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Adapting the Formal to the Substantive: Constrained Tucker3-HICLAS

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Abstract: Ceulemans, Van Mechelen, and Leenen (2003) recently presented the Tucker3 hierarchical classes model for three-way three-mode binary data. This model includes a hierarchical classification of the elements of each mode involved in the data, and a linking structure among the three hierarchies. In substantive applications of this model, one may wish to incorporate substantive knowledge in the data analysis. In this paper, we show how the latter may be achieved by imposing constraints on the model. As the number of possible Tucker3-HICLAS constraints is huge, we present a comprehensive taxonomy of a wide range of constrained Tucker3-HICLAS models. Furthermore, we investigate which features of the existing Tucker3-HICLAS algorithm have to be adapted for fitting the different types of constrained Tucker3-HICLAS models. Finally, the constrained Tucker3-HICLAS approach is illustrated with applications from psychiatric diagnosis and personality research.

Keywords: Three-way three-mode data; Binary data; Hierarchical classes analysis; Constraints.

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1. Introduction

In this paper, we focus on the modeling of three-way three-mode binary data. An example of such data, which we will use throughout the paper, is a binary situation by behavior by person data array $\underline{\mathbf{D}}$ with $d_{ijk} = 1$ if situation i elicits behavior j from person k and 0 otherwise. For the modeling of such data, Ceulemans, Van Mechelen, and Leenen (2003) recently proposed the Tucker3-HICLAS model as a new member of the family of hierarchical classes models for n-way n-mode binary data (De Boeck and Rosenberg, 1988; Van Mechelen, De Boeck, and Rosenberg, 1995; Leenen, Van Mechelen, De Boeck, and Rosenberg, 1999; Leenen, Van Mechelen, and De Boeck, 2001; Ceulemans et al., 2003; Ceulemans and Van Mechelen, in press).The Tucker3-HICLAS model reduces each of the three modes of $\underline{\mathbf{D}}$ to a few binary variables, called bundles, and links the three sets of bundles in a three-mode binary core array; the bundles are further restricted to represent the quasi-order relations among the elements of a mode. Obviously, the Tucker3-HICLAS model is the hierarchical classes counterpart of the Tucker3/3MPCA model for three-way three-mode real-valued data (Tucker, 1966; Kroonenberg and De Leeuw, 1980; Kroonenberg, 1983) which, as a generalization of two-way two-mode principal component analysis (PCA), reduces each mode of a three-mode real-valued data array to a few components and interrelates the three sets of components by means of a three-mode real-valued core array. Both the Tucker3-HICLAS and the Tucker3/3MPCA model have been successfully applied in various substantive contexts (e.g., Kuppens, Van Mechelen, Smits, De Boeck, and Ceulemans, 2003; Realo, Koido, Ceulemans, and Allik, 2002; Kroonenberg, 1983).

An algorithm has been proposed to fit the Tucker3-HICLAS model to data. The resulting solutions can be considered unconstrained in that the algorithm may look in the whole solution space for the best fitting solution. However, in some substantive applications it may be desirable to search only a part of the solution space as one may wish to incorporate substantive knowledge or hypotheses into the analysis. For the Tucker3/3MPCA model, several authors have shown that the latter may be achieved by imposing constraints on the model and by developing an algorithm for fitting the constrained model to data (see e.g., Bro, 1998; Kiers, Ten Berge, and Rocci, 1997). For example, in the area of chemometrics one may wish to estimate physical properties like concentrations by means of a Tucker3/3MPCA model. As concentrations can only have non-negative values, this implies that one wishes to consider Tucker3/3MPCA solutions with non-negative component scores only. Bro and De Jong (1997) showed that the latter can be accomplished by means of an algorithm that fits Tucker3/3MPCA models that are constrained to include non-negative component scores only.

In this paper, we describe how in Tucker3-HICLAS applications the existing Tucker3-HICLAS model (i.e., 'the formal') may be adapted to substantive questions and hypotheses associated with specific data sets (i.e., 'the substantive'). In particular, we show that one may take such substantive knowledge on the data into account by imposing constraints on the model. Considering some of the constraints that have been proposed for the real-valued counterpart of the Tucker3-HICLAS model - non-negative component scores (Bro and De Jong, 1997), component scores with equal values (Kiers and Smilde, 1998), unimodal component scores (Bro and Sidiropoulos, 1998), fixing a number of core entries to zero (Kiers, 1992; Kiers et al., 1997), and smooth component scores (Timmerman and Kiers, 2002) -, one may realize that the number and variety of possible Tucker3-HICLAS constraints is huge. Therefore, we organize a wide range of possible Tucker3-HICLAS constraints into a taxonomy; this taxonomy may also be useful for classifying a variety of Tucker3/3MPCA constraints. Furthermore, we investigate which features of the existing Tucker3-HICLAS algorithm have to be adapted for fitting the different types of constrained Tucker3-HICLAS models, and propose three examples of appropriately adapted algorithms for fitting three specific constraints.

The remainder of this paper is organized as follows: In Section 2, the existing Tucker3-HICLAS model is briefly recapitulated and a taxonomy of Tucker3-HICLAS constraints is proposed. In Section 3, we describe the existing Tucker3-HICLAS algorithm and report an algorithmic analysis. In Section 4, we illustrate constrained Tucker3-HICLAS with three applications from research on psychiatric diagnosis and on personality. Section 5 contains some concluding remarks.

2. Model

2.1 The Existing Tucker3-HICLAS Model

The Tucker3-HICLAS model approximates an I (situations) $\times$ J (behaviors) $\times$ K (persons) binary data array $\underline{\mathbf{D}}$ by an $I \times J \times K$ binary model array $\underline{\mathbf{M}}$, which can be further decomposed into an $I \times P$ binary situation bundle matrix $\mathbf{A}$, a $J \times Q$ binary behavior bundle matrix $\mathbf{B}$, a $K \times R$ binary person bundle matrix $\mathbf{C}$, and a $P \times Q \times R$ binary core array $\underline{\mathbf{G}}$, where (P, Q, R) denotes the rank of the model. In the following, the hypothetical situation by behavior by person array $\underline{\mathbf{M}}$ in Table 1 will serve as a guiding example; Table 2 presents a (2,2,2) Tucker3-HICLAS decomposition of $\underline{\mathbf{M}}$.

As all hierarchical classes models, a Tucker3-HICLAS model represents two types of structural relations in $\underline{\mathbf{M}}$: the association relation among the three modes and the quasi-order relation on each of the three modes.

Association. The association relation is the ternary relation among the

Table 1. Hypothetical Tucker3-HICLAS reconstructed data array

Pers. 1					Pers. 2					Pers. 3				
	Beh.					Beh.					Beh.			
Sit.	1	2	3	4	Sit.	1	2	3	4	Sit.	1	2	3	4
1	1	0	0	1	1	0	0	0	0	1	1	0	0	1
2	1	0	0	1	2	0	0	0	0	2	1	0	0	1
3	0	1	1	1	3	1	1	1	1	3	1	1	1	1
4	1	1	1	1	4	1	1	1	1	4	1	1	1	1

situations, behaviors, and persons as defined by the 1-entries of the array $\underline{\mathbf{M}}$. The Tucker3-HICLAS model represents the association relation by the following association rule:

$$m_{ijk} = \bigoplus_{p=1}^{P} \bigoplus_{q=1}^{Q} \bigoplus_{r=1}^{R} a_{ip} b_{jq} c_{kr} g_{pqr}, \tag{1}$$

where $\bigoplus$ denotes the Boolean sum. The latter implies that a situation i, a behavior j, and a person k are associated in $\underline{\mathbf{M}}$ iff a situation bundle, a behavior bundle, and a person bundle exist, to which i, j, and k respectively belong, and that are associated in $\underline{\mathbf{G}}$. For example, in Table 2, Situation 3 elicits Behavior 1 from Person 2, because the second situation bundle (SB_2), the first behavior bundle (BB_1), and the second person bundle (PB_2), to which Situation 3, Behavior 1, and Person 2 belong, respectively, are associated in $\underline{\mathbf{G}}$.

Quasi-order. A quasi-order $\leq$ is defined on each mode of $\underline{\mathbf{M}}$. In the case of the situation mode, situation $i \leq$ situation i' in $\underline{\mathbf{M}}$ iff the set of (behavior, person) pairs associated with i constitutes a subset of the set of (behavior, person) pairs associated with i'. The Tucker3-HICLAS model represents the quasi-order relation among the situations in that $i \leq i'$ iff $a_{i.} \leq a_{i'.}$ (i.e., in terms of subset-superset relations among the corresponding bundle patterns). For example, Situation 1 and Situation 2 have identical association patterns in Table 1; consequently, Situations 1 and 2 have identical bundle patterns in the Tucker3-HICLAS model of Table 2. Furthermore, in Table 1, the association pattern of Situation 1 is a proper subset of that of Situation 4; hence, in Table 2, the bundle pattern of Situation 1 is a proper subset of the bundle pattern of Situation 4. The quasi-order relations among the behaviors and persons are defined and represented similarly.

Ceulemans et al. (2003) also proposed a comprehensive graphical repre-

Table 2. Tucker3-HICLAS Model for the Data in Table 1

Bundle matrices									Core array			
	Sit. bundle			Beh. bundle			Pers. bundle				Pers. bundle	
Sit.	SB_1	SB_2	Beh.	BB_1	BB_2	Pers.	PB_1	PB_2	Sit. bundle	Beh. bundle	PB_1	PB_2
1	1	0	1	1	0	1	1	0	SB_1	BB_1	1	0
2	1	0	2	0	1	2	0	1	SB_1	BB_2	0	0
3	0	1	3	0	1	3	1	1	SB_2	BB_1	0	1
4	1	1	4	1	1				SB_2	BB_2	1	1

sentation of a Tucker3-HICLAS model from which the two types of structural relations can be read; the latter will be introduced in the illustrative applications section.

2.2 Taxonomy of Constraints

Imposing a constraint on a Tucker3-HICLAS model may be formalized as follows: One requires **A**, **B**, **C** and/or $\underline{\mathbf{G}}$ to belong to a precisely defined subset of the set of Boolean arrays of the prespecified size. To obtain a firmer grip on the wide range of possible Tucker3-HICLAS constraints, we propose to classify them into a taxonomy based on four features of the constraints. (1) What is the *locus* of the constraint: does it pertain to a bundle matrix or to the core array? (2) What is the *nature* of the constraint: are the values of the parameters constrained - i.e., is the value of specific bundle matrix/core entries fixed -, or is the structure of the parameter set constrained - i.e., do the bundle matrix/core entries have to fulfil a specific structural property, without their values being fixed (similar to Thurstonian simple structure in factor analysis or to the binary relations described in Coombs' theory of data, which in matrix form, upon an appropriate permutation of the rows and columns, come down to a specific geometric pattern of ones such as a triangle or a parallelogram) - ? (3) What is the *extent* of the constraint: is the constraint imposed on the whole bundle matrix/core array or just on a part of it? (4) Is the constraint imposed with or without making use of *external information* - i.e., information that is not part of the actual three-way data array under study? Combining these four features, we end up with a $2 \times 2 \times 2 \times 2$ taxonomy of Tucker3-HICLAS constraints.

In the following paragraphs, we will make the latter taxonomy more concrete by providing some examples and formalizations of different types of concrete by providing some examples and formalizations of different types of constrained Tucker3-HICLAS models. For clarity's sake, we will primarily focus on the first two features of the taxonomy: locus and nature. In particular, we will give examples and formalizations of each of the resulting 2×2 types of constrained models, these examples, however, also differing with respect to the last two features of the taxonomy: extent and external information. Throughout, we will use a fixed substantive context as a basis of our examples, that is, a context of personality psychology research in which binary data are available on the (non)occurrence of different types of anger behaviors for different persons in a series of frustrating situations.

2.2.1 Value Constraints on a Bundle Matrix

This type includes all Tucker3-HICLAS constraints that (with or without making use of external information) specify the exact value of one or more bundle matrix entries. For example, the bundle matrix entries of all or a subset of the situations may be fixed to the values that were obtained in a previous study (value constraint on the whole or a part of a bundle matrix depending on external information); for the whole bundle matrix this constraint may be formalized as follows:

$$\mathbf{A}^{current} = \mathbf{A}^{previous}. \tag{2}$$

When applied to a subset of the situations, this constraint may be useful, amongst other cases, if one wishes to expand a set of situations used in previous studies, as it allows to investigate the relations between an already well-studied subset of situations and a new subset.

As a second example, one may consider fixing the number of person bundles R to 1 as well as all person bundle matrix entries to 1 (value constraint on the whole bundle matrix without using external information); formally, this constraint may be written as

$$\forall k : 1 \ldots K : c_{k1} = 1. \tag{3}$$

The latter constraint is useful if one hypothesizes that there are no differences in the situation - behavior profiles of the persons, implying that the persons may be considered replications of one another.

2.2.2 Structure Constraints on a Bundle Matrix

This type includes all Tucker3-HICLAS constraints that (with or without making use of external information) specify a structural property that (part of) a bundle matrix has to satisfy. As a first example, consider the property that a bundle matrix has to take the form of a Guttman scale (Guttman, 1944) (structure constraint on the whole bundle matrix without making use of external information):

$$\forall k_1, k_2 : 1 \ldots K : (c_{k_1.} \subseteq c_{k_2.}) \vee (c_{k_1.} \supseteq c_{k_2.}). \quad (4)$$

Such a Guttman scale can be considered as a quantitative dimension (Gati and Tversky, 1982). In personality research, such a quantitative dimension may be postulated for the person mode, as an obvious formalization of a personality trait.

As a second example, consider the constraint that the person bundle matrix $\mathbf{C}$ is the Boolean matrix product of a given $K \times C$ partition matrix $\mathbf{P}$, in which each person is assigned to one of C partition classes, and a $C \times R$ partition class bundle matrix $\mathbf{C}^*$ (structure constraint on the whole bundle matrix based on external information):

$$\mathbf{C} = \mathbf{P} \otimes \mathbf{C}^*. \quad (5)$$

Such a property may be of substantive interest when additional data are available on the grouping of the persons into a number of partition classes like personality disorders, cultures or education levels, and one is interested in studying the situation - behavior profiles characterizing each of these partition classes.

2.2.3 Value Constraints on the Core Array

This type includes all Tucker3-HICLAS constraints that (with or without making use of external information) specify the exact value of one or more core entries. As a first example, the core entries may be fixed to the values that were obtained in a previous study (value constraint on the whole core array depending on external information):

$$\underline{\mathbf{G}}^{current} = \underline{\mathbf{G}}^{previous}; \quad (6)$$

usually, such a constraint will be supplemented by constraints that also fix the entries of the situation and behavior bundle matrices to the values that were found in this previous study. Such constraints may be considered when one wishes to replicate a situation hierarchy, a behavior hierarchy and the linking structure that characterizes the person hierarchy in terms of specific situation - behavior profiles. Also, such constraints may be useful if one wishes to classify a number of persons into a person typology that is defined in terms of a set of well-established situation - behavior profiles.

As a second example, the core array may be constrained to take the form of a 'unit superdiagonal' array $\underline{\mathbf{I}}$:

$$\underline{\mathbf{G}} = \underline{\mathbf{I}}, \quad (7)$$

with $\underline{\mathbf{I}}$ being defined by (1) $P = Q = R$ and (2) $g_{pqr} = 1$ iff $p = q = r$ (value constraint on the whole core array without making use of external information). The latter constraint implies that the Tucker3-HICLAS model reduces to the more simple INDCLAS model (Leenen, Van Mechelen, De Boeck, and Rosenberg, 1999), and, hence, that the linking structure among the situation, behavior and person bundles takes the form of a one-to-one correspondence. Note that a unit superdiagonal constraint could also be considered a structure constraint; however, by way of convention, we classify all constraints that imply fixing the value of (at least some) specific bundle matrix/core entries, as value constraints.

2.2.4 Structure Constraints on the Core Array

This type includes all Tucker3-HICLAS constraints that (with or without making use of external information) specify a structural property that (part of) the core array has to satisfy. As a first example, consider the property that the core array can be further decomposed into a $P \times R$ binary matrix $\mathbf{G}^1$ and a $Q \times R$ binary matrix $\mathbf{G}^2$ as follows:

$$g_{pqr} = g^1_{pr} g^2_{qr} \tag{8}$$

(structure constraint on the whole core array without making use of external information). In personality research, this could formalize the mechanism that each person type r reacts to each situation type p that it deems frustrating (i.e., $g^1_{pr} = 1$) with all the behavior types q that belong to the behavioral repertorium of that person type (i.e., $g^2_{qr} = 1$).

As a second example, one may think of the constraint that the core array includes a small, prespecified number n of 1-entries (structure constraint on the whole core array without making use of external information):

$$\sum_{p=1}^{P} \sum_{q=1}^{Q} \sum_{r=1}^{R} g_{pqr} = n. \tag{9}$$

Such a constraint may be interesting from an interpretational point of view, as a core array that implies fewer associations among situation, behavior and person bundles may imply a model that is easier to interpret. From a technical point of view, such a constraint also implies a more parsimonious model, which, therefore, may prove to be more stable in replication research.

3. Algorithm

3.1 The Existing Tucker3-HICLAS Algorithm

Given an $I \times J \times K$ data array $\underline{\mathbf{D}}$ and a rank (P, Q, R), the existing Tucker3-HICLAS algorithm searches by means of two routines for arrays **A**, **B**, **C** and $\underline{\mathbf{G}}$ that combine by (1) to an $I \times J \times K$ model array $\underline{\mathbf{M}}$ that has a minimal value on the loss function

$$f(\underline{\mathbf{M}}) = \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K}(d_{ijk} - m_{ijk})^2. \tag{10}$$

The first routine is an alternating least squares routine, in which **A**, **B**, **C** and $\underline{\mathbf{G}}$ are re-estimated conditional upon all the others by means of Boolean regression (Leenen and Van Mechelen, 1998). This routine starts from an initial configuration for **A**, **B** and **C** that can be obtained rationally (by a built-in heuristic) or randomly, and continues until no updating of a bundle matrix or core array further improves the loss function (10). Whereas $\underline{\mathbf{G}}$ has to be updated array-wise, note that, due to a separability property of the loss function (Chaturvedi and Carroll, 1994), **A**, **B** and **C** can be updated row-wise by successively optimizing each of the bundle patterns $a_{i.}$, $b_{j.}$ and $c_{k.}$.

As the thus obtained **A**, **B**, **C** are only restricted to represent the association relation in $\underline{\mathbf{M}}$, the second routine transforms these arrays, without altering $\underline{\mathbf{M}}$, such that they also represent the quasi-order relations. The latter is achieved by applying a closure operation to **A**, **B**, **C**, which boils down to changing 0-entries of the bundle matrices into 1-entries if these modifications do not alter $\underline{\mathbf{M}}$.

3.2 Adapting the Algorithm for Fitting Constrained Models: Algorithmic Analysis

In this subsection, we will investigate which features of the existing Tucker3-HICLAS algorithm should be adapted for fitting the different types of constrained models. As a starting point for this algorithmic analysis, one should bear in mind that the existing Tucker3-HICLAS algorithm implies structural options on different levels. On the highest level (level 1), the algorithm implies the option of a consecutive combination of an alternating least squares routine pertaining to the association relation and a closure operation routine pertaining to the quasi-order relations. At an intermediate level (level 2), within the alter-

Table 3: Overview of algorithmic possibilities and problems

Type of constraint		Adaptation of the algorithm		
Nature	Locus	Level of change	Solution	Application
Value=1	Bundles	3	simple	-
Value=0	Bundles	1	somewhat more involved, but feasible	1
Value=0/1	Core	3	simple	1
Structure: Closure-compatible	Bundles	2	sometimes available	2
Structure: Closure-incompatible	Bundles	1	sometimes available	-
Structure	Core	3	somewhat more involved, but feasible	3

nating least squares routine, it was opted to update the bundle matrices row-wise and the core array array-wise (depending on the existence of a separability property). Finally, on the lowest level (level 3), Boolean regression was chosen as estimation method for the bundle patterns and the core array. Below, we will show that adapting the Tucker3-HICLAS algorithm for fitting the different types of constrained Tucker3-HICLAS models boils down to reconsidering some of the latter options; obviously, the higher the level of the option to be reconsidered, the more fundamental the adaptation of the algorithm becomes. As the first two features of our taxonomy are the most decisive from an algorithmic point of view, we will again primarily focus on the different locus-nature combinations. Table 3 summarizes the results of the algorithmic analysis by specifying for the different types of constraints (1) the level on which the algorithm has to be adapted, (2) the difficulty of the involved adaption, and (3) the application in which an example of an appropriately adopted algorithm is provided.

Value constraints on the bundle matrix. As the closure operation routine may alter 0-entries of a bundle matrix into 1-entries, but not vice versa, the level on which the Tucker3-HICLAS algorithm has to be adapted depends on the value of the fixed bundle matrix entries. More specifically, whereas constraints that fix bundle matrix entries to 1 may simply be fitted by fixing the corresponding Boolean regression weights to the prespecified values when optimizing the bundle patterns - i.e., a level 3 change -, constraints that fix bundle matrix entries to 0 require a level 1 change of the algorithm: the development of an algorithm that simultaneously fits the value constraints and the quasi-order relations. In the context of the first illustrative application, an example of the latter type of algorithm will be given.

Structure constraints on the bundle matrix. The level on which the Tucker3-HICLAS algorithm has to be altered for fitting structure constraints on the bundle matrix, depends on the structural property, or, more precisely, on whether applying the closure operation routine to appropriately constrained estimates resulting from the alternating least squares routine, may yield final estimates that no longer satisfy the structural property. If the fulfilment of the structural property is jeopardized by applying the closure operation, a level 1 adaptation of the algorithm is required; otherwise, a level 2 adaptation is necessary as, due to the structural constraint, the separability property no longer holds (i.e., the best update of the bundle pattern of a specific element depends on the updates of the bundle patterns of the other elements), implying that the constrained bundle matrix has to be estimated as a whole. Examples of structure constraints that require a level 2 adaptation only, include the Guttman and partition constraints as discussed above. For, the Guttman constraint comes down to the requirement that the quasi-order relation between the rows of the bundle matrix is total, whereas the partition constraint comes down to the requirement that the same quasi-order includes a number of equivalences (i.e., for specific pairs (k_1,k_2) it should hold that $c_{k_1.} = c_{k_2.}$). Such constraints are not affected by the closure operation as the latter can only add and not delete links of the quasi-order among the rows of the bundle matrix. An example of a level 2 adaptation is described for the second illustrative application.

Value constraints on the core array. All these constraints may be fitted by a simple adaptation of the core array updating step of the alternating least squares routine - i.e., a level 3 change. More specifically, the Boolean regression weights that correspond to the constrained core entries must be fixed to their prespecified values. Note that the latter implies that, if all core entries are fixed, the core array updating step of the alternating least squares routine can be skipped.

Structure constraints on the core array. As was the case for the value constraints on the core array, adapting the Tucker3-HICLAS algorithm for fitting structure constraints on the core array, requires a level 3 modification. Indeed, for this purpose a tailor-made core updating procedure has to be developed. An example of such a procedure will be provided when discussing the third illustrative application.

4. Illustrative Applications

In this section, we illustrate constrained Tucker3-HICLAS analysis with three applications, two from personality psychology research and one on decision making in psychiatric diagnosis. For each application, we will successively discuss (1) the substantive questions and hypotheses that guided the Tucker3-HICLAS analysis, (2) the formalization of the guiding hypotheses into a constrained Tucker3-HICLAS model, (3) the adapted version of the Tucker3-HICLAS algorithm that was developed for fitting the constrained Tucker3-HICLAS model, and (4) the obtained results.

4.1 Application 1: Individual Differences in Self-reported Hostile Behavior in Frustrating Situations

4.1.1 Substantive Questions and Hypotheses

According to Bem (1983), a fundamental scientific task for personality psychology is to construct linked triple typologies of situations, behaviors, and persons. If binary situation by behavior by person data are available, Vansteelandt and Van Mechelen (1998) showed that the latter may be achieved by applying three-way three-mode hierarchical classes models to the data set, as these models yield a hierarchical classification of each mode and a linking structure, which interrelates the three hierarchies. However, an important question concerns the replicability of the obtained linked triple typology: To which extent will the linked triple typology show up in the analysis of a data set that is obtained by gathering the same situation - behavior profiles in a second sample of persons? This application shows how the replicability of Tucker3-HICLAS results may be checked in practice.

In particular, we will consider data that were gathered by Vansteelandt and Van Mechelen (1998) in two samples of 54 and 316 persons that rated 23 frustrating situations with respect to the display of 15 hostile behaviors, yielding a $23 \times 15 \times 54$ and a $23 \times 15 \times 316$ binary data array respectively. Ceulemans et al. (2003) reported a (2,3,2) Tucker3-HICLAS solution for the 54 persons data set, which is graphically represented in Figure 1. More specifically, the hierarchical classification of the situations, as defined by the quasi-order on this mode, shows up in the upper half of Figure 1. This situation hierarchy takes the form of a total order, which may be conceived as a quantitative dimension (Gati and Tversky, 1982); note that the situations have been indicated by the key words presented in Table 4. Similarly, the behavior hierarchy is represented upside down in the lower half of Figure 1. One may conclude that, except for 'Grimace', the behaviors also constitute a quantitative dimension, which, in part, reflects different levels of physiological arousal. In the middle part of Figure 1, lines and hexagons (the latter containing the person bundle labels) represent the association relation among the situations, behaviors and persons. More specifically, a situation i, a behavior j and a person k are associated iff a downward path exists from situation i to behavior j across a hexagon that

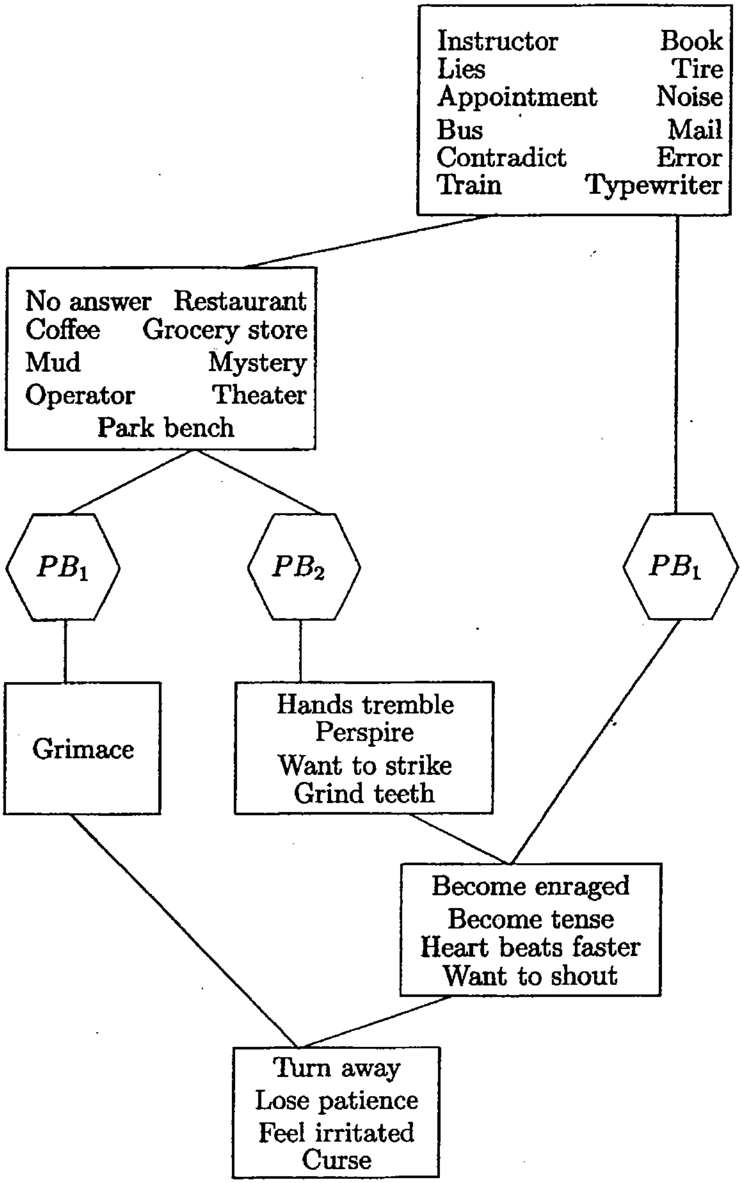

Figure 1. Overall graphical representation of the unconstrained Tucker3-HICLAS model for the 54 persons sample.

Table 4: Key words for the 21 frustrating situations in the graphical representations of the Tucker3-HICLAS models for the hostility data

Key word	Full situation description
instructor	Your instructor unfairly accuses you of cheating on an examination
book	Someone has lost an important book of yours
lies	You have just found out that someone has told lies about you
tire	You are driving to a party and suddenly your car has a flat tire
appointment	You arrange to meet someone and he (she) doesn't show up
noise	You are trying to study and there is incessant noise
bus	You are waiting at the bus stop and the bus fails to stop for you
mail	Someone has opened your personal mail
contradict	Someone persistently contradicts you when you know you are right
error	Someone makes an error and blames it on you
train	You miss your train because the clerk has given you faulty information
typewriter	You are typing a term paper and your typewriter breaks
no answer	You are talking to someone and he (she) does not answer you
restaurant	You are in a restaurant and have been waiting a long time to be served
coffee	You are carrying a cup of coffee to the table and someone bumps into you
grocery store	The grocery store closes just as you are about to enter
mud	Someone has splashed mud over your new clothing
mystery	You are reading a mystery and find that the last page of the book is missing
operator	You use your last 10 c to call a friend and the operator disconnects you
theater	Someone pushes ahead of you in a theater ticket line
park bench	You accidently bang your shins against a park bench

includes a person bundle person k belongs to. For example, it is clear that the situation with the label 'No answer' elicits the behavior 'Grimace' from the persons belonging to the first person bundle (PB_1), since 'No answer' and 'Grimace' are connected in Figure 1 by a downward path that includes PB_1.

In order to check the extent to which the latter results may be replicated in a Tucker3-HICLAS analysis of the 316 persons data set, we will first impose the full situation-behavior structure that resulted from the 54 persons data set; this boils down to fixing (1) the whole situation bundle matrix, (2) the whole behavior bundle matrix, and (3) the whole core array for the 316 persons data set to the arrays found for the 54 persons data set. Next, we will successively remove one or more of the latter three constraints, in order to investigate the replicability of the different aspects of the linked triple typology. In particular, we will first withdraw the constraint on the core array, as it is plausible that the person typology (which is defined by the core array in terms of situation - behavior profiles) may change from sample to sample. Since fixing only the core array and either the situation bundle matrix or the behavior bundle matrix makes no sense (as the meaning of the core array as definition of the person typology depends on both the situation and the behavior bundle matrix), the other two constrained models to be considered imply either a fixed situation or a fixed behavior bundle matrix. Comparing the fit values of the four obtained constrained models to the fit value of the unconstrained model, it will become clear which aspects of the model for the 54 persons data set also hold for the 316 persons data set.

4.1.2 Formalization of the Hypotheses

Given the binary frustrating situation by hostile behavior by person data array that was obtained from the 316 persons sample, the replicability of the Tucker3-HICLAS results for the 54 persons sample may be checked by successively imposing the four combinations of constraints that were discussed above: (1) fixing the situation bundle matrix, the behavior bundle matrix and the core array of the Tucker3-HICLAS model for the 316 persons sample to the corresponding arrays of the Tucker3-HICLAS model for the 54 persons sample, (2) fixing the situation bundle matrix and the behavior bundle matrix, (3) fixing the situation bundle matrix only, and (4) fixing the behavior bundle matrix only. All these constraints are value constraints on the whole bundle matrix/core array that depend on external information.

4.1.3 Algorithm

As discussed in Subsection 3.2, adapting the Tucker3-HICLAS algorithm for fitting value constraints on the whole core array boils down to a level 3 change - i.e., fixing all Boolean regression weights to their prespecified value, which implies that the core array updating step of the alternating least squares routine is skipped -, whereas the value constraints on the whole situation and behavior bundle matrices imply a level 1 change - i.e., the development of an algorithm that simultaneously fits the value constraints and the quasi-order relations -. In particular, we developed the following algorithm: If unconstrained, the bundle matrices and core array are estimated by means of an alternating least squares procedure (i.e., the updating steps of fixed arrays are skipped). In each step of this alternating least squares routine, the closure operation routine was performed on the current estimates for the unconstrained bundle matrices as well as on the fixed bundle matrices. If the latter operation did not alter the fixed matrices (implying that the current Tucker3-HICLAS model is valid, that is, correctly represents all quasi-orders in the corresponding model array $\underline{\mathbf{M}}$), we went on to the next step. Otherwise, a small proportion of the entries of the array that was being updated was randomly changed of value, until an estimate was obtained such that applying the closure operation did not change the fixed matrices; the latter procedure was repeated a high number of times (e.g., 100 times), after which the update that minimized the loss function was retained. To evaluate the performance of this new algorithm, a small simulation study was set up, the results of which are reported in the Appendix.

4.1.4 Results

Given the 316 persons data set, the (2,3,2) Tucker3-HICLAS model with a fixed situation bundle matrix, behavior bundle matrix and core array has a proportion of discrepancies between $\underline{\mathbf{D}}$ and $\underline{\mathbf{M}}$ of .248. The model with value constraints on the situation and behavior bundle matrices yielded a proportion of discrepancies of .241. Finally, the models with either a fixed situation bundle matrix or a fixed behavior bundle matrix had a proportion of discrepancies of .234 and .241, respectively. Comparing the latter proportions with the proportion of discrepancies of .234 of the unconstrained (2,3,2) Tucker3-HICLAS model, we decided to retain the model with a fixed situation bundle matrix, as this is the only constrained model that fits the data equally well as the unconstrained model; the selected model is graphically represented in Figure 2. We must conclude that only the situation typology of the 54 persons data set is replicated in the analysis of the 316 persons dataset.

Investigating more closely what happened to the other aspects of the linked triple typology, one may derive from Figure 2 that the behavior typology now seems to indicate the existence of two separate hostile behavior channels: a facial channel ('Grimace' and 'Turn away') and a verbal channel ('Want to shout' and 'Curse'). Furthermore, we may differentiate between two types of

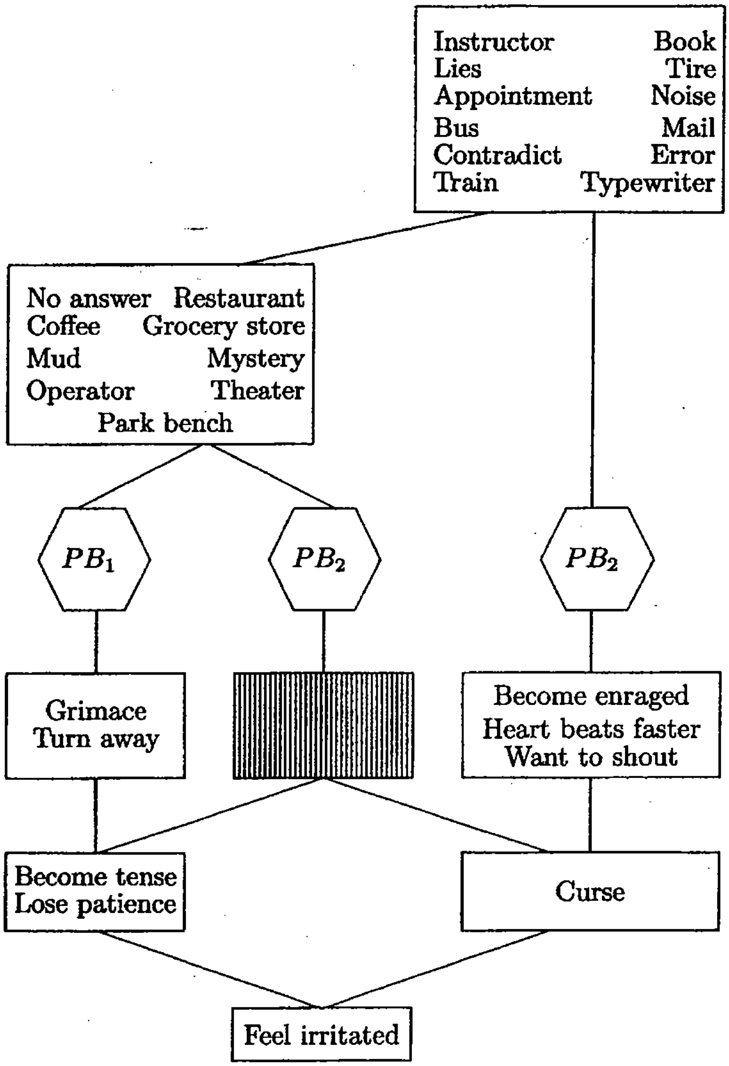

Figure 2. Overall graphical representation of the constrained Tucker3-HICLAS model for the 316 persons sample.

persons: The first type (PB_1) reacts to all frustrating situations with facial hostile behavior; the second type (PB_2) draws a distinction between mildly and strongly frustrating situations: in mildly frustrating situations the persons of this type only display 'mild' verbal hostile behavior ('Curse'); in strongly frustrating situations they, on top of that, also want to shout and become enraged.

4.2 Application 2: Types of Anger-related Behavior as a Function of Status and Liking

4.2.1 Substantive Questions and Hypotheses

Anger behavior has traditionally been conceptualized in terms of general traits referring to anger-out (overt expression of anger) and anger-in (suppressing the expression of anger) (Funkenstein, King, and Drolette, 1954; Spielberger et al., 1985). However, recently, several voices have risen that have questioned such a trait dichotomy to describe anger behavior. First, it has been argued that the dichotomy may be too narrow: Other behaviors (among which more prosocial, constructive behavior) should be considered as well in order to capture the variety of behaviors that may possibly follow the experience of anger (Linden et al., 2003). Second, research suggests that anger behavior may be strongly context-dependent (Bongard and al'Absi, 2003). In an attempt to meet these considerations, Kuppens, Van Mechelen, and Meulders (2003) have constructed a contextual anger behavior questionnaire in which the display of a wide variety of anger behaviors is assessed as a function of situation characteristics that are hypothesized to produce distinctive anger reactions. Regarding anger behavior, the questionnaire included seven behavior types: anger-out, anger-in, assertive behavior, reconciliation, avoidance, indirect anger behavior, and social sharing, each of them being assessed by means of two items. Regarding situation characteristics, the questionnaire assesses the display of anger behavior in six recalled situations, in which the targets of anger were either of a higher, equal or lower status, and either liked or disliked; both status and liking have been documented to influence anger behavior (Allan and Gilbert, 2002; Babad and Wallbott, 1986).

Kuppens et al. (2003) administered the questionnaire to 114 participants who were asked to indicate for each situation whether or not they had displayed each of the behavior items. To investigate the structure and the context-dependence of anger behavior, unconstrained Tucker3-HICLAS models in rank (1,1,1) through (5,5,5) were fitted to the resulting 6 situation $\times$ 14 behavior $\times$ 114 participant data array. Applying the rank selection heuristics described by Ceulemans et al. (2003) resulted in the selection of the (2,3,3) model, which has a proportion of discrepancies of .302. From the graphical representation

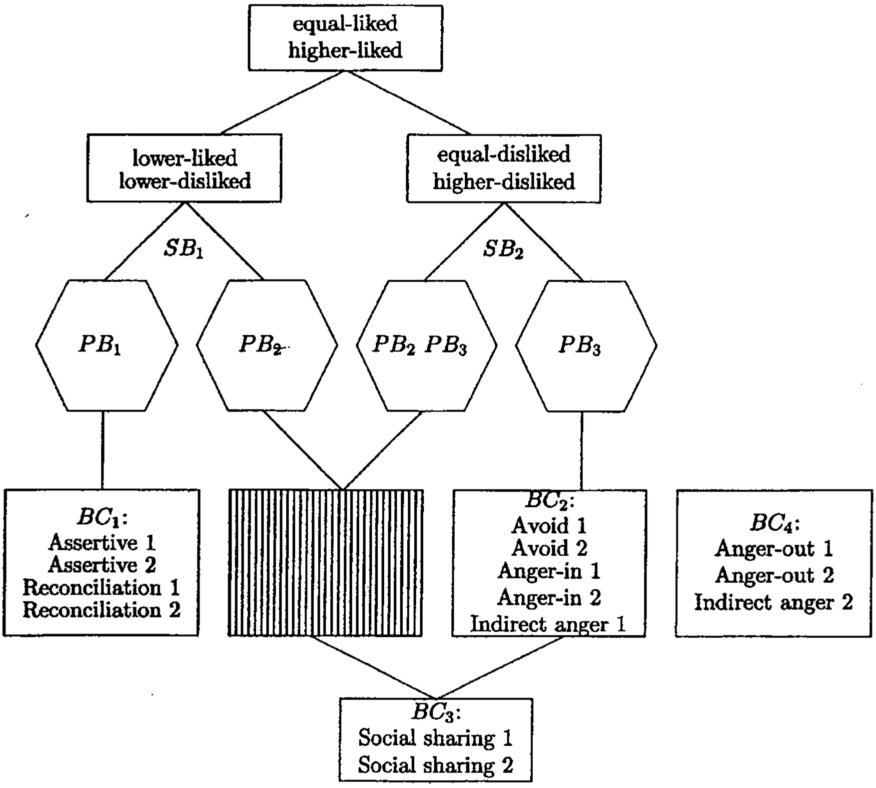

Figure 3. Overall graphical representation of the unconstrained Tucker3-HICLAS model for the anger expression data.

of the selected model, which is shown in Figure 3, one may read that for all but one of the seven included behavior types (i.e., indirect anger behavior) the corresponding two items were placed in the same behavior class (i.e., they have identical bundle patterns). The question arises whether imposing same class-membership to the two items referring to each of the seven behavior types would yield a model that fits the data (almost) equally well, implying that also the items referring to indirect anger behavior reflect a single behavior type.

4.2.2 Formalization of the Hypotheses

For each of the seven considered behavior types, one may check whether the two corresponding items indeed reflect the behavior type in question by imposing the constraint mentioned above: The two items are required to have an identical bundle pattern. Formally, this constraint implies that the behavior bundle matrix may be further decomposed into a $J \times C$ binary partition matrix **P** and a $C \times Q$ partition class bundle matrix $\mathbf{B}^*$:

$$\forall j = 1 \dots J, q = 1 \dots Q : b_{jq} = \bigoplus_{c=1}^{C} p_{jc} b^*_{cq} \tag{11}$$

where for **P** holds that C=7 and that, iff behaviors j and j' assess the same behavior type, $p_{j.} = p_{j'.}$. Clearly, the latter constraint is a structure constraint on the whole behavior bundle matrix that depends on external information.

4.2.3 Algorithm

As applying the closure operation routine to an estimate of the behavior bundle matrix **B** constrained according to (11), will always yield final estimates that still satisfy the constraint in question (see Subsection 3.2), we developed the following level 2 adaptation of the algorithm: When updating **B** in the alternating least squares routine, we successively optimized the bundle patterns of the seven partition classes defined by the partition matrix **P**, by means of Boolean regression. More specifically, to estimate the bundle pattern of partition class c, $b^*_{c.}$, the values of the criterion variable were the data entries d_{ijk} $(\forall i = 1 \dots I, k = 1 \dots K; \forall j : p_{jc} = 1)$ and the values of the q-th predictor variable were the sums $\bigoplus_{p=1}^{P} \bigoplus_{r=1}^{R} a_{ip} c_{kr} g_{pqr}$ $(\forall i = 1 \dots I, k = 1 \dots K)$. Some simulation results for this new algorithm are given in the appendix.

4.2.4 Results

A constrained Tucker3-HICLAS model of rank (2,3,3), in which the two items reflecting a particular behavior type were required to have an identical bundle pattern, was fitted to $\underline{\mathbf{D}}$. The proportion of discrepancies of the resulting constrained model, which amounts to .306, is only .004 higher than that of the unconstrained model. Together with the finding that, except for the bundle pattern of two participants only, the arrays **A**, **C** and $\underline{\mathbf{G}}$ were not altered by constraining **B**, the former result suggests that all item pairs can indeed be considered to reflect a particular type of anger behavior. Figure 4 displays the overall graphical representation of the constrained (2,3,3) model, and Figure 5 represents the participant hierarchy; note that, unlike for the behaviors, the participants with a zero bundle pattern have not been included in the representations.

Regarding the structure of the behavior types that may follow anger experiences, the hierarchical classification of the behavior items may be interpreted

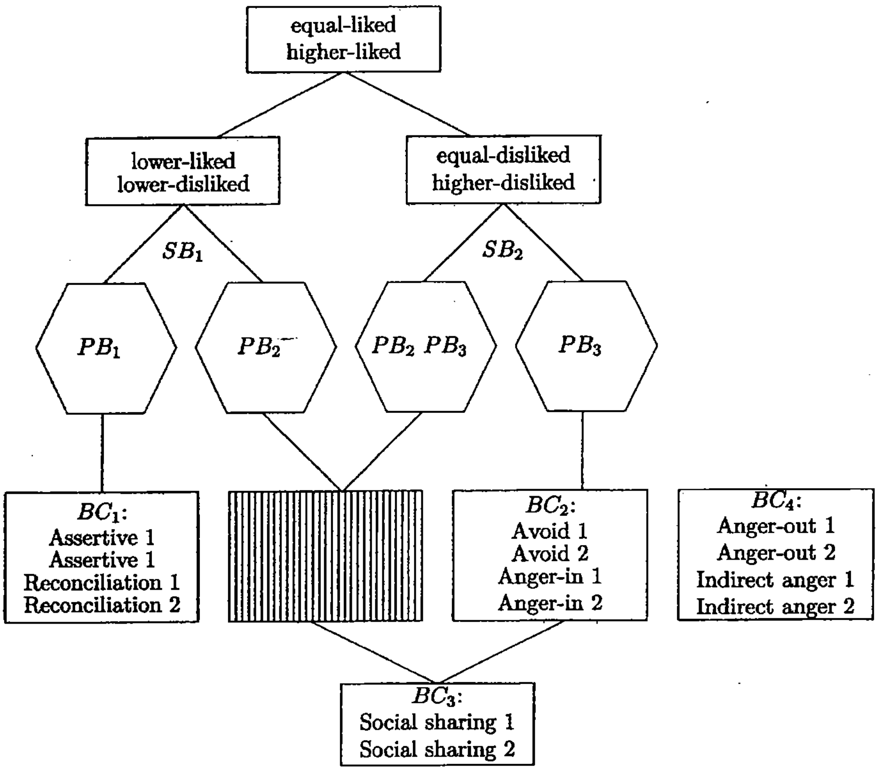

Figure 4. Overall graphical representation of the constrained Tucker3-HICLAS model for the anger expression data.

as follows: Behavior class (BC_1) contains behaviors that imply approaching the target of anger without aggressive intentions (assertive behavior and reconciliation). Behavior class (BC_2) consists of behaviors that imply avoiding a confrontation with the target of anger (avoid, anger-in). The latter behavior class further implies the third behavior class (BC_3): socially sharing the anger experience with others. Finally, the anger-out and indirect anger behavior types that constitute the fourth behavior class (BC_4) imply approaching the target in an antisocial way. Such a characterization in terms of approach and avoidance is in line with suggestions made by other authors regarding the organization of interpersonal behavior (Elliot and Trash, 2002). Interestingly, the results suggest that if one suppresses one's anger and avoids the person one is angry at, one will revert to social sharing, possibly to cope with the anger incident.

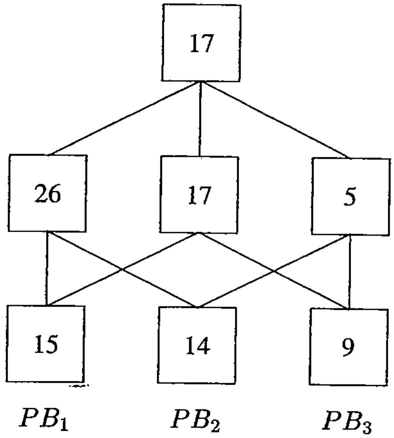

Figure 5. Participant structure of the constrained Tucker3-HICLAS model for the anger expression data.

Regarding the context-dependence of anger behavior, the analysis suggests two situation features that may differentiate between various types of anger behavior: 'the target is of lower status or liked' (SB_1) and 'the target is of higher or equal status' (SB_2).

4.3 Application 3: Decision Making in Psychiatric Diagnosis

4.3.1 Substantive Questions and Hypotheses

An important research question in psychiatric diagnosis research pertains to individual differences among clinicians' symptom judgements. It has been suggested that the latter differences may be explained by considering the cognitive structures and processes that underly the symptom judgements (e.g., Van Mechelen and De Boeck, 1989). For example, one may assume that symptom judgements involve a cognitive structure in the head of the clinician, in particular, an implicit taxonomy of syndromes that are defined in terms of clusters of symptoms; such an implicit taxonomy of syndromes may have been constructed on the basis of the study and work experiences of the clinician. One may then hypothesize that assigning symptoms to patients implies the following three-step cognitive process: In the first step, the clinician determines which types of evidence may be derived from the case description of the patient. In the second step, the clinician decides which of the derived types of evidence he will take into account. In the third step, the clinician classifies the patient, based on the retained clinical evidence, into his implicit taxonomy of syndromes; the taxonomy being defined in terms of clusters of symptoms, this classification immediately yields the symptoms to assign to the patient. Given this assumed process, individual differences among clinicians in symptom judgements may be explained by individual differences in the clinicians' implicit taxonomies and/or in one or more of the steps of the process in question. In this application, we will check the extent to which we can already satisfactorily approximate the data by assuming individual differences in the second step of the cognitive process only, by analyzing a 30 case description of psychiatric inpatient $\times$ 23 symptom $\times$ 15 clinician binary data array that was gathered by Van Mechelen and De Boeck (1990); $d_{ijk} = 1$ implies that clinician k indicated that symptom j was presumably present for inpatient i.

4.3.2 Formalization of the Hypotheses

Given a binary case description of psychiatric inpatient by symptom by clinician data array, the hypothesis discussed above may be formalized by a (P, Q, R) Tucker3-HICLAS model with a constrained core array. More in particular, the inpatient bundle matrix **A** shows which clinical evidence may be derived from each of the case descriptions (step 1 of the cognitive process), the symptom bundle matrix **B** yields the clusters of symptoms that define the Q syndromes of the implicit taxonomy, and the clinician bundle matrix **C** denotes membership of the R overlapping clinician types. Steps 2 and 3 of the cognitive process can be formalized by means of a core array $\underline{\mathbf{G}}$ that is constrained to be further decomposable into a $P \times R$ binary matrix $\mathbf{G}^1$ and a $P \times Q$ binary matrix $\mathbf{G}^2$ as follows:

$$\forall p = 1..P, q = 1..Q, r = 1..R : g_{pqr} = g^1_{pr} g^2_{pq}. \tag{12}$$

In (12), $\mathbf{G}^1$ represents the second step of the three-step cognitive process, that is, the willingness of each of the R clinician types to take each of the P clinical evidence types into account; $\mathbf{G}^2$ represents the third step, that is, which of the Q implicit syndromes is diagnosed on the basis of each of the P clinical evidence types. From the above description, it is obvious that the imposed constraint is a structure constraint on the whole core array that is not based on external information.

4.3.3 Algorithm

As discussed in Subsection 3.2, a structure constraint on the core array may be fitted by a level 3 adaptation of the Tucker3-HICLAS algorithm, with the adaptation boiling down to the development of a tailor-made procedure for

Table 5: Core array $\underline{G}$ of the unconstrained (4,4,2) Tucker3-HICLAS model for the psychiatrists data

Clinician type 1					Clinician type 2				
	Syndromes					Syndromes			
Evidence types	1	2	3	4	Evidence types	1	2	3	4
1	1	1	0	0	1	0	0	0	0
2	1	1	0	0	2	0	1	0	0
3	1	0	0	0	3	0	0	1	0
4	1	0	0	1	4	0	0	0	1

updating the core array in the alternating least squares routine. For the constraint given by (12), the following tailor-made procedure was developed. In the first substep, $\mathbf{G}^2$ was filled randomly, subject to the restriction that no row or column of $\mathbf{G}^2$ was a zero-vector or identical to another row or column; this restriction was imposed in order to obtain a Tucker3-HICLAS model of full rank. In the second substep, an optimal estimate of $\mathbf{G}^1$ was calculated conditionally upon $\mathbf{G}^2$ and the current estimates of **A**, **B** and **C** by means of Boolean regression. These two substeps (i.e., random generation of $\mathbf{G}^2$ and estimation of $\mathbf{G}^1$) are repeated a high number of times (e.g., 100 times); out of the resulting ($\mathbf{G}^1$,$\mathbf{G}^2$) pairs, the pair that minimized the loss function is retained and combined to $\underline{G}$ by (12). Note that this is just one possible procedure; for example, the roles of $\mathbf{G}^1$ and $\mathbf{G}^2$ can easily be reversed, that is, random generation of $\mathbf{G}^1$ and estimation of $\mathbf{G}^2$. Some simulation results for this algorithm are shown in the appendix.

4.3.4 Results

First, it was checked whether unconstrained Tucker3-HICLAS analyses yield a model that is in line with our hypothesis of a three-step cognitive process with individual differences in the second step only. In particular, unconstrained Tucker3-HICLAS models in ranks (1,1,1) through (5,5,5) were fitted to $\underline{\mathbf{D}}$. Applying the rank selection heuristics described by Ceulemans et al. (2003) resulted in the selection of the (4,4,2) model, which has a proportion of discrepancies of .187. From Table 5, it may be derived that the core array of the selected model is not of the hypothesized form as described by (12).

Therefore, in order to check whether imposing the constraint (12) would imply a large increase of the proportion of discrepancies and, hence, would

Table 6: $\mathbf{G}^1$ and $\mathbf{G}^2$ of the constrained (4,4,2) Tucker3-HICLAS model for the psychiatrists data

$\mathbf{G}^1$			$\mathbf{G}^2$				
	Clinician types			Syndromes			
Evidence types	1	2	Evidence types	1	2	3	4
1	1	1	1	1	0	0	0
2	0	1	2	0	1	0	0
3	1	1	3	0	0	1	0
4	1	1	4	0	0	0	1

falsify our hypothesis, we fitted an appropriately constrained (4,4,2) Tucker3-HICLAS model. The proportion of discrepancies of the resulting model equals .189, implying a .002 increase only of that of the unconstrained model. The latter finding suggests that the individual differences in clinicians' symptom judgements may indeed be explained by assuming our three-step cognitive process with individual differences in the second step only, that is, in terms of differences in willingness to take the different clinical evidence types into account. Table 6 presents the matrices $\mathbf{G}^1$ and $\mathbf{G}^2$, which can be combined by (12) to the constrained core array $\underline{\mathbf{G}}$. Furthermore, Figure 6 shows the overall graphical representation of the (4,4,2) model and Figure 7 represents the clinician hierarchy, with the inpatient and clinician classes indicating the number of elements that belong to the class; note that the inpatients, symptoms and clinicians with a zero bundle pattern have not been included in the representations and that the hatched boxes represent empty base classes. In the following paragraphs, we will give a substantive interpretation of this (4,4,2) solution.

Regarding the clinical evidence types that may be derived from the case descriptions of the inpatients (Step 1 of the cognitive process), we conclude from these case descriptions that the first type of evidence (ET_1) pertains to blocking of speech and interpersonal contact, whereas the second type of evidence (ET_2) pertains to disorganization of emotion, cognition and motor behavior. Inpatients showing evidence of the third and fourth type (ET_3 and ET_4) both reported problems of severe negative affect, but differ in that patients of the third type also reported suicidal tendencies and social isolation, whereas those of the fourth type showed augmented arousal and verbally expressed their negative affect.We tentatively label these four evidence types 'Social and speech blocking', 'Disorganized cognition, affect and motor behavior', 'Negative affect combined with suicidality and social isolation' and 'Negative affect com-

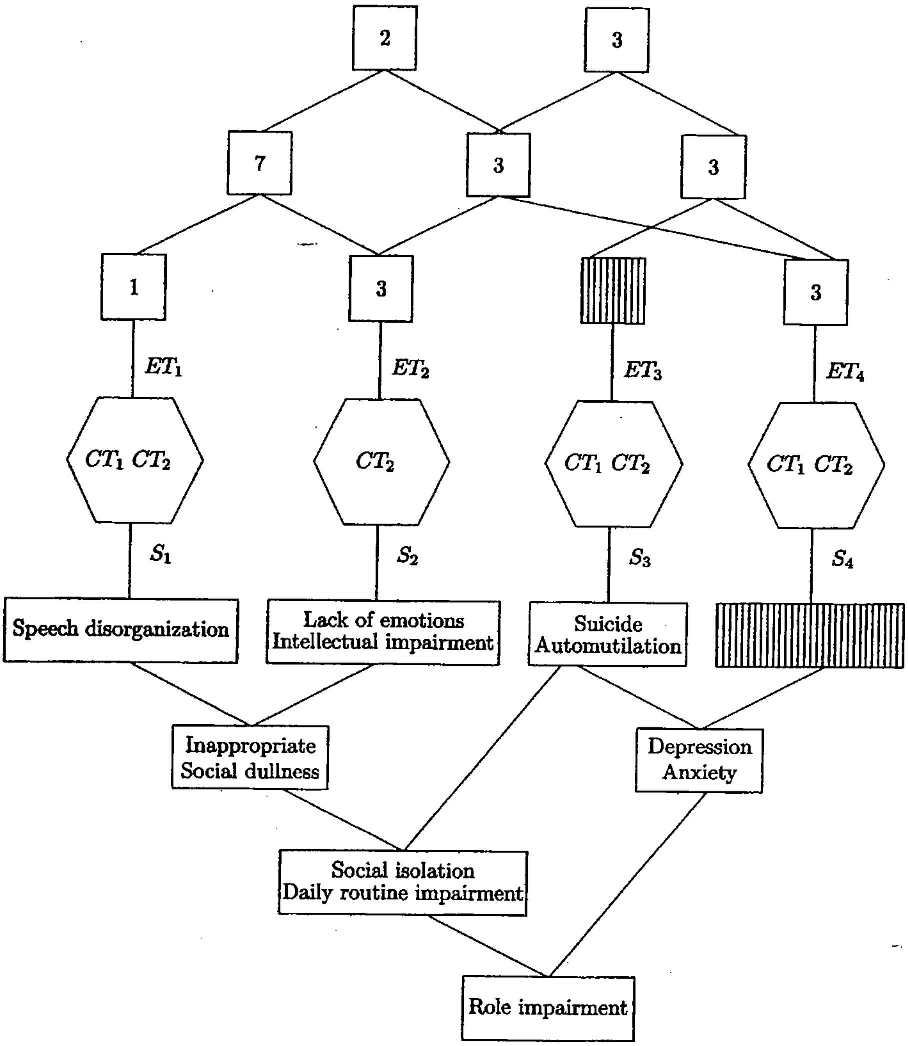

Figure 6. Overall graphical representation of the constrained Tucker3-HICLAS model for the psychiatrists data.

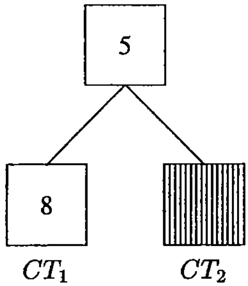

Figure 7. Clinician structure of the constrained Tucker3-HICLAS model for the psychiatrists data.

bined with arousal and verbal expression', respectively.

Turning our attention to Step 2 of the cognitive process, Figure 7 shows that there are two types of clinicians involved: a first type (CT_1) to which almost all clinicians belong and a second type (CT_2) to which only five of them belong. As stated above, the difference between these two clinician types can be understood in terms of willingness to take the different clinical evidence types into account: More specifically, one may read from the matrix $\mathbf{G}^1$ in Table 6 that the second clinician type takes all evidence types into account, whereas the first clinician type does not consider 'Disorganized cognition, affect and motor behavior' (ET_2).

Finally, to assign the symptoms on the basis of the retained clinical evidence (Step 3 of the cognitive process), an implicit taxonomy consisting of four syndromes was used. The first and second syndromes (S_1 and S_2), which are diagnosed on the basis of ET_1 and ET_2 (see $\mathbf{G}^2$ in Table 6), both contain psychotic symptoms. The first syndrome however also includes a specific symptom of interpersonal dysfunctioning (Speech disorganization) whereas the second syndrome also includes symptoms of intrapersonal dysfunctioning (e.g., Intellectual impairment); we therefore label them as psychotic/interpersonal and psychotic/intrapersonal, respectively. The third and fourth syndromes (S_3 and S_4), which are based on ET_3 and ET_4, are both defined by the depression and anxiety symptoms of a major affective disorder; however, only the third syndrome also includes suicidality. Hence, we may call them affective/suicidal and affective/non-suicidal, respectively.

5. Discussion

Constrained Tucker3-HICLAS modeling may be desirable for substantive as well as more technical reasons. From a substantive point of view, constrained Tucker3-HICLAS may be useful for investigating hypotheses on the structure of a data set. In particular, one may wish to test an a priori hypothesis obtained from substantive theory or from previous empirical research, implying a purely confirmatory analysis of the data set under study. Also, a hypothesis may arise from the analysis of the data set itself, which fits a strategy of modeling a data set alternatingly in an exploratory and confirmatory way. Finally, one may combine a priori and a posteriori hypotheses in one and the same analysis. In all cases, it is recommended to compare the fit of the constrained model with that of the unconstrained model of the same rank, in order to check whether the hypotheses are supported by the data. Other reasons for considering constrained Tucker3-HICLAS modeling are more technical: For example, due to the constraints on the values or the structure of the Tucker3-HICLAS parameters, constrained Tucker3-HICLAS models may be more parsimonious; therefore, constrained Tucker3-HICLAS modeling may yield results that are more stable in replication research.

For ease of explanation, in this paper the constrained Tucker3-HICLAS approach was primarily illustrated with hypothetical and real examples from the substantive context of personality psychology; however, it is obvious that the approach is also relevant for other substantive contexts. As a first example, note that we illustrated in this paper the usefulness of constrained Tucker3-HICLAS for research on psychiatric diagnosis. For another example, we consider a problem of developmental psychology; more specifically, the study of how cognitive skills develop over time in different types of children. Within this context, one may hypothesize that once a child acquires a specific cognitive skill, he will never loose it. If binary child by cognitive task by time point data are available, this hypothesis could be incorporated in a Tucker3-HICLAS analysis of the data set by restricting the time point bundle matrix to take the form of an ordered Guttman scale, that is, by imposing that the bundle pattern of each time point is a superset of all the previous time points (structure constraint on a whole bundle matrix that implies external information, i.e., time order).

As the number and variety of possible Tucker3-HICLAS constraints is huge, we proposed to organize them into a taxonomy based on four features of the constraints, which provides a generic framework for considering constrained Tucker3-HICLAS analysis and for investigating the interrelations of the different constraints. Although it is indeed possible to apply any constrained model to a given data array without knowing about this taxonomy, the benefits of using it are twofold: Firstly, the taxonomy gives an overview that may help researchers in finding or/and developing the constraint(s) that best match their analysis aims. Secondly, classifying a specific constraint in the taxonomy yields indications about the type of algorithm needed for fitting this constraint. Moreover, the proposed taxonomy may also be inspiring for real-valued

Tucker3/3MPCA research as it can also be used to classify Tucker3/3MPCA constraints. For example, the unimodality constraint described by Bro and Sidiropoulos (1998) can be considered a structure constraint on a whole component matrix that does not depend on external information, whereas Kiers et al.'s (1997) suggestion of fixing core entries to zero is a parameter constraint on part of the core array without making use of external information.

Possible future work in this area includes a further expansion of the family of constrained hierarchical classes models. The taxonomy proposed in this paper comprises constraints that pertain to a Tucker3-HICLAS analysis of a single data set. However, it may be worthwhile to consider other types of hierarchical classes constraints as well, including constraints that may be imposed when analyzing two data sets simultaneously. As an example of such a constraint, assume that a study from personality psychology research yields the following two data sets: a binary person × person characteristic data matrix and a binary situation × behavior × person data array, which have the person mode in common. In such a case, it would be interesting to analyze each of these data sets in such a way that the obtained person typology based on situation - behavior profiles can be immediately linked to the typology of the person characteristics. The latter can be achieved by simultaneously fitting a two-mode HICLAS model (De Boeck and Rosenberg, 1988) to the person × person characteristic data matrix and a Tucker3-HICLAS model to the situation × behavior × person data array, subject to the constraint that the person bundle matrices of the two models have to be identical; note that the latter type of constrained hierarchical classes analysis of two data sets is closely related to the multiway covariates regression analysis as proposed by Smilde and Kiers (1999).

Appendix

In this appendix, we briefly present some simulation results for the three constrained algorithms that were proposed in the Illustrative applications Section for fitting partition, decomposable core and value constraints. In this simulation study, we distinguish between three different types of $I \times J \times K$ binary arrays: true arrays $\underline{\mathbf{T}}$, data arrays $\underline{\mathbf{D}}$ and model arrays $\underline{\mathbf{M}}$. A true array $\underline{\mathbf{T}}$, which is constructed by the simulation researcher, can be perfectly represented by a constrained Tucker3-HICLAS model. A data array $\underline{\mathbf{D}}$ is a true array $\underline{\mathbf{T}}$ perturbed with error. A model array $\underline{\mathbf{M}}$ can be perfectly represented by a constrained Tucker3-HICLAS model of a specific rank, as it is obtained by analyzing $\underline{\mathbf{D}}$ with the associated constrained algorithm in the respective rank.

In the simulation study, we used two true array types: in particular, a partition constraint on **B** type and a decomposable core constraint type. Three parameters were further systematically varied:

(1) the *Size*, $I \times J \times K$, of $\underline{\mathbf{T}}$, $\underline{\mathbf{D}}$ and $\underline{\mathbf{M}}$, at 2 levels: $15 \times 15 \times 15$, $30 \times 20 \times 10$.

(2) the *True rank* of the constrained Tucker3-HICLAS model for $\underline{\mathbf{T}}$; for the partition type 2 levels were used: (2,2,2), (4,3,2); for the decomposable core type 2 levels were used: (2,2,2), (3,3,2).

(3) the *Error level*, ε, which is the proportion of cells d_{ijk} differing from t_{ijk}, at 5 levels: .00, .05, .10, .20, .30.

For the partition type, a fourth parameter - number of partition classes - was varied at three levels: 1/4, 2/4 and 3/4 of the number of columns.

For each combination of size, true rank, error level and, if applicable, number of partition classes, 20 true arrays $\underline{\mathbf{T}}$ were generated randomly; the generation procedure was similar to the procedure used in the unconstrained Tucker3-HICLAS simulation study (Ceulemans et al., 2003). Next, a data array $\underline{\mathbf{D}}$ was constructed from each true array $\underline{\mathbf{T}}$ by randomly altering the values of a proportion ε of the entries of $\underline{\mathbf{T}}$. On each of the resulting data arrays, a constrained Tucker3-HICLAS analysis of the true array type was performed in a rank equal to the True rank.

To evaluate the partition and decomposable core constraint algorithms, we first studied how well the constrained algorithms succeed in minimizing the loss function by calculating $BOF - \varepsilon$, i.e., the difference between the proportion of discrepancies between $\underline{\mathbf{D}}$ and $\underline{\mathbf{M}}$ on the one hand and the error level ε on the other hand. The mean value of the latter statistic equals .004 and .007 across the 1200 partition and 400 decomposable core observations, indicating that the obtained solutions are about as close to the data as the truth is. To assess the recovery of the association relation, we calculated as a badness of recovery (BOR) measure the proportion of discrepancies between $\underline{\mathbf{T}}$ and $\underline{\mathbf{M}}$, and found mean values of .010 and .012 respectively, implying that the models yielded by the algorithms differ on average about 1 % from the underlying truth. These results are comparable to the corresponding values of the unconstrained Tucker3-HICLAS simulation study.

To evaluate the value constraints algorithm, we analyzed all 1600 data arrays subject to the constraint that the behavior bundle matrix yielded by the algorithm equals the true behavior bundle matrix. In particular, we first used a regular two routine Tucker3-HICLAS algorithm in which the updating step for **B** was skipped to get an impression of how often the closure operation routine would violate the constraint: The latter happened for 298 (18.6%) data arrays only. The arrays in question were subsequently subjected to the constrained Tucker3-HICLAS algorithm that simultaneously optimizes the association and quasi-order relations. On average, the $BOF - \varepsilon$ and BOR values of the latter one routine algorithm were .0015 lower than those of the two routine algorithm. As the two routine algorithm already yielded solutions with on average lower

$BOF - \varepsilon$ and BOR values than the partition constraint and decomposable core constraint algorithms, we conclude that the one routine algorithm works well.

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