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Kruskal's condition for uniqueness in Candecomp/Parafac when ranks and k-ranks coincide

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Abstract

A key feature of the analysis of three-way arrays by Candecomp/Parafac is the essential uniqueness of the trilinear decomposition. Kruskal has previously shown that the three component matrices involved are essentially unique when the sum of their k-ranks is at least twice the rank of the decomposition plus 2. It was proved that Kruskal's sufficient condition is also necessary when the rank of the decomposition is 2 or 3. If the rank is 4 or higher, the condition is not necessary for uniqueness. However, when the k-ranks of the component matrices equal their ranks, necessity of Kruskal's condition still holds in the rank-4 case. Ten Berge and Sidiropoulos conjectured that Kruskal's condition is necessary for all cases of rank 4 and higher where ranks and k-ranks coincide. In the present paper we show that this conjecture is false.

Keywords: Candecomp; Parafac; Three-way arrays; Uniqueness; k-rank

1. Introduction

Carroll and Chang (1970) and Harshman (1970) have independently proposed the same method for component analysis of three-way arrays, and christened it Candecomp and Parafac, respectively. For a given three-way array $\underline{\mathbf{X}}$ and a fixed number of r components, Candecomp/Parafac (CP) provides a trilinear decomposition as follows. When $\underline{\mathbf{X}}$ contains

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K slices of order $I \times J$, CP yields component matrices $\mathbf{A}$ $(I \times r)$, $\mathbf{B}$ $(J \times r)$ and $\mathbf{C}$ $(K \times r)$ such that $\sum_{k=1}^{K} tr(\mathbf{E}_k'\mathbf{E}_k)$ is minimized in the decomposition

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

where $\mathbf{C}_k$ is the diagonal matrix containing the elements of kth row of $\mathbf{C}$. The smallest number of components r for which there exists a CP decomposition with perfect fit is equal to the three-way rank of the array.

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 a CP decomposition, i.e., a 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, rescaling columns of $\mathbf{A}$ or $\mathbf{B}$ or $\mathbf{C}$ by a diagonal matrix $\mathbf{L}$ is allowed, provided that the inverse of $\mathbf{L}$ is accounted for elsewhere. For instance, $\mathbf{A}\mathbf{C}_k\mathbf{B}' = \mathbf{A}\mathbf{L}\mathbf{L}^{-1}\mathbf{C}_k\mathbf{B}' = (\mathbf{A}\mathbf{L})\mathbf{C}_k(\mathbf{B}\mathbf{L}^{-1})'$, which shows that replacing $\mathbf{A}$ by $\mathbf{AL}$ is allowed when paired with replacing $\mathbf{B}$ by $\mathbf{B}\mathbf{L}^{-1}$. Also, simultaneous permutations of columns of $\mathbf{A}$, $\mathbf{B}$ and diagonal elements of $\mathbf{C}_k$, $k = 1, 2, \ldots, K$, are allowed. Usually, these are the only transformational indeterminacies in CP. 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*.

Kruskal (1977) has shown that (essential) uniqueness holds under relatively mild conditions, to be discussed below. Ten Berge and Sidiropoulos (2002) have shown that Kruskal's condition is necessary and sufficient for $r = 2$ and 3, but not for $r > 3$. They conjectured that necessity still holds if the ranks of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ equal their k-ranks (a notion to be defined below) and proved the conjecture to hold for the case $r = 4$. In the present paper two counterexamples to the conjecture will be given, one for $r = 5$ and another for $r = 6$. That is, Kruskal's condition is not satisfied in the examples, while the solutions are (essentially) unique and the ranks of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ equal their k-ranks.

2. Kruskal's condition for uniqueness

The most general sufficient condition for (essential) uniqueness of a CP solution 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 by Harshman and Lundy (1984). The k-rank of a matrix is the largest value of m such that every subset of m columns of the matrix is linearly independent.

By definition, the k-rank of a matrix cannot exceed its rank. The k-rank is 1 if there is a pair of proportional columns. Kruskal's condition is now: in CP the component matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are essentially unique if

$$k_A + k_B + k_C \geqslant 2r + 2, \tag{2}$$

where k_A, k_B and k_C are the k-ranks of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$, respectively. Ten Berge and Sidiropoulos (2002) have shown that Kruskal's sufficient condition (2) is also necessary for $r=2$ and 3, but not for $r > 3$. In practice, (2) is almost invariably met, because the number of components r is usually small enough. Note that (2) cannot be satisfied when $r = 1$. For this case, however, conditions for essential uniqueness are trivial.

Harshman (1972) has shown that it is sufficient for (essential) uniqueness to have **A** and **B** of full column rank and **C** of k-rank 2 or higher. When $r = 2$, Harshman's condition is equivalent to Kruskal's condition. For $r > 2$, however, Kruskal's condition may be satisfied when Harshman's is not.

Ten Berge and Sidiropoulos (2002) conjectured that Kruskal's condition (2) is necessary for essential uniqueness if the k-ranks of **A**, **B** and **C** equal their ranks. They also proved this for the case $r = 4$. Below, we give two examples with $r > 4$ in which k-ranks are ranks, the solution is essentially unique, but (2) is not satisfied. This shows that the conjecture is not true for $r > 4$. In the first example $r = 5$ and in the second example $r = 6$. The difference between the two examples is the following. For a random array (sampled from a continuous distribution) the first example occurs with probability zero, while the second example occurs with probability 1.

The concepts "with probability 1" and "with probability zero" are used throughout the paper and may need some explanation. Suppose property x holds with probability 1 for an array which is randomly sampled from a continuous distribution. Then this means that arrays not satisfying property x occur with probability zero. For example, a $2 \times 2 \times 1$ array with its elements randomly sampled from a 4-dimensional continuous distribution, has nonzero determinant with probability 1. Notice that this does not imply that property x holds for all arrays. It may still be possible to contrive arrays for which property x does not hold. For example, there are infinitely many $2 \times 2 \times 1$ arrays with determinant zero. However, such arrays have probability zero of occurring when randomly sampled from a continuous distribution. Notice that if property y holds with probability zero for a random array, then the negative of property y holds with probability 1.

Next, we start with our first example.

Example 1. $3 \times 3 \times 5$ arrays with $r = 5$

Let $I = J = 3$ and $K = r = 5$. Let the component matrices **A**, **B**, and **C** of order 3×5, 3×5, and 5×5, respectively, be randomly sampled from a continuous distribution. Then the implied $3 \times 3 \times 5$ array will have rank 5 with probability 1. This can be seen as follows. Let $\mathbf{X}_i = \mathbf{C}\mathbf{A}_i\mathbf{B}'$ for $i = 1, 2, 3$, where $\mathbf{A}_i$ is the diagonal matrix containing the elements of the ith row of **A**. Then, with probability 1, the rank of $[\mathbf{X}_1|\mathbf{X}_2|\mathbf{X}_3]$ equals 5, which implies that the rank of the $3 \times 3 \times 5$ array is at least 5. However, since **A**, **B**, and **C** represent a decomposition in 5 components, the array is at most of rank 5. Therefore, the implied $3 \times 3 \times 5$ array has rank 5 with probability 1.

There will hold $k_A = \text{rank}(\mathbf{A}) = 3$, $k_B = \text{rank}(\mathbf{B}) = 3$ and $k_C = \text{rank}(\mathbf{C}) = 5$. This implies that Kruskal's condition (2) is not satisfied, since $k_A + k_B + k_C = 11$ and $2r + 2 = 12$. Hence, if **A**, **B** and **C** were essentially unique our first counterexample would have been a fact. However, Ten Berge (2004) proved that in this case the CP decomposition is partially unique with probability 1. That is, there exist six possible CP solutions, any two of which have four of the five components in common. This means that any solution (**A**,**B**,**C**) which is essentially unique occurs with probability zero. Ten Berge (2004) first showed that a random $3 \times 3 \times 5$ array has rank {5 or 6} with probability 1 and then considers a random $3 \times 3 \times 5$ array under the assumption that it has rank 5. In order to find an essentially unique solution we will give an alternative proof of partial uniqueness for $3 \times 3 \times 5$ arrays with

$r=5$ by starting with random matrices **A**, **B** and **C**. This approach allows us to determine in which cases essential uniqueness occurs and results in our first counterexample. Our proof of partial uniqueness is presented in the next section. After the proof we formulate our first counterexample.

3. Partial uniqueness for $3 \times 3 \times 5$ arrays with $r = 5$

Let **A**, **B** and **C** be randomly sampled from a continuous distribution. Then, with probability 1, we are able to transform them into $\mathbf{C} = \mathbf{I}_5$,

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 1 & a_1 \\ 0 & 1 & 0 & 1 & a_2 \\ 0 & 0 & 1 & 1 & a_3 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 1 & 0 & 0 & 1 & b_1 \\ 0 & 1 & 0 & 1 & b_2 \\ 0 & 0 & 1 & 1 & b_3 \end{bmatrix}. \tag{3}$$

This can be seen as follows (also see the appendix of Ten Berge and Sidiropoulos (2002)). First, transform **A** and **B** such that they have $\mathbf{I}_3$ in their first three columns. Denote their fourth columns by **a** and **b**, respectively. Next, premultiply the new **A** and **B** by the inverses of diag(**a**) and diag(**b**), respectively. This preserves diagonal matrices in the first three columns, but transforms the fourth columns to $(1\,1\,1)'$. Then rescale the first three columns of the present **A** and **B** to restore the identity matrices, now absorbing the inverses of the necessary constants in the columns of **C**. Finally, premultiply **C** by its inverse. Although these transformations do change the array and its CP solution, they leave the ranks, k-ranks, and uniqueness properties unaffected.

Next, we will show that, with probability 1, there exist five other solutions than (3). We will make use of a necessary condition for essential uniqueness due to Liu and Sidiropoulos (2001). Let $\mathbf{Y}_k$ denote the fitted part of $\mathbf{X}_k$ in (1), i.e. $\mathbf{Y}_k = \mathbf{A}\mathbf{C}_k\mathbf{B}'$. Let **Y** be the matrix having Vec($\mathbf{Y}_k$) as its kth column, $k = 1, 2, \ldots, K$, where the Vec is taken row wise. Then **Y** can be written as

$$\mathbf{Y} = (\mathbf{A} \bullet \mathbf{B})\mathbf{C}', \tag{4}$$

where $\mathbf{A} \bullet \mathbf{B}$ is the Khatri–Rao product (the column-wise Kronecker product) of **A** and **B**. Suppose that $\mathbf{A} \bullet \mathbf{B}$ is not of full column rank. Then there exists a linear combination of the columns of $\mathbf{A} \bullet \mathbf{B}$ which equals **0**. Suppose the (nonzero) vector **n** contains the coefficients of this linear combination. Then **n** is orthogonal to the rows of $\mathbf{A} \bullet \mathbf{B}$. Adding **n** to any column of $\mathbf{C}'$ preserves (4), but produces a different solution for **C**. It follows that full column rank of $\mathbf{A} \bullet \mathbf{B}$ is necessary for essential uniqueness.

As mentioned above, we consider the case $K = r = 5$ and $\mathbf{C} = \mathbf{I}_5$. Suppose there exists an alternative solution $\mathbf{Y} = (\mathbf{G} \bullet \mathbf{H})\mathbf{D}'$ and $\mathbf{A} \bullet \mathbf{B}$ is of full column rank, then $\mathbf{A} \bullet \mathbf{B} = (\mathbf{G} \bullet \mathbf{H})\mathbf{D}'$, with **D** nonsingular. Hence, $\mathbf{A} \bullet \mathbf{B}$ and $\mathbf{G} \bullet \mathbf{H}$ span the same spaces and, consequently, every column of $\mathbf{G} \bullet \mathbf{H}$ must be a linear combination of the columns of $\mathbf{A} \bullet \mathbf{B}$. This implies that five linearly independent vectors $\mathbf{w}_j$ can be found such that $(\mathbf{A} \bullet \mathbf{B})\mathbf{w}_j = \mathbf{g}_j \bullet \mathbf{h}_j = \text{Vec}(\mathbf{h}_j \mathbf{g}_j')$. Clearly, if the only possible set of five linearly independent vectors $\mathbf{w}_j$ constitutes a rescaled permutation matrix, the solution $\mathbf{Y} = (\mathbf{A} \bullet \mathbf{B})\mathbf{I}_5$ has been proven essentially unique (see also Jiang and Sidiropoulos, 2004). Below, we show that for **A** and **B** in (3) six rather than five of such vectors $\mathbf{w}_j$ can be found, namely

$$\begin{pmatrix}\lambda_1\\0\\0\\0\\0\end{pmatrix},\quad \begin{pmatrix}0\\\lambda_2\\0\\0\\0\end{pmatrix},\quad \begin{pmatrix}0\\0\\\lambda_3\\0\\0\end{pmatrix},\quad \begin{pmatrix}0\\0\\0\\\lambda_4\\0\end{pmatrix},\quad \begin{pmatrix}0\\0\\0\\0\\\lambda_5\end{pmatrix} \quad \text{and} \quad \begin{pmatrix}x_1\mu\\x_2\mu\\x_3\mu\\x_4\mu\\\mu\end{pmatrix}, \tag{5}$$

where $\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \mu$ are arbitrary nonzero constants and the x_i depend on the elements in the fifth columns of **A** and **B**. Since any five of the six vectors in (5) are linearly independent, this proves that exactly six different solutions exist and that any two different solutions share four of the five components. Notice that if the sixth vector in (5) is not a solution then essential uniqueness has been established.

We are now ready to present our proof of the existence of a solution (5). For **A** and **B** in (3) we have

$$(\mathbf{A} \bullet \mathbf{B}) = \left[\begin{array}{ccccc} 1 & 0 & 0 & 1 & a_1b_1\\ 0 & 0 & 0 & 1 & a_1b_2\\ 0 & 0 & 0 & 1 & a_1b_3\\ \hline 0 & 0 & 0 & 1 & a_2b_1\\ 0 & 1 & 0 & 1 & a_2b_2\\ 0 & 0 & 0 & 1 & a_2b_3\\ \hline 0 & 0 & 0 & 1 & a_3b_1\\ 0 & 0 & 0 & 1 & a_3b_2\\ 0 & 0 & 1 & 1 & a_3b_3 \end{array}\right], \tag{6}$$

which has full column rank with probability 1. For a general vector $\mathbf{w} = (\alpha\beta\gamma\delta\varepsilon)'$ the 3×3 matrix form of $(\mathbf{A} \bullet \mathbf{B})\mathbf{w}$ is

$$\mathbf{W} = \mathbf{hg}' = \begin{bmatrix} \alpha + \delta + a_1b_1\varepsilon & \delta + a_1b_2\varepsilon & \delta + a_1b_3\varepsilon\\ \delta + a_2b_1\varepsilon & \beta + \delta + a_2b_2\varepsilon & \delta + a_2b_3\varepsilon\\ \delta + a_3b_1\varepsilon & \delta + a_3b_2\varepsilon & \gamma + \delta + a_3b_3\varepsilon \end{bmatrix}. \tag{7}$$

We determine all solutions $(\alpha\beta\gamma\delta\varepsilon)'$ for which **W** has indeed rank 1. We will use the fact that the determinant of any minor of **W** has to be zero. This yields nine equations. When all elements of **W** are nonzero, only four minors have to be checked. However, elements of **W** are often zero in the solutions presented below. Therefore, we start with the equations for all nine minors. The minor of **W** obtained by deleting row i and column j is denoted by $\mathbf{M}_{i,j}$.

$$\det(\mathbf{M}_{2,3}) = \alpha(\delta + a_3b_2\varepsilon) + \delta\varepsilon(a_1 - a_3)(b_1 - b_2) = 0, \tag{8}$$

$$\det(\mathbf{M}_{3,2}) = \alpha(\delta + a_2b_3\varepsilon) + \delta\varepsilon(a_1 - a_2)(b_1 - b_3) = 0, \tag{9}$$

$$\det(\mathbf{M}_{1,3}) = -\beta(\delta + a_3b_1\varepsilon) + \delta\varepsilon(a_2 - a_3)(b_1 - b_2) = 0, \tag{10}$$

$$\det(\mathbf{M}_{3,1}) = -\beta(\delta + a_1b_3\varepsilon) + \delta\varepsilon(a_1 - a_2)(b_2 - b_3) = 0, \tag{11}$$

$$\det(\mathbf{M}_{1,2}) = \gamma(\delta + a_2b_1\varepsilon) + \delta\varepsilon(a_2 - a_3)(b_1 - b_3) = 0, \tag{12}$$

$$\det(\mathbf{M}_{2,1}) = \gamma(\delta + a_1 b_2 \varepsilon) + \delta\varepsilon(a_1 - a_3)(b_2 - b_3) = 0, \tag{13}$$

$$\det(\mathbf{M}_{3,3}) = \alpha\beta + \alpha(\delta + a_2 b_2 \varepsilon) + \beta(\delta + a_1 b_1 \varepsilon) + \delta\varepsilon(a_1 - a_2)(b_1 - b_2) = 0, \tag{14}$$

$$\det(\mathbf{M}_{2,2}) = \alpha\gamma + \alpha(\delta + a_3 b_3 \varepsilon) + \gamma(\delta + a_1 b_1 \varepsilon) + \delta\varepsilon(a_1 - a_3)(b_1 - b_3) = 0, \tag{15}$$

$$\det(\mathbf{M}_{1,1}) = \beta\gamma + \beta(\delta + a_3 b_3 \varepsilon) + \gamma(\delta + a_2 b_2 \varepsilon) + \delta\varepsilon(a_2 - a_3)(b_2 - b_3) = 0. \tag{16}$$

Notice that all terms $(a_i - a_j)$ and $(b_i - b_j)$ are nonzero with probability 1 for $i \neq j$. Suppose that $\alpha = 0$. From (8) it follows that $\delta\varepsilon = 0$. There are three possibilities. If $\delta = 0$ and $\varepsilon \neq 0$, then (10) and (12) yield $\beta = \gamma = 0$. This also holds when $\delta \neq 0$ and $\varepsilon = 0$. Finally, if $\delta = \varepsilon = 0$, it follows from (16) that $\beta\gamma = 0$, so either $\beta = 0$ or $\gamma = 0$. Hence, the second, third, fourth and fifth vector in (5) have been found. It is easy to see that in these cases $\mathbf{W}$ has indeed rank 1. Suppose next that $\alpha \neq 0$. Together, Eqs. (8) and (9) are equivalent to

$$\frac{-\delta\varepsilon}{\alpha} = \frac{\delta + a_3 b_2 \varepsilon}{(a_1 - a_3)(b_1 - b_2)} = \frac{\delta + a_2 b_3 \varepsilon}{(a_1 - a_2)(b_1 - b_3)}. \tag{17}$$

If $\delta\varepsilon = 0$, then (17) implies that $\delta = \varepsilon = 0$ and (14) and (15) yield $\beta = \gamma = 0$. It can be seen that $\mathbf{W}$ has indeed rank 1 in this case. This fifth solution is equivalent to the first vector in (5). From now on we assume that $\alpha \neq 0$ and $\delta\varepsilon \neq 0$. We make use of the following fact. For any 3×3 matrix of rank 1 with all elements nonzero, there holds that if $\det(\mathbf{M}_{i,j}) = 0$ for all $i \neq j$, then $\det(\mathbf{M}_{i,i}) = 0$, $i = 1, 2, 3$. Moreover, if all elements are nonzero and $\det(\mathbf{M}_{2,3}) = \det(\mathbf{M}_{3,2}) = \det(\mathbf{M}_{1,3}) = \det(\mathbf{M}_{1,2}) = 0$, then it follows that $\det(\mathbf{M}_{3,1}) = \det(\mathbf{M}_{2,1}) = 0$. Hence, if (8)–(10) and (12) are satisfied and all elements of $\mathbf{W}$ are nonzero, then also (11), (13) and (14)–(16) hold. We now determine all vectors $(\alpha\beta\gamma\delta\varepsilon)'$ satisfying (8)–(10) and (12), or equivalently (10), (12) and (17). Since $\delta\varepsilon \neq 0$ the second equality in (17) can be written as

$$\frac{\delta}{\varepsilon} = \frac{(a_1 - a_3)(b_1 - b_2)a_2 b_3 - (a_1 - a_2)(b_1 - b_3)a_3 b_2}{(a_1 - a_2)(b_1 - b_3) - (a_1 - a_3)(b_1 - b_2)} = x_4. \tag{18}$$

Both the numerator and the denominator of the second term in (18) are analytical real-valued functions of the six parameters a_j and b_j. Since they are not identically zero, it follows from Fisher (1966, Theorem 5.A.2) that they are nonzero with probability 1. From the first equality in (17) it follows that:

$$\frac{-\alpha}{\varepsilon} = \frac{x_4(a_1 - a_3)(b_1 - b_2)}{x_4 + a_3 b_2} = -x_1. \tag{19}$$

Using the result of Fisher (1966) as above, it can be shown that the denominator of the second term in (19) is nonzero with probability 1. From (10) it follows that:

$$\frac{\beta}{\varepsilon} = \frac{x_4(a_2 - a_3)(b_1 - b_2)}{x_4 + a_3 b_1} = x_2. \tag{20}$$

Analogous to (19) the denominator of the second term in (20) is nonzero with probability 1. From (12) it follows that:

$$\frac{-\gamma}{\varepsilon} = \frac{x_4(a_2 - a_3)(b_1 - b_3)}{x_4 + a_2 b_1} = -x_3. \tag{21}$$

The denominator of the second term in (21) is nonzero with probability 1. As stated above, Eqs. (11), (13) and (14)–(16) hold automatically when using (18)–(21). It remains to verify that all elements of **W** are nonzero with probability 1. The matrix **W** is

$$\mathbf{W} = \begin{bmatrix} x_1 + x_4 + a_1 b_1 & x_4 + a_1 b_2 & x_4 + a_1 b_3 \\ x_4 + a_2 b_1 & x_2 + x_4 + a_2 b_2 & x_4 + a_2 b_3 \\ x_4 + a_3 b_1 & x_4 + a_3 b_2 & x_3 + x_4 + a_3 b_3 \end{bmatrix} \varepsilon. \tag{22}$$

Notice that, since $\text{rank}(\mathbf{W}) = 1$, if the element in row i and column j is zero, then either row i is $(0\,0\,0)$ or column j is $(0\,0\,0)'$ or both. This yields equalities of the form $a_i = a_j$ with $i \neq j$ or $b_i = b_j$ with $i \neq j$, which have probability zero. Hence, all elements of **W** are nonzero. The solution (18)–(21) with $\varepsilon \neq 0$ is equivalent to the sixth vector in (5). Since we have shown that exactly six different solutions **w** exist, this concludes our proof of partial uniqueness.

Example 1. construction of a case of essential uniqueness

Recall that our goal is to determine a CP solution $(\mathbf{A},\mathbf{B},\mathbf{C})$ for a $3 \times 3 \times 5$ array with $r = 5$, which is essentially unique. Above, we showed that if $(\mathbf{A},\mathbf{B},\mathbf{C})$ are randomly sampled from a continuous distribution, then there exist exactly six different solutions with probability 1. Each solution can be constructed from five of the six vectors **w** in (5) for which the 3×3 matrix form of $(\mathbf{A} \bullet \mathbf{B})\mathbf{w}$ has rank 1. If the sixth vector in (5) cannot be used, the solution is essentially unique. We will now show how to pick an **A** and **B** where this happens.

Above, we considered all vectors $(\alpha\beta\gamma\delta\varepsilon)'$ for which **W** in (7) has rank 1. The sixth vector in (5) was discovered by starting with the assumptions $\alpha \neq 0$ and $\delta\varepsilon \neq 0$. This yielded the Eqs. (18)–(21) characterizing the sixth vector in (5). Suppose we choose the numbers a_i and b_i such that either the numerator or the denominator of the expression in (18) is zero. Then $\delta = \varepsilon = 0$ has to hold if $\alpha \neq 0$ and the sixth vector in (5) cannot be used anymore. In this case, the only set of five linearly independent vectors **w** such that the matrix **W** in (7) has rank 1, are the first five vectors in (5), which constitute a rescaled permutation matrix. Hence, the CP solution is essentially unique. From the proof above it follows that these situations have probability zero. A numerical example of such a solution is the following. Let $\mathbf{C} = \mathbf{I}_5$,

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 2 \\ 0 & 0 & 1 & 1 & 3 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 3 \\ 0 & 0 & 1 & 1 & 5 \end{bmatrix}, \tag{23}$$

then the numerator in (18) equals 4, while the denominator is zero. It can be verified that $k_A = \text{rank}(\mathbf{A}) = 3$, $k_B = \text{rank}(\mathbf{B}) = 3$ and $k_C = \text{rank}(\mathbf{C}) = 5$. Moreover, the implied $3 \times 3 \times 5$ array has rank 5. This is a case of essential uniqueness, which is a first counterexample to the conjecture of Ten Berge and Sidiropoulos (2002).

It is instructive to examine this counterexample in terms of the analysis of partial uniqueness by Ten Berge (2004). In his proof of partial uniqueness for random $3 \times 3 \times 5$ arrays of rank 5, Ten Berge shows that the component matrices **A**, **B** and **C** can be constructed from five roots of a 7th degree polynomial. This polynomial has seven real roots, one of which is to be discarded. Hence, there remain six roots, five of which are used. This yields six possible CP solutions, any two of which have four of the five components in common. Applying the approach of Ten Berge to our example in (23) yields the following. After transforming the $3 \times 3 \times 5$ array implied by (23) to the form Ten Berge starts from, we find that the coefficient of the leading term of the 7th degree polynomial is zero. Hence, we obtain a 6th degree polynomial. Since one root has to be discarded, only five roots remain and only one CP solution is possible. However, we cannot conclude that our analysis of the $3 \times 3 \times 5$ arrays of rank 5 is fully compatible with that of Ten Berge (2004). This can be seen as follows. We use a transformation of (**A**,**B**,**C**) to the form (3) which is possible with probability 1. Ten Berge transforms the random $3 \times 3 \times 5$ array to a simple form, which is also possible with probability 1. Therefore, it may happen that the implied array of an essentially unique solution (**A**,**B**,**C**) of the form (3), which has probability zero, cannot be transformed to the form Ten Berge starts from.

It may be noted that our analysis of the $3 \times 3 \times 5$ arrays of rank 5 can be readily adapted to the case where the five slices are *symmetric* matrices. Ten Berge et al. (2004) have shown that also symmetric $3 \times 3 \times 5$ arrays, when randomly sampled from a continuous distribution, have rank $\{5 \text{ or } 6\}$ with probability 1. They found that, when the symmetric $3 \times 3 \times 5$ array has rank 5, then there exist infinitely many CP solutions. Our proof above allows the same inference from a different perspective. That is, if we set $\mathbf{A} = \mathbf{B}$ in (3) a symmetric $3 \times 3 \times 5$ array of rank 5 is obtained. Again, we may consider vectors $\mathbf{w} = (\alpha\beta\gamma\delta\varepsilon)'$ for which the matrix **W** in (7) has rank 1. Hence, Eqs. (8)–(16) must hold. Since $\mathbf{A} = \mathbf{B}$, (8) is equivalent to (9), (10) is equivalent to (11) and (12) is equivalent to (13). Note that this implies that we cannot use (18); both numerator and denominator being zero. From (8)–(13) it follows that α, β and γ are completely determined by δ and ε. Next, use the fact that for any 3×3 matrix of rank 1 with nonzero elements and $\det(\mathbf{M}_{i,j}) = 0$ for all $i \neq j$, there holds $\det(\mathbf{M}_{i,i}) = 0$, $i = 1, 2, 3$. Hence, if (8)–(13) are satisfied and all elements of **W** are nonzero, then also (14)–(16) hold. In this way, it can be verified that there exist infinitely many pairs (δ, ε) that constitute a vector **w** for which **W** has rank 1 (excluding cases of probability zero). This shows that indeed infinitely many CP solutions exist in the symmetric case.

Example 2. $3 \times 4 \times 6$ arrays with $r = 6$

Here we present our second counterexample to the conjecture that Kruskal's condition (2) is necessary for essential uniqueness when the *k*-ranks of **A**, **B** and **C** equal their ranks. This example concerns $3 \times 4 \times 6$ arrays of rank $r = 6$. We adopt the same approach as in the previous section, i.e. we start with component matrices **A**, **B**, and**C** of order 3×6, 4×6, and 6×6, respectively, which are randomly sampled from a continuous distribution. The implied $3 \times 4 \times 6$ array will have rank 6 with probability 1. This can be seen as follows. Let $\mathbf{X}_i = \mathbf{C}\mathbf{A}_i\mathbf{B}'$ for $i = 1, 2, 3$, where $\mathbf{A}_i$ is the diagonal matrix containing the elements of the *i*th row of **A**. Then, with probability 1, the rank of $[\mathbf{X}_1|\mathbf{X}_2|\mathbf{X}_3]$ equals 6, which implies that the rank of the $3 \times 4 \times 6$ array is at least 6. However, since **A**, **B**, and **C** represent a decomposition in 6 components, the array is at most of rank 6. Therefore, the implied $3 \times 4 \times 6$ array has rank 6 with probability 1.

There will hold $k_A = \text{rank}(\mathbf{A}) = 3$, $k_B = \text{rank}(\mathbf{B}) = 4$ and $k_C = \text{rank}(\mathbf{C}) = 6$. This implies that Kruskal's condition (2) is not satisfied, since $k_A + k_B + k_C = 13$ and $2r + 2 = 14$. Next, we show that **A**, **B** and **C** are essentially unique with probability 1, thus establishing our second counterexample. Analogous to Example 1, the component matrices **A**, **B** and **C** may be transformed, with probability 1, into $\mathbf{C}=\mathbf{I}_6$ and

$$\mathbf{A}=\begin{bmatrix}1&0&0&1&x_1&y_1\\0&1&0&1&x_2&y_2\\0&0&1&1&x_3&y_3\end{bmatrix}\quad\text{and}\quad\mathbf{B}=\begin{bmatrix}1&0&0&0&1&z_1\\0&1&0&0&1&z_2\\0&0&1&0&1&z_3\\0&0&0&1&1&z_4\end{bmatrix},\tag{24}$$

where x_i, y_i and z_i are nonzero with probability 1. We have

$$(\mathbf{A}\bullet\mathbf{B})=\left[\begin{array}{cccccc}1&0&0&0&x_1&y_1z_1\\0&0&0&0&x_1&y_1z_2\\0&0&0&0&x_1&y_1z_3\\0&0&0&1&x_1&y_1z_4\\\hline 0&0&0&0&x_2&y_2z_1\\0&1&0&0&x_2&y_2z_2\\0&0&0&0&x_2&y_2z_3\\0&0&0&1&x_2&y_2z_4\\\hline 0&0&0&0&x_3&y_3z_1\\0&0&0&0&x_3&y_3z_2\\0&0&1&0&x_3&y_3z_3\\0&0&0&1&x_3&y_3z_4\end{array}\right],\tag{25}$$

which has full column rank with probability 1. For a general vector $\mathbf{w}=(\alpha\beta\gamma\delta\varepsilon\varphi)'$ the 3×4 matrix form of $(\mathbf{A}\bullet\mathbf{B})\mathbf{w}$ is

$$\begin{aligned}\mathbf{W}&=\mathbf{hg}'\\&=\begin{bmatrix}\alpha+x_1\varepsilon+y_1z_1\varphi & x_1\varepsilon+y_1z_2\varphi & x_1\varepsilon+y_1z_3\varphi & \delta+x_1\varepsilon+y_1z_4\varphi\\ x_2\varepsilon+y_2z_1\varphi & \beta+x_2\varepsilon+y_2z_2\varphi & x_2\varepsilon+y_2z_3\varphi & \delta+x_2\varepsilon+y_2z_4\varphi\\ x_3\varepsilon+y_3z_1\varphi & x_3\varepsilon+y_3z_2\varphi & \gamma+x_3\varepsilon+y_3z_3\varphi & \delta+x_3\varepsilon+y_3z_4\varphi\end{bmatrix}.\end{aligned}\tag{26}$$

Next we determine all solutions $(\alpha\beta\gamma\delta\varepsilon\varphi)'$ for which $\text{rank}(\mathbf{W})=1$. Suppose first that $\varphi=0$ and $\varepsilon\neq 0$. Then $\alpha=\beta=\gamma=0$. Moreover, since $x_i\neq x_j$ for $i\neq j$ with probability 1, also $\delta=0$. This yields the first solution $\mathbf{w}_1=(0\,0\,0\,0\,\varepsilon\,0)'$. Suppose next that $\varphi=0$ and $\varepsilon=0$. Then only one of α, β, γ, δ can be nonzero. This yields the four solutions $\mathbf{w}_2=(\alpha\,0\,0\,0\,0\,0)'$, $\mathbf{w}_3=(0\,\beta\,0\,0\,0\,0)'$, $\mathbf{w}_4=(0\,0\,\gamma\,0\,0\,0)'$ and $\mathbf{w}_5=(0\,0\,0\,\delta\,0\,0)'$. Now suppose that $\varphi\neq 0$ and $\varepsilon=0$. Then there must hold, with probability 1, that $\alpha=\beta=\gamma=\delta=0$. The sixth solution is thus $\mathbf{w}_6=(0\,0\,0\,0\,0\,\varphi)'$.The vectors $\mathbf{w}_i$ constitute a rescaled permutation matrix. Therefore, if no more solutions are possible we have shown that **A**, **B** and **C** in (24) are essentially unique with probability 1. Thus it remains to show that $\varphi\neq 0$ and $\varepsilon\neq 0$ yields a contradiction with probability 1.

The proof of this is as follows. Suppose that $\varphi\neq 0$ and $\varepsilon\neq 0$. Define $\tilde{w}_{ij}=x_i\varepsilon+y_iz_j\varphi$ for $i=1,2,3$ and $j=1,2,3,4$. Then

$$\mathbf{W}=\begin{bmatrix}\alpha+\tilde{w}_{11} & \tilde{w}_{12} & \tilde{w}_{13} & \delta+\tilde{w}_{14}\\ \tilde{w}_{21} & \beta+\tilde{w}_{22} & \tilde{w}_{23} & \delta+\tilde{w}_{24}\\ \tilde{w}_{31} & \tilde{w}_{32} & \gamma+\tilde{w}_{33} & \delta+\tilde{w}_{34}\end{bmatrix}.\tag{27}$$

Notice that no more than one $\tilde{w}_{ij}$ can be zero. Indeed, if $\tilde{w}_{ij} = \tilde{w}_{kl} = 0$ with $(i, j) \neq (k, l)$, then (with probability 1) we have a system of two linear independent and homogenous equations in ε and φ, which can only be solved by $\varepsilon = \varphi = 0$. This implies that no column of $\mathbf{W}$ equals $(0\,0\,0)'$ and no row of $\mathbf{W}$ equals $(0\,0\,0\,0)$. Together with the fact that $\text{rank}(\mathbf{W}) = 1$ this implies that we must have $\tilde{w}_{21} \neq 0$, $\tilde{w}_{31} \neq 0$, $\tilde{w}_{32} \neq 0$. Analogously, also $\tilde{w}_{12} \neq 0$, $\tilde{w}_{13} \neq 0$, $\tilde{w}_{23} \neq 0$. Moreover, there exist nonzero constants c_1 and c_2 such that row 1 of $\mathbf{W}$ equals c_1 times row 2 and row 2 equals c_2 times row 3. For each column of $\mathbf{W}$ this yields two equations. From the equations for columns 1 and 3 it follows that:

$$c_1 = \frac{\tilde{w}_{13}}{\tilde{w}_{23}} \quad \text{and} \quad c_2 = \frac{\tilde{w}_{21}}{\tilde{w}_{31}}, \tag{28}$$

$$\alpha = c_1 \tilde{w}_{21} - \tilde{w}_{11} \quad \text{and} \quad \gamma = \frac{\tilde{w}_{23}}{c_2} - \tilde{w}_{33}. \tag{29}$$

From the second column we obtain the following two equations for β

$$\beta = \frac{\tilde{w}_{12}}{c_1} - \tilde{w}_{22} \quad \text{and} \quad \beta = c_2 \tilde{w}_{32} - \tilde{w}_{22}. \tag{30}$$

Using (28), it can be seen that for (30) to hold we must have $\tilde{w}_{12}\tilde{w}_{23}\tilde{w}_{31} = \tilde{w}_{13}\tilde{w}_{21}\tilde{w}_{32}$. This expression is equivalent to

$$\frac{\varepsilon}{\varphi} = \frac{x_2 y_1 y_3 z_2 (z_3 - z_1) + x_3 y_1 y_2 z_3 (z_1 - z_2) + x_1 y_2 y_3 z_1 (z_2 - z_3)}{x_1 x_2 y_3 (z_1 - z_2) + x_1 x_3 y_2 (z_3 - z_1) + x_2 x_3 y_1 (z_2 - z_3)}. \tag{31}$$

Hence, by choosing α, β, γ, ε, φ as in (29)–(31) the matrix consisting of the first three columns of $\mathbf{W}$ will have rank 1.

Next, we show that adding the equations for the fourth column of $\mathbf{W}$ leads to a contradiction. From the fourth column we obtain the following two equations for δ:

$$(1 - c_1)\delta = c_1 \tilde{w}_{24} - \tilde{w}_{14} \quad \text{and} \quad (1 - c_2)\delta = c_2 \tilde{w}_{34} - \tilde{w}_{24}. \tag{32}$$

Both $c_1 = 1$ and $c_2 = 1$ would yield (with probability 1) a ratio ε/φ different from (31). Therefore, we may assume that $c_1 \neq 1$ and $c_2 \neq 1$. Using (28), it can be seen that (32) can only hold if

$$\tilde{w}_{14}\tilde{w}_{23}(\tilde{w}_{21} - \tilde{w}_{31}) + \tilde{w}_{24}(\tilde{w}_{23}\tilde{w}_{31} - \tilde{w}_{21}\tilde{w}_{13}) + \tilde{w}_{34}\tilde{w}_{21}(\tilde{w}_{13} - \tilde{w}_{23}) = 0. \tag{33}$$

We write $\varepsilon = d\varphi$, where the constant d is defined by the right-hand side of (31). Consequently, we may write $\tilde{w}_{ij} = e_{ij}\varphi$ where $e_{ij} = x_i d + y_i z_j$ are constants. In this notation (33) is equivalent to $\varphi^3 \tilde{e} = 0$, with

$$\tilde{e} = e_{14}e_{23}(e_{21} - e_{31}) + e_{24}(e_{23}e_{31} - e_{21}e_{13}) + e_{34}e_{21}(e_{13} - e_{23}). \tag{34}$$

By Fisher (1966) we have $\tilde{e} \neq 0$ with probability 1. Hence $\varphi = 0$ must hold, which contradicts the assumption of $\varphi \neq 0$. This shows that $\varphi \neq 0$ and $\varepsilon \neq 0$ cannot occur and completes the proof of our second counterexample.

4. Discussion

The examples of this paper refute the conjecture, stated in Ten Berge and Sidiropoulos (2002), that Kruskal's condition will be necessary and sufficient when ranks and k-ranks coincide, for $r > 4$. Two counterexamples have been given. Example 1, in which $r=5$, occurs with probability zero and Example 2, in which $r = 6$, occurs with probability 1. Since we have not found a counterexample for $r = 5$ which occurs with positive probability, it might still be true that the conjecture holds for $r = 5$ with probability 1. However, $4 \times 4 \times 3$ arrays of rank 5 invariably do seem to yield unique solutions in numerical experiments. These arrays represent cases where ranks and k-ranks coincide, for which Kruskal's condition is not met. Although we have no mathematical proof for uniqueness in these cases, it does seem safe to conclude that the conjecture by Ten Berge and Sidiropoulos (2002) is incorrect for $r = 5$ generically, and not just in cases which occur with probability zero.

References

Carroll, J.D., Chang, J.J., 1970. Analysis of individual differences in multidimensional scaling via an *n*-way generalization of Eckart–Young decomposition. Psychometrika 35, 283–319.

Fisher, F.M., 1966. The Identification Problem in Econometrics. McGraw-Hill, New York.

Harshman, R.L., 1970. Foundations of the Parafac procedure: models and conditions for an "explanatory" multimodal factor analysis. UCLA Work. Pap. Phonetics 16, 1–84.

Harshman, R.L., 1972. Determination and proof of minimum uniqueness conditions for Parafac-1. UCLA Work. Pap. Phonetics 22, 111–117.

Harshman, R.A., Lundy, M.E., 1984. The PARAFAC model for three-way factor analysis and multidimensional scaling. In: Law, H.G., Snyder, C.W., Hattie, J.A., McDonald, R.P. (Eds.), Research Methods for Multimode Data Analysis. Praeger, New York, pp. 122–215.

Jiang, T., Sidiropoulos, N.D., 2004. Kruskal's permutation lemma and the identification of Candecomp/Parafac and bilinear models with constant modulus constraints. IEEE Trans. Signal Process. 52, 2625–2636.

Kruskal, J.B., 1977. Three-way arrays: rank and uniqueness of trilinear decompositions, with applications to arithmetic complexity and statistics. Linear Algebra Appl. 18, 95–138.

Liu, X., Sidiropoulos, N.D., 2001. Cramer–Rao lower bounds for low-rank decomposition of multidimensional arrays. IEEE Trans. Signal Process. 49, 2074–2086.

Ten Berge, J.M.F., 2004. Partial uniqueness in Candecomp/Parafac. J. Chemometr. 18, 12–16.

Ten Berge, J.M.F., Sidiropoulos, N.D., 2002. On uniqueness in Candecomp/Parafac. Psychometrika 67, 399–409.

Ten Berge, J.M.F., Sidiropoulos, N.D., Rocci, R., 2004. Typical rank and Indscal dimensionality for symmetric three-way arrays of order $I \times 2 \times 2$ or $I \times 3 \times 3$. Linear Algebra Appl. 388, 363–377.