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ON UNIQUENESS IN CANDECOMP/PARAFAC

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One of the basic issues in the analysis of three-way arrays by CANDECOMP/PARAFAC (CP) has been the question of uniqueness of the decomposition. Kruskal (1977) has proved that uniqueness is guaranteed when the sum of the k-ranks of the three component matrices involved is at least twice the rank of the solution plus 2. Since then, little has been achieved that might further qualify Kruskal's sufficient condition. Attempts to prove that it is also necessary for uniqueness (except for rank 1 or 2) have failed, but counterexamples to necessity have not been detected. The present paper gives a method for generating the class of all solutions (or at least a subset of that class), given a CP solution that satisfies certain conditions. This offers the possibility to examine uniqueness for a great variety of specific CP solutions. It will be shown that Kruskal's condition is necessary and sufficient when the rank of the solution is three, but that uniqueness may hold even if the condition is not satisfied, when the rank is four or higher.

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

Let $\mathbf{X}$ be a three-way data array of order $I \times J \times K$, containing K frontal slices $\mathbf{X}_1, \ldots, \mathbf{X}_K$ of order $I \times J$. CANDECOMP/PARAFAC (CP), see Carroll and Chang (1970) and Harshman (1970), in R dimensions decomposes the slices as

$$\mathbf{X}_k = \mathbf{A}\mathbf{C}_k\mathbf{B}' + \mathbf{E}_k, \tag{1}$$

where $\mathbf{A}$ is an $I \times R$ matrix, $\mathbf{B}$ is a $J \times R$ matrix, $\mathbf{C}_k$ is a diagonal matrix, containing the elements of row k of a $K \times R$ matrix $\mathbf{C}$, $k = 1, \ldots K$, and $\mathbf{E}_k$ is a matrix of residuals. The decomposition is fully symmetric in $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$. That is, they may switch places in (1) if we switch the modes of the array and residual array accordingly.

Suppose there exists an alternative solution of the form

$$\mathbf{X}_k = \mathbf{G}\mathbf{D}_k\mathbf{H}' + \mathbf{E}_k \tag{2}$$

with $\mathbf{G}$ and $\mathbf{H}$ of the same order as $\mathbf{A}$ and $\mathbf{B}$, respectively, and $\mathbf{D}_k$ diagonal, containing the elements of row k of a $K \times R$ matrix $\mathbf{D}$, $k = 1, \ldots, K$. A solution for CP is said to be *unique* when, for every other solution of the form (2), $\mathbf{G} = \mathbf{A}\Pi\mathbf{\Lambda}_1$, $\mathbf{H} = \mathbf{B}\Pi\mathbf{\Lambda}_2$, and $\mathbf{D} = \mathbf{C}\Pi\mathbf{\Lambda}_3$, for some permutation matrix Π and diagonal matrices $\mathbf{\Lambda}_1$, $\mathbf{\Lambda}_2$, and $\mathbf{\Lambda}_3$, with $\mathbf{\Lambda}_1\mathbf{\Lambda}_2\mathbf{\Lambda}_3 = \mathbf{I}_R$. It is obvious that the residuals play no role at all, in the present context. They will be ignored in the sequel. As a matter of convenience, we shall consider them to vanish, which means that $\mathbf{X}_k$ does not denote a slice of the original array, but merely the CP fitted part of it.

This paper is concerned with conditions for uniqueness of CP decompositions. Kruskal (1977) has shown that uniqueness holds under relatively mild conditions, to be discussed shortly. These conditions are necessary and sufficient for uniqueness when $R = 2$, but they are not necessary when $R = 1$. It has long been conjectured that these conditions are generally necessary

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and sufficient for $R > 1$. This paper will prove that Kruskal's condition is indeed necessary and sufficient for $R = 2$ and $R = 3$, but not for $R > 3$. We start with a review of the available conditions.

Previous Results on Uniqueness

The simplest case of nonuniqueness arises when **A** or **B** or **C** has two proportional columns. For instance, let $R = 2$, and $\mathbf{C} = [\mathbf{c}|\lambda\mathbf{c}]$, for some scalar λ and some vector $\mathbf{c} = [c_1, \ldots, c_K]'$. Then $\mathbf{X}_k = \mathbf{AC}_k\mathbf{B}' = c_k\mathbf{a}_1\mathbf{b}_1' + \lambda c_k\mathbf{a}_2\mathbf{b}_2' = c_k[\mathbf{a}_1|\lambda\mathbf{a}_2]\mathbf{B}' = c_k[\mathbf{a}_1|\lambda\mathbf{a}_2]\mathbf{TT}^{-1}\mathbf{B}'$, for any nonsingular **T**. If we choose **T** other than the product of a diagonal and a permutation matrix, alternative solutions, with $[\mathbf{a}_1|\lambda\mathbf{a}_2]\mathbf{T}$ instead of **A**, become readily available. This argument can be extended to the case $R > 2$: Whenever two columns of **C** are proportional, the corresponding columns of **A** and **B** can be mixed without loss of fit. In general, it is necessary for uniqueness that neither **A**, nor **B**, nor **C** has a pair of proportional columns (Krijnen, 1993, p. 28).

Another necessary condition for uniqueness is due to Liu and Sidiropoulos (2001). Let **X** be the matrix having $\text{Vec}(\mathbf{X}_k)$ as its k-th column, $k = 1, \ldots, K$. Then the expression (1), again dropping $\mathbf{E}_k$, can be written equivalently as

$$\mathbf{X} = (\mathbf{A} \bullet \mathbf{B})\mathbf{C}', \tag{3}$$

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 nonzero vector **n** orthogonal to the rows of $\mathbf{A} \bullet \mathbf{B}$. Adding **n** to any column of $\mathbf{C}'$ preserves (3), but produces a different solution for **C**. It follows that full column rank for $\mathbf{A} \bullet \mathbf{B}$ (and $\mathbf{A} \bullet \mathbf{C}$ and $\mathbf{B} \bullet \mathbf{C}$) is necessary for uniqueness.

Kruskal (1977) has proposed a sufficient condition for uniqueness which relies on the following definition:

Definition 1. The k-rank of a matrix is the largest value of k such that every subset of k columns of the matrix is linearly independent.

Note that the k-rank is 1 if there is a pair of proportional columns in a matrix. Kruskal has proven that the condition $k_A + k_B + k_C \geq 2R + 2$ is sufficient for uniqueness in CP, where k_A is the k-rank of **A**, and so on. Sidiropoulos and Bro (2000) have generalized this sufficient condition to N-way arrays. Harshman (1972) has shown that it is sufficient for uniqueness to have **A** and **B** of full column rank, and **C** of k-rank 2 or higher. To be precise, Harshman considered the case where at least one of the diagonal matrices $\mathbf{C}_k$ in (1), (or a linear combination thereof), $\mathbf{C}_1$, say, is nonsingular and, in addition, there is another diagonal matrix $\mathbf{C}_2$ such that $\mathbf{C}_1^{-1}\mathbf{C}_2$ has all diagonal elements distinct. This is equivalent to the case where the k-rank of **C** is greater than 1.

When $R = 2$, Harshman's conditions are equivalent to Kruskal's condition (and, in fact, necessary and sufficient for uniqueness). For $R = 1$, Kruskal's condition is never met even when Harshman's are (Kruskal did provide a separate necessary and sufficient condition for $R = 1$). For $R > 2$, Kruskal's condition may be satisfied even when Harshman's are not.

It has been conjectured (Kruskal, 1989, Conjecture 4a) that Kruskal's condition is generally necessary and sufficient for uniqueness when $R > 1$, but a proof has never been given (except for $R = 2$) nor has a counterexample been produced. In the present paper, a method is proposed to generate, for any given CP solution (1) with specified ranks and k-ranks, the class of alternative solutions (2), or at least part of that class. As soon as an alternative solution has been found, different from the original one, nonuniqueness has been established. However, whenever the class of alternative solutions is proven empty, we have proven uniqueness for the case under consideration. This approach will be used to show that Kruskal's sufficient condition is indeed necessary and sufficient for uniqueness when $R = 3$, but not necessary when $R > 3$. First, preliminary simplifications of CP solutions will be discussed.

Simplifying a CP Solution

It is clear that any two matrices **A** and **G** have proportional columns, up to a permutation, if and only if **SA** and **SG** have proportional columns up to the same permutation, for every nonsingular matrix **S**. It is also clear that, for $k = 1, \ldots, K$,

$$\mathbf{AC}_k\mathbf{B}' = \mathbf{GD}_k\mathbf{H}' \Leftrightarrow \mathbf{SAC}_k\mathbf{B}' = \mathbf{SGD}_k\mathbf{H}'$$

for any nonsingular **S**. Using the symmetry of the CP decomposition to apply the same principle to **B** and **C**, it follows that a decomposition based on **A**, **B**, and **C** is identical (up to permutation and scale) to one based on **G**, **H**, and **D**, if and only if the decomposition based on **SA**, **TB**, and **UC** is identical (up to permutation and scale) to the one based on **SG**, **TH**, and **UD**, for arbitrary nonsingular matrices **S**, **T**, and **U**. That is, premultiplying the matrices **A**, **B**, or **C** of any CP solution by nonsingular matrices in no way changes the uniqueness properties of that solution. In addition, it affects neither the rank nor the k-rank of the matrices involved. Because such transformations greatly simplify the manipulation of ranks and k-ranks of **A**, **B**, and **C**, we shall use them throughout.

Firstly, when **A**, say, is an $I \times R$ matrix of rank R_A, the singular value decomposition of **A** yields a nonsingular **S** such that **SA** has all rows zero except the first R_A. Next, removing these zero rows from **SA**, and the corresponding zero slices from the array, does not affect the uniqueness properties of the decomposition. Specifically, when the reduced array has a non-unique CP decomposition, then so does the full array, because restoring the zero rows in **SA** and the zero slices in the array does not impose any further constraints on **B** and **C**. Conversely, when the reduced array does have a unique CP decomposition, the Khatri-Rao product $\mathbf{B} \bullet \mathbf{C}$ is of full column rank (the Liu & Sidiropoulos condition, explained above) which implies that it has no zero linear combinations of columns (the removed slices of the array) unless when zero weights are used (the removed rows of **SA**), thus uniquely restoring the removed rows of **SA**.

After transforming **A** and/or **B**, and/or **C** to reduced versions of full row rank, we may further simplify them. Take any nonsingular $R_A \times R_A$ submatrix of the reduced version of **A**, and premultiply the latter by the inverse of that submatrix. We end up with an identity submatrix form, for instance,

$$\mathbf{A} = \left[\begin{array}{ccc|c} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{array}\right].$$

This matrix has k-rank 2 because column 4 is a linear combination of columns 1 and 3 (the zero element in the fourth column reveals this at once). Note that this k-rank is also the k-rank of the original version of **A**, because neither premultiplying a matrix by a nonsingular matrix, nor removing zero rows, has an impact on the k-rank. We are now ready to show that Kruskal's condition is indeed necessary when $R = 3$.

Necessity of Kruskal's Condition for $R = 3$

For $R = 3$, Kruskal's sufficient condition for uniqueness reads $k_A + k_B + k_C \geq 8$. To prove necessity, we shall consider all possible cases where this condition is not met, and show, for each case, that alternative solutions exist. The specific cases to be considered are

a. when the k-rank of **A**, **B**, or **C** is less than 2,
b. when the k-ranks of **A**, **B**, and **C** are (2,2,2), and
c. when the k-ranks of **A**, **B**, and **C** are (2,2,3), (2,3,2) or (3,2,2).

Case a. When one of the three component matrices have k-rank 1, nonuniqueness is immediate, as has been explained above.

Case b. Let $k_A = k_B = k_C = 2$. Because $R = 3$, the ranks are also 2 (They cannot be 3 because a matrix of full column rank is also of full k-rank). Hence, without loss of generality, we may pretransform the array in two directions to have

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & a_1 \\ 0 & 1 & a_2 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 1 & 0 & b_1 \\ 0 & 1 & b_2 \end{bmatrix}, \tag{4}$$

with a_1, a_2, b_1, and b_2 nonzero because the k-ranks are 2. We consider the CP solution in the form $\mathbf{X} = (\mathbf{A} \bullet \mathbf{B})\mathbf{C}'$, see (3), and examine whether or not $\mathbf{A} \bullet \mathbf{B}$ is the only Khatri-Rao product which generates the columns of $\mathbf{X}$ as linear combinations. Noting that

$$\mathbf{A} \bullet \mathbf{B} = \begin{bmatrix} 1 & 0 & a_1b_1 \\ 0 & 0 & a_1b_2 \\ 0 & 0 & a_2b_1 \\ 0 & 1 & a_2b_2 \end{bmatrix}, \tag{5}$$

it can be seen that, in the third column of $\mathbf{A} \bullet \mathbf{B}$, the first and the last element do not have any impact on the column space. Hence, we can change them, as long as we maintain the Khatri-Rao form. Specifically, we can replace the third column by

$$\mathbf{g} \bullet \mathbf{h} = \begin{bmatrix} x \\ a_1b_2 \\ a_2b_1 \\ y \end{bmatrix} \tag{6}$$

where x is arbitrary (but nonzero), and y is the value that produces a $\mathbf{g} \bullet \mathbf{h}$ in Khatri-Rao form. Equivalently, because $\text{Vec}(\mathbf{hg}') = \mathbf{g} \bullet \mathbf{h}$, y has to yield a determinant zero for the matrix

$$\mathbf{gh}' = \begin{bmatrix} x & a_1b_2 \\ a_2b_1 & y \end{bmatrix}. \tag{7}$$

That is, $y = a_1a_2b_1b_2/x$. We then have $\mathbf{g} = [1 \;\; a_2b_1/x]'$ and $\mathbf{h} = [x \;\; a_1b_2]'$ to replace the third columns of $\mathbf{A}$ and $\mathbf{B}$, respectively. Any nonzero choice for x other than $x = a_1b_1$ will render $\mathbf{g}$ nonproportional to the vector $[a_1 \;\; a_2]'$, implying a different solution from the one we started with. We have thus found a new basis $\mathbf{G} \bullet \mathbf{H}$ for the column space of $\mathbf{A} \bullet \mathbf{B}$. If a complete alternative solution is desired, it remains to find $\mathbf{D}$ such that $(\mathbf{G} \bullet \mathbf{H})\mathbf{D}' = (\mathbf{A} \bullet \mathbf{B})\mathbf{C}'$. This is an elementary matrix problem.

Case c. Although we have three different k-rank distributions to consider, it suffices to consider any one of these three. The symmetry of the CP solution, discussed below (1), guarantees that the other two distributions are equivalent, as far as uniqueness is concerned, to the first. We shall pick the distribution with $k_A = k_B = 2$, and $k_C = 3$. Although $\mathbf{C}$ now has rank and k-rank 3, the rank and k-rank of both $\mathbf{A}$ and $\mathbf{B}$ remain unchanged compared with Case b, and the same alternative solution for $\mathbf{g}$ and $\mathbf{h}$ as was found in (7) can be used to construct an alternative CP solution.

Having shown nonuniqueness in all possible cases of $k_A + k_B + k_C < 8$, it can be concluded that Kruskal's condition is indeed necessary and sufficient for R =3.The next issue to address is the case $R = 4$. Here it will be shown that Kruskal's condition is no longer necessary.

The Case $R = 4$, When Kruskal's Condition Is Not Met

When $R = 4$, it becomes possible to have matrices of k-rank 2, that have a rank greater than 2. This offers the possibility of constructing arrays where the CP solution has k-ranks 2, 2, and 4, while the ranks are 3, 3, and 4. In fact, this allows us to create cases where uniqueness holds in spite of failure to satisfy Kruskal's sufficient condition. First, we consider a case where the preliminary simplifying transformations yield a zero element in the last column of **A** in a different place than for **B**. That is, suppose we have

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & a_1 \\ 0 & 1 & 0 & a_2 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 1 & 0 & 0 & b_1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & b_3 \end{bmatrix}, \tag{8}$$

with a_1, a_2, b_1, and b_3 nonzero, and $\mathbf{C} = \mathbf{I}_4$. The k-rank of both **A** and **B** is 2, as can be seen from the zero elements in the last columns, $\mathbf{A} \bullet \mathbf{B}$ has full column rank (see (9)), and **C** has k-rank 4. Let there be another CP solution, so $\mathbf{AC}_k\mathbf{B}' = \mathbf{GD}_k\mathbf{H}'$, $k = 1, \ldots, 4$. It will be shown that the columns of **A** are essentially those of **G**, and so on.

In Khatri-Rao notation, we have $(\mathbf{A} \bullet \mathbf{B}) = (\mathbf{G} \bullet \mathbf{H})\mathbf{D}'$, with **D** nonsingular, so $\mathbf{A} \bullet \mathbf{B}$ and $\mathbf{G} \bullet \mathbf{H}$ span the same spaces. Hence, every column of $\mathbf{G} \bullet \mathbf{H}$ must be a linear combination of the columns of $\mathbf{A} \bullet \mathbf{B}$. Accordingly, we consider all solutions to the equation $(\mathbf{A} \bullet \mathbf{B})\mathbf{w} = \mathbf{g} \bullet \mathbf{h}$. Because

$$\mathbf{A} \bullet \mathbf{B} = \begin{bmatrix} 1 & 0 & 0 & a_1b_1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a_1b_3 \\ \hline 0 & 0 & 0 & a_2b_1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & a_2b_3 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \tag{9}$$

these solutions are, written as a matrix, of the general form

$$\mathbf{gh}' = \begin{bmatrix} w_1 + w_4a_1b_1 & 0 & w_4a_1b_3 \\ w_4a_2b_1 & w_2 & w_4a_2b_3 \\ 0 & 0 & w_3 \end{bmatrix}. \tag{10}$$

The question is how $\mathbf{w} = [w_1\, w_2\, w_3\, w_4]'$ can be chosen to have $\mathbf{gh}'$ of rank one. Clearly, if $w_4 = 0$, only single diagonal elements of $\mathbf{gh}'$ can be nonzero, which retrieves the first three columns of **A** and **B**. If w_4 is nonzero, w_2 and w_3 must be zero, and w_1 must render a determinant zero for the 2×2 submatrix of $\mathbf{gh}'$ that is left upon deleting row 3 and column 2. It appears that w_1 must be zero also, which retrieves the fourth columns of **A** and **B**, respectively. It follows that the solution we had is the only possible solution, whence uniqueness for **A** and **B** has been proven. Clearly, **D** can only be a rescaled permutation matrix, which establishes uniqueness for **C** also.

It can be concluded that, in the case under consideration, Kruskal's sufficient condition is not necessary for uniqueness. In general, for $R > 3$, it is not necessary. This can be explained as follows: When we start with matrices **A**, **B** and **C**, with ranks equal to k-ranks, and $k_A + k_B + k_C < 2R + 2$, we can append $R - k_A - 1$ rows to **A**, say, and to the corresponding frontal slices of the array, in such a way that we *increase the rank of* **A** *without changing its k-rank.* Adding slices this way makes the number of constraints increase faster than the number of free parameters. This should, at some point, enforce uniqueness, without affecting the k-ranks. Indeed, this is what happens. It explains why having $k_A + k_B + k_C \geq 2R + 2$ is sufficient, but not necessary for uniqueness, when $R > 3$. In the final section of this paper, further support to this explanation will be offered.

From the example in (8), it may be tempting to infer that necessary and sufficient conditions for uniqueness might be derived from assumptions on rank and k-rank jointly. However, it is even more complicated than that. Consider what happens if we change (8) to have the zero elements in column 4 of **A** and **B** in the same place. For instance, we may take the element (3,4) zero in both matrices. Then we can again find all possible alternative solutions. We have

$$\mathbf{A} \bullet \mathbf{B} = \begin{bmatrix} 1 & 0 & 0 & a_1b_1 \\ 0 & 0 & 0 & a_1b_2 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & a_2b_1 \\ 0 & 1 & 0 & a_2b_2 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{11}$$

All possible vectors $(\mathbf{A} \bullet \mathbf{B})\mathbf{w} = \mathbf{g} \bullet \mathbf{h}$, written as a matrix, are now of the form

$$\mathbf{gh}' = \begin{bmatrix} w_1 + w_4a_1b_1 & w_4a_1b_2 & 0 \\ w_4a_2b_1 & w_2 + w_4a_2b_2 & 0 \\ 0 & 0 & w_3 \end{bmatrix}. \tag{12}$$

When we set $w_1 = w_2 = w_3 = 0$, we retrieve the fourth columns of **A** and **B**. However, this time, alternative solutions do exist: Upon taking any w_1 and w_4 with w_1, w_4, and $w_1 + w_4a_1b_1$ nonzero, and $w_3 = 0$, we still have w_2 to get a zero determinant for the upper left 2×2 submatrix of $\mathbf{gh}'$. Hence, an infinite number of alternative solutions exist. We thus have nonuniqueness in a case with k-ranks 2, 2, and 4, and ranks 3, 3, 4, due to the fact that the nonzero elements in the fourth columns of **A** and **B** now occur in exactly the same place.

Necessity of Kruskal's Condition for $R = 4$ When Ranks are k-Ranks

The counterexample to necessity of Kruskal's condition, given in the previous section, seems to capitalize on the possibility that k-ranks can be smaller than ranks. If this explanation is valid, then, assuming that ranks and k-ranks coincide, we should have that Kruskal's condition is necessary and sufficient for uniqueness. To investigate this conjecture, we examine the $R = 4$ case in greater detail, when all cases with k-ranks less than ranks are excluded. It will be proven that Kruskal's condition is indeed necessary and sufficient for uniqueness in this special case. Specifically, we show how to construct alternative solutions when $k_A + k_B + k_C < 10$, and $k_A = \text{rank}(\mathbf{A})$, $k_B = \text{rank}(\mathbf{B})$, and $k_C = \text{rank}(\mathbf{C})$. The following cases need to be treated:

a. when one of the matrices has rank less than 2,
b. when two matrices have rank 2, and the third has at least rank 2,
c. when one matrix has rank 2, one has rank 3, and the third has rank 3 or 4,
d. when all ranks are 3.

Case a. We can discard this case at once, as has been explained above.

Case b. When two ranks are 2, we can, without loss of generality, take **A** and **B** to have rank 2. They can be brought in the form

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & a_{13} & a_{14} \\ 0 & 1 & a_{23} & a_{24} \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 1 & 0 & b_{13} & b_{14} \\ 0 & 1 & b_{23} & b_{24} \end{bmatrix}, \tag{13}$$

whence

$$\mathbf{A} \bullet \mathbf{B} = \begin{bmatrix} 1 & 0 & a_{13}b_{13} & a_{14}b_{14} \\ 0 & 0 & a_{13}b_{23} & a_{14}b_{24} \\ 0 & 0 & a_{23}b_{13} & a_{24}b_{14} \\ 0 & 1 & a_{23}b_{23} & a_{24}b_{24} \end{bmatrix}. \tag{14}$$

Note that all elements in columns 3 and 4 are nonzero because the ranks are also k-ranks, and that these two columns are not proportional.

Again, like in (5), the column space of $\mathbf{A}\bullet\mathbf{B}$ is insensitive to changing the elements (1,3) and (4,3), or (1,4) and (4,4). They can be replaced by arbitrary elements preserving the Khatri-Rao form. That is, as long as the product of (1,3) and (4,3) remains equal to $a_{13}a_{23}b_{13}b_{23}$, and that of (1,4) and (4,4) remains equal to $a_{14}a_{24}b_{14}b_{24}$, the column space of $\mathbf{A} \bullet \mathbf{B}$ is left unchanged, and alternative solutions arise in the same column space.

Case c. When one rank is 2, and another is 3, we can bring **A** and **B** in the form

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & a_{13} & a_{14} \\ 0 & 1 & a_{23} & a_{24} \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 1 & 0 & 0 & b_1 \\ 0 & 1 & 0 & b_2 \\ 0 & 0 & 1 & b_3 \end{bmatrix}, \tag{15}$$

with

$$\mathbf{A} \bullet \mathbf{B} = \left[\begin{array}{cccc} 1 & 0 & 0 & a_{14}b_1 \\ 0 & 0 & 0 & a_{14}b_2 \\ 0 & 0 & a_{13} & a_{14}b_3 \\ \hline 0 & 0 & 0 & a_{24}b_1 \\ 0 & 1 & 0 & a_{24}b_2 \\ 0 & 0 & a_{23} & a_{24}b_3 \end{array}\right]. \tag{16}$$

All possible vectors $(\mathbf{A} \bullet \mathbf{B})\mathbf{w} = \mathbf{g} \bullet \mathbf{h}$, written as a matrix, are now of the form

$$\mathbf{gh}' = \begin{bmatrix} w_1 + w_4a_{14}b_1 & w_4a_{14}b_2 & w_3a_{13} + w_4a_{14}b_3 \\ w_4a_{24}b_1 & w_2 + w_4a_{24}b_2 & w_3a_{23} + w_4a_{24}b_3 \end{bmatrix}.$$

Setting only w_1, w_2, w_3, or w_4 nonzero retrieves the four rank-one matrices associated with the columns of $\mathbf{A} \bullet \mathbf{B}$. To find a different rank one matrix, take any nonzero w_3 and w_4 such that $w_3a_{13} + w_4a_{14}b_3$ and $w_3a_{23} + w_4a_{24}b_3$, respectively, are nonzero. This fixes the third column of $\mathbf{gh}'$. Then pick w_1 to get the first column of $\mathbf{gh}'$ proportional to the third column, and w_2 to get the second column proportional to the third. The resulting rank-one matrix $\mathbf{gh}'$ can be used to replace columns 4 of **A** and **B** by **g** and **h**, respectively, which shows nonuniqueness.

Case d. The last case to be dealt with is the case 3-3-3. This case cannot be solved as the previous cases, by finding a different Khatri-Rao basis in the column space of $\mathbf{A} \bullet \mathbf{B}$. To see this, suppose that we add one slice to the array, to have the 3-3-4 case, with **C** nonsingular. Then we would have uniqueness. Uniqueness implies that there cannot be another Khatri-Rao basis for the column space of $\mathbf{A} \bullet \mathbf{B}$. It follows that, to construct alternative solutions for the 3-3-3 case, we shall have to find them outside the column space of $\mathbf{A} \bullet \mathbf{B}$. This can be done by manipulating the coefficients of a certain quartic equation to the effect that it has four distinct real roots. The details of this problem are explained in the appendix. We conclude that Kruskal's condition is necessary and sufficient for uniqueness when $R = 4$, and ranks are equal to k-ranks.

Discussion

The approach of finding alternative solutions for any given CP solution has proven useful for the study of uniqueness. Twenty-five years after Kruskal' seminal paper, it has become clear that Kruskal's sufficient condition for uniqueness is necessary when $R = 3$, but not when $R > 3$. The reason is that, when $R > 3$, the possibility arises that **A**, **B**, and **C**, while having k-ranks 2 or more, have larger ranks than k-ranks. Indeed, when $R = 4$, and the k-ranks are equal to the ranks, Kruskal's condition is necessary and sufficient.

It has also been shown that, in cases of small k-rank, the particular pattern of zeros, after pretransformations to have identity submatrices in **A**, **B**, and **C**, may have a decisive impact on uniqueness. This implies that attempts to derive necessary and sufficient conditions for uniqueness are doomed to fail unless they take that very pattern into account.

Paatero (1999) has suggested a *numerical* method for assessing *local* uniqueness of a given CP decomposition, by evaluating the Jacobian of the model in (1) and counting zero singular values. The approach developed above assesses *global* uniqueness, and it is *analytical*: It proves or disproves uniqueness for a class of models obeying certain rank conditions.

Appendix

Constructing Alternative CP Solutions When Ranks and k-Ranks Are 3, and $R = 4$

Without loss of generality, we first transform the problem to one where **A**, **B**, and **C** have $\mathbf{I}_3$ in their first three columns and a fourth column **a**, **b**, **c** without zero elements. Next, premultiply the new **A**, **B**, and **C** by the inverses of diag(**a**), diag(**b**), and diag(**c**), respectively. This keeps diagonal matrices in the first three columns, but transforms the fourth columns to $[1\ 1\ 1]'$. Finally, 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**. We thus start from

$$\mathbf{A} = \mathbf{B} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \quad \text{and} \quad \mathbf{C} = \begin{bmatrix} x & 0 & 0 & 1 \\ 0 & y & 0 & 1 \\ 0 & 0 & z & 1 \end{bmatrix}, \tag{A1}$$

for certain nonzero constants x, y, and z. As a result of the transformations, the three frontal slices of the array have become symmetric. They can be further simplified by subtracting row 3 of **C** from row 1 and from row 2. It follows that the slices of the transformed array are now of the form

$$\mathbf{X}_1 = \begin{bmatrix} x & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -z \end{bmatrix}, \quad \mathbf{X}_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & y & 0 \\ 0 & 0 & -z \end{bmatrix}, \quad \text{and} \quad \mathbf{X}_3 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & z+1 \end{bmatrix} \tag{A2}$$

with x, y, and z nonzero. Because all transformations used are nonsingular, they do not affect (non)uniqueness. We shall now examine how an alternative solution $\{\mathbf{G}, \mathbf{H}, \mathbf{D}\}$ can be found.

Although there is no necessity to impose that $\mathbf{G} = \mathbf{H}$, CP fitting invariably seems to yield such solutions for data as given in (A2). Accordingly, we shall also derive alternative solutions $\{\mathbf{G}, \mathbf{H}, \mathbf{D}\}$ subject to the constraint $\mathbf{G} = \mathbf{H}$, and with row 1 rescaled to $[1\ 1\ 1\ 1]$. The latter constraint means that the first row of **G** has no zero elements. Hence, if such a solution can be found, it differs from **A** in (A1). Let the notation be

$$\mathbf{G} = \mathbf{H} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ b_1 & b_2 & b_3 & b_4 \\ c_1 & c_2 & c_3 & c_4 \end{bmatrix}, \tag{A3}$$

and $\mathbf{D}' = [\mathbf{u}|\mathbf{v}|\mathbf{w}]$, of order 4×3. We want to solve $(\mathbf{G} \bullet \mathbf{G})\mathbf{D}' = \mathbf{X}_{93}$, with $\mathbf{X}_{93}$ (the vectorized data) defined as

$$\mathbf{X}_{93} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \\ \mathbf{X}_3 \end{bmatrix}, \tag{A4}$$

see (A2), for arbitrary fixed nonzero constants x, y, and z. Remove the three redundant equations, and rearrange the remaining rows of $\mathbf{G} \bullet \mathbf{G}$ and $\mathbf{X}_{93}$ into matrices

$$\mathbf{G}_6 = \begin{bmatrix} b_1 & b_2 & b_3 & b_4 \\ c_1 & c_2 & c_3 & c_4 \\ b_1c_1 & b_2c_2 & b_3c_3 & b_4c_4 \\ \hline 1 & 1 & 1 & 1 \\ b_1^2 & b_2^2 & b_3^2 & b_4^2 \\ c_1^2 & c_2^2 & c_3^2 & c_4^2 \end{bmatrix} \quad \text{and} \quad \mathbf{X}_6 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ \hline x & 0 & 1 \\ 0 & y & 1 \\ -z & -z & z+1 \end{bmatrix}. \tag{A5}$$

Note that solving $(\mathbf{G} \bullet \mathbf{G})\mathbf{D}' = \mathbf{X}_{93}$ is equivalent to solving $\mathbf{G}_6\mathbf{D}' = \mathbf{X}_6$.

Because the first two columns of $\mathbf{X}_6$ are nonproportional, so are $\mathbf{u}$ and $\mathbf{v}$. Hence, the first three rows of $\mathbf{G}_6$, being orthogonal to $\mathbf{u}$ and $\mathbf{v}$, are linearly dependent. This means that they satisfy, for some λ and δ, $b_ic_i = \lambda b_i + \delta c_i$, $i = 1, \ldots, 4$. Because, in $\mathbf{X}_6$, row 3 must then equal λ times row 1 plus δ times row 2, we must have $\lambda + \delta = 1$. Hence, $b_ic_i = \lambda b_i + (1-\lambda)c_i$. This expression implies that

$$c_i(b_i + \lambda - 1) = \lambda b_i. \tag{A6}$$

When $b_i \neq 1 - \lambda$, we can write c_i explicitly as

$$c_i = \frac{\lambda b_i}{b_i + \lambda - 1} \tag{A7}$$

for some scalar λ. Although this implies loss of generality, we shall set $\lambda = 2$. As will become clear later, this choice still allows solving $\mathbf{G}_6\mathbf{D}' = \mathbf{X}_6$. Note that, as a result of (A7), $\mathbf{G}_6$ is fully determined by the elements of its first row.

Because of the linear dependency implied by (A6), we can remove the third rows of $\mathbf{G}_6$ and $\mathbf{X}_6$, and continue with solving $\mathbf{G}_5\mathbf{D}' = \mathbf{X}_5$, with

$$\mathbf{G}_5 = \begin{bmatrix} b_1 & b_2 & b_3 & b_4 \\ c_1 & c_2 & c_3 & c_4 \\ 1 & 1 & 1 & 1 \\ b_1^2 & b_2^2 & b_3^2 & b_4^2 \\ c_1^2 & c_2^2 & c_3^2 & c_4^2 \end{bmatrix} \quad \text{and} \quad \mathbf{X}_5 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ x & 0 & 1 \\ 0 & y & 1 \\ -z & -z & 1+z \end{bmatrix}. \tag{A8}$$

We shall now see under what choice of b_1, b_2, b_3, and b_4 $\mathbf{X}_5$ is in the column-space of $\mathbf{G}_5$. Note that the orthogonal complement space of $\mathbf{X}_5$ is spanned by vectors of the form

$$\mathbf{n} = \begin{bmatrix} -.5w + \alpha \\ -.5w - \alpha \\ yz \\ xz \\ xy \end{bmatrix} \tag{A9}$$

where $w = xy + xz + yz + xyz$, and α is a free scalar. If we take the four columns of $\mathbf{G}_5$ orthogonal to $\mathbf{n}$ and linearly independent, then they span the same column space as $\mathbf{X}_5$ and a solution for $\mathbf{G}_5\mathbf{D}' = \mathbf{X}_5$ exists. Any column of $\mathbf{G}_5$ (ignoring the subscript), using $\lambda = 2$, can be written as $[b \quad 2b/(b+1) \quad 1 \quad b^2 \quad 4b^2/(b+1)^2]'$, which is proportional to

$$\mathbf{g} = [b(b+1)^2 \quad 2b(b+1) \quad (b+1)^2 \quad b^2(b+1)^2 \quad 4b^2]'. \tag{A10}$$

Asking that, for arbitrary but fixed α, each column of $\mathbf{G}_5$ be orthogonal to $\mathbf{n}$ of (A9) amounts to asking that each column satisfy $\mathbf{n}'\mathbf{g} = 0$. We then seek four real valued roots to the quartic equation $\mathbf{n}'\mathbf{g} = c_4b^4 + c_3b^3 + c_2b^2 + c_1b + c_0 = 0$, with coefficients

$$\begin{aligned} c_4 &= xz \\ c_3 &= -.5w + \alpha + 2xz \\ c_2 &= -2w + xz + 4xy + yz \\ c_1 &= -1.5w - \alpha + 2yz \\ c_0 &= yz. \end{aligned} \tag{A11}$$

Upon dividing all coefficients by α, it can be seen that, when α tends to infinity, three roots of the polynomial tend to the roots of

$$(b^3 - b) = 0, \tag{A12}$$

which has roots 1, -1 and 0. Therefore, by taking α sufficiently large, three roots b_1, b_2, and b_3 of the polynomial will tend to 1, -1, and 0, respectively. The fourth root is implied by the well known relationship

$$-c_3/c_4 = (.5w - \alpha - 2xz)/xz = b_1 + b_2 + b_3 + b_4. \tag{A13}$$

The right hand side tends to b_4 as α tends to infinity, whence b_4 will tend to plus or minus infinity, depending on the sign of xz. Because no pair of these roots tend to equality, it follows that four distinct nonzero real roots can indeed be obtained by picking α large enough (a proof for this, suggested by Tom Snijders, is available on request). These roots can be used to fill the second row of a solution for **G**, see (A3). The third row follows at once from (A7), with $\lambda = 2$. The implied columns of $\mathbf{G}_5$ are orthogonal to $\mathbf{n}$. In addition, they are linearly independent. Specifically, by elementary row operations, the four columns of $\mathbf{G}_5$ can be transformed to the form $[1 \quad b_i \quad b_i^2 \quad b_i^3 \quad b_i^4]'$, $i = 1, 2, 3, 4$. The first four rows of the transformed matrix define a Vandermonde matrix, which is nonsingular because the four roots are distinct.

An example may be instructive. Let (A1) be given with $x = 1$, $y = 2$, $z = 9$, so $w = 47$. Solving $\mathbf{n}'\mathbf{g} = 0$ can be done by the Matlab command roots ([9 $\quad \alpha - 5.5 \quad -59 \quad -\alpha - 34.5$ 18]). When $\alpha = 0$, the roots are 3.0774, $-1.3988 + .0684i$, $-1.3988 - .0684i$, and .3313. So let us step up α to 5.5, say. The roots of [9 0 -59 -40 18] are 2.8080, -1.9257, -1.1925, and .3102. They fill the second row of **G**. From (A7) we find the third row as [1.4748 4.1606 12.3911 .4735]. Hence,

$$\mathbf{G} = \begin{bmatrix} 1.0000 & 1.0000 & 1.0000 & 1.0000 \\ 2.8080 & -1.9257 & -1.1925 & .3102 \\ 1.4748 & 4.1606 & 12.3911 & .4735 \end{bmatrix}. \tag{A14}$$

From

$$\mathbf{G} \bullet \mathbf{G} = \begin{bmatrix} 1.0000 & 1.0000 & 1.0000 & 1.0000 \\ 2.8080 & -1.9257 & -1.1925 & .3102 \\ 1.4748 & 4.1606 & 12.3911 & .4735 \\ 2.8080 & -1.9257 & -1.1925 & .3102 \\ 7.8847 & 3.7082 & 1.4220 & .0962 \\ 4.1412 & -8.0119 & -14.7761 & .1469 \\ 1.4748 & 4.1606 & 12.3911 & .4735 \\ 4.1412 & -8.0119 & -14.7761 & .1469 \\ 2.1750 & 17.3105 & 153.5403 & .2242 \end{bmatrix} \text{ and } \mathbf{X}_{93} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 2 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ -9 & -9 & 10 \end{bmatrix} \tag{A15}$$

we solve $\mathbf{D}' = \{(\mathbf{G} \bullet \mathbf{G})'(\mathbf{G} \bullet \mathbf{G})\}^{-1}(\mathbf{G} \bullet \mathbf{G})'\mathbf{X}_{93}$ to find

$$\mathbf{D} = \begin{bmatrix} -.0573 & .1610 & .1781 \\ .1239 & .2386 & -.1631 \\ -.0732 & -.0873 & .0797 \\ 1.0067 & -.3123 & .9053 \end{bmatrix}. \tag{A16}$$

It can be verified that indeed $(\mathbf{G} \bullet \mathbf{G})\mathbf{D}' = \mathbf{X}_{93}$, which constitutes an alternative solution to (A1).

It may be noted that the roots we have used, based on $\alpha = 5.5$, do not yet approach their asymptotic values. However, when we take $\alpha = 1005.5$, the roots of [9 1000 -59 -1040 18] are -111.1607, 1.0362, -1.0039, and 0.0173. Now the asymptotic pattern of the roots does begin to show up, one root being very large in magnitude, one close to 1, one close to -1, and one close to 0, respectively.

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