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The Carroll and Chang conjecture of equal Indscal components when Candecomp/Parafac gives perfect fit

Jos M.F. Ten Berge^{a,*}, Alwin Stegeman^{a,1}, Mohammed Bennani Dosse^b

^a University of Groningen, Netherlands ^b Université de Rennes 2, France

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ABSTRACT

The Candecomp/Parafac algorithm approximates a set of matrices $X_1, ..., X_I$ by products of the form AC_iB' , with C_i diagonal, i = 1, ..., I. Carroll and Chang have conjectured that, when the matrices are symmetric, the resulting **A** and **B** will be column wise proportional. For cases of perfect fit, Ten Berge et al. have shown that the conjecture holds true in a variety of cases, but may fail when there is no unique solution. In such cases, obtaining proportionality by changing (part of) the solution seems possible. The present paper extends and further clarifies their results. In particular, where Ten Berge et al. solved all $I \times 2 \times 2$ cases, now all $I \times 3 \times 3$ cases, and also the $I \times 4 \times 4$ cases for I = 2, 8, and 9 are clarified. In a number of cases, **A** and **B** necessarily have column wise proportionality when Candecomp/Parafac is run to convergence. In other cases, proportionality can be obtained by using specific methods. No cases were found that seem to resist proportionality.

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1. Introduction

As a generalization of Principal Component Analysis, Carroll and Chang [2] and Harshman [3] proposed the so-called Candecomp/Parafac (CP) algorithm. It decomposes an $I \times J \times K$ array with slices \mathbf{X}_i , i = 1, ..., I, as

$$\mathbf{X}_i = \mathbf{A}\mathbf{C}_i\mathbf{B}' + \mathbf{E}_i$$

(1)

* Corresponding author. Address: Heymans Institute, Grote Kruisstraat 2/1, 9712 TS Groningen, Netherlands.

E-mail addresses: j.m.f.ten.berge@rug.nl (J.M.F. Ten Berge), a.w.stegeman@rug.nl (A. Stegeman), mohammed.bennani@uhb.fr (M.B. Dosse).

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with $\sum \|\mathbf{E}_i\|^2$ as small as possible. In Indscal-related applications of CP, see [2], the *I* slices are symmetric, and we need to have a CP decomposition with **A** and **B** equal. In the absence of a direct method to fit (1) subject to this constraint, Carroll and Chang proposed using CP (unconstrained). In theory, we may then end up with a decomposition (1), with **A** and **B** different. There is no problem when **A** and **B** are column wise proportional. In that case, it is just a matter of rescaling the columns of **B** to become equal to those of **A**, with counter scaling of the columns of a matrix **C**, the rows of which hold the diagonal elements of $\mathbf{C}_1, \ldots, \mathbf{C}_I$. We shall say that **A** and **B** are *equivalent* when they are equal up to rescaling. When they are *not equivalent*, there is no way of scaling **A** and **B** to become equal. This is a serious problem for Indscal because it needs **A** and **B** to be equal.

The use of CP in the Indscal-related applications is based on the conjecture [2] that CP will converge to equivalent matrices **A** and **B**, when the slices are symmetric. In standard applications, where the data are randomly sampled from continuous distributions, and the number of components (the number of columns of **A**, **B**, and **C**) is too small to admit perfect fit, there seems to be no problem with this conjecture. Still, a general proof has not been given, and, in fact, cannot be given. For one thing, Ten Berge and Kiers [7] have given some partial results for the case where the number of components is small. They presented counterexamples to equivalence, which were deliberately constructed for that purpose. These examples represented non-optimal points (in fact, Bennani Dosse and Ten Berge [1] have shown that they are saddle points), with asymmetric products **AC**_i**B**'. Conceivably, they never occur in real-life situations. We conjecture that, under the condition of random sampling of the data, asymmetric solutions arise with probability zero at the global minimum of the CP function, when the number of components is small.

More recently, the problem of non-equivalence has also been examined for the case of perfect fit. Ten Berge et al. [8] have given partial results for this case, where it is granted that $E_1, ..., E_I$ vanish. This means that, unlike the counterexamples discussed above, which pertained to situations of imperfect fit, we now do have AC_iB' symmetric, i = 1, ..., I. Specifically, they examined cases with J = 2 and J = 3, where the number of components equals the so-called *typical rank values*, which are the ranks that arise with positive probability when the array is randomly sampled from a continuous distribution. They found that, in situations of perfect fit, equivalence was immediate in certain cases, but cases of nonequivalence also arise with positive probability. An important question then becomes when and how we can obtain equivalence, when a non-equivalent solution has been found. Ten Berge et al. [8] have specified how to find alternative solutions that do have equivalence for $I \times 2 \times 2$ arrays. This paper is meant to give an answer for all $I \times 3 \times 3$ cases. In addition, we treat the $2 \times 4 \times 4$ case, the $8 \times 4 \times 4$ case, and the $9 \times 4 \times 4$ case.

The organization of this paper is as follows. First, we consider some basic expressions and derive three preliminary results. Result 1 allows us to discard all cases where the number of slices *I* exceeds or is equal to the rank *R*, because such cases necessarily have equivalence almost surely. Result 2 is an improved version of Result 8 by Ten Berge et al. [8], giving a sufficient condition for equivalence. Result 3 deals with the impossibility of three symmetric matrices admitting a linear combination of rank 1, a result to be used for the $3 \times 3 \times 3$ case. Next, we treat (non-)equivalence for all $I \times 3 \times 3$ cases. Finally, the $2 \times 4 \times 4$ case, the $8 \times 4 \times 4$ case, and the $9 \times 4 \times 4$ cases are considered.

2. Basic expressions and preliminary results

Throughout, it is assumed that arrays have symmetric slices $X_1, ..., X_l$ of order $J \times J$, and that we have perfect fit using *R* components, where *R* is the rank of the array. Rank values of probability zero, when the slices are randomly sampled from a continuous distribution, will be ignored. This implies that the slices $X_i = AC_iB'$ will have rank *J*, so *A* and *B* are $J \times R$ matrices, $J \leq R$, of rank *J*.

In searching for non-equivalence, the symmetry of

$$\mathbf{X}_i = \mathbf{A}\mathbf{C}_i\mathbf{B}' = \mathbf{B}\mathbf{C}_i\mathbf{A}',\tag{2}$$

i = 1, ..., I, plays a key role. First of all (2) can be expressed as

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

where • is the Khatri-Rao (column wise Kronecker) product, and $\mathbf{X} = [\text{Vec}(\mathbf{X}_1)|\cdots|\text{Vec}(\mathbf{X}_l)]$, of order $J^2 \times I$, with .5J(J + 1) unrepeated rows. Let $\mathbf{U} = (\mathbf{B} \bullet \mathbf{A})$ and $\mathbf{V} = (\mathbf{A} \bullet \mathbf{B})$. Then we can write (3) as

$$\mathbf{X} = \mathbf{U}\mathbf{C}' = \mathbf{V}\mathbf{C}' \tag{4}$$

and hence

$$(\mathbf{U} - \mathbf{V})\mathbf{C}' = \mathbf{0}.$$
 (5)

Note that **A** and **B** are equivalent if and only if $\mathbf{U} = \mathbf{V}$. Clearly, (non-)equivalence of **A** and **B** is not affected when **C**' and **X** are postmultiplied by a nonsingular slice-mixing matrix **N**. So when I > R, implying linear dependence in the columns of **C**' and **X**, we may transform the problem into an equivalent one with R - I zero rows in **N**'**C**. That is, by mixing the slices we obtain R - I zero columns in **C** and **X**. Because they do not affect the validity of (5), we may leave them out.

The bottom line is that cases with I > R can be reduced to cases with I = R, without loss of generality. On the other hand, for cases with I = R, Ten Berge et al. [8] have proven that equivalence will hold almost surely. In our search for non-equivalence, we may thus limit our attention entirely to cases with I < R. We record this as

Result 1. Almost surely, equivalence is granted when $I \ge R$.

We also rephrase Result 8 of Ten Berge et al. [8], as Result 2. It relies on the concept of k-rank (Kruskal rank), which is defined as the largest number of columns of a matrix that are always linearly independent, no matter which columns are picked.

Result 2. When I < R and **C** has at least *k*-rank R - J + 2, equivalence is guaranteed almost surely.

Proof. Upon premultiplying **A** and **B** by the same nonsingular matrix, to create an identity submatrix in **A**, as was done in the proof of Result 8 of Ten Berge et al. [8], there will be at most R - J + 2 nonzero elements in every row of **U** – **V**. When the zeros of any of these rows are removed, the remaining vector is orthogonal to the columns of a submatrix holding R - J + 2 rows of **C**', see (5). Because **C** has a *k*-rank of at least R - J + 2, those rows are linearly independent, so the submatrix has rank R - J + 2. It follows that all rows of **U** – **V** vanish. This implies that **A** and **B** are equivalent.

It may be noted that Ten Berge et al. [8] used the additional condition $I \ge R - J + 2$. We have omitted that condition, because it is redundant when I < R. That is, when R - J + 2 columns of **C** are linearly independent, it follows that rank(**C**) $\ge R - J + 2$. Because **C** is an $I \times R$ matrix, I < R, we have $I \ge \text{rank}(\mathbf{C})$, so $I \ge R - J + 2$ is already implied.

Results 1 and 2 give sufficient conditions for equivalence. Non-equivalence can only arise when neither of these is met. That is, we need to consider cases where I < R (see Result 1) and **C** has *k*-rank less than R - J + 2 (see Result 2). Because we are only interested in cases that arise with positive probability, we looked into the known typical rank values reported in Table 1 of Ten Berge et al. [8]. For cases of J = 2, all possibilities of non-equivalence and ways of avoiding that have been discussed by Ten Berge et al., so we focus on cases with J = 3. Within these cases, we have I < R only for $2 \times 3 \times 3$ arrays when R = 3 or 4, for $3 \times 3 \times 3$ arrays when R = 4, for $4 \times 3 \times 3$ arrays when R = 5, and for $5 \times 3 \times 3$ when R = 6. It will now be examined which of these cases may admit low *k*-rank for **C**, and hence have **A** and **B** possibly non-equivalent. Also, it will be shown how to attain alternative solutions which do have equivalence, in such cases.

The following result is crucial in determining whether or not low k-rank for C is possible.

Result 3. Almost surely, three symmetric $J \times J$ matrices, $J \ge 3$, do not admit a linear combination of rank one.

Proof. First, consider the case J = 3. Suppose that two of the three matrices **X**, **Y**, **Z** can be diagonalized simultaneously. Then replace the slices by **D**, **E**, **F**, with **D** and **E** diagonal, and **F** symmetric. This does

not change the rank of all possible linear combinations of the three matrices. Suppose there is a linear combination $\mathbf{L} = u\mathbf{D} + v\mathbf{E} + w\mathbf{F}$ of rank one. When this is possible with w = 0, \mathbf{D} and \mathbf{E} have two corresponding pairs of diagonal elements satisfying a condition of proportionality, an event of probability zero. Hence, we may assume $w \neq 0$. Because \mathbf{L}/w also has rank one, set w = 1 without loss of generality. The off-diagonal elements of \mathbf{L} (given by \mathbf{F}) imply a unique set of diagonal elements, which are needed to get \mathbf{L} of rank one. Let the vector \mathbf{g} hold these diagonal elements, and let \mathbf{d} , \mathbf{e} and \mathbf{f} hold the diagonal elements of \mathbf{D} , \mathbf{E} , and \mathbf{F} , respectively. Then we must have $\mathbf{g} = u\mathbf{d} + v\mathbf{e} + \mathbf{f}$ so $u\mathbf{d} + v\mathbf{e} = \mathbf{g} - \mathbf{f}$. Because $\mathbf{g} - \mathbf{f}$ is in the column space of $[\mathbf{d}|\mathbf{e}]$ with probability zero, we arrive at a contradiction almost surely.

Next, suppose that no pair of **X**, **Y**, and **Z** can be diagonalized simultaneously. Then we may transform the matrices to

$$\mathbf{D} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \mathbf{E} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \text{ and } \mathbf{F} \text{ symmetric}$$
(6)

[6,9], without changing the ranks that can be attained by linear combinations of the matrices. Again, let $\mathbf{L} = u\mathbf{D} + v\mathbf{E} + w\mathbf{F}$ be of rank one. When w = 0, $u\mathbf{D} + v\mathbf{E}$ has a 2 × 2 submatrix with determinant $-u^2 - v^2$, hence it cannot have rank 1. So we may set w = 1. Without loss of generality, also rescale \mathbf{F} to have $f_{12} = f_{21} = 1$. Setting the determinant of \mathbf{L} , with row 1 and column 3 discarded, to zero yields $f_{23} + v = f_{13}(f_{22} + u)$, so

$$\mathbf{L} = \begin{bmatrix} f_{11} + u & 1 & f_{13} \\ 1 & f_{22} + u & f_{13}(f_{22} + u) \\ f_{13} & f_{13}(f_{22} + u) & f_{33} - u \end{bmatrix}.$$
 (7)

Setting the determinant of **L**, with row 2 and column 1 discarded, to zero yields $f_{33} - u = f_{13}^2(f_{22} + u)$, so $u = (f_{33} - f_{13}^2f_{22})/(1 + f_{13}^2)$. Setting the determinant of **L** with row 3 and column 3 discarded to zero yields $u^2 + u(f_{11} + f_{22}) + f_{11}f_{22} - 1 = 0$, which implies at most two possible values for *u*, that generically differ from $u = (f_{33} - f_{13}^2f_{22})/(1 + f_{13}^2)$. This proves the result for J = 3. The proof generalizes immediately to matrices of higher order, because any linear combination of rank one has submatrices of smaller order which are also linear combinations of rank one.

It should be noted, however, that the result does not generalize to more than three slices. \Box

In the next sections, we examine the issue of equivalence for $I \times 3 \times 3$ arrays in cases of perfect fit. It will be shown that equivalence (having **A** and **B** column wise proportional) is either granted, or can be found by appropriate methods that will be explained.

3. Equivalence for 2 × 3 × 3 arrays of rank 3 or 4

The $2 \times 3 \times 3$ array has typical rank {3,4}. When it has rank 3, the solution is almost surely unique, and equivalence follows from Result 6 of Ten Berge et al. [8]. When the array has rank 4, equivalence is not granted, but a solution displaying equivalence can be derived.

Although Ten Berge et al. [8, Result 7] have already shown how to obtain equivalence in the R = 4 case, we take a different approach here, that will be easier to generalize. Let X_1 and X_2 be the slices of the array. By mixing the slices, it can be arranged that one slice (X_2 , say) has rank 2. Let N be a nonsingular matrix with third column orthogonal to the columns and rows of X_2 . Then $N'X_2N$ has zeros in row and column 3. We can obtain zeros in row and column 3 of $N'X_1N$ also, by subtracting a certain symmetric rank one matrix from it. That rank one matrix is constructed by copying row 3 and column 3 of $N'X_1N$, and picking the remaining four elements in such a way that all rows become proportional (J.B. Kruskal, personal communication, June 1991). Subtracting it implies that one column of the matrix A to be derived and one column of the matrix B to be derived are already fixed and equal. What remains is a $2 \times 2 \times 2$ array, which is known to have maximum rank 3. It also has minimum rank 3 because otherwise the original $2 \times 3 \times 3$ array would have a rank less than 4. It is easy to construct a

solution with full equivalence for this $2 \times 2 \times 2$ array, e.g. [5]. Reverting the entire process and restoring the symmetric rank one matrix that was subtracted gives an R = 4 solution with full equivalence for the original array.

4. Equivalence for 3 × 3 × 3 arrays of rank 4

The typical rank of symmetric slice $3 \times 3 \times 3$ arrays is 4, so CP solutions for these arrays have a 3×4 matrix **C** of rank 3. When its *k*-rank, written as k_{C} , is as high as 3, we have equivalence by virtue of Result 2. Suppose its *k*-rank is less than 3. Premultiply **C** by the inverse of the matrix that holds three linearly independent columns of **C**, the first three columns of **C**, say. This operation is equivalent to mixing the slices of the array in an invertible way. The resulting **C*** will be of the form

$$\mathbf{C}^* = \begin{bmatrix} 1 & 0 & 0 & x \\ 0 & 1 & 0 & y \\ 0 & 0 & 1 & z \end{bmatrix}$$
(8)

with at least one element (x, y, or z) of the last column zero because $k_c < 3$. Then at least one row of C^* has just one nonzero element, implying that the three slices admit a linear combination of rank 1. By Result 3, this has probability zero. Hence we have $k_c = 3$ and A = B almost surely. We have thus eliminated a possibility of non-equivalence, left open by Ten Berge et al. [8, p. 375].

5. Equivalence for 4 × 3 × 3 arrays of rank 5

The typical rank of $4 \times 3 \times 3$ arrays of symmetric slices is {4, 5}. Suppose the array has rank 4. Then I = R, and a CP solution has equivalence almost surely (Result 1). Henceforth, consider the $4 \times 3 \times 3$ arrays of rank 5. In theory, we have four cases to consider, namely, **C** may have *k*-rank 1, 2, 3, or 4. We need not discuss the case of $k_c = 4$ because it has equivalence by virtue of Result 2. We start with the case $k_c = 1$.

Ten Berge et al. [8, p. 368] developed a necessary and sufficient condition for $4 \times 3 \times 3$ arrays to be of rank 4. That is, they derived a fourth degree polynomial equation from the premise that the four slices admit a linear combination of rank one. The number of distinct real valued roots of the equation is the number of independent linear combinations of rank 1. The array has rank 4 if there are four distinct real valued roots, and rank 5 if at least one root is complex. We ignore the case of equal real valued roots, because it arises with probability zero. It will now be shown that *k*-rank 1 for **C** is impossible in the case under consideration.

Result 4. When a $4 \times 3 \times 3$ array has rank 5, it does not admit a CP solution with $k_{\rm C} = 1$.

Proof. Suppose **C** has *k*-rank 1. Then two columns, the first two, say, are proportional. Because **C** has rank 4 almost surely, there is a nonsingular matrix **N** such that

	Γλ	1	0	0	07		
N'C =	0	0	1	0	0		(0)
	0	0	0	1	0	. ((9)
	0	0	0	0	1		

Note that **N** mixes the slices of the data array, without affecting rank and *k*-rank of **C**. That is, $\mathbf{X} = \mathbf{UC'}$ if and only if $\mathbf{XN} = \mathbf{UC'N}$, see (4). This means that the last three slices of the array which has vec-form **XN** are of rank 1. Because the original slices admit three independent linear combinations of rank 1, three roots of the polynomial equation are real. That means that the fourth root is also real, and the array had rank 4 to begin with. \Box

Having excluded the possibility of $k_c = 1$, the next case to consider is when **C** has *k*-rank 2. This seems to occur quite often in practice. In particular, it may happen that three columns of **C**, the first

three, say, are linearly dependent, and only the fourth and fifth column of **A** and **B** are proportional. The appendix gives a numerical example of a randomly generated array, the solution for **A** and **B**, and the vector orthogonal to the rows of **C**, with $k_c = 2$. Clearly, it has equivalence only for two components. It will now be explained why that is, and how an alternative solution with full equivalence of **A** and **B** can be retrieved.

Suppose **C** has *k*-rank 2, with linear dependence in the first three columns. Then there exists a slice mix which transforms **C** to

$$\mathbf{C}^* = \begin{vmatrix} x & 1 & 0 & 0 & 0 \\ y & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{vmatrix}$$
(10)

with *x* and *y* nonzero. Let **A** and **B** be partitioned as $\mathbf{A} = [\mathbf{A}_1|\mathbf{A}_2]$ and $\mathbf{B} = [\mathbf{B}_1|\mathbf{B}_2]$, respectively, with \mathbf{A}_1 and \mathbf{B}_1 of order 3×3 . Because the last two slices of the transformed array are now of rank 1, \mathbf{A}_2 and \mathbf{B}_2 are equivalent. We ignore these slices and continue with the first two, which we call \mathbf{Y}_1 and \mathbf{Y}_2 . They form a $2 \times 3 \times 3$ array of rank 3. When \mathbf{A}_1 and \mathbf{B}_1 have rank 3, we have $k_A + k_B + k_C = 8 = 2R + 2$, implying uniqueness of the solution [4]. Hence, by Result 6 of Ten Berge et al. [8] we have equivalence at once. This happens quite often in practice, but we also encounter exceptions.

Indeed, it sometimes does happen that \mathbf{A}_1 (or \mathbf{B}_1) has rank less than 3. Then there is a vector \mathbf{n} orthogonal to the columns of \mathbf{A}_1 (or \mathbf{B}_1). Let \mathbf{N} be an orthonormal matrix with \mathbf{n} as third column. Then the third row of $\mathbf{N}'\mathbf{A}_1$ (or $\mathbf{N}'\mathbf{B}_1$) is zero. Let $\mathbf{N}'\mathbf{Y}_1\mathbf{N} = \mathbf{Z}_1$ and $\mathbf{N}'\mathbf{Y}_2\mathbf{N} = \mathbf{Z}_2$. Because \mathbf{Z}_1 and \mathbf{Z}_2 are symmetric, their third rows and columns vanish. It is easy (e.g. [5]) to find a solution with equivalence for a $2 \times 2 \times 2$ array with symmetric slices, using three components. Thus, we attain full equivalence for the mixed slices. Unmixing preserves the equivalence. We have thus adjusted the non-equivalent part of the solution (viz. \mathbf{A}_1 and \mathbf{B}_1) and obtained full equivalence.

Finally, suppose we have k-rank 3 for C. Then there will be a slice mix of the form

$$\mathbf{C}^* = \begin{bmatrix} 1 & 0 & 0 & 0 & x \\ 0 & 1 & 0 & 0 & y \\ 0 & 0 & 1 & 0 & z \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix},$$
(11)

x, *y*, and *z* nonzero. Clearly, the array now has one slice of rank 1, implying equivalence for column 4 of **A** and **B**. Leaving out that slice, we are left with a $3 \times 3 \times 3$ array of R = 4 and $k_C = 3$. For this array, we have equivalence almost surely from Result 2.

It may be noted that those arrays which admit solutions with *k*-rank 3 for **C** are also those that admit solutions with *k*-rank 2 for **C**, when CP is started repeatedly from different initializations. This is because, when one root of the fourth degree polynomial equation of Ten Berge et al. [8] is real, as can be seen from the fact that the slices admit a linear combination of rank 1, two roots will be real. In other words, when an array admits solutions allowing a slice mix of the form (11), it admits solutions allowing a slice mix of the form (10), and vice versa. Still, whenever CP yields a solution with $k_C = 3$, **A** and **B** are necessarily equivalent. In cases where CP, applied to the same array, produces a solution with $k_C = 2$, **A** and **B** are often equivalent but sometimes they happen to have three non-proportional columns, as has been explained above.

6. Equivalence for 5 × 3 × 3 arrays of rank 6

The 5 × 3 × 3 arrays have typical rank {5, 6}. When the rank is 5, Result 1 implies equivalence. When the rank is 6, and $k_c = 5$, Result 2 implies equivalence. It will now be shown that $k_c < 5$ is impossible when the rank is 6. Ten Berge et al. [8, p. 370] noted that a 5 × 3 × 3 array has rank 5 if and only if its five slices admit five linearly independent linear combinations of rank one. Such linear combinations exist when a certain quadratic equation has real roots, while the discriminant depends continuously on a free parameter. Specifically, the discriminant is $(f_3 + df_5)^2 + 4(f_1 + df_2 + d^2f_4)$, with *d* free, and

 f_1, \ldots, f_5 fixed. Now suppose that the array admits a solution with $k_c < 5$. Then the slices admit at least one linear combination of rank one, which means that it is possible to pick *d* in such a way that the discriminant is non-negative. But then, almost surely, an infinite number of other linear combinations of rank one can be found by slightly changing *d*, which means that the array had rank 5 to begin with. It can be concluded that $k_c = 5$ when a $5 \times 3 \times 3$ array has rank 6. Equivalence of **A** and **B** is thus guaranteed.

At this point, all possible cases where CP applied to $I \times 3 \times 3$ arrays might give non-equivalence have been dealt with. Solutions with full equivalence either occur necessarily, or can be derived. This means that, in the Indscal-related application of CP to $I \times 3 \times 3$ arrays, no serious problems can arise with the assumption of equivalence in cases of perfect fit. Our next step might be a treatment of $I \times J \times J$ arrays with J > 3. However, for these arrays the typical ranks are largely unknown. Only partial results are available. Specifically, the $2 \times 4 \times 4$ array is known to have typical rank {4, 5}, and we shall treat the question of (non-)equivalence in the next section. Also, the typical rank of $8 \times 4 \times 4$ arrays and $9 \times 4 \times 4$ arrays is {8, 9} and {9, 10}, respectively. A proof for this, and a treatment of the (non-)equivalence issue for these two array formats will be given in the last sections. Finally, it is also known that $I \times 4 \times 4$ arrays have typical rank 10 when $I \ge 10$ [8] but this requires no further treatment, because equivalence is granted by Result 1 above.

7. Equivalence for 2 × 4 × 4 arrays of rank 4 or 5

The 2 × 4 × 4 array has typical rank {4, 5}. When the rank is 4, the CP solution is almost surely unique, and equivalence is implied [8, Result 6]. When the rank is five, we have either 2 or 4 complex eigenvalues for $X_1^{-1}X_2$, where X_1 and X_2 are the two slices of the array. First, suppose that two eigenvalues are complex. A solution with equivalence can easily be constructed by the method that was used to solve the 2 × 3 × 3 case. Because the slices admit linear combinations of rank 3, X_2 can be assumed to be of rank 3, and there exists an orthonormal nonsingular matrix N such the last row and column of N'X₂N vanish. Next, we use one component to clear row 4 and column 4 of N'X₁N. We are left with the problem of finding a rank-4 solution for a 2 × 3 × 3 array. A solution with full equivalence has been discussed above.

It remains to deal with the case where all four eigenvalues of $X_1^{-1}X_2$ are complex. We offer a method which uses a symmetric rank-one perturbation of one slice, rendering it simultaneously diagonizable with the other slice. Then the remaining array has rank 4, so it has four unique CP components with equivalence granted. Because the perturbation also has equivalence, a 5 component solution with full equivalence will be obtained.

By an adaptation of a procedure by Rocci and Ten Berge [6], we transform and mix the slices to obtain

$$\mathbf{Z}_{1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \text{ and } \mathbf{Z}_{2} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & b \\ 0 & 0 & b & 0 \end{bmatrix}$$
(12)

with $b \neq 0$ and $b^2 \neq 1$. To attain this form, we first evaluate the eigenvalues $\alpha_1 + i\beta_1, \alpha_1 - i\beta_1, \alpha_2 + i\beta_2$, and $\alpha_2 - i\beta_2$ of $\mathbf{X}_1^{-1}\mathbf{X}_2$. Then solve equations A4 and A2 of Rocci and Ten Berge [6] to find

$$u_{21} = \frac{\alpha_2^2 + \beta_2^2 - \alpha_1^2 - \beta_1^2 + \sqrt{(\alpha_1 - \alpha_2)^4 + (\beta_1^2 - \beta_2^2)^2 + 2(\beta_1^2 + \beta_2^2)(\alpha_1 - \alpha_2)^2}}{2\alpha_2(\alpha_1^2 + \beta_1^2) - 2\alpha_1(a_2^2 + \beta_2^2)}$$
(13)

and

$$u_{12} = \frac{-u_{21}\beta_1^2 - \alpha_1 - u_{21}\alpha_1^2}{1 + u_{21}\alpha_2}$$

Define $\mathbf{Y}_1 = \mathbf{X}_1 + u_{21}\mathbf{X}_2$ and $\mathbf{Y}_2 = u_{12}\mathbf{X}_1 + \mathbf{X}_2$ and compute the eigendecomposition $\mathbf{Y}_1^{-1}\mathbf{Y}_2 = \mathbf{KLK}^{-1}$. Next, define $\mathbf{T} = [real(\mathbf{k}_1) \ imag(\mathbf{k}_2) \ real(\mathbf{k}_3) \ imag(\mathbf{k}_4)]$, where \mathbf{k}_j is column j of \mathbf{K} . Then we have

$$\mathbf{T}'\mathbf{Y}_{1}\mathbf{T} = \begin{bmatrix} a & 0 & 0 & 0\\ 0 & c & 0 & 0\\ 0 & 0 & -c & 0\\ 0 & 0 & 0 & -a \end{bmatrix} \text{ and } \mathbf{T}'\mathbf{Y}_{2}\mathbf{T} = \begin{bmatrix} 0 & 0 & 0 & d\\ 0 & 0 & e & 0\\ 0 & e & 0 & 0\\ d & 0 & 0 & 0 \end{bmatrix}$$
(14)

for certain real scalars *a*, *c*, *d*, and *e*. By rescaling and permuting (14) can be brought in the form (12), yielding \mathbf{Z}_1 and \mathbf{Z}_2 .

Next, construct a vector $\mathbf{a} = [a_1 \ a_2 \ a_3 \ a_4]'$ with $a_1^2 = a_2^2$, and $a_3^2 = a_4^2$, such that

$$a_1 a_2 = \left[\frac{1+b^2}{1-b^2}\right] \text{ and } a_3 a_4 = \left[\frac{-b(1+b^2)}{(1-b^2)}\right].$$
 (15)

This yields **a** uniquely, up to sign changes of a_1 and a_2 jointly, and a_3 and a_4 jointly. We want to show that Z_1 and $Z_2 - aa'$ form a rank 4 array, by showing that $(Z_1)^{-1}(Z_2 - aa')$ has eigenvalues 1, -1, *b*, and -*b*. The eigenvalues solve the equation $|Z_1^{-1}(Z_2 - aa') - \lambda I_4| = 0$. Equivalently, they are the roots of

$$|\lambda \mathbf{Z}_1 - \mathbf{Z}_2 + \mathbf{a}\mathbf{a}'| = 0. \tag{16}$$

In general, when **Z** is nonsingular, $|\mathbf{Z} + \mathbf{a}\mathbf{a}'| = (1 + \mathbf{a}'\mathbf{Z}^{-1}\mathbf{a})|\mathbf{Z}|$. Therefore, having $|\lambda \mathbf{Z}_1 - \mathbf{Z}_2 + \mathbf{a}\mathbf{a}'| = 0$ is equivalent to having $|\lambda \mathbf{Z}_1 - \mathbf{Z}_2|\{1 + \mathbf{a}'(\lambda \mathbf{Z}_1 - \mathbf{Z}_2)^{-1}\mathbf{a}\} = 0$. Note that $|\lambda \mathbf{Z}_1 - \mathbf{Z}_2| = (\lambda^2 + 1)(\lambda^2 + b^2)$, and

$$(\lambda \mathbf{Z}_{1} - \mathbf{Z}_{2})^{-1} = \begin{bmatrix} \frac{\lambda}{\lambda^{2}+1} & \frac{-1}{\lambda^{2}+1} & 0 & 0\\ \frac{-1}{\lambda^{2}+1} & \frac{-\lambda}{\lambda^{2}+1} & 0 & 0\\ 0 & 0 & \frac{\lambda}{\lambda^{2}+b^{2}} & \frac{-b}{\lambda^{2}+b^{2}} \\ 0 & 0 & \frac{-b}{\lambda^{2}+b^{2}} & \frac{-\lambda}{\lambda^{2}+b^{2}} \end{bmatrix}.$$
(17)

It is readily verified that

$$\mathbf{a}'(\lambda \mathbf{Z}_1 - \mathbf{Z}_2)^{-1} \mathbf{a} = (\lambda^2 + 1)^{-1} (\lambda a_1^2 - \lambda a_2^2 - 2a_1 a_2) + (\lambda^2 + b^2)^{-1} (\lambda a_3^2 - \lambda a_4^2 - 2ba_3 a_4).$$
(18)

Using that $a_1^2 = a_2^2$ and $a_3^2 = a_4^2$, and (15) gives

$$\mathbf{a}'(\lambda \mathbf{Z}_{1} - \mathbf{Z}_{2})^{-1}\mathbf{a} = -2(1+b^{2})/\{(1-b^{2})(\lambda^{2}+1)\} + 2b^{2}(1+b^{2})/\{(1-b^{2})(\lambda^{2}+b^{2})\}$$

$$= \frac{-2(1+b^{2})(\lambda^{2}+b^{2}) + 2b^{2}(1+b^{2})(\lambda^{2}+1)}{(1-b^{2})(\lambda^{2}+1)(\lambda^{2}+b^{2})}$$

$$= \frac{(1+b^{2})(-2\lambda^{2}-2b^{2}) + (1+b^{2})(2b^{2}\lambda^{2}+2b^{2})}{(1-b^{2})(\lambda^{2}+1)(\lambda^{2}+b^{2})}$$

$$= \frac{(1+b^{2})(-2\lambda^{2}+2b^{2}\lambda^{2})}{(1-b^{2})(\lambda^{2}+1)(\lambda^{2}+b^{2})} = \frac{2\lambda^{2}(1+b^{2})(b^{2}-1)}{(1-b^{2})(\lambda^{2}+1)(\lambda^{2}+b^{2})}$$

$$= \frac{-2\lambda^{2}(1+b^{2})}{(\lambda^{2}+1)(\lambda^{2}+b^{2})}.$$
(19)

Therefore, $|\lambda \mathbf{Z}_1 - \mathbf{Z}_2|(1 + \mathbf{a}'(\mathbf{Z}_1 - \lambda \mathbf{Z}_2)^{-1}\mathbf{a}) = (\lambda^2 + 1)(\lambda^2 + b^2) - 2\lambda^2(1 + b^2) = (\lambda^2 - 1)(\lambda^2 - b^2)$. Setting this expression to zero yields the roots 1, -1, *b*, and -*b*. Combining the component \mathbf{aa}' with the four components of the array with slices \mathbf{Z}_1 and $\mathbf{Z}_2 - \mathbf{aa}'$, we have found a five component solution with **A** and **B** fully equivalent when all four roots of $\mathbf{X}_1^{-1}\mathbf{X}_2$ are complex.

8. Typical rank and equivalence for 8 × 4 × 4 arrays

Tendeiro et al. [9] have offered a method for transforming $8 \times 4 \times 4$ arrays with symmetric slices to simple forms, with a vast majority of zero elements. The transformation involves slice mixing, and

pre and postmultiplying the slices by a matrix \mathbf{T}' and \mathbf{T} , respectively, thus preserving the symmetry of the slices. They found only three distinct cases that arise with positive probability. The first two cases are when the matrix \mathbf{X} , holding the Vecs of the slices in its columns, can be transformed to (20), with δ either 1 or -1:

	 72a	0	0	0	0	0	0	ר0
	0	0	0	1	0	0	0	0
	0	0	0	0	1	0	0	0
	0	0	0	0	0	1	0	0
	0	0	0	1	0	0	0	0
	b	1	1	0	0	0	0	0
	0	0	0	0	0	0	1	0
v	0	0	0	0	0	0	0	1
Λ =	0	0	0	0	1	0	0	0
	0	0	0	0	0	0	1	0
	0	а	0	0	0	0	0	0
	C C	0	0	0	0	0	0	0
	0	0	0	0	0	1	0	0
	0	0	0	0	0	0	0	1
	c	0	0	0	0	0	0	0
	LΟ	0	аδ	0	0	0	0	0_

(20)

Rank less than 8 for this array has probability zero. A rank 8 solution exists if and only if **X** admits 8 linearly independent linear combinations of Khatri-Rao form **b** • **a**. Postmultiplying **X** by a vector **w** which generates a product of the form **b** • **a** shows that such a vector exist only when **a** and **b** are proportional. Upon rescaling both **a** and **b** to $\begin{bmatrix} 1 & x & y & z \end{bmatrix}'$, it follows that $\mathbf{w} = \begin{bmatrix} \frac{1}{2a} & \frac{y^2}{a} & \frac{\delta z^2}{a} & x & y & z & xy & xz \end{bmatrix}'$. The equation $\mathbf{Xw} = \mathbf{a} \cdot \mathbf{a}$ amounts to solving the equations yz = c/(2a) and $\frac{b}{2a} + \frac{y^2}{a} + \frac{\delta z^2}{a} = x^2$. Substituting c/(2az) for y yields $\frac{b}{2a} + \frac{c^2}{4a^3z^2} + \frac{\delta z^2}{a} = x^2$. This always has a solution when δ has the same sign as *a*. By picking large enough values for z^2 (eight times) to find solutions for x^2 , a rank 8 solution is easily obtained. The solution has equivalence. On the other hand, when a < 0, $\delta = 1$, and b > 0, the equation cannot be solved. In this case we have at least rank 9. An easy way to attain a rank 9 solution when $a\delta < 0$ is by adding $-2a\delta$ to element (16, 3) of **X**. This changes the sign of $a\delta$, and yields an array that has rank 8. To account for the sign change, however, we need one additional component, so we have attained a rank 9 solution. Note that the 8 solutions for **a** and **w** form the columns of **A** and (**C**)⁻¹.

respectively, in a CP decomposition. The additional ninth component, if needed, will appear in column 9 of **A** and **C**. Again, we have attained a solution with **A** and **B** equivalent.

Next, we need to treat the third simple form that we may have. That is, we consider

	г1	1	1	0	0	0	0	ך0
	0	0	0	1	0	0	0	0
	0	0	0	0	1	0	0	0
	0	0	0	0	0	1	0	0
	0	0	0	1	0	0	0	0
	1	0	0	0	0	0	0	0
	0	0	0	0	0	0	1	0
v	0	0	0	0	0	0	0	1
A =	0	0	0	0	1	0	0	0
	0	0	0	0	0	0	1	0
	0	a_1	0	0	0	0	0	0
	0	0	0	b	0	0	0	0
	0	0	0	0	0	1	0	0
	0	0	0	0	0	0	0	1
	0	0	0	b	0	0	0	0
	_0	0	$-a_2$	0	0	0	0	0_

(21)

It should be noted that $a_1 = a_2$ [9], but we label these elements independently because we will adjust only a_2 when we need to. Proceeding like before, we find that a vector **w** that generates a product $\mathbf{X}\mathbf{w} = \mathbf{a} \cdot \mathbf{b}$ has elements $\begin{bmatrix} x^2 & \frac{y^2}{a_1} & \frac{-z^2}{a_2} & x & y & z & xy & xz \end{bmatrix}'$, with $\mathbf{a} = \mathbf{b} = \begin{bmatrix} 1 & x & y & z \end{bmatrix}'$. We need to solve bx = yz and $x^2 + \frac{y^2}{a_1} - \frac{z^2}{a_2} = 1$. So we need to solve $\frac{y^2z^2}{b^2} + \frac{y^2}{a_1} - \frac{z^2}{a_2} = 1$, or $y^2 \left(\frac{z^2}{b^2} + \frac{1}{a_1}\right) = 1 + \frac{z^2}{a_2}$. When $a_2 > 0$, we can pick any z large enough to render $\left(\frac{z^2}{b^2} + \frac{1}{a_1}\right) > 0$, solve for y^2 , pick a sign for y, and find x = yz/b. This readily gives a rank 8 solution. When $a_2 < 0$, we can use one additional component to change the sign of a_2 , to have a rank 9 solution. It may be noted that all solutions derived here have equivalence. For CP, equivalence is guaranteed when the rank is 8 (see Result 1) but not when it is 9.

9. Typical rank and equivalence for 9 × 4 × 4 arrays

Following Tendeiro et al. [9], we can almost surely simplify a $9 \times 4 \times 4$ array to the form

	Г−а	-b	-c	0	0	0	0	0	ר0
	0	0	0	1	0	0	0	0	0
	0	0	0	0	1	0	0	0	0
	0	0	0	0	0	1	0	0	0
	0	0	0	1	0	0	0	0	0
	1	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	1	0	0
v	0	0	0	0	0	0	0	1	0
A =	0	0	0	0	1	0	0	0	0
	0	0	0	0	0	0	1	0	0
	0	1	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	1
	0	0	0	0	0	1	0	0	0
	0	0	0	0	0	0	0	1	0
	0	0	0	0	0	0	0	0	1
	L 0	0	1	0	0	0	0	0	0_

Rank less than 9 for this array has probability zero. Finding a **w** such that $Xw = b \cdot a$ yields $a = b = [1 \ x \ y \ z]$ and $w = [x^2 \ y^2 \ z^2 \ x \ y \ z \ xy \ xz]$. The only equation to be solved is $-ax^2 - by^2 - cz^2 = 1$. Clearly, there is a positive probability that this works. For instance, when *a*, *b*, and *c* are negative, we can pick any pair of values for *y* and *z* and solve for *x*, in nine different ways, to have a rank 9 solution. There are also cases where rank 9 is impossible. For instance, when *a*, *b*, and *c* are positive, there is no solution. This shows that a rank above 9 has positive probability. A rank 10 solution is always available from Rocci and Ten Berge [5]. This completes the proof that the typical rank for $9 \times 4 \times 4$ arrays is {9, 10}.

Having settled the typical rank issue, it remains to consider the question of equivalence. Suppose the rank is 9. Then I = R and equivalence almost surely is implied by Result 1. Indeed, the solutions we found did have equivalence. When the rank is 10, equivalence is not granted for CP, but a closed-form solution with equivalence is available from Rocci and Ten Berge [5].

The approach used above applies in general to $I \times J \times J$ arrays with symmetric slices, when the number of slices I is the number of free parameters in the slices minus 1. That is, when I = .5J(J + 1) - 1, the array has typical rank $\{I, I + 1\}$. So the $14 \times 5 \times 5$ array has typical rank $\{14, 15\}$, the $20 \times 6 \times 6$ array has typical rank $\{20, 21\}$, and the $27 \times 7 \times 7$ array has typical rank $\{27, 28\}$. Also, finding a solution with equivalence is straightforward in these cases.

10. Discussion

A key result of this paper is that non-equivalence for $I \times 3 \times 3$ arrays with symmetric slices can only occur when a $4 \times 3 \times 3$ array has rank 5, with $k_c = 2$. This settles some issues that were left undecided

(22)

by Ten Berge et al. [8]. Result 3 is also new. It clarifies why cases like the $2 \times 3 \times 3$ array of rank 4 have almost surely a solution with equivalence. Interestingly, our analysis of $4 \times 3 \times 3$ and $5 \times 3 \times 3$ arrays reveals that four or five randomly generated symmetric 3×3 matrices admit a linear combination of rank 1 with a positive probability less than one. But six of these matrices do admit a linear combination of rank one almost surely, because they are space filling.

This paper has focused on cases of non-equivalence when CP gives a perfect fit solution. Nonequivalent solutions occur quite often, in cases where CP has no unique solution. So far, it has never been a problem to find an alternative solution which does have equivalence. It seems, therefore, that the cause of non-equivalent solutions (non-uniqueness) also paves the way for its remedy.

Further extension of our analysis is severely hampered by the absence of typical rank results. For instance, as long as the typical rank values of $I \times 4 \times 4$ arrays, $3 \le I \le 7$, are unknown, there is no way of settling the equivalence issue for $I \times 4 \times 4$ arrays in general.

Appendix: Restoring equivalence for a $4 \times 3 \times 3$ array of rank 5 when $k_c = 2$

Consider these slices of a randomly generated $4 \times 3 \times 3$ array of rank 5

1.1346	0.1630	1.8262
0.1630	0.1299	1.9809
1.8262	1.9809	2.1604
-2.1353	-0.2361	1.2687
-0.2361	2.3622	0.0724
1.2687	0.0724	0.9238
2.0254	-0.3567	0.1805
-0.3567	2.2626	0.5967
0.1805	0.5967	0.2767
3.4732	-0.2749	-0.9870
-0.2749	-0.4460	1.1702
-0.9870	1.1702	5.1791

A possible CP solution has this **A**, **B**, and null(**C**):

Α	.5601	.2075	.0717	1597	.9106
	.4775	.2568	.1646	.9832	0684
	.6770	.9439	.9838	0880	4077
В	.3798	.7954	.3549	–.1597	.9106
	.1659	.5854	.3529	.9832	0684
	–.9101	.1570	.8657	–.0880	4077
null(C)	.7040	.6594	.2636	.0000	.0000

Three columns of **A** and **B** are non-equivalent, which implies low *k*-rank of **C**. Indeed, columns 1, 2, and 3 of **C** are linearly dependent, as can be seen from null(**C**). Premultiplying **C** by the inverse of the matrix holding columns 2-3-4-5 of **C** yields this **C**^{*}, see (10)

9366	1.0000	.0000	.0000	.0000
.5500	1.0000	.0000	.0000	.0000
3744	.0000	1.0000	.0000	.0000
	.0000	1.0000	.0000	.0000
.0000	.0000	.0000	1.0000	.0000
.0000	.0000	.0000	1.0000	.0000
.0000	.0000	.0000	.0000	1.0000
.0000	.0000	.0000	.0000	1.0000

so slices 3 and 4 are now of rank one. They can be ignored, and we continue with slices \mathbf{Y}_1 and \mathbf{Y}_2 . The vector $\mathbf{n} = [.5781 - .8106 .0935]'$ is orthogonal to column 3 and row 3 of \mathbf{Y}_1 and \mathbf{Y}_2 . An orthonormal

matrix **N** with **n** as third column will reduce the problem to a $2 \times 2 \times 2$ problem, with slices **Z**₁ and **Z**₂ for which a CP solution with equivalence is easily found by the method of Rocci and Ten Berge [5].

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