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Uniqueness of real-valued hierarchical classes models

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ABSTRACT

Two novel uniqueness theorems are derived for the family of hierarchical classes (HICLAS) models, a family of structural decomposition models for N-way N-mode data that imply simultaneous hierarchically organized classifications of all modes involved in the data. The theorems generalize earlier results on binary HICLAS models to the integer- and real-valued cases. In addition, they allow for a shorter and insightful proof of a result on Boolean matrix invertibility that goes back to earlier work of Luce (1952) and Rutherford (1963).

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1. Introduction

In psychological research one often encounters objects by variables data. Typically, these data can be arranged into a matrix in which the rows refer to the objects and in which the columns refer to the variables. A wealth of information is included in such a data matrix. This includes not only information on the association between object i and variable j (i.e., the value contained in row i and column j), but also on the relation between pairs of objects and between pairs of variables. A concrete example is a patient by symptom data matrix in which the entries indicate the presence/absence of each symptom in each patient. In this case, presence/absence may be represented by a binary variable with 1 indicating presence and 0 indicating absence. Information included in such a data set comprises information on which symptoms are associated to a given patient, information on which patients display similar symptom patterns, as well as information on which symptoms typically co-occur within the set of patients.

A challenge is then to simultaneously capture these types of information as included in a data set at hand. For this purpose, two-mode clustering methods that imply a discrete reduction of both the set of objects and the set of variables are especially suitable (for a comprehensive overview of this family, see Van Mechelen, Bock, & De Boeck, 2004). An important subclass within this family are hierarchical classes models. A distinctive characteristic of these models (as opposed to other two-mode clustering methods) is that they allow for a representation of if-then relations. In many applications these relations are of substantive interest. For example, in case one wishes to capture the internal structure of disease processes, relevant information may be of the following type: if a patient suffers from symptom j, then he/she will also suffer from symptom j'.

Originally, the HICLAS model was developed as a decomposition model for binary (e.g., presence/absence) objects by variables data, that is, binary two-way two-mode data (Carroll & Arabie, 1980). Recently, however, new members of the HICLAS family have been developed for data that take values from the set of positive integers (Van Mechelen, Lombardi, & Ceulemans, 2007) and for data that take values from the set of positive reals (Schepers & Van Mechelen, submitted for publication). These two types of data may be encountered, for example, in case the association between patients and symptoms is not simply characterized by presence/absence but rather by symptom severity.

An important question concerning HICLAS models is to what extent the decompositions are unique, as nonuniqueness may imply the existence of different substantive interpretations for a single data set. In this regard, one may note that HICLAS models are also closely related (see Section 2) to multi-mode component analysis (MMCA) models, including the well-known principal component analysis (PCA) model as one specific case. From this relatedness, one might in general expect an infinite number of HICLAS decompositions to yield the same reproduced data values (given the rotational freedom in many MMCA models). This, however, is not true in that many HICLAS decompositions are unique upon a permutation of the order of the components (see Section 2 for permutational freedom). The major remaining challenge on the level of uniqueness then pertains to identifying conditions under which uniqueness upon permutational freedom does hold indeed.

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Up until now, the challenge as mentioned above has only been dealt with for binary HICLAS models. In particular, Van Mechelen, De Boeck, and Rosenberg (1995) derived a theorem (see 3.1.1) that gives a sufficient condition for uniqueness of binary two-mode HICLAS decompositions. Subsequently, Ceulemans and Van Mechelen (2003) have generalized the theorem of Van Mechelen et al. (1995) to binary Tucker*N*-HICLAS models (see 3.1.2). Both of these proofs rely heavily on a result by Luce (1952) and Rutherford (1963) involving the existence of Boolean matrix inverses.

In this paper we will derive novel and more general conditions to deal with the uniqueness issue in the more general case of integer- and real-valued HICLAS models. As the result obtained by Luce and Rutherford only pertains to matrices over a Boolean algebra, the results of Van Mechelen et al. (1995) and Ceulemans and Van Mechelen (2003) cannot be readily generalized to the integer- and real-valued cases, as such cases do not involve a purely binary decomposition (see Section 2.2). To overcome this problem, we will need to take a more general approach.

The remainder of this paper is organized as follows: In Section 2, we will first briefly recapitulate two important members of the subclass of binary HICLAS models (2.1) and next explain the recently developed integer- and real-valued models (2.2). In Section 3, uniqueness conditions for the binary models will be recapitulated (3.1) and two novel, more general uniqueness conditions are derived that also hold for integer- and real-valued HICLAS models (3.2). In Section 4, we show that an intermediate result from Section 3 leads to an alternative and insightful proof of the result of Luce and Rutherford (which plays a key role in the proofs of Van Mechelen et al., 1995 and Ceulemans & Van Mechelen, 2003) on the existence of Boolean matrix inverses.

2. Models

All HICLAS models imply an approximate decomposition of the data in terms of a number of component matrices (one for each mode in the data, e.g., the set of objects) and possibly a linking array that connects components corresponding to different modes. An important characteristic of these models is that structural relations (e.g., which objects show similar patterns; if-then relations) are represented by the individual component matrices. As decomposition models, HICLAS models are closely related to multi-mode component analysis (MMCA) models (see e.g. Carroll & Chang, 1970; Harshman, 1970; Kiers, 1991; Kiers & Van Mechelen, 2001; Kroonenberg & De Leeuw, 1980; Tucker, 1966). The difference is that in HICLAS models (1) the component matrices are binary, meaning that the reduction for each mode implies a (discrete) clustering instead of a representation of each element (e.g., object) in a low-dimensional space, and (2) the mathematical structure being used is the semiring $(\mathbb{R}^+, \max, \times)$ instead of the well-known field $(\mathbb{R}, +, \times)$.

2.1. Binary HICLAS models

In this section, we briefly recapitulate two important representatives of the subclass of binary HICLAS models: the original (disjunctive) hierarchical classes model (HICLAS) as introduced by De Boeck and Rosenberg (1988) and the Tucker3-HICLAS model as introduced by Ceulemans, Van Mechelen, and Leenen (2003).

2.1.1. HICLAS

The original HICLAS model (De Boeck & Rosenberg, 1988) has been introduced as a model for two-mode $I \times J$ binary objects by attributes data matrices **D**. These data are approximated by an $I \times J$ matrix **M** of binary reconstructed data values that can be represented by a rank P HICLAS model. Such a model includes a binary $I \times P$ matrix **A** and a binary $J \times P$ matrix **B**. The columns in **A** and **B** represent (possibly overlapping) clusters/components of objects and attributes, which will further be called bundles; correspondingly, **A** and **B** will be called bundle matrices. As a guiding example, we will make use of the hypothetical reconstructed data matrix **M** in Table 1, and the bundle matrices **A** and **B** of the HICLAS solution for these data in Table 2.

Table 1
Hypothetical binary reconstructed data matrix **M**.

Objects	Attributes					
	a_1	a_2	a_3	a_4	a_5	a_6
o_1	0	0	1	1	0	1
o_2	1	0	0	0	1	0
o_3	1	0	0	0	1	0
o_4	0	0	1	1	0	1
o_5	1	1	0	0	1	1
o_6	1	1	1	1	1	1
o_7	1	1	0	0	1	1

Table 2
HICLAS model for **M** in Table 1.

Bundle matrices							
A				**B**			
Objects	A_1	A_2	A_3	Attributes	B_1	B_2	B_3
o_1	1	0	0	a_1	0	0	1
o_2	0	0	1	a_2	0	1	0
o_3	0	1	0	a_3	1	0	0
o_4	1	0	0	a_4	1	0	0
o_5	0	1	1	a_5	0	1	1
o_6	1	1	1	a_6	1	1	0
o_7	0	1	1				

Three types of relations implied by **M** are represented by the bundle matrices **A** and **B**: association, equivalence and hierarchy.

The *association relation* is the binary relation that links the objects and the attributes. It is represented by the decomposition rule of the HICLAS model:

$$m_{ij} = \bigoplus_{p=1}^{P} a_{ip} b_{jp} \quad \forall i, j, \tag{1}$$

where m_{ij} is the entry in row i and column j of **M**, $\bigoplus$ denotes the Boolean sum, a_{ip} is the entry in row i and column p of the bundle matrix **A** and b_{jp} is the entry in row j and column p of the bundle matrix **B**. The decomposition rule in (1) implies that object i is associated to attribute j iff they share at least one corresponding bundle. Note that the Boolean sum in (1) may just as well be replaced by the maximum operator. However, in this paper, in order to make the distinction between binary models and integer- or real-valued ones more clear we will keep using the symbol $\bigoplus$ whenever all parts involved in the decomposition rule are binary. From (1) it should be clear that a permutation of the columns of **A** does not affect **M**, as long as the columns of **B** are permuted in the same way. This is why any HICLAS decomposition can only be unique up to a permutation of the bundles. Such permutations, however, do not imply different substantive interpretations, but merely a relabeling of the bundles.

An *equivalence relation* is defined on the objects and attributes: Letting S^x denote the set of elements from the other mode that x is related with in **M**, it holds that object i is equivalent to object i' in **M** iff $S^i = S^{i'}$. For example, from Table 1 it can be read that $S^{o_1} = \{a_3, a_4, a_6\}$ and $S^{o_2} = \{a_1, a_5\}$. From the definition it follows that objects o_1 and o_4 are equivalent, as well as objects o_5 and o_7. Similarly, attribute j is equivalent to attribute j' in **M** iff $S^j = S^{j'}$. For example, from Table 1 it can be read that $S^{a_1} = \{o_2, o_3, o_5, o_6, o_7\}$ and $S^{a_2} = \{o_5, o_6, o_7\}$. From the definition it follows that attributes a_3 and a_4 are equivalent. Equivalence relations are represented by the bundle matrices of the HICLAS model (see Table 2) in terms of identical binary row patterns for two equivalent objects (attributes). By the representation of the equivalence relations and

their implied equivalence classes, the HICLAS model includes a partition of the two modes of the data.

A *hierarchical relation* is defined on the objects and attributes. It holds for objects i and i' that $i \preceq i'$ in $\mathbf{M}$ iff $S^i \subseteq S^{i'}$. Similarly, for attributes j and j' it holds that $j \preceq j'$ in $\mathbf{M}$ iff $S^j \subseteq S^{j'}$. For example, in Table 1 it holds, among others, that $o_1 \preceq o_6$ (because $S^{o_1} \subseteq S^{o_6}$), and that $a_4 \preceq a_6$ (because $S^{a_4} \subseteq S^{a_6}$). Hierarchical relations represent if-then rules. For example, it follows from $a_4 \preceq a_6$ that if attribute a_4 is associated to a certain object, then attribute a_6 also is. Hierarchical relations are represented by the bundle matrices of the HICLAS model (see Table 2) in terms of subset–superset relations between the binary patterns corresponding to two objects (attributes). By the representation of the hierarchical relations, the classifications included in a HICLAS model turn into hierarchically organized partitions.

These three types of relations correspond to the ones that were discussed in light of the patients by symptoms presence/absence data in the introduction. In particular, the association relation in this case may comprise information on which symptoms are associated to a given patient; the equivalence relation may comprise information on which patients display similar symptom patterns, and on which symptoms typically co-occur within the set of patients; and the hierarchical relation may represent information of the type: If a patient suffers from symptom j, then he/she will also suffer from symptom j'.

A HICLAS solution captures the major pattern of these relations within a data set (note that this is also the case for all generalizations of the HICLAS model that are discussed further in this paper). For a given rank P, a model is looked for that fits the observed data as good as possible in terms of a least absolute deviations loss function. In general this results in discrepancies between reconstructed data entries m_{ij} and observed data entries d_{ij}. Hence, the association relation in $\mathbf{D}$ (the observed data matrix) is only approximated by the association relation in $\mathbf{M}$. This further implies that equivalence and hierarchy relations are represented exactly on the level of the reconstructed data $\mathbf{M}$, but only approximately on the level of the observed data $\mathbf{D}$. This means that in $\mathbf{M}$ an equivalence (hierarchy) relation may hold between, say, two objects, but that violations to equivalence (hierarchy) between the same two objects may occur in the observed data. If the fit of the model to the observed data is acceptable, however, one may then nonetheless conclude that an equivalence (hierarchy) relation represents the major pattern of the relation between these two objects.

2.1.2. Tucker3-HICLAS

Ceulemans et al. (2003) presented a generalization of HICLAS, the Tucker3-HICLAS model, for binary three-mode $I \times J \times K$ objects by attributes by sources data arrays $\underline{\mathbf{D}}$ (see also Leenen, Van Mechelen, De Boeck, & Rosenberg, 1999). These data are approximated by an $I \times J \times K$ array $\underline{\mathbf{M}}$ of binary reconstructed data entries that can be represented by a rank (P, Q, R) Tucker3-HICLAS model. Such a model includes a binary $I \times P$ matrix $\mathbf{A}$, a binary $J \times Q$ matrix $\mathbf{B}$, a binary $K \times R$ matrix $\mathbf{C}$ and a $P \times Q \times R$ binary linking array $\underline{\mathbf{G}}$. $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are called object, attribute and source bundle matrices, respectively, $\underline{\mathbf{G}}$ is called the core.

As in the original HICLAS model, three types of relations implied by $\underline{\mathbf{M}}$ are represented by the Tucker3-HICLAS model: association, equivalence and hierarchy.

The *association relation* is represented by the decomposition rule:

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

meaning that m_{ijk} equals 1 iff an object, attribute and source bundle exist, to which i, j, and k respectively belong and that are interrelated in $\underline{\mathbf{G}}$. Note that if P, Q and R are equal and $\underline{\mathbf{G}}$ is a 'unit superdiagonal' array (Kiers, 2000), Tucker3-HICLAS reduces to INDCLAS (Leenen et al., 1999). In the latter case, a one-to-one correspondence between bundles of different modes is implied, just as in the two-way two-mode HICLAS case. In generalizations of the HICLAS model that involve a core array with nonzero off-(super)diagonal entries (i.e., Tucker3-HICLAS, Tucker$N$-HICLAS, HICLAS-R and RV-HICLAS), however, one object bundle, say, may be linked to more than one attribute bundle and/or to more than one source bundle. The relaxations that are implied by these generalizations of the HICLAS model make sense from a substantive point of view because there is often no a priori reason for the object, attribute and source structure to have the same number of bundles, let alone for a one-to-one correspondence between object, attribute and source bundles (Ceulemans et al., 2003).

An *equivalence relation* is defined on each mode. Letting S^x denote the set of *pairs of elements* of the other two modes x is related with in $\underline{\mathbf{M}}$, it holds that element x is equivalent to element y in $\underline{\mathbf{M}}$ iff $S^x = S^y$. Equivalence relations are represented by the bundle matrices of the Tucker3-HICLAS model in the same way as in HICLAS.

A *hierarchical relation* is defined on each mode. In particular, it holds for elements x and y that $x \preceq y$ in $\underline{\mathbf{M}}$ iff $S^x \subseteq S^y$. Hierarchical relations are represented by the bundle matrices of the Tucker3-HICLAS model in the same way as in HICLAS.

2.1.3. Tucker N-HICLAS

An N-way N-mode extension of Tucker3-HICLAS was briefly discussed in Ceulemans and Van Mechelen (2003). It implies the decomposition of a binary $I_1 \times I_2 \times \cdots \times I_N$ model array $\underline{\mathbf{M}}$ into $I_n \times P_n$ bundle matrices $\mathbf{A}^n$ $(n = 1 \ldots N)$ and a binary $P_1 \times P_2 \times \cdots \times P_N$ core array $\underline{\mathbf{G}}$, with $(P_1, P_2, \ldots, P_N)$ denoting the rank of the model. The decomposition rule associated to this model is:

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

The relations of equivalence and hierarchy between two elements of the same mode, say x and y, are straightforward generalizations from the Tucker3-HICLAS case by letting S^x, resp. S^y, denote the set of $(N-1)$-*tuples* of elements of the other $N-1$ modes x, resp. y, are related with in $\underline{\mathbf{M}}$.

2.2. Integer- and real-valued HICLAS

In this section we first summarize the integer- and real-valued HICLAS models that were developed specifically for positive integer- and positive real-valued two-way two-mode data, respectively. Subsequently we will discuss their N-way N-mode extension.

2.2.1. HICLAS-R and RV-HICLAS

Van Mechelen et al. (2007) have recently presented the HICLAS-R model for positive integer-valued two-mode $I \times J$ objects by attributes data matrices $\mathbf{D}$. These data are approximated by an $I \times J$ matrix $\mathbf{M}$ of positive integer-valued reconstructed data entries that can be represented by a rank (P, Q, R) HICLAS-R model. This model includes a binary $I \times P$ matrix $\mathbf{A}$, a binary $J \times Q$ matrix $\mathbf{B}$ and a $P \times Q$ linking matrix $\mathbf{G}$ with R $(R \leq P \times Q)$ distinct positive integer values. $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{G}$ are called object and attribute bundle matrices, and the core, respectively. Schepers and Van Mechelen (submitted for publication) have further generalized the HICLAS-R model to the so-called RV-HICLAS model by allowing the core $\mathbf{G}$ to contain positive real-valued entries, and thus permitting the reconstruction of positive real-valued data. In RV-HICLAS, no restriction is imposed on the number of distinct values in $\mathbf{G}$. The rank of an RV-HICLAS decomposition therefore can be

Table 3
Hypothetical positive real-valued reconstructed data matrix **M**.

Objects	Attributes			
	a_1	a_2	a_3	a_4
o_1	3.12	2.17	3.12	1.17
o_2	1.11	3.16	3.16	1.19
o_3	3.12	3.16	3.16	1.19
o_4	0.16	1.04	2.07	2.07
o_5	1.11	3.16	3.16	1.19
o_6	3.12	3.16	3.16	2.07
o_7	3.12	2.17	3.12	1.17

summarized by the ordered pair (P, Q). Within the argument of the present paper, the distinction between the HICLAS-R and RV-HICLAS models is not relevant. Therefore, we will further describe them simultaneously. As a guiding example, we will make use of the hypothetical reconstructed data matrix **M** in Table 3, and the bundle matrices **A** and **B** and linking matrix **G** of the RV-HICLAS solution for these data in Table 4.

Generalizations of the three types of relations implied by **M** as in HICLAS, are represented by the RV-HICLAS (HICLAS-R) model: association, equivalence and hierarchy. In particular, the generalized relations and their representation are as follows:

The generalized *association relation* is the mapping that links each object–attribute pair to its corresponding value in **M**. This relation is represented by the following decomposition rule:

$$m_{ij} = \max_{p=1}^{P} \max_{q=1}^{Q} a_{ip} b_{jq} g_{pq} \quad \forall i, j, \tag{2}$$

where max denotes the maximum operator, a_{ip} and b_{jq} are defined as before, and g_{pq} is the value in row p and column q of the linking matrix **G**. This rule implies that object i is associated to attribute j with strength g_{pq} (integer-valued in HICLAS-R, real-valued in RV-HICLAS) iff g_{pq} is the largest value in **G** for which it holds that object i and attribute j belong to bundles p and q, respectively. Note that the max-operator rather than the Boolean sum is needed in (2) because non-binary values (g_{pq}) show up in the decomposition rule.

A generalized *equivalence relation* is defined on the objects as well as on the attributes. To define it, let S^x denote the *vector of values* by which x is associated to the elements of the other mode in **M**. Then, element x is equivalent to element y in **M** iff $S^x = S^y$. For example, from Table 3 it can be read that $S^{o_1} = (3.12\ 2.17\ 3.12\ 1.17)$, that $S^{a_1} = (3.12\ 1.11\ 3.12\ 0.16\ 1.11\ 3.12\ 3.12)$, and that objects o_2 and o_5 are equivalent (because $S^{o_2} = S^{o_5}$). Note that the equivalence relation as defined in RV-HICLAS (HICLAS-R) includes the equivalence relation for the binary HICLAS model as a special case. Equivalence relations are represented by the bundle matrices of the RV-HICLAS (HICLAS-R) model (see Table 4) in the same way as in HICLAS.

A generalized *hierarchical relation* is defined on the objects as well as on the attributes: $x \preceq y$ in **M** iff $S^x \leq S^y$ in terms of a pointwise order, which means that the inequality is true for every entry-by-entry value comparison between S^x and S^y. For example, in Table 3, $o_2 \preceq o_3$ (because $S^{o_2} \leq S^{o_3}$), and $a_1 \preceq a_3$ (because $S^{a_1} \leq S^{a_3}$). Note that this generalized hierarchical relation again includes the hierarchical relation in the HICLAS model as a special case. Hierarchical relations are represented by the bundle matrices of the RV-HICLAS (HICLAS-R) model (see Table 4) in the same way as in HICLAS. The hierarchical relation as defined here is a generalized if-then relation. In particular, it follows from $a_1 \preceq a_3$ that if attribute a_1 is associated with some strength to a certain object, then attribute a_3 is associated to that object with the same strength or more. To make things more clear, let us assume that the objects and attributes of the reconstructed data matrix **M** in Table 3 represent patients and symptoms, respectively. Further assume that the data entries in this matrix represent symptom severity. From $a_1 \preceq a_3$ it then follows that if a patient suffers from symptom a_1 by some severity, then that patient suffers from symptom a_3 by at least the same severity.

2.2.2. N-way N-mode generalizations

Analogous to Tucker$N$-HICLAS models, N-way N-mode extensions of RV-HICLAS (HICLAS-R) imply the decomposition of a positive real-valued (integer-valued) $I_1 \times I_2 \times \cdots \times I_N$ model array $\underline{\mathbf{M}}$ into $I_n \times P_n$ bundle matrices $\mathbf{A}^n$ $(n = 1 \ldots N)$ and a positive real-valued (integer-valued) $P_1 \times P_2 \times \cdots \times P_N$ core array $\underline{\mathbf{G}}$, with $(P_1, P_2, \ldots, P_N)$ denoting the rank of the N-way N-mode RV-HICLAS model ($(P_1, P_2, \ldots, P_N, Q)$ denoting the rank of the N-way N-mode HICLAS-R model with Q distinct values in the core). The decomposition rule associated to this model is:

$$m_{i_1 i_2 \ldots i_N} = \max_{p_1=1}^{P_1} \max_{p_2=1}^{P_2} \ldots \max_{p_N=1}^{P_N} \left(\prod_{n=1}^{N} a^n_{i_n p_n} \right) g_{p_1 p_2 \ldots p_N} \quad \forall i_1, i_2 \ldots i_N, \tag{3}$$

with $g_{p_1 p_2 \ldots p_N}$ positive real-valued in the case of N-way N-mode RV-HICLAS and positive integer-valued in the case of N-way N-mode HICLAS-R. The relations of equivalence and hierarchy between two elements of the same mode, say x and y, are straightforward generalizations from RV-HICLAS (HICLAS-R) by letting S^x, resp. S^y, now denote the *array of values* by which x, resp. y, is associated to the elements of the *Cartesian product* of the other $N - 1$ modes in $\underline{\mathbf{M}}$.

3. Uniqueness

In this section, we first go over three uniqueness conditions that were derived for the binary HICLAS models. In the second part, two novel uniqueness conditions for positive real-valued (integer-valued) HICLAS models are presented that include the conditions for the binary models as special cases.

3.1. Binary models

3.1.1. Uniqueness of HICLAS

An important concept in the study of uniqueness of HICLAS models is that of a permutation matrix. We therefore first recapitulate the definition of permutation matrices (Kim, 1982).

Definition 1. A square matrix is called a permutation matrix if every row and every column contains exactly one 1.

Table 4
RV-HICLAS model for **M** in Table 3.

A				**B**				**G**			
Objects	A_1	A_2	A_3	Attributes	B_1	B_2	B_3		B_1	B_2	B_3
o_1	1	0	0	a_1	1	0	0	A_1	3.12	1.17	2.17
o_2	0	1	0	a_2	0	0	1	A_2	1.11	1.19	3.16
o_3	1	1	0	a_3	1	1	1	A_3	0.16	2.07	1.04
o_4	0	0	1	a_4	0	1	0				
o_5	0	1	0								
o_6	1	1	1								
o_7	1	0	0								

In Van Mechelen et al. (1995) the following sufficient condition for uniqueness of a rank P HICLAS decomposition was derived:

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

For a formal proof of Theorem 1, we refer to Van Mechelen et al. (1995). An essential part of it relies on the following result by Luce (1952) and Rutherford (1963) (see also Section 4):

Theorem 2 (*Luce and Rutherford*). *The only Boolean matrices that have an inverse are permutation matrices.*

Van Mechelen et al. (1995) showed that a decomposition that satisfies the condition in Theorem 1 implies that the associated matrix of reconstructed values $\mathbf{M}$ contains a $P \times P$ identity submatrix, possibly upon permutations of the rows and columns of $\mathbf{M}$. Using the result by Luce and Rutherford, this submatrix can only be decomposed into permutation matrices. Uniqueness of the decomposition upon permutations of the bundles then follows.

3.1.2. Uniqueness of Tucker3-HICLAS

Ceulemans and Van Mechelen (2003) have generalized Theorem 1 to a sufficient condition for uniqueness of a (P, Q, R) Tucker3-HICLAS decomposition:

Theorem 3. *If a (P, Q, R) Tucker 3-HICLAS decomposition of an $I \times J \times K$ binary array* $\underline{\mathbf{M}}$ *exists, such that (1) all bundle-specific object (resp. attribute, source) classes are non-empty, 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 bundles.*

For a formal proof of Theorem 3, we refer to Ceulemans and Van Mechelen (2003). Here it suffices to say that the proof involves a rewriting of the Tucker3-HICLAS model as a HICLAS model for a matricized version of array $\underline{\mathbf{M}}$. The result of Luce and Rutherford further again plays a key role in the proof in question.

3.1.3. Uniqueness of TuckerN-HICLAS

Ceulemans and Van Mechelen (2003) also derived a general sufficient condition for uniqueness of a $(P_1, P_2, \ldots, P_N)$ Tucker$N$-HICLAS decomposition:

Theorem 4. *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) all bundle-specific classes, for each mode, are non-empty, 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 bundles.*

The formal proof of Theorem 4 is a straightforward extension of that for Theorem 3.

3.2. Integer- and real-valued HICLAS models

It has been shown in Section 2.2 that the decomposition rule in integer- and real-valued HICLAS models no longer only involves strictly binary elements. As a consequence, the framework of Theorems 1, 3 and 4 is no longer sufficient for studying the uniqueness of these models. Below we will present two new theorems to overcome this problem. For the sake of simplicity, we will only present these theorems for the real-valued models, but as the integer-valued models are special cases of them, the new uniqueness theorems apply to them as well.

3.2.1. Uniqueness of RV-HICLAS

In the following, it is convenient to use matrix notation. We denote by $\otimes$ a (max, $\times$) matrix multiplication, and by T matrix transpose. Eq. (2) may then be rewritten as:

$$\mathbf{M} = \mathbf{A} \otimes \mathbf{G} \otimes \mathbf{B}^T. \tag{4}$$

To specify sufficient conditions for the uniqueness of RV-HICLAS decompositions, we will extensively make use of a property of positive real-valued matrices that is defined below.

Definition 2. A positive real-valued $I \times J$ matrix $\mathbf{X}$ is called *left Boolean unique* iff

$$v \otimes \mathbf{X} = v^* \otimes \mathbf{X} \Leftrightarrow v = v^*,$$

where v and v^* are Boolean $1 \times I$ vectors. Similarly, a matrix $\mathbf{X}$ is called *right Boolean unique* iff $\mathbf{X} \otimes v = \mathbf{X} \otimes v^* \Leftrightarrow v = v^*$, where v and v^* are Boolean $J \times 1$ vectors.

From this definition, the following lemma immediately follows:

Lemma 1. *If $\mathbf{X} \otimes \mathbf{Z}$ is left Boolean unique, then $\mathbf{X}$ is left Boolean unique. Similarly, if $\mathbf{Y} \otimes \mathbf{X}$ is right Boolean unique, then $\mathbf{X}$ is right Boolean unique.*

Proof. Assume $\mathbf{X}$ is not left Boolean unique. Then, two non-identical Boolean vectors v and v^* exist for which it holds that:

$$v \otimes \mathbf{X} = v^* \otimes \mathbf{X}.$$

It then follows that

$$v \otimes \mathbf{X} \otimes \mathbf{Z} = v^* \otimes \mathbf{X} \otimes \mathbf{Z}.$$

Hence, $\mathbf{X} \otimes \mathbf{Z}$ is not left Boolean unique. The proof for right Boolean uniqueness is similar. □

A sufficient condition for uniqueness of a (P, Q) RV-HICLAS decomposition can be derived, making use of the definition of left and right Boolean uniqueness.

Theorem 5. *If a (P, Q) RV-HICLAS decomposition of an $I \times J$ positive real-valued matrix* $\mathbf{M}$ *exists, such that (1) all bundle-specific object and attribute classes are non-empty, and (2)* $\mathbf{G}$ *is left and right Boolean unique, this decomposition is unique upon a permutation of the object and attribute bundles.*

For the proof of this theorem we will rely on a lemma that will also appear to be useful to prove other theorems (see Section 4).

Lemma 2. *A square $n \times n$ Boolean matrix* $\mathbf{X}$ *is a permutation matrix iff* $\mathbf{X}$ *is left and right Boolean unique.*

Proof. $\Rightarrow$ Assume that $\mathbf{X}$ is a permutation matrix that is not left Boolean unique. Then, a pair of non-identical Boolean $1 \times n$ vectors v and v^* exist, such that

$$v \otimes \mathbf{X} = v^* \otimes \mathbf{X}. \tag{5}$$

As $v \neq v^*$, for at least one entry i, a 1 appears in one of these vectors, whereas a zero appears in the other. Assume, without loss of generality, that $v_i = 1$ and $v_i^* = 0$. Note that premultiplication of $\mathbf{X}$ by v^* is equivalent to taking the Boolean sum of a subset of the rows of $\mathbf{X}$, excluding row i. From (5) it then follows that row i of $\mathbf{X}$ is less than or equal (in terms of a pointwise order) to the Boolean sum of the other rows of $\mathbf{X}$ (otherwise the equality in (5) would not hold). Now, as $\mathbf{X}$ is a permutation matrix it follows that $x_{ij} = 1$ for some j. But as row i of $\mathbf{X}$ is less than or equal to the Boolean sum of the other rows of $\mathbf{X}$, it further follows that for some $i' \neq i$, $x_{i'j}$ should equal 1 as well. This follows because one can never obtain a 1 for entry j of the Boolean sum of all rows other than row i unless for some $i' \neq i$, $x_{i'j} = 1$. But then column j in $\mathbf{X}$ contains at least two ones (viz., in rows i and i'), which contradicts $\mathbf{X}$ to be a permutation matrix.

$\Leftarrow$ We first note that square Boolean matrices $\mathbf{X}$ that are not permutation matrices may be categorized into three mutually

exclusive types: Type (a), one or more rows of $\mathbf{X}$ are zero vectors; Type (b), $\mathbf{X}$ does not include zero vectors, but two or more rows of $\mathbf{X}$ are equal; and Type (c), $\mathbf{X}$ includes neither zero vectors nor equal rows, but at least one of the rows of $\mathbf{X}$ contains more than one 1. Assume now that $\mathbf{X}$ is left Boolean unique but not a permutation matrix. It then follows that $\mathbf{X}$ is of Type (a), (b) or (c). We will now show that each of these three types is incompatible with the property of left Boolean uniqueness, which will complete this part of the proof by contradiction.

Type (a): One or more rows of $\mathbf{X}$ are zero vectors. Assume, without loss of generality, that the first row of $\mathbf{X}$ is a zero vector. Then it follows

$$(011\ldots1)\otimes\mathbf{X}=(111\ldots1)\otimes\mathbf{X},$$

which contradicts that $\mathbf{X}$ is left Boolean unique.

Type (b): Two or more rows of $\mathbf{X}$ are equal. Assume, without loss of generality, that this is the case for the first and second row of $\mathbf{X}$. Then:

$$(011\ldots1)\otimes\mathbf{X}=(111\ldots1)\otimes\mathbf{X},$$

which contradicts that $\mathbf{X}$ is left Boolean unique.

Type (c): At least one of the rows of $\mathbf{X}$ contains more than one 1, and $\mathbf{X}$ does not contain zero rows. Assume, without loss of generality, that a 1 appears in the first two columns of the first row of $\mathbf{X}$. Furthermore, every row i ($i=2,\ldots,n$) should contain a 1 in a column that contains zeroes in all $i-1$ previous rows (because otherwise, $\mathbf{X}$ would not be left Boolean unique). However, given that a 1 appears in the first two columns of the first row of $\mathbf{X}$, only $n-2$ such free columns in $\mathbf{X}$ remain after the first row, whereas in that case $n-1$ rows are left in $\mathbf{X}$. As a consequence, $\mathbf{X}$ is not left Boolean unique. □

We now turn to the proof of Theorem 5, making use of Lemma 2.

Proof of Theorem 5. Assume a decomposition that satisfies the conditions of Theorem 5 exists. Assume further, without loss of generality, that the submatrix $\mathbf{A}_P$ consisting of the first P rows of $\mathbf{A}$, equals $\mathbf{I}_P$ (i.e., the $P\times P$ identity matrix). Likewise, assume that the submatrix $\mathbf{B}_Q$ consisting of the first Q rows of $\mathbf{B}$, equals $\mathbf{I}_Q$ (i.e., the $Q\times Q$ identity matrix). This implies that the submatrix $\mathbf{M}_{P\times Q}$, consisting of the first P rows and the first Q columns of $\mathbf{M}$, equals

$$\mathbf{M}_{P\times Q}=\mathbf{I}_P\otimes\mathbf{G}\otimes\mathbf{I}_Q^T=\mathbf{G}. \tag{6}$$

Because $\mathbf{G}$ satisfies the conditions of Theorem 5, this further implies that $\mathbf{M}_{P\times Q}$ is left and right Boolean unique. It is then easy to derive that $\mathbf{M}_P$, consisting of the first P full rows of $\mathbf{M}$, is left Boolean unique and $\mathbf{M}_Q$, consisting of the first Q full columns of $\mathbf{M}$, is right Boolean unique.

We will prove now the uniqueness of $\mathbf{A}$ by contradiction (the proof of the uniqueness of $\mathbf{B}$ is similar). Assume that a second decomposition of $\mathbf{M}$ involving $\mathbf{A}^*$ exists, i.e.,

$$\mathbf{M}=\mathbf{A}^*\otimes\mathbf{G}^*\otimes(\mathbf{B}^*)^T, \tag{7}$$

with $\mathbf{A}^*$ not being equal to a mere permutation of the columns of $\mathbf{A}$. Consider then the submatrix $\mathbf{A}_P^*$ consisting of the first P rows of $\mathbf{A}^*$. It follows immediately that

$$\mathbf{M}_P=\mathbf{A}_P^*\otimes\mathbf{G}^*\otimes(\mathbf{B}^*)^T. \tag{8}$$

We will now successively consider the cases that $\mathbf{A}_P^*$ is (a) and is not (b) a permutation matrix.

(a) Assume that $\mathbf{A}_P^*$ is a permutation matrix. In that case, it follows from (8) that

$$(\mathbf{A}_P^*)^T\mathbf{M}_P=\mathbf{G}^*\otimes(\mathbf{B}^*)^T.$$

It then follows that $\mathbf{G}^*\otimes(\mathbf{B}^*)^T$ is left Boolean unique. Further, as $\mathbf{A}_P=\mathbf{I}_P$, it follows from (4) that:

$$\mathbf{M}_P=\mathbf{G}\otimes\mathbf{B}^T,$$

and hence

$$\mathbf{M}=\mathbf{A}\otimes\mathbf{M}_P. \tag{9}$$

Plugging (8) into (9) gives

$$\mathbf{M}=\mathbf{A}\otimes\mathbf{A}_P^*\otimes\mathbf{G}^*\otimes(\mathbf{B}^*)^T. \tag{10}$$

But, from (7) and (10), and the fact that $\mathbf{G}^*\otimes(\mathbf{B}^*)^T$ is left Boolean unique, it follows that

$$\mathbf{A}\otimes\mathbf{A}_P^*=\mathbf{A}^*,$$

which contradicts the assumption that $\mathbf{A}^*$ is not a permutation of $\mathbf{A}$.

(b) Assume that $\mathbf{A}_P^*$ is not a permutation matrix. From Lemma 2, it then follows that $\mathbf{A}_P^*$ is not left Boolean unique. However, applying Lemma 1 to (8), this would imply that $\mathbf{M}_P$ is not left Boolean unique too, which is not the case.

With respect to the core $\mathbf{G}$ it should be clear from (6) that any change in $\mathbf{G}$ would cause a change in $\mathbf{M}_{P\times Q}$, implying that $\mathbf{G}$ is unique (upon a permutation of its rows and columns). □

Interestingly, for a particular RV-HICLAS decomposition, left and right Boolean uniqueness of $\mathbf{G}$ can easily be verified:

Corollary 1. *A positive real-valued matrix $\mathbf{G}$ is left Boolean unique iff every row of $\mathbf{G}$ contains an entry that is strictly larger than the other entries in the same column as that entry (i.e., $\forall i,\exists j: g_{ij}>\max_{i'\neq i}g_{i'j}$).*

$\Rightarrow$ Assume that $\mathbf{G}$ is left Boolean unique and that not every row of $\mathbf{G}$ contains an entry that is strictly larger than the other entries in the same column as that entry. Then, for some row i, it holds that

$$g_{ij}\leq\max_{i'\neq i}g_{i'j}\quad\forall j.$$

But then it follows that a pair of non-identical Boolean $n\times1$ vectors v and v^* exist, for which it holds that $v_i=1$ and $v_i^*=0$, such that

$$v\otimes\mathbf{G}=v^*\otimes\mathbf{G},$$

which contradicts that $\mathbf{G}$ is left Boolean unique.

$\Leftarrow$ Assume that every row of $\mathbf{G}$ contains an entry that is strictly larger than the other entries in the same column as that entry and that $\mathbf{G}$ is not left Boolean unique. Then, a pair of non-identical Boolean $n\times1$ vectors v and v^* exist, such that

$$v\otimes\mathbf{G}=v^*\otimes\mathbf{G}. \tag{11}$$

As $v\neq v^*$, for at least one entry i, a 1 appears in one of these vectors, whereas a zero appears in the other. Assume, without loss of generality, that $v_i=1$ and $v_i^*=0$. Then it follows that

$$g_{ij}\leq\max_{i'\neq i}g_{i'j}\quad\forall j,$$

otherwise the equality in (11) would not hold. But this contradicts that row i of $\mathbf{G}$ contains an entry that is strictly larger than the other entries in the same column as that entry.

It can be proven similarly that a positive real-valued matrix $\mathbf{G}$ is right Boolean unique iff every column of $\mathbf{G}$ contains an entry that is strictly larger than the other entries in the same row as that entry.

3.2.2. Uniqueness of N-way N-mode RV-HICLAS

First, we generalize the definition of Boolean uniqueness to multidimensional arrays.

Definition 3. A positive real-valued array $\underline{\mathbf{X}}$ is *Boolean unique with respect to mode n* iff

$$v\otimes\mathbf{X}_{I_n(I_1I_2\ldots I_{n-1}I_{n+1}\ldots I_N)}=v^*\otimes\mathbf{X}_{I_n(I_1I_2\ldots I_{n-1}I_{n+1}\ldots I_N)}\Leftrightarrow v=v^*,$$

with $\mathbf{X}_{I_n(I_1I_2\ldots I_{n-1}I_{n+1}\ldots I_N)}$ denoting a matricized form of the N-dimensional array $\underline{\mathbf{X}}$ in which the rows correspond to the elements of mode n of $\underline{\mathbf{X}}$, and the columns to the elements of the Cartesian product of the other modes.

Note that the restriction on binary core arrays $\underline{\mathbf{G}}$ as assumed in Theorems 3 and 4 (i.e., that no core plane of $\underline{\mathbf{G}}$ is a subset of the Boolean sum of the other core planes of the same mode) is a special case of Boolean uniqueness as specified in Definition 3.

Definition 3 allows us to formulate a sufficient condition for uniqueness of a rank $(P_1, P_2, \ldots, P_N)$ RV-HICLAS decomposition.

Theorem 6. *If a $(P_1, P_2, \ldots, P_N)$ RV-HICLAS decomposition of an $I_1 \times I_2 \times \cdots \times I_N$ positive real-valued array $\underline{\mathbf{M}}$ exists, such that* (1) *for each mode all bundle-specific classes are non-empty, and* (2) *$\underline{\mathbf{G}}$ is Boolean unique with respect to all of its N modes, then this decomposition is unique upon permutations of the N sets of bundles.*

Proof. The formal proof of Theorem 6 is a straightforward extension of that of Theorem 5. An essential part of it includes rewriting (3) in matrix notation as follows:

$$\mathbf{M}_{I_n(I_1I_2\ldots I_{n-1}I_{n+1}\ldots I_N)} = \mathbf{A}^n \otimes \mathbf{G}_{P_n(P_1P_2\ldots P_{n-1}P_{n+1}\ldots P_N)} \otimes (\tilde{\mathbf{B}}_n)^T,$$

where $\mathbf{M}_{I_n(I_1I_2\ldots I_{n-1}I_{n+1}\ldots I_N)}$ denotes a matricized form of $\underline{\mathbf{M}}$ such that its rows correspond to the elements of mode n of $\underline{\mathbf{M}}$, and its columns correspond to the elements of the Cartesian product of the other modes of $\underline{\mathbf{M}}$, $\mathbf{G}_{P_n(P_1P_2\ldots P_{n-1}P_{n+1}\ldots P_N)}$ is a similarly matricized form of $\underline{\mathbf{G}}$, and $\tilde{\mathbf{B}}_n$ is a binary matrix equalling $\mathbf{A}^N \bigotimes \mathbf{A}^{N-1} \cdots \bigotimes \mathbf{A}^{n+1} \bigotimes \mathbf{A}^{n-1} \cdots \bigotimes \mathbf{A}^1$, where we have used $\bigotimes$ to denote Kronecker product, instead of the perhaps more conventional $\otimes$, because the latter was already defined in this paper to denote a (max, $\times$) matrix product (note also that the subscript n in $\tilde{\mathbf{B}}_n$ is used to denote that $\mathbf{A}^n$ is not involved in that Kronecker product).

The proof of uniqueness of $\mathbf{A}^n$, and of $\underline{\mathbf{G}}$, is then completely analogous to that of $\mathbf{A}$ and $\mathbf{G}$, respectively, in the two-mode case. □

4. Invertibility of Boolean matrices

Interestingly, Lemma 2 can also be used to give an alternative and insightful proof for Theorem 2, that is the theorem by Luce and Rutherford on Boolean matrix invertibility:

Proof. If a square $n \times n$ Boolean matrix $\mathbf{A}$ is a permutation matrix, then it immediately follows that $\mathbf{A}$ is invertible, with $\mathbf{A}^{-1} = \mathbf{A}^T$. Conversely, assume $\mathbf{A}$ is invertible, with $\mathbf{A}^{-1} = \mathbf{B}$. Then it follows that $\mathbf{A} \otimes \mathbf{B} = \mathbf{I}_n$ (with $\mathbf{I}_n$ denoting the $n \times n$ identity matrix). We will now prove, by contradiction, that $\mathbf{A}$ should be a permutation matrix. Assume that $\mathbf{A}$ is not a permutation matrix. Lemma 2 then implies that $\mathbf{A}$ is not left Boolean unique. From Lemma 1, it then follows that $\mathbf{A} \otimes \mathbf{B}$ $(=\mathbf{I}_n)$ is not left Boolean unique. However, using again Lemma 2, this would further imply that $\mathbf{A} \otimes \mathbf{B}$ is not a permutation matrix, which is contradicted by $\mathbf{I}_n$ being the identity matrix. □

5. Summary

In this paper, we derived two novel uniqueness theorems for the family of hierarchical classes models. These theorems give sufficient conditions for uniqueness of real-valued hierarchical classes decompositions and are more general than those obtained earlier by Van Mechelen et al. (1995) and Ceulemans and Van Mechelen (2003). As such, the results presented in this paper apply to decompositions for binary and integer-valued hierarchical classes models as well. In addition, from a mathematical point of view, an interesting secondary outcome of our work is a shorter and insightful proof of a result on Boolean matrix invertibility.

Studying the uniqueness of real-valued hierarchical classes models proved to be challenging because of the fact that the associated decompositions do not involve binary components only. As the earlier results that apply to binary HICLAS models heavily relied on invertibility of Boolean matrices, a different, more general, approach had to be taken for the real-valued case. In this regard, the notions of left and right Boolean uniqueness have been introduced. In order to allow for an easy check on the uniqueness of any given real-valued hierarchical classes solution, we have shown how left and right Boolean uniqueness can be verified for positive real-valued matrices.

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