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SUFFICIENT CONDITIONS FOR UNIQUENESS IN CANDECOMP/PARAFAC AND INDSCAL WITH RANDOM COMPONENT MATRICES

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A key feature of the analysis of three-way arrays by Candecomp/Parafac is the essential uniqueness of the trilinear decomposition. We examine the uniqueness of the Candecomp/Parafac and Indscal decompositions. In the latter, the array to be decomposed has symmetric slices. We consider the case where two component matrices are randomly sampled from a continuous distribution, and the third component matrix has full column rank. In this context, we obtain almost sure sufficient uniqueness conditions for the Candecomp/Parafac and Indscal models separately, involving only the order of the three-way array and the number of components in the decomposition. Both uniqueness conditions are closer to necessity than the classical uniqueness condition by Kruskal.

Key words: Candecomp, Parafac, Indscal, three-way arrays, uniqueness.

1. Introduction

Carroll and Chang (1970) and Harshman (1970) have independently proposed the same method for component analysis of three-way arrays, and named it Candecomp and Parafac, respectively. In the sequel, we will denote column vectors as $\mathbf{x}$, matrices as $\mathbf{X}$, and three-way arrays as $\underline{\mathbf{X}}$. For a given real-valued three-way array $\underline{\mathbf{X}}$ of order $I \times J \times K$ and a fixed number of R components, Candecomp/Parafac (CP) yields component matrices $\mathbf{A}$ $(I \times R)$, $\mathbf{B}$ $(J \times R)$, and $\mathbf{C}$ $(K \times R)$ such that $\sum_{k=1}^{K} \mathrm{tr}\,(\mathbf{E}_k^T \mathbf{E}_k)$ is minimized in the decomposition

$$\mathbf{X}_k = \mathbf{A}\,\mathbf{C}_k \mathbf{B}^T + \mathbf{E}_k, \qquad k = 1, 2, \ldots, K, \tag{1}$$

where $\mathbf{X}_k$ denotes the kth slice of order $I \times J$ and $\mathbf{C}_k$ is the diagonal matrix containing the elements of the kth row of $\mathbf{C}$.

The concept of rank is the same for matrices and three-way arrays. The three-way rank of $\underline{\mathbf{X}}$ is defined as the smallest number of rank-1 arrays whose sum equals $\underline{\mathbf{X}}$. A three-way array $\underline{\mathbf{Y}}$ has rank 1 if it is the outer product of three vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$, i.e., $y_{ijk} = a_i b_j c_k$. Notice that (1)

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can also be written as

$$\underline{\mathbf{X}} = \sum_{r=1}^{R} \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r + \underline{\mathbf{E}}, \tag{2}$$

where $\mathbf{a}_r$, $\mathbf{b}_r$, and $\mathbf{c}_r$ are the rth columns of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$, respectively, $\circ$ denotes the outer vector product, and $\underline{\mathbf{E}}$ is the residual array with slices $\mathbf{E}_k$, $k = 1, 2, \ldots, K$. Hence, CP decomposes $\underline{\mathbf{X}}$ into R arrays having three-way rank 1. The smallest number of components R for which there exists a CP decomposition with perfect fit (i.e., $\underline{\mathbf{E}}$ is all-zero) is by definition equal to the three-way rank of $\underline{\mathbf{X}}$.

The uniqueness of a CP solution is usually studied for given residuals $\mathbf{E}_k$, $k = 1, 2, \ldots, K$. It can be seen that the fitted part of a CP decomposition, i.e., a full decomposition of the matrices $\mathbf{X}_k - \mathbf{E}_k$, $k = 1, 2, \ldots, K$, can only be unique up to rescaling and jointly permuting columns of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$. Indeed, the residuals will be the same for the solution given by $\bar{\mathbf{A}} = \mathbf{APT}_a$, $\bar{\mathbf{B}} = \mathbf{BPT}_b$, and $\bar{\mathbf{C}} = \mathbf{CPT}_c$, for a permutation matrix $\mathbf{P}$ and diagonal matrices $\mathbf{T}_a$, $\mathbf{T}_b$, and $\mathbf{T}_c$ with $\mathbf{T}_a\mathbf{T}_b\mathbf{T}_c = \mathbf{I}_R$. When, for given residuals $\mathbf{E}_k$, $k = 1, 2, \ldots, K$, the matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are unique up to these indeterminacies, the solution is called *essentially unique*.

The first uniqueness results of CP date back to Jennrich (in Harshman, 1970) and to Harshman (1972). The most general sufficient condition for essential uniqueness is due to Kruskal (1977). Kruskal's condition relies on a particular concept of matrix rank that he introduced, which has been named k-rank (Kruskal rank) after him. Specifically, the k-rank of a matrix is the largest number x such that every subset of x columns of the matrix is linearly independent. We denote the k-rank of a matrix $\mathbf{A}$ as k_A. For a CP solution $(\mathbf{A}, \mathbf{B}, \mathbf{C})$, Kruskal (1977) proved that the condition

$$k_A + k_B + k_C \geq 2R + 2 \tag{3}$$

is sufficient for essential uniqueness. More than two decades later, the study of uniqueness has been revived in two different ways. On the one hand, additional results on Kruskal's condition have been obtained and, on the other, alternative conditions have been examined for the case where one of the component matrices, $\mathbf{C}$ say, is of full column rank.

Additional results on Kruskal's condition started with Sidiropoulos and Bro (2000) who offered a short-cut proof for the condition, and generalized it to n-way arrays ($n > 3$). Next, Ten Berge and Sidiropoulos (2002) have shown that Kruskal's *sufficient* condition is also *necessary* for $R = 2$ or 3, but not for $R > 3$. It may be noted that the condition cannot be met when $R = 1$. However, uniqueness for that case has already been proven by Harshman (1972). Ten Berge and Sidiropoulos (2002) conjectured that Kruskal's condition might be necessary and sufficient for $R > 3$, provided that k-ranks of the component matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ coincide with their ranks. However, Stegeman and Ten Berge (2005) refuted this conjecture.

Alternative uniqueness conditions came from De Lathauwer (2004) and Jiang and Sidiropoulos (2004). They independently examined the case where one of the component matrices (for which they picked $\mathbf{C}$) is of full column rank. Uniqueness of the CP solution then only depends on $(\mathbf{A}, \mathbf{B})$. De Lathauwer (2004) assumed that:

(A1) $(\mathbf{A}, \mathbf{B})$ are randomly sampled from an $((I + J)R)$-dimensional continuous distribution F with $F(S) = 0$ if and only if $L(S) = 0$, where L denotes the Lebesgue measure and S is an arbitrary Borel set in $\Re^{(I+J)R}$;

(A2) $\mathbf{C}$ has full column rank;

(A3) $\dfrac{R(R-1)}{2} \leq \dfrac{I(I-1)J(J-1)}{4}$.

De Lathauwer proved that a CP solution $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ satisfying (A1)–(A3) is essentially unique "almost surely," i.e., with probability 1 with respect to the distribution F. Incidentally, De Lathauwer's proof yields an algorithm, based on simultaneous matrix diagonalization, to compute the CP solution $(\mathbf{A}, \mathbf{B}, \mathbf{C})$. Notice that the requirement on F under (A1) guarantees that $F(S) = 0$ if and only if the set S has dimensionality lower than $(I + J)R$. In this context, the phrase "essentially unique with probability 1" means that the set of $(\mathbf{A}, \mathbf{B})$, corresponding to nonunique CP solutions, has dimensionality lower than $(I + J)R$.

Jiang and Sidiropoulos (2004) do not consider random component matrices. They examined a matrix $\mathbf{U}$ filled with products of 2×2 minors of $\mathbf{A}$ and $\mathbf{B}$, and proved that it is sufficient for uniqueness that (A2) holds and $\mathbf{U}$ is of full column rank. In the present paper, we assume that (A1) and (A3) hold and show that the matrix $\mathbf{U}$ of Jiang and Sidiropoulos (2004) has full column rank with probability 1 with respect to the distribution F. Hence, (A1)–(A3) implies uniqueness almost surely. This establishes a link between the condition of Jiang and Sidiropoulos (2004) and the result of De Lathauwer (2004), which is of importance for understanding CP uniqueness. By making use of the tools of Jiang and Sidiropoulos (2004), we offer an alternative approach to proving De Lathauwer's result. Contrary to De Lathauwer (2004), our proof does not involve fourth-order tensors and requires only a basic understanding of linear algebra. Therefore, it is likely to increase the accessibility of De Lathauwer's result.

By extending our analysis, we are able to propose a uniqueness condition for the Indscal decomposition in which the array has symmetric slices and the constraint $\mathbf{A} = \mathbf{B}$ is imposed. Here, we assume:

(B1) $\mathbf{A}$ is randomly sampled from an IR-dimensional continuous distribution F with $F(S) = 0$ if and only if $L(S) = 0$, where L denotes the Lebesgue measure and S is an arbitrary Borel set in $\Re^{I\,R}$;

(B2) $\mathbf{B} = \mathbf{A}$ and $\mathbf{C}$ has full column rank;

(B3) $\dfrac{R\,(R-1)}{2} \leq \dfrac{I\,(I-1)}{4}\;[\dfrac{I\,(I-1)}{2} + 1] - \binom{I}{4}\; I_{\{I\geq 4\}},$

where $I_{\{I\geq 4\}} = \begin{cases} 0 \text{ if } & I < 4, \\ 1 \text{ if } & I \geq 4. \end{cases}$

We conjecture that if (B1) and (B3) hold, then the matrix $\mathbf{U}$ of Jiang and Sidiropoulos (2004) has full column rank with probability 1 with respect to the distribution F. Hence, (B1)–(B3) would imply essential uniqueness almost surely for the Indscal decomposition. Although we were not able to give a complete proof of this, we will show it holds for a range of pairs (I, R) and indicate how a proof for any R and I satisfying (B3) can be obtained.

To our knowledge, this is the first time that distinct general uniqueness conditions, i.e., (A3) and (B3), have been derived for the CP and Indscal models, respectively (as opposed to Kruskal's condition (3) with $\mathbf{A} = \mathbf{B}$). In the Indscal case, a stricter uniqueness condition (in terms of R) is obtained, since the model contains less parameters than the CP model. Under (A1) and (A2), we can compare our uniqueness condition (A3) with Kruskal's condition (3). The latter boils down to $R + 2 \leq \min(I,\ R) + \min(J,\ R)$ in our context. It can be seen that condition (A3) is implied by this version of Kruskal's condition. Hence, condition (A3) is more relaxed than Kruskal's condition if (A1) and (A2) are assumed. The same is true for the Indscal decomposition. Under assumptions (B1) and (B2), Kruskal's condition becomes $R + 2 \leq 2\min(I,\ R)$, which implies our uniqueness condition (B3).

In the majority of cases (see also the Discussion section below), solutions obtained from CP and Indscal algorithms can be regarded as randomly sampled from a continuous distribution. Hence, our sufficient uniqueness conditions (A3) and (B3) apply. Since (A3) and (B3) are closer to necessity than Kruskal's condition (3), the practical relevance is immediate.

In the sequel, we denote the column space and the null space (i.e., the kernel) of an arbitrary matrix $\mathbf{Z}$ by span($\mathbf{Z}$) and null($\mathbf{Z}$), respectively. Hence,

$$\text{span}(\mathbf{Z}) = \{\mathbf{y}\text{: there exists an } \mathbf{x} \text{ such that } \mathbf{Z}\mathbf{x} = \mathbf{y}\},$$

and

$$\text{null}(\mathbf{Z}) = \{\mathbf{x}\text{: there holds } \mathbf{Zx} = \mathbf{0}\}.$$

The Khatri–Rao product (i.e., the column-wise Kronecker product) of two matrices **X** and **Y**, with an equal number of columns, is denoted by $\mathbf{X} \bullet \mathbf{Y}$. To prove our results, we will make use of the following result by Fisher (1966, Theorem 5.A.2). We state it here without a proof.

Lemma 1. *Let S be an n-dimensional subspace of $\Re^n$ and let g be a real-valued analytic function defined on S. If g is not identical to zero, then the set $\{\mathbf{x} : g(\mathbf{x}) = 0\}$ is of Lebesgue measure zero in $\Re^n$.*

2. Almost Sure Uniqueness in Candecomp/Parafac

Before we formulate our main result, we first consider the structure of the matrix **U** of Jiang and Sidiropoulos (2004). It has elements of the following form:

$$\begin{vmatrix} a_{i,g} & a_{i,h} \\ a_{j,g} & a_{j,h} \end{vmatrix} \cdot \begin{vmatrix} b_{k,g} & b_{k,h} \\ b_{l,g} & b_{l,h} \end{vmatrix}, \tag{4}$$

where $1 \le g < h \le R$ and $1 \le i,\ j \le I$ and $1 \le k,\ l \le J$. In each row of **U** the value of (i, j, k, l) is fixed and in each column of **U** the value of (g, h) is fixed. So **U** has $I^2 J^2$ rows and $R(R-1)/2$ columns. We order the columns of **U** such that index g runs slower than h. The following facts can be observed:

- Rows of **U** with $i = j$ and/or $k = l$ are the zero vector.
- Rows (i, j, k, l) and (i, j, l, k) sum up to the zero vector.
- Rows (i, j, k, l) and (j, i, k, l) sum up to the zero vector.
- Rows (i, j, k, l) and (j, i, l, k) are identical.

This yields the conclusion that, when determining the rank of **U**, we only have to consider rows for which $1 \le i < j \le I$ and $1 \le k < l \le J$. From now on, this reduced matrix will be referred to as $\mathbf{U}^{(1)}$. It has $I(I-1)J(J-1)/4$ rows and $R(R-1)/2$ columns. This implies that (A3) is equivalent to $\mathbf{U}^{(1)}$ being a vertical or square matrix, which is necessary for full column rank.

Next, we define the following two matrices. Let $\tilde{\mathbf{A}}$ have elements of the form

$$\begin{vmatrix} a_{i,g} & a_{i,h} \\ a_{j,g} & a_{j,h} \end{vmatrix}, \qquad \text{with} \quad 1 \le i < j \le I \quad \text{and} \quad 1 \le g < h \le R, \tag{5}$$

where in each row of $\tilde{\mathbf{A}}$ the value of $(i,\ j)$ is fixed and in each column of $\tilde{\mathbf{A}}$ the value of $(g,\ h)$ is fixed. Then $\tilde{\mathbf{A}}$ has $I(I-1)/2$ rows and $R(R-1)/2$ columns. The columns of $\tilde{\mathbf{A}}$ are ordered such that index g runs slower than h. The rows of $\tilde{\mathbf{A}}$ are ordered such that index i runs slower than j. Let $\tilde{\mathbf{B}}$ have elements of the form

$$\begin{vmatrix} b_{k,g} & b_{k,h} \\ b_{l,g} & b_{l,h} \end{vmatrix}, \qquad \text{with} \quad 1 \le k < l \le J \quad \text{and} \quad 1 \le g < h \le R, \tag{6}$$

where in each row of $\tilde{\mathbf{B}}$ the value of $(k,\ l)$ is fixed and in each column of $\tilde{\mathbf{B}}$ the value of (g, h) is fixed. Then $\tilde{\mathbf{B}}$ has $J(J-1)/2$ rows and $R(R-1)/2$ columns. The columns of $\tilde{\mathbf{B}}$ are ordered such that index g runs slower than h. The rows of $\tilde{\mathbf{B}}$ are ordered such that index k runs slower than l. It can be seen that each row of $\mathbf{U}^{(1)}$ is the Hadamard (i.e., element-wise) product of a row of $\tilde{\mathbf{A}}$ and a row of $\tilde{\mathbf{B}}$. Moreover, the Hadamard products of all row pairs of $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{B}}$ are included in $\mathbf{U}^{(1)}$. Therefore, the rows of $\mathbf{U}^{(1)}$ can be ordered such that $\mathbf{U}^{(1)}$ is the Khatri–Rao product of $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{B}}$, i.e., $\mathbf{U}^{(1)} = \tilde{\mathbf{A}} \bullet \tilde{\mathbf{B}}$. A different ordering of the rows of $\mathbf{U}^{(1)}$ yields $\mathbf{U}^{(1)} = \tilde{\mathbf{B}} \bullet \tilde{\mathbf{A}}$.

The uniqueness condition of Jiang and Sidiropoulos (2004) boils down to both $\mathbf{C}$ and $\mathbf{U}^{(1)}$ having full column rank. Our main result is the following.

Theorem 1. *If* (A1) *and* (A3) *hold, then* $\mathbf{U}^{(1)} = \tilde{\mathbf{A}} \bullet \tilde{\mathbf{B}}$ *has full column rank with probability 1 with respect to the distribution* F. *Hence, if* (A1)–(A3) *hold, then the CP solution* ($\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$) *is essentially unique with probability 1.*

The rest of this section contains the proof of Theorem 1. First, we consider the case where $R \leq I$ or $R \leq J$ or both. Lemma 2 below shows that Theorem 1 holds in this case. A proof of Lemma 2 can be found in Leurgans, Ross, and Abel (1993). Below, we offer an alternative proof, which is more straightforward in our context. Notice that if both $R \leq I$ and $R \leq J$, the result of Lemma 2 follows from the uniqueness condition in Harshman (1972).

Lemma 2. *Suppose* (A1) *and* (A3) *hold. If* $R \leq I$ *or* $R \leq J$ *or both, then* $\mathbf{U}^{(1)}$ *has full column rank with probability 1.*

Proof. Suppose (A1) and (A3) hold and $R \leq I$. Premultiplying $\mathbf{A}$ or $\mathbf{B}$ by a nonsingular matrix does not affect the uniqueness of the decomposition. If $R \leq I$ there exists (with probability 1) a nonsingular matrix $\mathbf{S}$ such that $\mathbf{SA} = \begin{bmatrix} \mathbf{I}_R \\ \mathbf{O} \end{bmatrix}$. The associated matrix $\tilde{\mathbf{A}}$ then equals $\begin{bmatrix} \mathbf{I}_{R(R-1)/2} \\ \mathbf{O} \end{bmatrix}$. Since $\tilde{\mathbf{B}}$ has at least one row with all elements nonzero (with probability 1), it follows that $\text{rank}(\mathbf{U}^{(1)}) = \text{rank}(\tilde{\mathbf{B}} \bullet \tilde{\mathbf{A}}) = \text{rank}(\tilde{\mathbf{A}}) = R(R-1)/2$. From the symmetry of the problem it follows analogously that also $R \leq J$ yields $\text{rank}(\mathbf{U}^{(1)}) = R(R-1)/2$. □

In the remaining part of the proof of Theorem 1 we assume that $R > I$ and $R > J$. A roadmap of the upcoming proof is as follows. We write the matrix $\mathbf{U}^{(1)}$ as

$$\mathbf{U}^{(1)} = \tilde{\mathbf{A}} \bullet \tilde{\mathbf{B}} = \begin{bmatrix} \tilde{\mathbf{a}}_1^T \bullet \tilde{\mathbf{B}} \\ \vdots \\ \tilde{\mathbf{a}}_{I(I-1)/2}^T \bullet \tilde{\mathbf{B}} \end{bmatrix}, \tag{7}$$

where $\tilde{\mathbf{a}}_s^T$ denotes row s of $\tilde{\mathbf{A}}$. If the columns of $\mathbf{U}^{(1)}$ are linearly dependent, there exists a nonzero vector $\mathbf{d}$ such that $\mathbf{U}^{(1)}\mathbf{d} = \mathbf{0}$. This implies that $\mathbf{d}$ lies in the null spaces of $\tilde{\mathbf{a}}_s^T \bullet \tilde{\mathbf{B}}$, $s = 1, \ldots, I(I-1)/2$. Below, we find a matrix $\mathbf{N}$, the columns of which constitute a basis for $\text{null}(\tilde{\mathbf{B}})$, i.e., $\text{null}(\tilde{\mathbf{B}}) = \text{span}(\mathbf{N})$. With probability 1, the rows $\tilde{\mathbf{a}}_s^T$ do not contain zeros. It follows that $\text{null}(\tilde{\mathbf{a}}_s^T \bullet \tilde{\mathbf{B}}) = \text{null}(\tilde{\mathbf{B}}\mathbf{T}_s) = \text{span}(\mathbf{T}_s^{-1}\mathbf{N})$, where $\mathbf{T}_s = \text{diag}(\tilde{\mathbf{a}}_s^T)$. Hence, a vector $\mathbf{d}$ in $\text{null}(\mathbf{U}^{(1)})$ must lie in the intersection of $\text{span}(\mathbf{T}_s^{-1}\mathbf{N})$, $s = 1, \ldots, I(I-1)/2$. We will show that, with probability 1, this intersection contains only the all-zero, vector, if (A1) and (A3) hold.

We denote the column of $\tilde{\mathbf{B}}$ involving columns g and h of $\mathbf{B}$ as (g, h). We need the following lemma to determine the dimensionality of $\text{null}(\tilde{\mathbf{B}})$.

Lemma 3. *Suppose* (A1) *holds and* $R > J$. *Then* $\tilde{\mathbf{B}}$ *has full row rank with probability* 1. *Also, the columns* (i, j) *of* $\tilde{\mathbf{B}}$, $1 \leq i < j \leq J$, *are linearly independent with probability* 1.

Proof. Let $\mathbf{W}$ denote the square matrix consisting of the columns (i, j) of $\tilde{\mathbf{B}}$, $1 \leq i < j \leq J$. Then $\det(\mathbf{W})$ is an analytic function of the elements of the first J columns of $\mathbf{B}$. From Lemma 1 it follows that if $\det(\mathbf{W})$ is nonzero for one particular $\mathbf{B}$, then it is nonzero with probability 1. Let the first J columns of $\mathbf{B}$ be equal to $\mathbf{I}_J$. Then $\mathbf{W} = \mathbf{I}_{J(J-1)/2}$ and $\det(\mathbf{W}) = 1$. Hence, it follows that $\det(\mathbf{W})$ is nonzero with probability 1, which proves both statements of the lemma. □

It follows from Lemma 3 that, with probability 1, the dimensionality of null($\tilde{\mathbf{B}}$) equals $R(R-1)/2 - J(J-1)/2$. Next, we characterize null($\tilde{\mathbf{B}}$) by a basis. For this, we need the following lemma which specifies a relationship between the columns of **B** and the columns of $\tilde{\mathbf{B}}$.

Lemma 4. *Suppose the columns with indices $g_1, g_2, \ldots, g_m$, $m \leq R$, of* **B** *are linearly dependent. Then the columns $(g_1, g_2), (g_1, g_3), \ldots, (g_1, g_m)$ of* $\tilde{\mathbf{B}}$ *are linearly dependent.*

Proof. Write $\mathbf{b}_{g_2} = c_1\mathbf{b}_{g_1} + c_3\mathbf{b}_{g_3} + \cdots + c_m\mathbf{b}_{g_m}$ with coefficients c_j, where $\mathbf{b}_s$ denotes the sth column of **B**. Then, for the row of $\tilde{\mathbf{B}}$ involving rows k and l of **B**, we have

$$\begin{vmatrix} b_{k,g_1} & b_{k,g_2} \\ b_{l,g_1} & b_{l,g_2} \end{vmatrix} = c_1 \begin{vmatrix} b_{k,g_1} & b_{k,g_1} \\ b_{l,g_1} & b_{l,g_1} \end{vmatrix} + c_3 \begin{vmatrix} b_{k,g_1} & b_{k,g_3} \\ b_{l,g_1} & b_{l,g_3} \end{vmatrix} + \cdots + c_m \begin{vmatrix} b_{k,g_1} & b_{k,g_m} \\ b_{l,g_1} & b_{l,g_m} \end{vmatrix}. \qquad (8)$$

Notice that the first term on the right-hand side of (8) equals zero. Since the coefficients of the linear combination (8) do not depend on k and l, it can be concluded that $(g_1, g_2) = c_3(g_1, g_3) + \cdots + c_m(g_1, g_m)$. This completes the proof. □

Notice that Lemma 4 implies that if $R > J$, then $k_{\tilde{\mathbf{B}}} \leq J - 1$. This is because every set of $J + 1$ different columns of **B** is linearly dependent and yields a set of J different columns of $\tilde{\mathbf{B}}$ which is also linearly dependent.

As stated above, we characterize null($\tilde{\mathbf{B}}$) by a basis. Set $n = R - J$. It can be seen that

$$R(R-1)/2 - J(J-1)/2 = nJ + n(n-1)/2. \qquad (9)$$

Below we will give nJ vectors **d** and $n(n-1)/2$ vectors **e** that are linearly independent elements of null($\tilde{\mathbf{B}}$) and, hence, constitute a basis for null($\tilde{\mathbf{B}}$). Define the following sets of columns of **B**:

$$S_m = \{\mathbf{b}_1, \ldots, \mathbf{b}_J, \mathbf{b}_{J+m}\}, \qquad m = 1, 2, \ldots, n, \qquad (10)$$

where $\mathbf{b}_s$ denotes column s of **B**. Each set S_m is linearly dependent and yields, according to Lemma 4, a set of J linearly dependent columns in $\tilde{\mathbf{B}}$. However, the role of column g_1 in Lemma 4 can be taken by each of the columns $\mathbf{b}_1, \ldots, \mathbf{b}_J$ (and also by $\mathbf{b}_{J+m}$ but we leave this possibility out of consideration here). Hence, for each set S_m we can find J different sets of J linearly dependent columns in $\tilde{\mathbf{B}}$. We denote the corresponding vectors in null($\tilde{\mathbf{B}}$) by $\mathbf{d}(g, m)$, where g is the column number taking the role of column g_1 in Lemma 4. Since the columns (i, j) of $\tilde{\mathbf{B}}$, $1 \leq i < j \leq J$, are linearly independent with probability 1 (see Lemma 3) and each $\mathbf{d}(g, m)$ represents a linear combination of $J - 1$ of these columns, together with column $(g, J + m)$ of $\tilde{\mathbf{B}}$, it follows that each of the nJ vectors $\mathbf{d}(g, m)$ uniquely contains a nonzero element for the column $(g, J + m)$ of $\tilde{\mathbf{B}}$. Hence, the vectors $\mathbf{d}(g, m)$ are linearly independent.

Since $\tilde{\mathbf{B}}$ is a horizontal matrix, it follows that any set of $J(J-1)/2 + 1$ different columns is linearly dependent. The vectors $\mathbf{d}(g, m)$ contain zero elements for the columns $(J + f, J + h)$ of $\tilde{\mathbf{B}}$ with $1 \leq f < h \leq n$. These are $n(n-1)/2$ columns of $\tilde{\mathbf{B}}$. It is possible to find $n(n-1)/2$ vectors $\mathbf{e}(f, h)$ in null($\tilde{\mathbf{B}}$) with nonzero elements for the columns (i, j) of $\tilde{\mathbf{B}}$, $1 \leq i < j \leq J$, and the column $(J + f, J + h)$ of $\tilde{\mathbf{B}}$. Since the columns (i, j) of $\tilde{\mathbf{B}}$, $1 \leq i < j \leq J$, are linearly independent with probability 1 (see Lemma 3), it follows that each vector $\mathbf{e}(f, h)$ uniquely has a nonzero element for column $(J + f, J + h)$ of $\tilde{\mathbf{B}}$. This implies that the set of vectors given by $\mathbf{d}(g, m)$ and $\mathbf{e}(f, h)$ is linearly independent and, by (9), spans the whole null($\tilde{\mathbf{B}}$). Hence, this set of vectors is a basis for null($\tilde{\mathbf{B}}$).

Let the matrix $\mathbf{N}$ contain the vectors $\mathbf{d}(g,m)$ and $\mathbf{e}(f,h)$ as columns, i.e., span($\mathbf{N}$) = null($\tilde{\mathbf{B}}$). In the illustration below we present $\mathbf{N}$ for the case where $J = 4$ and $R = 7$. In this case, null($\tilde{\mathbf{B}}$) has dimension 15. Nonzero elements are denoted by an *.

	d(1,1)	**d**(1,2)	**d**(1,3)	**d**(2,1)	**d**(2,2)	**d**(2,3)	**d**(3,1)	**d**(3,2)	**d**(3,3)	**d**(4,1)	**d**(4,2)	**d**(4,3)	**e**(1,2)	**e**(1,3)	**e**(2,3)
(1,2)	*	*	*	*	*	*							*	*	*
(1,3)	*	*	*				*	*	*				*	*	*
(1,4)	*	*	*							*	*	*	*	*	*
(1,5)	*														
(1,6)		*													
(1,7)			*												
(2,3)				*	*	*	*	*	*				*	*	*
(2,4)				*	*	*				*	*	*	*	*	*
(2,5)				*											
(2,6)					*										
(2,7)						*									
(3,4)							*	*	*	*	*	*	*	*	*
(3,5)							*								
(3,6)								*							
(3,7)									*						
(4,5)										*					
(4,6)											*				
(4,7)												*			
(5,6)													*		
(5,7)														*	
(6,7)															*

Recall the form of the matrix $\mathbf{U}^{(1)}$ in (7) and the discussion below (7). A vector $\mathbf{d}$ in null($\mathbf{U}^{(1)}$) must lie in the intersection of span($\mathbf{T}_s^{-1}\,\mathbf{N}$), $s = 1, \ldots, I(I-1)/2$. This implies that there exist vectors $\mathbf{x}_1,\ \mathbf{x}_2,\ \ldots,\mathbf{x}_{I\,(I-1)/2}$ such that

$$\mathbf{d}\ = \mathbf{T}_1^{-1}\mathbf{N}\,\mathbf{x}_1\ =\ \mathbf{T}_2^{-1}\mathbf{N}\,\mathbf{x}_2\ =\ \cdots\ =\ \mathbf{T}_{I(I-1)/2}^{-1}\mathbf{N}\,\mathbf{x}_{I(I-1)/2}. \tag{11}$$

Notice that, since $\mathbf{N}$ has full column rank, it follows that the matrices $\mathbf{T}_s^{-1}\mathbf{N}$ also have full column rank. The remaining part of the proof of Theorem 1 is devoted to showing that (11) implies $\mathbf{x}_s = \mathbf{0}$ for all s and, hence, $\mathbf{d} = \mathbf{0}$. Naturally, this yields $\mathbf{U}^{(1)}$ having full column rank.

From the construction of $\mathbf{N}$ above, it follows that there exists a row-permutation $\mathbf{P}$ such that $\mathbf{P}\,\mathbf{N} = \begin{bmatrix} \mathbf{D} \\ \mathbf{N}_2 \end{bmatrix}$, where $\mathbf{D}$ is a nonsingular diagonal matrix. We apply the same permutation to the diagonals of $\mathbf{T}_s^{-1}$ and write $\mathbf{P}\mathbf{T}_s^{-1}\,\mathbf{P}^T = \begin{bmatrix} \widehat{\mathbf{T}}_s^{-1} & \mathbf{O} \\ \mathbf{O} & \breve{\mathbf{T}}_s^{-1} \end{bmatrix}$, where $\widehat{\mathbf{T}}_s^{-1}$ is of the same order as $\mathbf{D}$. Let $\mathbf{P}\mathbf{d} = \begin{pmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \end{pmatrix}$, where $\mathbf{d}_1$ has the same number of rows as $\mathbf{D}$. It then follows from (11) that

$$\mathbf{d}_1 = \widehat{\mathbf{T}}_s^{-1}\,\mathbf{D}\,\mathbf{x}_s \quad \text{and} \quad \mathbf{d}_2 = \breve{\mathbf{T}}_s^{-1}\,\mathbf{N}_2\,\mathbf{x}_s, \quad \text{for s} = 1, \ldots, I(I-1)/2. \tag{12}$$

From the first part of (12), it follows that $\mathbf{x}_s = \mathbf{D}_s\,\mathbf{x}_1,\ s = 2, \ldots, I(I-1)/2$, where $\mathbf{D}_s = \mathbf{D}^{-1}\widehat{\mathbf{T}}_s\widehat{\mathbf{T}}_1^{-1}\,\mathbf{D}$ is a nonsingular diagonal matrix. From the second part of (12), it then follows that $\breve{\mathbf{T}}_1^{-1}\,\mathbf{N}_2\mathbf{x}_1 = \breve{\mathbf{T}}_s^{-1}\,\mathbf{N}_2\mathbf{D}_s\mathbf{x}_1$, $s = 2, \ldots, I(I-1)/2$. In matrix form, these equations in $\mathbf{x}_1$ can be written as

$$\mathbf{H}\,\mathbf{x}_1 = \begin{bmatrix} \breve{\mathbf{T}}_1^{-1}\mathbf{N}_2 - \breve{\mathbf{T}}_2^{-1}\mathbf{N}_2\mathbf{D}_2 \\ \vdots \\ \breve{\mathbf{T}}_1^{-1}\mathbf{N}_2 - \breve{\mathbf{T}}_{I(I-1)/2}^{-1}\mathbf{N}_2\mathbf{D}_{I(I-1)/2} \end{bmatrix}\mathbf{x}_1 = \mathbf{0}. \tag{13}$$

The matrix $\mathbf{H}$ has $(I(I-1)/2-1)\,J(J-1)/2$ rows and $R(R-1)/2 - J(J-1)/2$ columns. Assumption (A3) is thus equivalent to $\mathbf{H}$ being either square or vertical. Next, we argue that $\mathbf{H}$ has full column rank with probability 1. This yields $\mathbf{x}_1 = \mathbf{0}$ and we are done.

The matrix $\mathbf{N}_2$ has no all-zero rows or columns (see the example above). This implies that any dependencies in the rows or columns of $\mathbf{N}_2$ due to rank-deficiency, do not carry over to the matrices $\breve{\mathbf{T}}_1^{-1}\mathbf{N}_2 - \breve{\mathbf{T}}_s^{-1}\mathbf{N}_2\mathbf{D}_s$, $s = 2, \ldots, I(I-1)/2$. In fact, the latter have full rank with probability 1. Moreover, any dependencies in the columns of $\breve{\mathbf{T}}_1^{-1}\mathbf{N}_2 - \breve{\mathbf{T}}_s^{-1}\mathbf{N}_2\mathbf{D}_s$ do not carry over to $\begin{bmatrix} \breve{\mathbf{T}}_1^{-1}\mathbf{N}_2 - \breve{\mathbf{T}}_s^{-1}\mathbf{N}_2\mathbf{D}_s \\ \breve{\mathbf{T}}_1^{-1}\mathbf{N}_2 - \breve{\mathbf{T}}_t^{-1}\mathbf{N}_2\mathbf{D}_t \end{bmatrix}$, for $s \neq t$, unless the latter is a horizontal matrix. Analogously, the matrix $\mathbf{H}$, since it is either square or vertical, has full column rank with probability 1. This completes the proof of Theorem 1. □

3. Almost Sure Uniqueness in Indscal

Here we consider the Indscal decomposition, i.e., the CP decomposition (1) in which the array $\underline{\mathbf{X}}$ has symmetric slices and the constraint $\mathbf{A} = \mathbf{B}$ is imposed. Hence, also the fitted part of the Indscal decomposition has symmetric slices. For a discussion of the Indscal model, see Carroll and Chang (1970) and Ten Berge, Sidiropoulos, and Rocci (2004). We assume that (B1) and (B2) hold, i.e., $\mathbf{A}$ is randomly sampled from an IR-dimensional continuous distribution and $\mathbf{C}$ has full column rank. Analogous to the CP decomposition, an Indscal solution $(\mathbf{A}, \mathbf{C})$ is essentially unique if the matrix $\mathbf{U}_{\text{sym}} = \tilde{\mathbf{A}}\bullet\tilde{\mathbf{A}}$ has full column rank. Our main result is the following.

Theorem 2. *If* (B1) *and* (B3) *hold, then* $\mathbf{U}_{\text{sym}} = \tilde{\mathbf{A}}\bullet\tilde{\mathbf{A}}$ *has full column rank with probability 1 with respect to the distribution* F. *Hence, if* (B1) – (B3) *hold, then the Indscal solution* $(\mathbf{A}, \mathbf{B})$ *is essentially unique with probability 1.*

As stated in the Introduction, we have not obtained a complete proof of Theorem 2. However, we will indicate how a proof can be obtained for any values of I and R satisfying (B3). As in the previous section, we start by deleting redundant rows from the matrix $\mathbf{U}_{\text{sym}}$.

Each row of $\mathbf{U}_{\text{sym}}$ is the Hadamard product of two (not necessarily different) rows of $\tilde{\mathbf{A}}$. However, some rows of $\mathbf{U}_{\text{sym}}$ appear twice. We denote a row of $\mathbf{U}_{\text{sym}}$ by (i, j, k, l), where (i, j) and (k, l) are the rows of $\tilde{\mathbf{A}}$ involving rows i, j and rows k, l of $\mathbf{A}$, respectively. The following can be observed:

- Rows (i, j, k, l) and (k, l, i, j) are identical.

When determining the rank $\mathbf{U}_{\text{sym}}$, we may delete one of every two identical rows. The identical rows described above are avoided by only taking, as rows of $\mathbf{U}_{\text{sym}}$, the Hadamard product of $\tilde{\mathbf{a}}_s^T$ with $\tilde{\mathbf{a}}_t^T$, $t \geq s$. Hence, instead of $I^2(I-1)^2/4$ rows we need to consider only $I\,(I-1)/4\,[I\,(I-1)/2+1]$ rows of $\mathbf{U}_{\text{sym}}$. We denote the matrix containing only these rows by $\mathbf{U}_{\text{sym}}^{(1)}$. The following lemma shows that there are still dependencies in the rows of $\mathbf{U}_{\text{sym}}^{(1)}$.

Lemma 5. *If (i, j, k, l) is a row of* $\mathbf{U}_{\mathrm{sym}}^{(1)}$ *and $j < k$, then*

$$\mathrm{row}(i,\ j,\ k,\ l) - \mathrm{row}\ (i,\ k,\ j,\ l) + \mathrm{row}\ (i,\ l,\ j,\ k) = \mathbf{0}^T. \tag{14}$$

Proof. We have $i < j < k < l$, which implies that (i, k, j, l) and (i, l, j, k) are indeed rows of $\mathbf{U}_{\mathrm{sym}}^{(1)}$. Evaluating (14) for the element in column (g, h) yields

$$\begin{vmatrix} a_{i,g} & a_{i,h} \\ a_{j,g} & a_{j,h} \end{vmatrix} \cdot \begin{vmatrix} a_{k,g} & a_{k,h} \\ a_{l,g} & a_{l,h} \end{vmatrix} - \begin{vmatrix} a_{i,g} & a_{i,h} \\ a_{k,g} & a_{k,h} \end{vmatrix} \cdot \begin{vmatrix} a_{j,g} & a_{j,h} \\ a_{l,g} & a_{l,h} \end{vmatrix} + \begin{vmatrix} a_{i,g} & a_{i,h} \\ a_{l,g} & a_{l,h} \end{vmatrix} \cdot \begin{vmatrix} a_{j,g} & a_{j,h} \\ a_{k,g} & a_{k,h} \end{vmatrix}, \tag{15}$$

which equals 0 for every value of (g, h). This completes the proof. □

Dependencies of type (14) can be removed by deleting all rows $(i,\ j,\ k,\ l)$ of $\mathbf{U}_{\mathrm{sym}}^{(1)}$ with $j < k$. Since we have $i < j < k < l$, the number of rows to be deleted is equal to the number of different ordered sets of four numbers we can choose from the set $\{1,\ 2,\ \ldots,\ I\}$, i.e., $\binom{I}{4}$ (provided that $I \geq 4$). The matrix in which these rows have been deleted is denoted by $\mathbf{U}_{\mathrm{sym}}^{(2)}$. The right and left-hand sides of (B3) are equal to the number of rows and columns of $\mathbf{U}_{\mathrm{sym}}^{(2)}$, respectively. Hence, assumption (B3) is equivalent to $\mathbf{U}_{\mathrm{sym}}^{(2)}$ being a square or vertical matrix, which is necessary for full column rank. From the discussion above, it follows that $\mathrm{null}(\mathbf{U}_{\mathrm{sym}}) = \mathrm{null}(\mathbf{U}_{\mathrm{sym}}^{(1)}) = \mathrm{null}(\mathbf{U}_{\mathrm{sym}}^{(2)})$. Hence, if one of these three matrices has full column rank, they all have full column rank. Notice that $\mathbf{U}_{\mathrm{sym}}^{(2)}$ plays the same role as $\mathbf{U}^{(1)}$ in the previous section.

The derivation above shows that in the Indscal decomposition a lower value of R is needed to guarantee essential uniqueness when compared to the CP decomposition. This is in line with Ten Berge et al. (2004) who found that arrays with symmetric slices often have lower typical rank values. Essential uniqueness usually occurs when R is smaller than the typical rank of the array.

Next, we continue our (partial) proof of Theorem 2. The following lemma treats the case $R \leq I$. Its proof follows from the uniqueness condition in Harshman (1972). Below, we offer an alternative proof, which is more straightforward in our context.

Lemma 6. *Suppose* (B1) *and* (B3) *hold. If $R \leq I$, then $\boldsymbol{U}_{\mathrm{sym}}$ has full column rank with probability 1.*

Proof. The proof is analogous to the proof of Lemma 2. Suppose that (B1) and (B3) hold and $R \leq I$. Premultiplying $\mathbf{A}$ by a nonsingular matrix does not affect the uniqueness of the decomposition. If $R \leq I$ there exists (with probability 1) a nonsingular matrix $\mathbf{S}$ such that $\mathbf{SA} = \begin{bmatrix} \mathbf{I}_R \\ \mathbf{O} \end{bmatrix}$. The associated matrix $\tilde{\mathbf{A}}$ then equals $\begin{bmatrix} \mathbf{I}_{R(R-1)/2} \\ \mathbf{O} \end{bmatrix}$ and $\mathbf{U}_{\mathrm{sym}} = \tilde{\mathbf{A}} \bullet \tilde{\mathbf{A}}$ can also be written (after a row permutation) as $\begin{bmatrix} \mathbf{I}_{R(R-1)/2} \\ \mathbf{O} \end{bmatrix}$. (Notice that the rows which are deleted when going from $\mathbf{U}_{\mathrm{sym}}$ to $\mathbf{U}_{\mathrm{sym}}^{(1)}$ to $\mathbf{U}_{\mathrm{sym}}^{(2)}$ are contained in the rows of zeros in $\mathbf{U}_{\mathrm{sym}}$.) This completes the proof. □

In the remaining part of our (partial) proof of Theorem 2, we assume that $R > I$. Using Lemma 1, we show that Theorem 2 holds for a range of values of I and R such that $R > I$ and (B3) holds.

TABLE 1.
Values of I and upper bounds for R which follow from (B3).

I	2	3	4	5	6	7	8	9
Upper bound for R	2	4	6	10	15	20	26	33

Notice that $\det(\mathbf{U}_{\text{sym}}^T\mathbf{U}_{\text{sym}})$ is a real-valued analytic function of the elements of $\mathbf{A}$. Moreover, $\det(\mathbf{U}_{\text{sym}}^T\mathbf{U}_{\text{sym}}) \neq 0$ is equivalent to $\mathbf{U}_{\text{sym}}$ being of full column rank. According to Lemma 1, there holds for fixed I and R that if $\det(\mathbf{U}_{\text{sym}}^T\mathbf{U}_{\text{sym}})$ is nonzero for one particular $\mathbf{A}$, then it is nonzero with probability 1. In Table 1, we give for values $I = 2, \ldots, 9$ the upper bound for R which follows from (B3). For all pairs (I, R) in Table 1 with $R > I$, we have generated a random matrix $\mathbf{A}$ and verified that $\det(\mathbf{U}_{\text{sym}}^T\mathbf{U}_{\text{sym}}) \neq 0$. Hence, using Lemma 1, we have proven Theorem 2 for these pairs (I, R). Lemma 6 above covers all cases for which $R \leq I$. To prove Theorem 2 for any pair (I, R) satisfying (B3), which is not considered in Lemma 6 or Table 1, it suffices to generate a random matrix $\mathbf{A}$ and to verify that $\det(\mathbf{U}_{\text{sym}}^T\mathbf{U}_{\text{sym}}) \neq 0$.

Notice that our proof of Theorem 1 cannot easily be adapted to prove Theorem 2. Indeed, if $\mathbf{A} = \mathbf{B}$ there exist deterministic relations between the diagonal matrices $\mathbf{T}_s = \text{diag}(\tilde{\mathbf{a}}_s^T)$ and the matrix $\mathbf{N}$, for which now holds $\text{span}(\mathbf{N}) = \text{null}(\tilde{\mathbf{A}})$. This makes the analysis a lot more complicated.

4. Discussion

We have obtained almost sure uniqueness conditions for the CP and Indscal decompositions when the component matrices $\mathbf{A}$ and $\mathbf{B}$ are randomly sampled from a continuous distribution and $\mathbf{C}$ has full column rank. By using the approach of Jiang and Sidiropoulos (2004) we were able to make a clear distinction between the CP and Indscal models. In the latter case, a stricter uniqueness condition (in terms of R) is obtained, since the Indscal model contains less parameters than the CP model. In our context, both uniqueness conditions are more relaxed than Kruskal's condition (3).

In the majority of cases, solutions obtained from CP and Indscal algorithms can be regarded as randomly sampled from a continuous distribution and our sufficient uniqueness conditions (A3) and (B3) apply. However, sometimes a solution obtained from a CP or Indscal algorithm may exhibit features which occur with probability zero in our analysis. The best known example are so-called degenerate solutions, in which the product of the correlations of two factors for the three modes tends to -1 (two-factor degeneracy, see Kruskal, Harshman, and Lundy, 1989). Such cases are outside the scope of analysis presented in this paper.

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