parsimony). The choice for a model should thus be seen as a subjective and free choice among an infinity of alternative possibilities, limited only by certain side conditions (e.g., not choosing equally parsimonious or interpretable models, which clearly fit more poorly). In this respect, descriptive data analysis is similar to journalism in that one has an infinity of possibilities for describing what has happened—limited, however, by the requirement that the descriptions be in line with all undebatable facts available. In a data analysis, the situation is not essentially different, except that the researcher's motivation for his or her choices must be made explicit. These motivations should not only clarify the researcher's preferences in choosing a model but should also clearly serve to distinguish undebatable facts (e.g., degree of fit, degree of stability, degree of parsimony) from subjective choices (what balance between fit and parsimony is chosen, how components are interpreted). In the remainder of this section, we discuss only some issues related to parsimony and fit. Interpretability and stability are discussed in later sections.

As mentioned in the *3MPCA* subsection of Three-Way Component Analysis Techniques (following Expression 3), the (global) fit of the model is defined as the sum of squares of the approximations to the data, often divided by the total sum of squares of the data to obtain a fit proportion (or percentage). Obviously, the chosen model should have a reasonable fit to the data, but usually it is hard to establish what is reasonable. Because the typical goal of the analyses is to describe the most important information in the data and to distinguish it from noise, in situations with much noise small amounts of fit can be reasonable, whereas in situations with little noise only models with very high fit values are useful. In practice, we do not know the amount of noise present in the data; thus, as far as fit values are concerned, we can use these only to compare different models and not in an absolute sense.

Using only fit values would lead to choosing the most complete and thus the most complex model, whereas in practice we wish to settle for a useful compromise between amount of information accounted for and parsimony of the model used. How one balances parsimony and fit depends on the purpose of the analysis of the data at hand and cannot be determined on the basis of external criteria. Thus, in this respect the choice of the model has a highly subjective aspect. As a guideline for this choice one may use the scree test (see Cattell, 1966) or a variant of it specially designed for 3MPCA by Timmerman and Kiers (2000). In the latter variant of the scree test, 3MPCA analyses are carried out for a large number of different triples of numbers of components (P, Q, R; e.g., all triples obtained by letting P, Q, and R run from 1 through 6), and the fit percentages for these triples are recorded. (In Tucker3.m such a series of analyses can be done with a single command and within a limited amount of time.) Next, solutions based on the same total number of components (i.e., $P + Q + R$) are compared, and the best of these are selected. The selected solutions are ordered with respect to the total numbers of components, and a scree test is applied to these by searching for those numbers of components that correspond to a considerable fit increase compared with the best solution with one component less but for which adding more components gives relatively small increases. This is illustrated below in detail in the section Three-Way Analysis of S-R Inventory Data.

Detailed Study of Fit and Residuals

On the basis of the balance of fit and parsimony, we get one or more solutions that may be useful as descriptions of the data. For these, it is useful to further study the model fit by partitioning the fit over the entries of the modes and by studying residuals.

Partitioning of fit. In addition to the fit of the full model, we can compute the partitioned fit for each entity of each mode (Ten Berge, De Leeuw, & Kroonenberg, 1987) and express this with respect to the total sum of squares of the data elements pertaining to this entity. This gives insight into which aspects of the data are represented well and which are not. If for certain entities poor fits are found, this may be caused both by relatively large amounts of noise for the associated data and by incomplete modeling of the data.

Analysis of residuals. To study to what extent a model is "complete," one can study the residuals ($x_{ijk} - \hat{x}_{ijk}$), that is, those aspects of the data not covered by the full model for the data. In this respect, rather than inspecting all residuals separately it is useful to search for structure in the residuals by means of PCAs on residuals collected in two-way matrices that may be set up for each of the three modes; for instance, one such matrix of residuals is set up to have the individuals in the rows and all combinations of variables and occasions in the columns, and a PCA may be carried out on this $I \times JK$ matrix of residuals. If strong components are found for these residuals, the model may be incomplete and description of the data may benefit from the use of additional components accounting for the structure in the matrices of residuals. It should be noted, however, that such components are rather complex because they pertain, for instance, to combinations of variables and occasions; hence, for simplicity, one may be satisfied with a model that still has some (but not too much) structure in the residuals.

Optimal Simple Structure Rotation

Clearly, because the goal of the three-way analyses as discussed here is description of the data, interpretability is of utmost importance: Uninterpretable solutions have no descriptive value whatsoever. The interpretability of a solution depends not only on the parameter values in the model but also on substantive theorizing, and it depends on the experience as well as the interest of the researcher. Thus, the interpretability criterion introduces a large amount of subjectivity into the choice of a model.

As has been mentioned earlier, the 3MPCA solution is by no means unique. Equivalent descriptions of the data can be obtained by rotations of **A**, **B**, and **C** when these are compensated for in the core. The next step in a three-way analysis (see Figure 1), therefore, is to choose among all such equally fitting representations—those solutions that are easiest to interpret. Sometimes, interpretability can be enhanced by transforming component matrices to optimally resemble target matrices, but if these are not available, rotation of the component matrices, of the core, or of both to optimal simplicity (in the sense of having parameters with absolute values that are as small or as large as possible) is recommended. For this purpose, in the case of two-way PCA, one often uses Kaiser's (1958) varimax orthogonal rotation (applied to the component loadings), but oblique rotations have also been proposed and are frequently used.

In 3MPCA, one may wish the three component matrices to be easily interpretable, and it is often useful if the core is simple as well. Although simplicity of each of the component matrices can be optimized independently, for the core to be simple one has to strike compromises between simplicity of the core and of the component matrices. The desired simplicity of each of the component matrices and of the core may differ between situations. Kiers (1998) has proposed a procedure for orthogonal rotation of the component matrices and the core so as to optimize any desired weighted sum of simplicity values for the component matrices and the core. Specifically, the criterion optimized over rotations of **A**, **B**, **C**, and $\underline{\mathbf{G}}$ is $w_aS(\tilde{\mathbf{A}}) + w_bS(\tilde{\mathbf{B}}) + w_cS(\tilde{\mathbf{C}}) + S(\tilde{\underline{\mathbf{G}}})$, where w_a, w_b, and w_c denote the relative simplicity weights for the component matrices in relation to simplicity of the core; $S(.)$ denotes a simplicity criterion value (e.g., the varimax value, normalized such that it is comparable across matrices of different size; see Kiers, 1998) for the matrix or core between parentheses; and $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$, and $\tilde{\underline{\mathbf{G}}}$ denote the rotated versions of **A**, **B**, **C**, and $\underline{\mathbf{G}}$. Thus, a relative weight smaller than 1 indicates that simplicity of the component matrix at hand is deemed less important than simplicity of the core, whereas values above 1 indicate that its simplicity is deemed more important than that of the core. Now, by optimizing this criterion over all possible rotations, high joint simplicity of all parts of the solution is attained in which, by varying the choice for the simplicity weights, one can ensure that simplicity of particular parts of the solution is given priority (e.g., by choosing large w_b and w_c and small w_a, the rotation will aim at high simplicity of **B** and **C**, if necessary at the cost of simplicity of **A** and $\underline{\mathbf{G}}$).

A procedure to systematically choose the relative weights is as follows. First, one should decide whether some component matrices need not be made simple at all, and for these the relative weight is set to 0. The remaining relative weights can then be varied systematically by trying a range of values while keeping the other values fixed. For instance, supposing no simplicity of the **A** is desired, one may start using $w_a = 0$, $w_b = 1$, and $w_c = 1$ and then gradually increase w_b. By inspecting the simplicity values (e.g., varimax values) for the different solutions, one will see that the simplicity of **B** gradually increases at the cost of that of **C** and $\underline{\mathbf{G}}$. One then selects a value of w_b after which simplicity of **B** hardly increases but simplicity of **C** and $\underline{\mathbf{G}}$ starts decreasing considerably. Similarly, one may fix w_b and gradually increase w_c. Also, if further simplicity of the core is desired, one may gradually decrease the values of w_b or w_c. It should be kept in mind that deciding on the weights to be used is not very critical: All rotated solutions are equally good in terms of fit, and the procedure is only meant to find a rotation that leads to a well-interpretable solution. Small variations in the weights will lead to somewhat differently rotated solutions, but these lead to virtually the same interpretation. Procedures for computing and comparing optimal simplicity values for a whole range of weights at once are available in Tucker3.m. A detailed illustration of this procedure has been given by Kiers (1998); the procedure is also mentioned, but in less detail, in the section Three-Way Analysis of S-R Inventory Data.

The above rotation procedure is limited to orthogonal rotations and as such leaves the component matrices orthogonal. However, sometimes nonorthogonal ("oblique") component matrices can be used to get more easily interpretable solutions. In particular, obliqueness of one component matrix can be profitable to simplify the interpretation of the other component matrices and the core. Therefore, if one component matrix does not have to be made simple, it can be useful to rotate this particular matrix obliquely rather than orthogonally. A useful form of oblique rotation can be carried out fairly easily with the above-described orthogonal rotation procedure, as follows. We start by rescaling the core such that it has unit sums of squares rowwise (i.e., we divide each element g_{pqr} by $\sigma_p = (\Sigma_q\Sigma_r g_{pqr})^{1/2}$), and we compensate for this by (inversely) rescaling the columns of **A** (i.e., by multiplying each element a_{ip} by σ_p). Second, an orthogonal simplicity rotation procedure is applied to the ensuing core and component matrices. Finally, the rotated **A** is normalized back to unit column sums of squares (i.e., by division of each element a_{ip} by $\sigma^*_p = (\Sigma_i a_{ip})^{1/2}$), and this is compensated for in the core (i.e., by multiplying each element g_{pqr} by σ^*_p). This procedure is very similar to the procedure used in Harris and Kaiser's (1964) "orthoblique" rotation. As in their procedure, this rotates **A** obliquely; thus, the columns of **A** will no longer be orthogonal.

The above oblique rotation procedure is particularly useful in cases in which the core has only a few large elements, corresponding to only one component (or to a few components) in **A**. In such cases, rotation of the core may not be able to redistribute the large core values in the rows corresponding to the first A-mode component(s) over the complete set of rows, and hence it does not reach simple structure. After first normalizing the rows of the core to unit sums of squares, however, it usually is indeed possible to find a relatively simple structure. This simple structure is left intact after "renormalization," and the only adverse effect is the nonorthogonality of the A-mode components. However, the nonorthogonality is only natural because in cases in which the data can to a large extent be summarized by one general A-mode component, the other A-mode components only serve to summarize differences in the A-mode entities in terms of some fine nuances (expressed in deviation from the general component). Such fine nuances typically pertain to aspects that are distinct conceptually but correlated rather strongly across individuals. The simple structure rotation redirects the A-mode components such that they describe these aspects themselves (rather than a general component and some components describing deviations between these aspects and the general component). As these aspects are correlated rather strongly, so are the associated rotated components.

It is possible that for the given numbers of components no interpretable solution can be found whereas a clearly interpretable solution can be found with either fewer or more components. In that case, one has to reconsider one's choice for the numbers of components (see the associated upward arrow in Figure 1) and must for the ensuing numbers select the best interpretable solution.

Studying Stability

Having found a well-fitting and interpretable solution, the next question is whether this solution is stable over trivial fluctuations in the sample. Stability is related to generalizability: Does the solution hold not merely for the present sample but also for other samples from the same population—that is, does it hold for the whole population? Usually, a solution is not deemed sensible if it is not reasonably stable over trivial modifications of the sample. Therefore, stability or generalizability is not a criterion that can be used in combination with the other criteria to find a best compromise: Reasonable stability should be used as a *sine qua non;* hence, a solution chosen should be maintained only if it is reasonably stable under trivial changes in the data. If it is not sufficiently stable, one should reconsider either the choice for the numbers of components or the choice for the simple structure rotation (see the associated upward arrows in Figure 1).

In practice, the stability or generalizability issue is a difficult one, first of all because it is hard to establish the appropriate population to generalize to (e.g., all possible individuals for the particular variables in the particular situations at hand, or all possible situations for the individuals and variables at hand, etc.). Here, we studied only stability across the entities of one mode, usually the individuals. Second, such inferences can only be made on the basis of assumptions, which, again, introduce subjective decisions. A more modest approach is to limit oneself to the data set at hand and only consider to what extent a model is stable, for instance, when the set of individuals is randomly split into two subsets of equal size (split-half procedure), when certain individuals are deleted from the total set (as in a jackknife procedure), or when there is a different composition of the set of individuals (as in bootstrap procedures). Similarly, split-half, jackknife, and bootstrap methods could be applied to variables or situations to study the stability of the results across different variables and situations (ideally, variation will be high). However, such studies are not very reliable in cases of small numbers of variables and situations. One may note that the jackknife and bootstrap procedures are based on resampling techniques (see, e.g., Efron & Tibshirani, 1993), which involve many complete reanalyses. Despite their potential usefulness for getting proper insight in the stability of the results, here we avoid complications and practical problems with resampling techniques and limit ourselves to the more practicable split-half procedure (for an extensive description of this procedure in the PARAFAC case, see Harshman & DeSarbo, 1984). It is worth mentioning that the outcome of the stability tests, as any accuracy measurement, will to some extent depend on the sample size (number of individuals). In case of very small samples (say, smaller than 20), resampling techniques as well as the split-half procedure will often indicate that the results are not very stable, simply because the subsamples used will easily differ considerably. This, however, is no reason not to use stability analysis in small- or moderate-size sample situations. To the contrary, these are the very situations in which stability is an issue, whereas in cases of very large samples there is little reason to study stability because one can expect to find stable results in almost any case. However, one should be careful in interpreting the outcomes of stability studies based on very small samples, because it is difficult to assess the stability accurately on the basis of very small samples (just as the accuracy of standard error estimates is small when these are based on small samples).

The split-half procedure starts by splitting the data into two halves by randomly partitioning the entities of one of the modes, usually the first mode pertaining to the individuals. In such a situation it is expected that any structure in **B** and **C** should be present for all subsets of the individuals. Thus, two half samples obtained by randomly assigning the individuals to two equally sized subsamples should give comparable three-way analysis solutions, as far as **B** and **C** are concerned. However, in 3MPCA, rotational indeterminacy may make solutions for different splits differ artificially. To eliminate this indeterminacy, several possibilities are available, each with its pros and cons. Here we propose to use the solution for the full data set (which has been made interpretable in the previous step) as a point of reference. We next rotate the solutions for **B** and **C** for the two splits optimally toward their full data set counterparts. For this purpose, we regress the full-sample component matrices on the subsample component matrices (i.e., by means of multiple regression), which boils down to a (possibly nonorthogonal) rotation of the subsample component matrices. To compare the rotated solutions of the splits, we propose to inspect Tucker's (1951) congruence coefficients (measuring proportionality of columns) for corresponding columns of the component matrices **B** and **C**. According to guidelines mentioned by Ten Berge (1986), congruence coefficients of .85 or more are considered to indicate stable solutions: Apparently, then, in each subsample, solutions for **B** and **C** can be found that are very similar to the full-data solutions for **B** and **C**. Congruence coefficients of .70–.85 are considered to be of intermediate value, and in such cases it is advisable to also verify whether the interpretations of the components in the two subsamples are different.

A study of split-half stability for the core can be carried out in several ways. One approach is to study to what extent the components obtained in the full set lead to the same optimal core matrices in the two subsets. To this end, we use the full-data component matrices **B** and **C** and we split the full-data component matrix **A** into submatrices $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(2)}$, using in each submatrix only the rows of **A** that are associated with the A-mode entities used in the split at hand. Now, to test the stability of the core, we first compute the core that leads to the best 3MPCA fit to the data of Subsample 1, using $\mathbf{A}^{(1)}$, **B**, and **C** as (fixed) component matrices. Hence, we search for the core array $\underline{\mathbf{G}}$ that minimizes Expression 3 using for x_{ijk} only the data values corresponding to the first subsample and keeping the component matrices fixed. Next, we similarly compute the core that leads to the best 3MPCA fit to the data of Subsample 2 by using $\mathbf{A}^{(2)}$, **B**, and **C** as (fixed) component matrices (again minimizing Expression 3, now using for x_{ijk} the data values corresponding to the second subsample). If the thus-computed cores are similar (e.g., in terms of absolute differences between corresponding elements of the cores), we conclude that the components for the full data set—which were well interpretable and appeared to be good summarizers for the whole data set—lead to stable core values, so that the conclusions based on the core values can be considered reliable or at least not very sensitive to sample fluctuations. Other, stronger ways of checking stability are possible, but the present one may suffice for most practical purposes.

Interpreting and Reporting the Solution

Having decided on which solution to retain as a useful description of one's data, one is in a position to interpret and report the results. First, interpret the components for all modes or for only the simple modes. Next, the core can be used to summarize the main interactions in the data. For interpretation of the component matrices **A**, **B**, and **C**, it should be noted that the component values can be compared only within components. Specifically, the component values are simply normalized to unit sums of squares columnwise; in this respect they differ, for instance, from component loadings in two-way PCA that in the orthogonal case can be interpreted as correlations between variables and components. The interpretations of the components, however, are not influenced by this normalization, because the interpretation of a component depends only on the relative differences of component values with respect to that component. Thus, whether a variable or situation is well represented cannot be read from these component values but should be read from the fit percentages that can be computed per A-mode, B-mode, and C-mode entity (see the *Balancing Fit and Parsimony to Choose the Numbers of Components* section).

As far as interpretation of the core is concerned, it should be noted that the core contains values that describe the full three-way data, reduced to the summarizing descriptions given by the components for the three modes. For example, the core value associated with components A1, B2, and C3 (A1 denoting the first A-mode component, etc.) indicates how a person scoring high on A1 responds to a variable associated strongly with B2, in a situation captured well by C3. Therefore, the core array summarizes the information in the original three-way array and will contain main effects and two- and three-way interactions, provided that these are present in the original three-way array. To interpret the core, it can therefore be helpful to draw line plots to visualize two- and three-way interactions. For instance, these plots can consist of a set of lines, one for each combination of an A-mode and

B-mode component and connecting core values for the respective C-mode components, as demonstrated in the example in the Three-Way Analysis of S-R Inventory Data section.

The core values can be compared meaningfully with each other. In fact, when all component matrices are orthogonal, the squared core values give the contributions of the associated combination of components to the total fit. When not all component matrices are orthogonal, this simple interpretation is no longer valid; however, interpretation of the sizes of the core values can be carried out, for instance, by inspecting contributions due to combinations of two (rather than three) components, as described in the example analysis in the next section.

When the simple structure rotations are successful, the interpretation of the solution can be done fairly easily with tabular information only, on the basis of which components are interpreted. Sometimes, however, the components are not easily interpretable. In such cases it may be more useful to plot several aspects of the 3MPCA solution. As described in detail by Kiers (2000), several possibilities exist: One may plot the entities of one mode only, plot combinations of entities of two modes and superimpose the entities of the third mode, or plot entities of two modes jointly, for each of the entities of the third mode (so-called "joint plots"; see Kroonenberg, 1983, pp. 164–165). An illustration of the last option is given in the Three-Way Analysis of S-R Inventory Data section.

Preliminary Stability and Interpretability Check

As a final note, we remark that in practice it is not very efficient to determine the most interpretable solution before one has any insight into the stability of such solutions. A quick preliminary check on stability and interpretability is therefore recommended. This check is to be carried out immediately after every choice of the numbers of components and proceeds as follows: First, rotate only parts of the solution to simple structure (e.g., rotate the component matrices for the variables and the occasions by varimax, when these are to be made well interpretable). Then study the stability of this rotated solution. If the solution is stable, it can be expected that a solution found by a more refined simple structure rotation will be similarly stable; if it is not stable, a solution rotated by a more refined method would probably also not be stable. Furthermore, if the rotated component matrices are not well interpretable, there is little reason to believe that a more refined rotation procedure would lead to an interpretable solution. This is because the more refined rotation procedure would simplify the overall solution (notably also the core) but could not further simplify the already optimally simple component matrices found with varimax. If this simple procedure shows that for the selected numbers of components a stable and interpretable solution can be obtained, one can take the trouble to carry out a more detailed study of the fit and determine which rotation gives the best interpretable solution. If the check turns out to give a negative result, a new solution (using different numbers of components) is to be determined (see Figure 1).

Three-Way Analysis of S-R Inventory Data

In this section a detailed analysis is given of an empirical three-way data set. In the analysis, we follow the steps described in The Three-Way Analysis Process section and displayed in Figure 1. The steps to be taken can be followed most easily in that flowchart. For details on the descriptions of the different steps, the reader may refer back to the relevant subsections of The Three-Way Analysis Process.

Problem and Data

The data analyzed in the present study have been collected in a contextualized study of personality (Van Mechelen & Kiers, 1999), that is, a study of individual differences in the personality domain that explicitly takes into account the situational context in which personality-relevant behaviors occur. The primary goal of that study was the search for parsimonious summary descriptions of individual differences in behavioral profiles across situations.

The data[1] are scores of 140 participants on the S-R Inventory of Anxiousness (developed by Endler, Hunt, & Rosenstein, 1962, and translated into Dutch for the present study). The inventory contains 14 anxiety-related responses to be rated for 11 different stressful situations. Back-translated and abbreviated descriptions of the responses are "heart beats faster," "uneasy feeling," "emotions disrupt action," "feel exhilarated and thrilled," "not want to avoid situation," "perspire," "need to urinate frequently," "enjoy the challenge," "mouth gets dry," "feel paralyzed," "full feeling in stomach," "seek experiences like this," "need to defecate," and "feel nausea." Back-translated

[1] We are grateful to Maes, Vandereycken, and Sutren at the University of Leuven, Leuven, Belgium, for collecting these data.

and abbreviated descriptions of the situations are "auto trip," "new date," "psychological experiment," "ledge high on mountainside," "speech before large group," "consult counseling bureau," "sail boat on rough sea," "match in front of audience," "alone in woods at night," "job interview," and "final exam." Each response had to be rated on a 5-point scale (1–5), with the labels along the scales specific to each of the scales and the label for 5 always pertaining to the most anxious reactions. However, to simplify interpretation of reactions, scales with positive, abbreviated descriptions (such as feel exhilarated) have been reversed (1 = 5, 2 = 4, . . ., 5 = 1) in all analyses. For example, for heart beats faster, 1 = *not at all* and 5 = *much faster;* for feel exhilarated and thrilled, 1 = *not at all* and 5 = *very much.*

Preliminary Analyses

As a first step in the three-way analysis of the data, the frequency distributions for all S-R combinations were inspected. Not surprisingly, some of these distributions were considerably skewed. However, the distributions for the same response differed considerably over situations and therefore were not deemed artificially skewed. Furthermore, we did not find any clear outliers and there were no missing data, so we saw no reason to adjust the data before the main analyses.

Three-Way ANOVA

Before carrying out a 3MPCA, we checked whether the data could reasonably well be analyzed by means of a two-way PCA on aggregated data. To do this, we performed a fixed-effects three-way ANOVA (see top of flowchart in Figure 1) on the 140 × 14 × 11 three-way data table, after subtraction of the grand mean. From the decomposition into sums of squares given in Table 6 it is clear that there are two sizable two-way interaction terms, as well as the three-way-interaction-plus-error term, which cannot be ignored. In fact, the latter has the highest contribution of all effects. Even though we cannot tell what part of this term is error, it cannot be excluded that an important three-way interaction is present in the data in addition to two important two-way interactions. Therefore, a three-way analysis is clearly indicated here. Moreover, when this reveals stable solutions representing a three-way interaction, we have clear indications that the three-way-interaction-plus-error term pertains to considerably more than error alone.

Table 6
Three-Way Analysis of Variance of Situation–Response Data After Subtraction of Grand Mean, With Individuals, Responses, and Situations as Fixed Factors

Effect	SS	%
Individuals	2,601	6.2
Variables	7,363	17.6
Situations	2,406	5.7
Individuals × Variables	7,160	17.1
Individuals × Situations	2,398	5.7
Variables × Situations	4,904	11.7
Individuals × Variables × Situations + error	15,096	36.0
Total	41,930	100

Note. SS = sum of squares.

Intermezzo: Two-Way PCA on Aggregated Data

Even though the three-way ANOVA pointed out that a 3MPCA of the present data is indicated, to illustrate the incompleteness of a two-way analysis (by offering a baseline that can help illustrate the gains produced by 3MPCA) we averaged the data across the individuals (see Table 7) and carried out a two-way PCA on these averaged data (see Table 8). From the ANOVA reported in Table 6 it can be seen that these averaged data, which only represent the variable and situation main effects, as well as their interaction carry only 35% (17.6% + 5.7% + 11.7%) of the variance in the original data. From Table 7 it can be seen which situations, on average, evoked most anxiousness or exhilaration, and so on. A PCA on these data (after standardizing the data across the situations) led to eigenvalues of 8.49, 3.63, 0.76, 0.61, 0.18, 0.12, 0.10, 0.08, 0.02, 0.01, and 0. From the eigenvalues, it can be deduced that the first two components (accounting for 87% of the variance) capture by far the greater part of the information in the data. We therefore considered only the first two components and subjected these to a varimax rotation. The resulting loadings for the variables and the component scores for the situations are given in Tables 8 and 9, respectively. As is discussed below, the structures obtained are partly related to the 3MPCA component matrices **B** and **C** reported in Tables 11 and 12. In fact, it can be seen in those tables that one of the components for the response scales is split into three different components; the present situation components resemble the 3MPCA situation components even less. All this is a direct implication of the fact

Table 7
Situation–Response Data Averaged Across Individuals

Situation	Heart beats faster	Uneasy feeling	Emotions disrupt action	Feel exhilarated and thrilled	Not want to avoid situation	Perspire	Need to urinate frequently	Enjoy the challenge	Mouth gets dry	Feel paralyzed	Full feeling in stomach	Seek experiences like this	Need to defecate	Feel nausea
	Response scale													
Auto trip	1.92	1.71	1.43	2.21	3.62	1.34	1.54	2.33	1.44	1.19	1.49	2.54	1.09	1.44
New date	4.13	2.99	3.04	2.54	3.24	2.40	1.60	2.71	1.84	1.79	1.66	2.79	1.14	1.39
Psychological experiment	1.39	1.59	1.27	0.91	1.94	1.39	1.17	1.14	1.31	1.16	1.24	0.94	1.08	1.25
Ledge high on mountainside	4.25	3.02	2.11	2.05	2.63	3.31	1.49	2.49	2.17	1.91	1.69	2.46	1.30	1.85
Speech before large group	4.41	3.82	2.97	1.35	1.56	3.43	2.34	1.69	2.96	2.31	2.21	1.41	1.41	2.16
Consult counseling bureau	3.11	3.01	2.20	0.84	1.99	2.43	1.67	0.84	2.19	1.74	1.76	0.81	1.16	1.51
Sail boat on rough sea	3.69	2.58	1.84	2.54	2.99	2.36	1.66	2.76	1.71	1.56	1.69	2.71	1.26	1.99
Match in front of audience	4.09	2.81	2.32	2.03	2.63	2.93	2.03	2.41	2.19	1.80	1.81	2.22	1.19	1.55
Alone in woods at night	3.79	3.56	2.45	1.08	1.35	2.88	1.58	1.35	2.20	2.26	1.93	1.15	1.46	1.64
Job interview	4.26	3.53	2.75	1.34	2.26	3.15	2.10	1.71	2.76	2.04	2.10	1.76	1.32	1.65
Final exam	4.26	3.56	2.72	0.87	1.66	3.22	2.34	1.20	2.41	1.99	2.33	1.15	1.34	1.85
Mean	3.57	2.93	2.28	1.61	2.35	2.62	1.77	1.88	2.11	1.79	1.81	1.81	1.25	1.66

Note. The questionnaire was taken from "An S-R Inventory of Anxiousness," by N. S. Endler, J. McV. Hunt, and A. J. Rosenstein, 1962, *Psychological Monographs, 76*(17, Whole No. 536). Copyright 1962 by the American Psychological Association. Adapted with permission of the author. The data were collected independently. Each response was rated on a 5-point scale, with 5 pertaining to the most anxious or excited reactions.

Table 8
Response Scale Loadings From Principal Components Analysis on Situation–Response Data Averaged Across Individuals

Variable loading	Component 1	Component 2
Heart beats faster	**.94**	.22
Uneasy feeling	**.95**	−.21
Emotions disrupt action	**.86**	.00
Feel exhilarated and thrilled	−.07	**.99**
Not want to avoid situation	**−.41**	**.86**
Perspire	**.95**	−.06
Need to urinate frequently	**.81**	−.11
Enjoy the challenge	.03	**.99**
Mouth gets dry	**.91**	−.25
Feel paralyzed	**.94**	−.20
Full feeling in stomach	**.91**	−.24
Seek experiences like this	−.03	**1.00**
Need to defecate	**.84**	−.23
Feel nausea	**.75**	.09

Note. For emphasis of the larger values, loadings exceeding .30 in the absolute sense are in bold.

Table 9
Component Scores for Situations From Principal Components Analysis on Situation–Response Data Averaged Across Individuals

Situation	Component 1	Component 2
Auto trip	**−.45**	.27
New date	−.01	**.42**
Psychological experiment	**−.64**	**−.38**
Ledge high on mountainside	.10	.25
Speech before large group	**.45**	−.13
Consult counseling bureau	−.13	**−.38**
Sail boat on rough sea	−.04	**.40**
Match in front of audience	.06	.20
Alone in woods at night	.14	**−.31**
Job interview	.25	−.06
Final exam	.27	−.28

Note. For emphasis of the larger values, scores exceeding .30 in the absolute sense are in bold.

that a PCA of the data averaged over individuals does not take into account any individual differences in response profiles across situations—neither in the form of a two-way interaction involving the individuals factor nor in the form of a three-way interaction of individuals, variables, and situations—whereas such interactions have been seen to be potentially very important in this data set. Clearly, if one is interested in summarizing such a three-way interaction, the above results are of no avail and a full three-way analysis is needed.

Preprocessing the Data

Having seen above that a three-way analysis is indicated, we now turn to the second main step (see Figure 1): preprocessing the data. As mentioned in the section on the three-way analysis process, the choice for a preprocessing procedure should depend on the presumed presence of neutral points in the data and on the associated form of the complete model that one supposes to underlie the data; consideration should also be given to whether to weight variables equally. For the present data, we assumed that there was a neutral point or "natural zero" for each response scale that was unknown and may have differed for each scale. The latter characteristic is a consequence of the fact that the response scales have incomparable labels, which makes it unreasonable to assume that the neutral point is at the same location of the 5-point scale for all variables. On the other hand, it does seem reasonable to assume that response scales are considered the same for each situation and thus, that the neutral point for the response scales does not differ across situations. Apart from the uncertainty on the neutral points of the scales, one could worry about possible response style differences among individuals. However, on the basis of the present data alone, these differences cannot be distinguished from real differences between the individuals in global anxiety level; in fact because it seemed likely that differences in global anxiety level were present, we chose to ignore response styles. Hence, we took into account only unknown neutral points for the response scales. As explained earlier, an adequate way of dealing with unknown neutral points is simply to eliminate them by centering over individuals and to fit the three-way model to the preprocessed data. Incidentally, we point out that because the data are centered, sums of squares are proportional to variances. Therefore, rather than defining fit contributions in terms of sums of squares accounted for, we can do this in terms of the more common concept of variance accounted for.

In addition to unknown neutral points, we have to deal with unknown differences in scale range use. In the present study we assumed that any individual differences in use of scale range were real (simply because we cannot distinguish real differences from response styles). Differences in scale-range use of different response scales, on the other hand, can be due to incomparability of the labels for the different scales. To eliminate such unwanted differences, we do normalize the response scales such that, after centering over individuals, the variances of all scores on each scale are normalized to unity (i.e., by dividing all elements $x_{ijk} - x_{.jk}$ by $\sigma_j = (\Sigma_i\Sigma_k(x_{ijk} - x_{.jk})^2/IK)^{1/2}$).

Balancing Fit and Parsimony to Choose the Numbers of Components

The next step (see Figure 1) in a three-way analysis is to balance fit and parsimony to choose the numbers of components. After some preliminary analyses, we soon found that for each mode we would use at least two components. To choose among the multitude of possible 3MPCA solutions, we performed 3MPCAs for all models using two, three, four, five, and six components for each of the modes and computed the associated fit values. We limited our search to six components for practical reasons and afterwards saw that this did not seem a serious limitation. We listed the fit values, ordered according to the value of $P + Q + R$, and checked the highest fit value per value of $P + Q + R$. A subset of all fit values obtained in this way is given in Table 10, where especially for the lower values of $P + Q + R$ different solutions are given (only for illustrative purposes). Using the variant of the scree test proposed by Timmerman and Kiers (2000), we selected four cases (indicated by bold and italics in Table 10) in which the last addition of a component (i.e., moving from $P + Q + R - 1$ to $P + Q + R$) led to a relatively large increase in fit but in which a further increase of the number of components led to a relatively low increase in fit. These were $P = 3$, $Q = 2$, $R = 2$ (fit = 31.3%); $P = 4$, $Q = 2$, $R = 3$ (fit = 34.8%); $P = 5$, $Q = 3$, $R = 3$ (fit = 37.9%); and $P = 6$, $Q = 4$, $R = 3$ (fit = 41.1%).

Preliminary Stability and Interpretability Check for a Number of Solutions

For each of the four above solutions, we carried out a preliminary stability and interpretability check. Specifically, in each case the solution was rotated by varimax applied to **B** and **C** because it was expected that the B- and C-mode components would indeed have an intrinsic simple structure. For these solutions, split-half stability and interpretability were checked only in terms of the component matrices **B** and **C**. In a later stage, stability and interpretability are also studied in terms of the core.

Table 10
Fit Percentages for a Subset of the Results of 3MPCA for Different Numbers of Components Applied to the Situation–Response Data

P	*Q*	*R*	*P* + *Q* + *R*	Fit (%)
2	**2**	**2**	**6**	**27.5**
2	2	3	7	27.7
2	3	2	7	27.7
3	***2***	***2***	***7***	***31.3***
2	2	4	8	27.8
2	3	3	8	28.3
2	4	2	8	27.7
3	2	3	8	31.8
3	3	2	8	31.9
4	**2**	**2**	**8**	**32.2**
4	***2***	***3***	***9***	***34.8***
4	3	2	9	34.4
3	2	5	10	32.1
3	3	4	10	32.8
4	2	4	10	35.2
4	3	3	10	35.5
5	**2**	**3**	**10**	**35.8**
5	3	2	10	35.4
5	***3***	***3***	***11***	***37.9***
6	**3**	**3**	**12**	**39.2**
6	***4***	***3***	***13***	***41.1***
6	**4**	**4**	**14**	**42.0**
6	**4**	**5**	**15**	**42.6**

Note. Rows with the highest fit for each value of $P + Q + R$ are in bold. Rows that, in addition, meet the scree test criterion proposed by Timmerman and Kiers (2000) have also been italicized. 3MPCA = three-mode principal components analysis.

For assessing the split-half stability, the sample of individuals was split into two halves by simply distinguishing the odd and even individual numbers, and the data for both splits were preprocessed and analyzed in the same way as the full data set. It was found that the $P = 3$, $Q = 2$, $R = 2$ solution was not very stable over split halves. Specifically, the second situation component led to a congruence over splits (φ) of .64, and on visual inspection it could be seen that the two splits indeed gave quite different second situation components. Thus, it can be concluded that this solution is unstable (despite the fact that the B-mode components were reasonably stable).

The $P = 4$, $Q = 2$, $R = 3$ solution was considerably more stable. The lowest φ value was .81 for one of the C-mode components, which implies a reasonable stability. This solution therefore merited a follow-up analysis. However, we soon realized that even when optimizing the simple structure rotation, the two-dimensional solution for the response scales could not be satisfactory from a substantive viewpoint: The optimally simple B-mode component matrix displayed a first component pertaining to a mixture of exhilaration-related variables and the distress variables heart beats faster, uneasy feeling, and emotions disrupt action, where the second component pertained to the other physiological anxiety reactions. Although the finding that exhilaration tends to go with certain distress variables is interesting, it seems an oversimplification to merge these into one component. In fact, the earlier results of the PCA on data averaged across individuals indicated that the exhilaration scales formed a subgroup on their own. Therefore, we searched for stable solutions with more than two B-mode components from then on.

The $P = 5$, $Q = 3$, $R = 3$ solution was next inspected, and it was found that it was rather unstable with respect to the B mode (congruences between .70 and .85). Furthermore, the B-mode component matrix was again not well interpretable: Whereas one of the three B-mode components did pertain to the exhilaration-related variables—and this component was reasonably stable—the other two components apparently distinguished between different aspects of physiological anxiety reactions, with different splits yielding different partitionings and each partitioning based on a different merging of three different subgroups of physiological reactions. These results suggested that one more component was needed for the B mode.

Finally, the $P = 6$, $Q = 4$, $R = 3$ solution was inspected. It was found that this solution was reasonably stable: The φ values for **B** were .93, .91, .95, and .90, and those for **C** were .95, .82, and .80. For the relatively unstable second and third C-mode components, we inspected the main component values on these components in each of the splits and found that in both splits, the main component values indicated the same partitioning of situations; the most important difference was that the relatively large negative loading of new date on the third component was recovered to only half the extent in one of the splits and therefore could hardly be considered salient.

Detailed Study of Fit and Residuals for Selected Solution

The above preliminary checks led us to consider the $P = 6$, $Q = 4$, $R = 3$ solution in more detail. First we inspected whether each of the B- and C-mode entities were fitted well enough. We saw that fit percentages (given in detail below) were reasonable for all response scales and for most of the situations; only auto trip and psychological experiment fitted rather poorly, but given the small number of situations at hand, increasing the number of components did not seem an adequate remedy.

To see to what extent the $P = 6$, $Q = 4$, $R = 3$ model covered the most important structural aspects in the data, we next studied the residuals for this model. Specifically, we calculated residuals by subtracting the 3MPCA estimates from the preprocessed data. To see whether they retained important structural information, we analyzed the residuals using PCA after constructing data matrices with one mode for the rows and the other two combined for the columns. By means of the three possible PCAs, we searched for remaining structure in the residuals with respect to relations between individuals, between response scales, and between situations. The first principal component of the $I \times JK$ residual matrix (with rows pertaining to the individuals) accounted for 6% of the sum of squares of the residuals, that of the $J \times IK$ residual matrix (with rows pertaining to the response scales) for 19%, and that of the $K \times IJ$ residual matrix (with rows pertaining to the situations) for 14%. Given that the residuals accounted for 59% of the variance in the data (100% − 41%), these percentages were all multiplied by .59 to get an idea of the contributions of the ensuing components to the total fit of the data. These values were then evaluated in light of the complexity of the components concerned (e.g., one individual component pertained to different component values for all Response Scale × Situation components). Given the complexity of such additional components, we concluded that the main, simple information in the data was adequately captured by the 3MPCA solution reported. On the other hand, a complicated interaction between response scales and situations did seem to exist and was missed by the present, more simple, description of the data. Taking all this information into account, we retained the $P = 6$, $Q = 4$, $R = 3$ model as our final choice.

Optimal Simple Structure Rotation of Selected Solution

In our preliminary checks, we focused on simplicity of the component matrices for the response scales (**B**) and for the situations (**C**) only, using varimax on both matrices. Having selected our model, however, we were in a position to optimize our choice for simple structure rotations of the solution. For the present data, we decided to rotate the solution in such a way that the core and the component matrices **B** and **C** jointly tended to simple structure. In fact, in preliminary investigations of the present data, we tried to find a simple structure for the mode of the individuals as well, but as this appeared hard to achieve we decided to ignore simplicity of this mode altogether.

On our first applications of the general procedure for optimizing a weighted sum of simplicity values across orthogonal rotations of the core and the component matrices **B** and **C**, the resulting rotated cores tended to have very high values in only one row (i.e., pertaining to only one A-mode component). This prompted us to consider an oblique rotation (as described earlier in this article). Specifically, we first normalized the slices of the core pertaining to the A-mode components to unit sums of squares and compensated for this in the component matrix for the individuals. With this normalization of the core, the observed unequal influences of A-mode components were effectively equalized. Next, we applied Kiers' (1998) procedure for joint varimax rotation of the core and component matrices a number of times, during which we varied the relative weights attached to simplicity of the (normalized) core and simplicity of **B** and **C**. Specifically, we gradually increased the relative weights for **B** and **C** from 1 to 5, leading to simplicity values of 2.31, 2.57, 2.91, 3.06, and 3.10 for **B** (for which the maximum was 3.14) and 2.98, 3.30, 3.46, 3.53, and 3.57 for **C** (maximum = 3.65). The simplicity values for the core decreased as follows: 9.82, 8.94, 7.71, 6.97, and 6.60. We concluded that increasing the relative weights beyond 4 made little sense for enhancing simplicity of **B** and **C**. Moreover, for the rotation with a relative weight of 4 for **B** and **C**, the core (after adjusting it for the renormalization of **A**) was still easily interpretable, so we considered this solution a useful representation of the data. We discuss this more in detail in the *Interpreting and Reporting the Solution* section later.

Studying the Stability of the Selected Solution

For the final solution, split-half stability was checked more fully, not only for **B** and **C** but also for the core. For **B** and **C**, the congruences were very similar as in the preliminary check (which was based on varimax of **B** and of **C** rather than on the weighted joint rotation procedure used here): The φ values for **B** were .95, .90, .94, and .90, and those for **C** were .97, .80, and .79. The intermediate-size congruence values found for **C** were associated with components that in both splits did lead to the same interpretation. To inspect the stability of the core, given the full data descriptions, we computed the cores for the two splits and observed that these were very similar indeed, especially in terms of the core elements with values exceeding 10 or −10 (which were the ones actually used in the interpretation [see next section]). Specifically, for these core elements, differences across the two splits were never larger than 3 and this hardly affected the interpretations. The biggest difference between corresponding core values was 4.6, and this was found for a case in which the actual core value was 1.7. This clearly demonstrates that interpretation of such small core values as pointing to nonnegligible contributions is not warranted.

Interpreting and Reporting the Solution

In this section, the final solution is interpreted and reported. The rotated component matrices for the response scales and the situations are given in Tables 11 and 12, respectively. The rotated core is given in Table 13. For the obliquely rotated A-mode components, we do not give the full (140 × 6) component matrix, but only the correlations between these components (Table 14).

We recall that the values in the component matrices contain only relative information, which suffices to interpret the components but cannot be used to assess whether a variable or situation is represented well. For the latter purpose, the fit percentages are given in the last columns of Tables 11 and 12.

The first component of the responses is called *approach–avoidance;* the second component is related to autonomic physiological reactions including heart beating faster and heavy perspiring and is therefore labeled *autonomic physiological reaction;* the third component pertains mainly to full feeling in stomach and feel nausea and is therefore labeled *sickness;* the fourth has highest component values on two response scales pertaining to an increased need for excretion and is therefore labeled *excretory need.*

The first situation relates to various contexts in which one's performance is judged by others, and it is denoted likewise; the second is called *inanimate danger,* being related mainly to the two inanimate dangers formed by being on the ledge of a mountainside and sailing on a rough sea; the third is almost completely covered by the single situation alone in woods

Table 11
Component Values for Response Scales, Resulting From 3MPCA of Situation–Response Data, With P = 6, Q = 4, and R = 3 Components for the Respective Modes

Response	Approach–avoidance	Autonomic physiological reaction	Sickness	Excretory need	Fit (%)
Heart beats faster	−.06	**.57**	−.07	−.18	38.9
Uneasy feeling	−.28	.25	.07	−.06	43.0
Emotions disrupt action	−.18	.20	.23	−.01	42.2
Feel exhilarated and thrilled	**.46**	.11	.05	.09	25.4
Not want to avoid situation	**.41**	−.11	.06	−.02	39.4
Perspire	−.07	**.52**	−.03	−.03	47.1
Need to urinate frequently	.06	.21	−.03	**.48**	42.0
Enjoy the challenge	**.48**	.09	.08	.01	29.5
Mouth gets dry	.08	**.36**	.00	**.32**	44.1
Feel paralyzed	−.06	.18	.28	.19	47.6
Full feeling in stomach	.00	.00	**.79**	−.12	56.2
Seek experiences like this	**.48**	.12	.09	−.03	28.9
Need to defecate	−.09	−.12	−.09	**.72**	49.0
Feel nausea	−.14	−.18	**.45**	.25	41.7

Note. For emphasis of the larger values, values exceeding .30 in the absolute sense are in bold. 3MPCA = three-mode principal components analysis.

at night and is labeled likewise. This component may seem limited because it pertains to only one situation, but it is worthwhile because it apparently elicits systematically different responses.

To describe the summarized interactions and to interpret the six components for the individuals (which can be considered individual difference dimensions), we used the core array. We focused on the sets of core values associated with a single individual component and compared these profiles across all individual components. From the viewpoint of a contextualized approach to the study of personality, these profiles could be considered a summary description of individual differences in behavior across situations. Thus, these core profiles concisely describe all three-way information ranging from main effects to three-way interaction. Figure 2 shows line plots of core values for the different components for the individuals. Spe-

Table 12
Component Values for Situations, Resulting From 3MPCA of Situation–Response Data, With P = 6, Q = 4, and R = 3 Components for the Respective Modes

Situation	Performance judged by others	Inanimate danger	Alone in woods at night	Fit (%)
Auto trip	.13	.15	−.11	13.0
New date	.26	.15	**−.30**	22.7
Psychological experiment	.04	.09	.13	6.8
Ledge high on mountainside	.04	**.77**	.09	54.7
Speech before large group	**.49**	−.14	−.11	44.0
Consult counseling bureau	.25	−.07	.19	29.7
Sail boat on rough sea	.15	**.53**	−.07	39.1
Match in front of audience	**.38**	.11	−.09	42.2
Alone in woods at night	.09	.05	**.89**	58.1
Job interview	**.48**	−.13	−.04	50.8
Final exam	**.46**	−.16	.16	51.1

Note. To emphasize the larger values, values exceeding .30 in the absolute sense are in bold. 3MPCA = three-mode principal components analysis.

Table 13
Core Array Resulting From 3MPCA of Situation–Response Data, With P = 6, Q = 4, and R = 3 Components for the Respective Modes

Individual component	Performance judged by others				Inanimate danger				Alone in woods at night			
	Approach–avoidance	Auto. phys.	Sickness	Excr. need	Approach–avoidance	Auto. phys.	Sickness	Excr. need	Approach–avoidance	Auto. phys.	Sickness	Excr. need
1	**36.4**	−1.0	−0.4	−0.2	1.6	3.4	2.0	1.0	2.5	4.3	1.7	−2.2
2	0.8	1.6	−0.3	2.2	**30.2**	**−11.1**	**−11.8**	−9.0	0.4	−0.4	0.8	2.4
3	0.5	−0.1	1.2	0.9	0.4	−2.6	1.9	1.9	**26.4**	**−18.5**	−8.4	−6.6
4	−1.0	**40.0**	1.2	1.2	2.7	**11.2**	0.5	−0.6	1.2	5.0	−4.8	−7.0
5	−0.4	1.0	**34.9**	0.2	−0.4	−4.0	6.5	−4.7	3.0	1.7	9.8	2.2
6	−0.2	0.7	−0.1	**36.9**	2.9	3.5	2.4	**15.2**	1.6	−0.5	3.9	**12.4**
Parts of fit (%)	6.6	7.9	5.8	6.2	4.0	1.5	1.1	1.4	3.0	1.9	0.9	0.9

Note. To emphasize the larger values, values exceeding 10.0 in the absolute sense are in bold. 3MPCA = three-mode principal components analysis; Auto. phys. = autonomic physiological reaction; Excr. = excretory.

Table 14
Correlations Between A-Mode Components, Resulting from 3MPCA of Situation–Response Data, With P = 6, Q = 4, and R = 3 Components for the Respective Modes

Component	Component 1	2	3	4	5	6
1	—	.27	.40	−.56	−.47	−.35
2	.27	—	.22	−.28	−.32	−.38
3	.40	.22	—	−.49	−.41	−.35
4	−.56	−.28	−.49	—	.60	.58
5	−.47	−.32	−.41	.60	—	.52
6	−.35	−.38	−.35	.58	.52	—

Note. 3MPCA = three-mode principal components analysis.

cifically, each of the 24 plots corresponds to one A-mode component and one B-mode component and thus displays the core values for the different situations for persons scoring high on the A-mode component at hand on the variables related most strongly to the B-mode component at hand. From these plots it can be seen that the lines are by no means parallel and that the patterns differ for both the different A- and B-mode components. Thus, in this summary description, we find a considerable three-way interaction, which we could assume to be rather free of error, having seen that the description was reasonably stable. By averaging the core values over one mode at a time (which is easier using Table 13 than Figure 2), we could verify the presence and shape of the two-way interactions between the other two modes.

To give a substantive interpretation of the information in the core, we refer to Table 13. It can be seen that A-mode Component 1 distinguished individuals in terms of their approach–avoidance behavior in situations in which one's performance is judged by others, with high scores pertaining to a higher tendency to be attracted to such situations. The second component pertained to approach–avoidance evoked by inanimate danger (again with high scores pertaining to a higher tendency to approach). The third component distinguished individuals with respect to approach–avoidance and, to some extent, to autonomic physiological reactions, in situations like being alone in the woods at night; on this, high scores pertained to high approach and weak autonomic physiological reactions. The fourth and fifth components pertained to autonomic physiological reactions and sickness, respectively, in response to judged performance situations (with high scores pertaining to strong reactions).

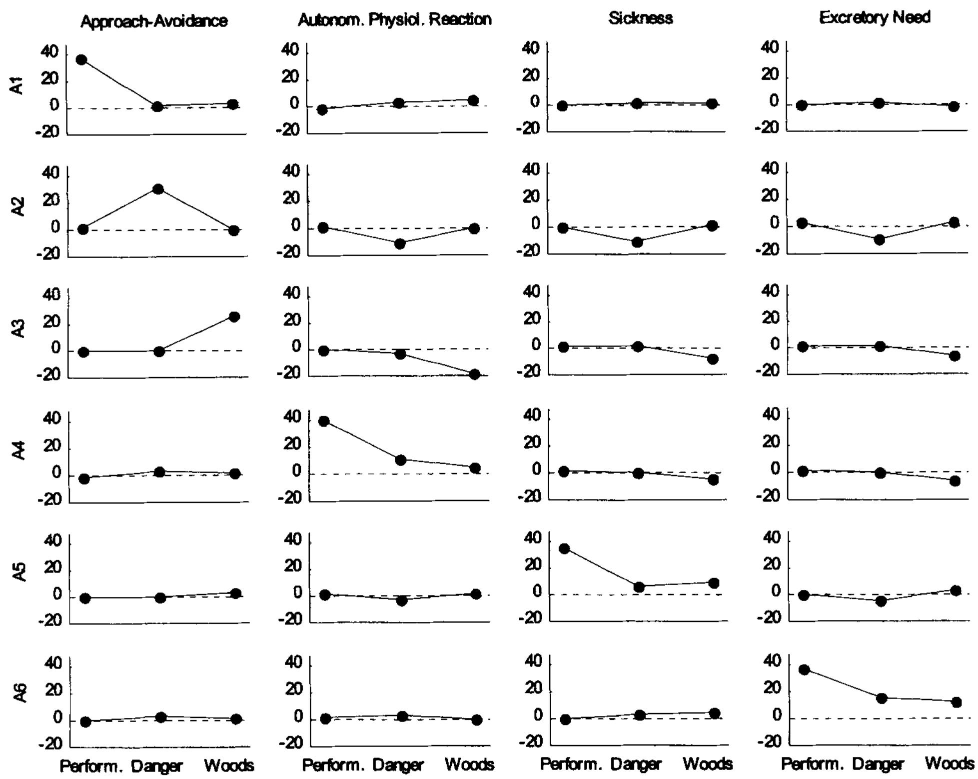

Figure 2. Line plots of core values, resulting from three-mode principal components analysis of situation–response data, with $P = 6$, $Q = 4$, and $R = 3$ components for the respective modes. Each line plot gives core values for one A-mode component (A1–A6) and one B-mode component (approach–avoidance, autonomic physiological [autonom. physiol.] reaction, sickness, or excretory need); the core values pertain to the three different situation components (performance judged by others [perform.], inanimate danger, and alone in woods). The dashed lines give the baseline value (0).

The sixth component distinguished individuals with increased need toward excretion (high scores) from others, especially in performance judgment situations but, to a lesser extent, also in other situations.

The fourth A-mode component showed a relatively complex pattern of core values. Rather than studying the information associated with this A-mode component only in terms of tabular information, one could also visualize this information as follows by a means of a "joint plot." We produced a joint plot (see Figure 3) representing the relations between the variables and the situations for persons scoring high on this fourth A-mode component. Specifically, a two-way matrix of scores on response scales for different situations was constructed that corresponded only to the fourth A-mode component (technically, this is the matrix product $\mathbf{BG}_4\mathbf{C}'$, where $\mathbf{G}_4$ denotes the fourth horizontal plane of the core $\underline{\mathbf{G}}$), and these scores were decomposed by a PCA. Next, the response scales and situations were plotted jointly, using only the first two components. It can be seen that for persons scoring high on the fourth A-mode component, situations like final exams, playing a match in front of an audience, and so forth are situations in which their hearts beat faster and they perspire heavily (as follows from their joint location to the far right in Figure 3); persons scoring low on this dimension have an increased need to defecate and feel nauseous in such situations (as follows from the fact that the situations and these responses are located at opposite sides in Figure 3). The latter holds not only in judgment situations but also notably in the situation in which one is alone in the woods. The joint plot thus displays the information in the fourth row of Table 13, combined with the interpretation of the B- and C-mode components. One should realize that the figure is based only on part of the variance explained by the fourth A-mode component (together with **B**, **C**, and the core), namely that part that could be expressed by its first two principal components. In this case, however, virtually no loss

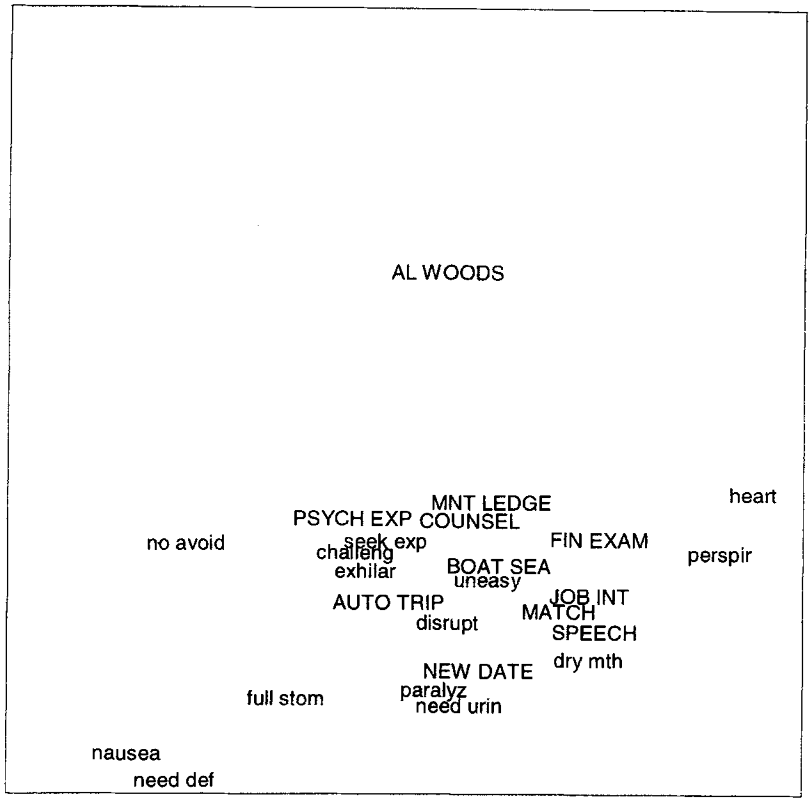

Figure 3. Joint plot for A-mode Component 4, resulting from three-mode principal components analysis of situation–response data, with $P = 6$, $Q = 4$, and $R = 3$ components for the respective modes. Response scales are given in lower case, and situations in capitals. The plot is based on the part of the data represented by the fourth A-mode component, as well as the full B- and C-mode component matrices and the associated core values. For persons scoring high on the fourth A-mode component, in a particular situation relatively high response scores can be expected on those response variables that lie close to the situation at hand and far from the origin. Al woods = alone in woods at night; boat sea = sail boat on rough sea; challeng = enjoy the challenge; counsel = consult counseling bureau; disrupt = emotions disrupt action; dry mth = mouth gets dry; exhilar = feel exhilarated and thrilled; fin exam = final exam; full stom = full feeling in stomach; heart = heart beats faster; job int = job interview; match = match in front of audience; mnt ledge = ledge high on mountainside; nausea = feel nausea; need def = need to defecate; need urin = need to urinate frequently; no avoid = not want to avoid situation; paralyz = feel paralyzed; perspir = perspire; psych exp = psychological experiment; seek exp = seek experiences like this; speech = speech before large group; uneasy = uneasy feeling.

was incurred because these components accounted for 99.6% of that variance.

The core array is not only used in interpreting the A-mode components, but it also indicates which combinations of situations and responses are most useful in distinguishing individuals. For this purpose, we computed per combination of a situation component (q) and a response component (r) the variance across individuals (i) of the values of

$$\sum_{p=1}^{P} a_{ip} g_{pqr};$$

the latter can be seen as the contributions of each combination of a situation component and a response component to the total amount of variance accounted for by the model (i.e., 41%). These variances have been converted to percentages and are listed in the bottom row of Table 13. It can be seen that in the performance judged by others situations each of the responses contributed considerably to the variance (and hence, the distinction between individuals), whereas for the other types of situations the approach–avoidance responses accounted for by far the greatest part of the variance.

Incidentally, the above fit values also help in interpreting the sizes of the individual core elements. For instance, the first core element (36.4) is by far the greatest in the first column, and hence the core value of 36.4 is predominantly responsible for the 6.6% fit of the total data fit accounted for by the components related to this column. Continuing in this way, one can see, for instance, that the core value of 26.4 relates to a little less than 3%, and one can conclude that a value of 10 contributes less than 1%. It should be noted, however, that, because of the correlatedness of the A-mode components we cannot simply associate a particular fit percentage to each core element: As in the case of correlated predictors in regression, in which fit contributions of different predictors depend on each other, in this case fit contributions associated with different core elements depend on each other. Only if the A-mode components were uncorrelated could the core elements be converted into fit contributions. In that case, this could be done by squaring the core elements, dividing by the total variance in the data (here IJK = 21,560), and multiplying by 100 to get percentages. To compare this with some core values found here, the value of 36.4 would then correspond to 6.2%, whereas that of 26.4 would correspond to 3.3%—values that do not differ much from the values given in Table 13.

We are now in a position to compare the results of 3MPCA on the full data to the results of two-way PCA on the data averaged over participants (see Tables 8 and 9). On comparison of Tables 8 and 11, it can be seen that the second component from PCA on averaged data resembles the approach–avoidance component found in our 3MPCA. The first component from PCA on averaged data is, in the 3MPCA solution, split into three components. This refinement into three components is due to the fact that 3MPCA takes into account individual differences. As to the situation component values, it can be seen that the values in Table 12 are only partly similar to those in Table 9. For instance, the first 3MPCA component covers all clear performance situations, whereas the first component from PCA on averaged data is hardly related to match in front of an audience, which clearly is a performance situation. Various similar differences can be found on comparison of the two solutions. This reveals not only that the PCA on averaged data ignores individual differences in responses to situations patterns but also that it misses worthwhile distinctions in groups of responses or situations, even though it analyzes responses by situation data.

Conclusion and Discussion

We have described how three-way analysis can be applied fruitfully in practice and can lead to interesting and interpretable results. Notably, it has been seen that 3MPCA concisely summarizes the three-way data in all its facets, that is, in terms of main effects but also in terms of two- and three-way interactions. It should be kept in mind that the representation of the three-way data analyzed here is only one of many possible different representations of the information in the data. However, the main phenomena encountered here can be expected to be found in any other good representation of these data.

The present article has illustrated the complete process of obtaining a concise description of one's three-way data. All basic three-way analysis steps (preprocessing, balancing fit and parsimony to choose the numbers of components, studying fit and residuals, optimization of simple structure rotation, and studying stability of the solution) can be carried out with Tucker3.m. Most of these steps can also be performed in 3WAYPACK.

Sometimes, in addition to the three-way data, external information on (for instance) the individuals is available, and one may wish to relate this information to the components found through 3MPCA. A straightforward way to do this is to relate the individuals scores on such external variables directly to the A-mode components. For quantitative external variables, one can simply use correlations between these variables and the components; in case of categorical external variables, one can compute category averages for each component. In both ways one gains further information for interpreting the A-mode components as well as for understanding the process that generated the three-way data. An example of a use of external information for the present data can be found in Van Mechelen and Kiers (1999).

The present example data set has been analyzed only with 3MPCA. We did, however, check whether a good PARAFAC solution could be found for this data set. It was found that PARAFAC with two components accounted for 28% of the variance in the data, three components accounted for 32%, and four components accounted for 36%. Although these values are reasonable, they are relatively low compared with the 3MPCA results, and more importantly, the solutions were rather uninteresting. For example, in the four-dimensional solution, the columns of **B** were very similar, and so were those of **C**. Thus, the solution by no means gives a useful grouping of response scales or situations. This also held for the three- and two-dimensional solutions. The columns of **A** did differ, but all in all the PARAFAC solutions did not appear useful. Therefore, 3MPCA seems better suited for these data.

The presented application was one in the area of personality psychology. As mentioned at the beginning of this article, three-way data can emerge in many different contexts in psychology, and modeling such data by PARAFAC or 3MPCA can be expected to be fruitful as soon as the data can be reduced through components. In all cases, three-way analyses have the advantage over two-way analyses in that they take differences along the three modes and all interactions into account; in addition, they summarize these differences by providing the main dimensions of within-mode differences and give a concise description of the interactions between all the modes.

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Received December 1, 1998
Revision received October 26, 2000
Accepted November 7, 2000 ■