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# Uniqueness of $N$-way $N$-mode hierarchical classes models

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**Abstract**

This paper presents two uniqueness theorems for the family of hierarchical classes models, a collection of order preserving Boolean decomposition models for binary $N$-way $N$-mode data. The theorems are compared with uniqueness results for the closely related family of $N$-way $N$-mode principal component models. It is concluded that the two-way two-mode PCA and $N$-way $N$-mode Tucker$N$ models suffer more from a lack of identifiability than their hierarchical classes analogues, whereas the uniqueness conditions for $N$-way $N$-mode PARAFAC/CANDECOMP models are less restrictive than the ones derived for their $N$-way $N$-mode hierarchical classes counterparts.



*Keywords:* Uniqueness; Hierarchical classes; PCA; TUCKER3; PARAFAC/CANDECOMP

## 1. Introduction

Hierarchical classes models are structural models for $N$-way $N$-mode binary data. The latter type of data often occurs in psychology. Examples of two-way two-mode binary data include person by item succes/failure data and psychiatric patient by symptom presence/absence data. Regarding three-way three-mode binary data, one may think of person by situation by behavior display/not display data and consumer by product by timepoint select/not select data.

Hierarchical classes analysis approximates the $I_1 \times I_2 \times \cdots \times I_N$ binary data array $\underline{\mathbf{D}}$ with a $I_1 \times I_2 \times \cdots \times I_N$ reconstructed data or model array $\underline{\mathbf{M}}$ that can be represented by a hierarchical classes model. Such a hierarchical classes model reduces each of the $N$ modes of $\underline{\mathbf{M}}$ to a few binary components and interrelates the $N$ sets of components by means of a linking structure. Furthermore, such a model represents two types of relations implied by $\underline{\mathbf{M}}$: (1) the $N$-ary relation defined by the 1-entries of $\underline{\mathbf{M}}$, and (2) the quasi order $\leqslant$ that is induced by $\underline{\mathbf{M}}$ on each of the $N$ modes. As to the latter, note that in the $N$-ary relation implied by $\underline{\mathbf{M}}$, each element $i$ of the $n$th mode is related with a subset $S^i$ of the Cartesian product of the other modes; we then define $i_1 \leqslant i_2$ iff $S^{i_1} \subseteq S^{i_2}$. In a hierarchical classes model, the $N$-ary relation is represented by a decomposition rule, which states how $\underline{\mathbf{M}}$ can be obtained from the $N$ sets of components and the linking structure. The quasi-orders are represented by subset–superset relations among the component patterns of the respective elements (i.e., the sets of components to which the elements belong).

The representations of the $N$-ary relation and of the quasi-orders are of substantive importance. Regarding the first, a hierarchical classes analysis of a $N$-way $N$-mode binary data array $\underline{\mathbf{D}}$ may uncover the structural mechanism underlying $\underline{\mathbf{D}}$. For example, a hierarchical classes analysis may reveal the latent choice requisites that underly consumer by product select/not select data, with a consumer selecting those products that satisfy all of his requisites (Van Mechelen & Van Damme, 1994). Similarly, such an analysis may reveal the latent pieces of clinical evidence and the latent syndromes behind psychiatric patient by symptom presence/absence data (Van Mechelen & De Boeck, 1989). The representation of the quasi-orders may be useful in that it implies a simultaneous classification of the elements of each of the modes involved in the data; this may, for instance, meet the substantive need of personality psychologists searching for simultaneous classifications or triple typologies of persons, situations and behaviors in binary person by situation by behavior display/not display data

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(Vansteelandt & Van Mechelen, 1998). Furthermore, the representation of the quasi-orders may also be used for retrieving if–then type relations among elements. Such relations are of key relevance in, for example, the study of person perception (e.g., Gara & Rosenberg, 1990); also, they constitute the core of the theory of knowledge spaces (Falmagne, Koppen, Vilano, Doignon, & Johannesen, 1990).

A possible problem in using hierarchical classes models is that hierarchical classes decompositions sometimes are not unique. The latter implies that several sets of components and a linking structure may account for the same $N$-ary relation, which may complicate a sound interpretation of the mechanism underlying the data. To handle this problem, one may derive uniqueness conditions for hierarchical classes decompositions. The latter has already been achieved for the two-way two-mode hierarchical classes model (Van Mechelen, De Boeck, & Rosenberg, 1995).

In the present paper we will prove two uniqueness theorems for two distinct types of three-way three-mode hierarchical classes models as well as their $N$-way $N$-mode extensions, that subsume the uniqueness results for the two-way two-mode model as a special case. Furthermore, we will compare the proposed uniqueness theorems for the hierarchical classes family with uniqueness results for the closely related family of principal component models (Tucker, 1966; Harshman, 1970; Carroll & Chang, 1970).

The remainder of this paper is organized as follows: Section 2 briefly recapitulates the two-way two-mode and three-way three-mode hierarchical classes models and shows how they can be extended to the $N$-way $N$-mode case. In Section 3, two general uniqueness theorems for $N$-way $N$-mode hierarchical classes models are derived. Section 4 compares the uniqueness theorems for the hierarchical classes models with uniqueness results for principal component models.

## 2. Theory of the hierarchical classes models

### 2.1. *De Boeck and Rosenberg's (1988) two-way two-mode HICLAS model*

De Boeck and Rosenberg's (1988) two-way two-mode hierarchical classes model (HICLAS) approximates an $I \times J$ objects by attributes binary data array $\mathbf{D}$ by an $I \times J$ binary model array $\mathbf{M}$ that can be decomposed into an $I \times R$ binary matrix $\mathbf{A}$ and a $J \times R$ binary matrix $\mathbf{B}$, where $R$ denotes the rank of the model. The columns of $\mathbf{A}$ and $\mathbf{B}$ define $R$ binary variables, called object and attribute components; therefore, $\mathbf{A}$ and $\mathbf{B}$ are called object and attribute component matrices, respectively.

The HICLAS model represents two types of structural relations implied by $\mathbf{M}$: the binary relation and quasi-orders on each of the modes implied by the data.

*Binary relation*: The HICLAS model represents the binary relation by the following decomposition rule:

$$\mathbf{M} = \mathbf{A} \otimes \mathbf{B}', \tag{1}$$

where $\otimes$ denotes the Boolean matrix product (Kim, 1982) and $'$ denotes transpose. This decomposition rule means that for an arbitrary entry $m_{ij}$ of $\mathbf{M}$,

$$m_{ij} = \bigoplus_{r=1}^{R} a_{ir} b_{jr}, \tag{2}$$

where $\oplus$ denotes the Boolean sum. Thus, an object $i$ is associated with an attribute $j$ in $\mathbf{M}$ iff a component exists to which both $i$ and $j$ belong. The decomposition rule further implies that the linking structure among the object and attribute components takes the form of a one-to-one correspondence between the respective components.

*Quasi-orders*: A quasi-order $\leqslant$ is defined on each mode of $\mathbf{M}$. Letting $S^x$ denote the set of elements from the other mode that $x$ is related with in $\mathbf{M}$, it holds that object $i_1 \leqslant$ object $i_2$ in $\mathbf{M}$ iff $S^{i_1} \subseteq S^{i_2}$. Similarly, attribute $j_1 \leqslant$ attribute $j_2$ in $\mathbf{M}$ iff $S^{j_1} \subseteq S^{j_2}$. These quasi-orders are represented in $\mathbf{A}$ and $\mathbf{B}$ in terms of subset–superset relations among the component patterns: object $i_1 \leqslant$ object $i_2$ iff $a_{i_1.} \subseteq a_{i_2.}$ and attribute $j_1 \leqslant$ attribute $j_2$ iff $b_{j_1.} \subseteq b_{j_2.}$.

Note that the representation of the quasi-orders on the object and attribute modes implies a simultaneous classification of both modes, in that objects and attributes with identical component patterns constitute object classes and attribute classes, respectively. Furthermore, from the representation of the quasi-orders one may derive if–then type relations among elements. More specifically, object $i_1 \leqslant$ object $i_2$ implies that *if* an attribute $j$ is related with $i_1$ in $\mathbf{M}$, *then* $j$ is also related with $i_2$ in $\mathbf{M}$. Similarly, attribute $j_1 \leqslant$ attribute $j_2$ implies that *if* an object $i$ is related with $j_1$ in $\mathbf{M}$, *then* $i$ is also related with $j_2$ in $\mathbf{M}$.

### 2.2. *The three-way three-mode INDCLAS and Tucker3-HICLAS models*

Two three-way three-mode hierarchical classes models have been proposed: the INDCLAS model (Leenen, Van Mechelen, De Boeck, & Rosenberg, 1999) and the more general Tucker3-HICLAS model (Ceulemans, Van Mechelen, & Leenen, in press).

#### 2.2.1. *The INDCLAS model*

Being a three-way three-mode extension of HICLAS, INDCLAS implies a decomposition of a binary $I \times J \times K$ objects by attributes by sources model array $\underline{\mathbf{M}}$ into an $I \times R$ object component matrix $\mathbf{A}$, a $J \times R$ attribute component matrix $\mathbf{B}$ and a $K \times R$ source component matrix $\mathbf{C}$, with $R$ denoting the rank of the model.

INDCLAS represents the ternary relation and the quasi-orders as follows:

*Ternary relation*: The INDCLAS model represents the ternary relation among the objects, attributes and sources in $\underline{\mathbf{M}}$ by the following decomposition rule:

$$m_{ijk} = \bigoplus_{r=1}^{R} a_{ir} b_{jr} c_{kr}. \tag{3}$$

This means that an object $i$, an attribute $j$ and a source $k$ are associated in $\underline{\mathbf{M}}$ iff a component exists to which $i$, $j$ and $k$ belong. Obviously, the linking structure among the object, attribute and source components takes the form of a one-to-one correspondence among the respective components.

*Quasi-orders*: A quasi-order $\leqslant$ is defined on the objects, attributes and sources. More specifically, element $x \leqslant$ element $y$ iff $S^x \subseteq S^y$, with $S^x$ denoting the set of pairs of elements of the other two modes $x$ is related with in $\underline{\mathbf{M}}$. The quasi-orders on the objects, attributes and sources are represented in terms of subset–superset relations among the component patterns in $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$, respectively.

The representation of the quasi-orders on the object, attribute and source mode implies (1) a simultaneous classification of the three modes, and (2) if–then type relations among elements. As to the latter, object $i_1 \leqslant$ object $i_2$ implies that *if* an attribute–source pair $(j,k)$ is related with $i_1$ in $\underline{\mathbf{M}}$, then $(j,k)$ is also related with $i_2$ in $\underline{\mathbf{M}}$.

#### 2.2.2. The Tucker3-HICLAS model

The INDCLAS model is quite restrictive in that it constrains (1) the number of components to be equal for each mode, and (2) the linking structure among the object, attribute and source components to constitute a one-to-one correspondence among the respective components. As the latter INDCLAS restrictions often make less sense from a substantive point of view (see Ceulemans et al., in press), the Tucker3-HICLAS model was proposed which allows (1) the number of components to differ across the three modes, and (2) all linking structures among the three sets of components that can be represented by an object components × attribute components × source components binary array. Formally, Tucker3-HICLAS decomposes $\underline{\mathbf{M}}$ into an $I \times P$ object component matrix $\mathbf{A}$, a $J \times Q$ attribute component matrix $\mathbf{B}$, a $K \times R$ source component matrix $\mathbf{C}$ and a $P \times Q \times R$ binary core array $\underline{\mathbf{G}}$, with $(P, Q, R)$ denoting the rank of the model and $\underline{\mathbf{G}}$ representing the linking structure among the three sets of components.

*Ternary relation*: The Tucker3-HICLAS decomposition rule is given by

$$m_{ijk} = \bigoplus_{p=1}^{P} \bigoplus_{q=1}^{Q} \bigoplus_{r=1}^{R} a_{ip} b_{jq} c_{kr} g_{pqr}, \tag{4}$$

implying that an object $i$, an attribute $j$ and a source $k$ are associated in $\underline{\mathbf{M}}$ iff an object, attribute and source component exist, to which $i$, $j$ and $k$, respectively, belong and that are interrelated in $\underline{\mathbf{G}}$. Note that Tucker3-HICLAS reduces to INDCLAS iff $P$, $Q$ and $R$ are equal and $\underline{\mathbf{G}}$ is a 'unit superdiagonal' array (i.e., $P = Q = R$, $g_{pqr} = 1$ iff $p = q = r$ and $g_{pqr} = 0$ otherwise; Kiers, 2000), and that every INDCLAS model can be rewritten as a Tucker3-HICLAS model by adding a $R \times R \times R$ 'unit superdiagonal' core array $\underline{\mathbf{G}}$.

*Quasi-orders*: The quasi-orders $\leqslant$ on the objects, attributes and sources are defined and represented as in the INDCLAS model.

### 2.3. N-way N-mode extensions of the INDCLAS and Tucker3-HICLAS models

$N$-way $N$-mode extensions of INDCLAS and Tucker3-HICLAS can be easily conceived. A $N$-way $N$-mode HICLAS model decomposes a binary $I_1 \times I_2 \times \cdots \times I_N$ model array $\underline{\mathbf{M}}$ into $I_n \times R$ component matrices $\mathbf{A}^n$ $(n = 1, \ldots, N)$, where $R$ denotes the rank of the model, and represents the $N$-ary relation in $\underline{\mathbf{M}}$ by the following decomposition rule

$$m_{i_1 i_2 \cdots i_N} = \bigoplus_{r=1}^{R} \left( \prod_{n=1}^{N} a^n_{i_n r} \right). \tag{5}$$

A $N$-way $N$-mode Tucker$N$-HICLAS model implies $I_n \times P_n$ component matrices $\mathbf{A}^n$ $(n = 1, \ldots, N)$ and a $P_1 \times P_2 \times \cdots \times P_N$ core array $\underline{\mathbf{G}}$, with $(P_1, P_2, \ldots, P_N)$ denoting the rank of the model, and takes the following decomposition rule:

$$m_{i_1 i_2 \cdots i_N} = \bigoplus_{p_1=1}^{P_1} \bigoplus_{p_2=1}^{P_2} \cdots \bigoplus_{p_N=1}^{P_N} \left( \prod_{n=1}^{N} a^n_{i_n p_n} \right) g_{p_1 p_2 \cdots p_n}. \tag{6}$$

Both models define a quasi-order $\leqslant$ on the $N$ modes in terms of the set of ($N$-1)-tuples of elements of the other $N$-1 modes an element of some mode is related with in $\underline{\mathbf{M}}$. The quasi-order on a mode is represented in the corresponding component matrix in terms of subset–superset relations among the component patterns.

## 3. Two uniqueness theorems for N-way N-mode hierarchical classes models

In this section we will derive sufficient conditions for the uniqueness of $N$-way $N$-mode hierarchical classes models, starting from uniqueness theorems for the two-way two-mode and three-way three-mode hierarchical classes models.

### *3.1. Uniqueness of the two-way two-mode HICLAS model*

Van Mechelen et al. (1995) have stated the following uniqueness theorem for the two-way two-mode HICLAS model:

**Theorem 1.** *If all component specific classes (i.e., classes of elements that belong to one component only) of a rank R HICLAS decomposition of an* $I \times J$ *binary array* $\mathbf{M}$ *are non-empty, this decomposition is unique upon a permutation of the components.*

**Proof.** Assume, without loss of generality, that the first $R$ rows of $\mathbf{A}$ and $\mathbf{B}$ are elements of the component specific classes. In particular, for $1 \leqslant i \leqslant R$, we assume $a_{ir} = 1$ iff $r = i$; similarly, for $1 \leqslant h \leqslant R$, $b_{jr} = 1$ iff $r = j$. In that case, given the HICLAS decomposition rule (1), the $R \times R$ submatrix $\mathbf{M}^*$ based on the first $R$ rows of $\mathbf{A}$ and $\mathbf{B}$ is an identity matrix. Formally,

$$\mathbf{M}^* = \mathbf{A}^* \otimes \mathbf{B}^{*'} = \mathbf{I}, \tag{7}$$

where $\mathbf{A}^*$ and $\mathbf{B}^*$ consist of the first $R$ rows of $\mathbf{A}$ and $\mathbf{B}$. Note that (7) implies that $\mathbf{A}^*$ and $\mathbf{B}^*$ are each other's inverse. Now, Luce (1952) and Rutherford (1963) have shown that the only Boolean matrices that have an inverse are permutation matrices. It therefore follows that the decomposition of $\mathbf{M}^*$ into $\mathbf{A}^*$ and $\mathbf{B}^*$ is unique upon a permutation of the components which, due to the representation of the binary relation in $\mathbf{M}$, then also holds for the decomposition of $\mathbf{M}$ into $\mathbf{A}$ and $\mathbf{B}$. □

### *3.2. Uniqueness of the three-way three-mode INDCLAS and Tucker3-HICLAS models*

#### *3.2.1. Uniqueness of the INDCLAS model*

As an extension of Theorem 1, Leenen et al. (1999) suggested, without a proof, the following sufficient condition for the uniqueness of an INDCLAS decomposition:

**Theorem 2.** *If the component matrices* $\mathbf{A}$, $\mathbf{B}$ *and* $\mathbf{C}$ *of a rank R INDCLAS decomposition of an* $I \times J \times K$ *binary array* $\underline{\mathbf{M}}$ *include all component specific patterns, this decomposition is unique (upon a permutation of the components).*

For this theorem we propose the following proof:

**Proof.** We will prove the uniqueness of $\mathbf{A}$; the uniqueness of $\mathbf{B}$ and $\mathbf{C}$ can be shown similarly. It follows from the INDCLAS decomposition rule (3) that, if $\underline{\mathbf{M}}$ is matricized into an $I \times JK$ matrix, the following HICLAS-decomposition exists:

$$m_{i(jk)} = \bigoplus_{r=1}^{R} a_{ir}\tilde{b}_{(jk)r},$$

where $\tilde{b}_{(jk)r} = b_{jr}c_{kr}$ is an entry of the $JK \times R$ (attributes × sources) component matrix $\tilde{\mathbf{B}}$. Theorem 1 states that this HICLAS decomposition is unique (upon a permutation of the components), if the component specific classes of $\mathbf{A}$ and $\tilde{\mathbf{B}}$ are non-empty. For $\mathbf{A}$, the latter is obvious. For $\tilde{\mathbf{B}}$, the non-emptiness of the component specific classes of $\mathbf{B}$ and $\mathbf{C}$ implies that for any component $b$ ($b = 1, \ldots, R$) an attribute $j$ and a source $k$ exist such that $\tilde{b}_{(jk)r} = b_{jr}c_{kr} = 1$ iff $r = b$; hence, $\tilde{\mathbf{B}}$ contains all component specific patterns. □

#### *3.2.2. Uniqueness of the Tucker3-HICLAS model*

For the three-way three-mode Tucker3-HICLAS model, the following novel uniqueness theorem can be stated:

**Theorem 3.** *If a* $(P, Q, R)$ *Tucker3-HICLAS decomposition of an* $I \times J \times K$ *binary array* $\underline{\mathbf{M}}$ *exists, such that (1) the component matrices* $\mathbf{A}$, $\mathbf{B}$ *and* $\mathbf{C}$ *include all component specific patterns, and (2) no object (resp. attribute, source) plane of* $\underline{\mathbf{G}}$ *is a subset of the Boolean sum of the other object (resp. attribute, source) planes of* $\underline{\mathbf{G}}$, *this decomposition is unique upon a permutation of the object, attribute and source components.*

**Proof.** Assume, without loss of generality, that the first $P$, $Q$ and $R$ rows of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$, respectively, are elements of the component specific classes. In particular, for $1 \leqslant i \leqslant P$, we assume $a_{ip} = 1$ iff $p = i$; similarly, for $1 \leqslant j \leqslant Q$, $b_{jq} = 1$ iff $q = j$ and, for $1 \leqslant k \leqslant R$, $c_{kr} = 1$ iff $r = k$. We will first prove the uniqueness of $\mathbf{A}$ (the proof is similar for $\mathbf{B}$ and $\mathbf{C}$) and next the uniqueness of $\underline{\mathbf{G}}$. The Tucker3-HICLAS decomposition rule (4) implies that the following HICLAS decomposition of the matricized $I \times JK$ array $\underline{\mathbf{M}}$ exists:

$$m_{i(jk)} = \bigoplus_{p=1}^{P} a_{ip}\tilde{b}_{(jk)p},$$

where $\tilde{b}_{(jk)p} = \bigoplus_{q=1}^{Q} \bigoplus_{r=1}^{R} b_{jq}c_{kr}g_{pqr}$ is an entry of the $JK \times P$ (attributes × sources) component matrix $\tilde{\mathbf{B}}$. This HICLAS decomposition is unique (upon a permutation of the object components) since the component specific classes of $\mathbf{A}$ and $\tilde{\mathbf{B}}$ are non-empty. To show the latter for $\tilde{\mathbf{B}}$ we first note that the assumption about $\mathbf{B}$ and $\mathbf{C}$ implies that the submatrix $\tilde{\mathbf{B}}^*$ based on the first $Q$ and $R$ rows of $\mathbf{B}$ and $\mathbf{C}$ equals the matricized $QR \times P$ core array $\underline{\mathbf{G}}$; that is, for all $1 \leqslant j \leqslant Q$ and $1 \leqslant k \leqslant R, \tilde{b}_{(jk)p} = g_{pjk}$. The non-emptiness of the component specific classes of $\tilde{\mathbf{B}}^*$, and hence of $\tilde{\mathbf{B}}$, further follows from the restriction on $\underline{\mathbf{G}}$ that no object core plane is a subset of the Boolean sum of the other object core planes. For this restriction implies that for any object component $p^*$ ($p^* = 1, \ldots, P$) an attribute component $q$ and a source component $r$ exist such that $g_{pqr} = 1$ iff $p = p^*$. With respect to the core array $\underline{\mathbf{G}}$, the assumption about **A**, **B** and **C** implies that for all $1 \leqslant i \leqslant P$, $1 \leqslant j \leqslant Q$ and $1 \leqslant k \leqslant R$ $m_{ijk} = g_{ijk}$. The latter means that no core entry can be modified without modifying $\underline{\mathbf{M}}$ and, therefore, that $\underline{\mathbf{G}}$ is unique. □

### *3.3. Uniqueness of N-way N-mode HICLAS and TuckerN-HICLAS models*

The uniqueness theorems for the three-way three-mode INDCLAS and Tucker3-HICLAS models can easily be generalized $N$-way $N$-mode, yielding two uniqueness theorems for the $N$-way $N$-mode hierarchical classes models. Since the proofs are also straightforward extensions of the proofs in Subsection 5.2 (making use of the HICLAS decompositions of the matricized $I_1 \times I_2 \cdots I_N$ array $\underline{\mathbf{M}}$), they will be omitted.

**Theorem 4.** *If all component specific classes of a rank $R$ HICLAS decomposition of an $I_1 \times I_2 \times \cdots \times I_N$ binary array $\underline{\mathbf{M}}$ are non-empty, this decomposition is unique upon a permutation of the components.*

**Theorem 5.** *If a $(P_1, P_2, \ldots, P_N)$ TuckerN-HICLAS decomposition of an $I_1 \times I_2 \times \cdots \times I_N$ binary array $\underline{\mathbf{M}}$ exists, such that* (1) *each component matrix includes all component specific patterns, and* (2) *no core plane of $\underline{\mathbf{G}}$ is a subset of the Boolean sum of the other core planes of the same mode, this decomposition is unique upon a permutation of the N sets of components.*

## 4. Comparison with uniqueness results for $N$-way $N$-mode principal component models

In this paper we presented two uniqueness theorems for the $N$-way $N$-mode hierarchical classes models, from which sufficient conditions for the uniqueness of any hierarchical classes decomposition can be derived. The family of hierarchical classes models closely resembles the family of principal component models (Tucker, 1966; Harshman, 1970; Carroll & Chang, 1970). In particular, PCA, PARAFAC/CANDECOMP and Tucker3 differ in three respects only from HICLAS, INDCLAS and Tucker3-HICLAS, respectively: (1) the component matrices and core array of a hierarchical classes model are restricted to be binary, (2) hierarchical classes models are based on Boolean algebra, whereas principal component models involve standard algebra (note that replacing the Boolean sum $\oplus$ in (2), (3) and (4) by the regular sum $\sum$ yields the PCA, PARAFAC/CANDECOMP and Tucker3 decomposition rules), and (3) hierarchical classes models represent the quasi-order relations $\leqslant$ in the model array. In view of this close relationship, we will compare the uniqueness results for the hierarchical classes and principal component models. Before, we note that, whereas non-uniqueness of a principal component decomposition implies that an infinite number of equally well-fitting decompositions exists, due to the Boolean nature of the hierarchical classes models, the number of alternative decompositions for a non-unique hierarchical classes decomposition is finite.

We will first focus on the uniqueness results for the principal component counterparts of the $N$-way $N$-mode HICLAS models. Since models with only one component are almost always unique (Kruskal, 1977, 1989), we will only discuss identifiability of models with several components (i.e., $R \geqslant 2$). In case of two-mode PCA, it is well known that any two-way two-mode PCA model with more than one component can be rotated without affecting the fit and hence is not unique. For three-mode PARAFAC/CANDECOMP, Kruskal (1977, 1989) has shown that a three-way three-mode PARAFAC/CANDECOMP model with $R$ components is unique up to permutation and rescaling of the components if

$$k_{\mathbf{A}} + k_{\mathbf{B}} + k_{\mathbf{C}} \geqslant 2R + 2, \tag{8}$$

where $k_{\mathbf{A}}$ denotes the $k$-rank (Kruskal-rank) of the component matrix **A** (with **A** having $k$-rank $r$ if in every set of $r$ components from **A** the components are linearly independent and if there is at least one set of $(r+1)$ components that includes linearly dependent components; the latter definition implies $k_{\mathbf{A}} \leqslant R$). The uniqueness condition stated in (8) is mild: unless one mode consists of mere replicates, almost every three-mode PARAFAC/CANDECOMP solution is unique (Harshman & Lundy, 1984; Carroll & Pruzansky, 1984). Extending Kruskal's theorem to the $N$-mode case, Sidiropoulos and Bro (2000) have proven a $N$-way $N$-mode PARAFAC/CANDECOMP model with $R$ components to be unique upon permutation and rescaling, provided that

$$\sum_{n=1}^{N} k_{\mathbf{A_n}} \geqslant 2R + (N-1). \tag{9}$$

It is clear from (9) that the already mild uniqueness conditions for three-mode PARAFAC/CANDECOMP become even less stringent when more modes are involved: By adding a mode that does not consist of mere replicates the left-hand side of (9) increases by at least two and the right-hand side by one only. Noting that the uniqueness conditions for $N$-way $N$-mode HICLAS models as included in Theorem 4 remain equally restrictive for higher values of $N$, we may conclude that, except for $N = 2$, the $N$-way $N$-mode HICLAS models suffer more from a lack of identifiability than their principal component counterparts.

As regards the principal component analogues of the $N$-way $N$-mode Tucker$N$-HICLAS models, the main result is that every $N$-way $N$-mode Tucker$N$ solution can be rotated without affecting the fit. More specifically, only some constrained Tucker$N$ models can be uniquely identified, where the constraints may, for instance, pertain to fixing the value of certain core entries or component scores (Kiers, Ten Berge, & Rocci, 1997; Kiers & Smilde, 1998) or to non-negativity or uni-modality of the component scores (Bro & De Jong, 1997; Bro & Sidiropoulos, 1998). Although the sufficient uniqueness conditions stated in Theorem 5 are rather restrictive, we may conclude that the $N$-way $N$-mode Tucker$N$-HICLAS models suffer less from identifiability problems than their principal component analogues.

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