JOURNAL OF CHEMOMETRICS
J. Chemometrics 2004; **18**: 17–21
Published online in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/cem.840

Simplicity and typical rank of three-way arrays, with applications to Tucker-3 analysis with simple cores

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Received 4 July 2003; Revised 5 December 2003; Accepted 24 December 2003

In chemometric applications of Tucker three-way principal component analysis, core arrays are often constrained to have a large majority of zero elements. This gives rise to questions of non-triviality (are the constraints active, or can any core of a given format be transformed to satisfy the constraints?) and uniqueness (can we transform the components in one or more directions without losing the given pattern of zero elements in the core?). Rather than deciding such questions on an *ad hoc* basis, general principles are to be preferred. This paper gives an overview of simplicity transformations on the one hand, and typical rank results on the other, which are suitable to determine whether or not certain constrained cores are trivial. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: CANDECOMP/PARAFAC; uniqueness, constrained tucker models

1. INTRODUCTION

It is well known that a square matrix $\mathbf{X}$ with SVD $\mathbf{X} = \mathbf{PDQ}'$ can be transformed to a diagonal matrix $\mathbf{D} = \mathbf{P}'\mathbf{XQ}$. The transformation brings about the maximum simplicity (in terms of the number of zero elements) that can be obtained by non-singular transformations. As a bonus, it also reveals the rank of $\mathbf{X}$ as the number of non-zero elements in $\mathbf{D}$. For three-way arrays consisting of K slices $\mathbf{X}_1, \ldots, \mathbf{X}_K$, similar transformations to simplicity are possible but typically more complicated. Such transformations can be helpful in finding the rank of the three-way array. The topics of simplicity and rank of three-way arrays have implications for the analysis of three-way arrays by Tucker three-way PCA (3PCA), for CANDECOMP/PARAFAC (CP) and, notably, for hybrid models in between the two. The present paper gives a summary of results.

The organization of this paper is as follows. First, the main features of CP, 3PCA and hybrid models in between will be reviewed. Next, maximal simplicity results and typical rank results for three-way arrays will be discussed. Finally, some applications, revolving around issues of *non-triviality* and *uniqueness* of hybrid models, will be discussed.

2. CANDECOMP/PARAFAC (CP)

Carroll and Chang [1] and Harshman [2] independently proposed CANDECOMP and PARAFAC respectively. Let X be a three-way array holding slices $\mathbf{X}_1, \ldots, \mathbf{X}_K$ of order $I \times J$. For any given number of components r, CP yields component matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$, with r columns, minimizing $\sum \mathrm{tr}(\mathbf{E}_k'\mathbf{E}_k)$ in the decomposition

$$\mathbf{X}_k = \mathbf{AC}_k\mathbf{B}' + \mathbf{E}_k \qquad (1)$$

where $\mathbf{C}_k$ is the diagonal matrix having the elements of row k of $\mathbf{C}$ in the diagonal, $k = 1, \ldots, K$.

Under mild conditions to be discussed below, CP has the property of *essential uniqueness*, which means that the columns of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are determined up to joint permutations and rescaling. Clearly, rescaling columns of $\mathbf{A}$ (or $\mathbf{B}$ or $\mathbf{C}$) by a diagonal matrix $\mathbf{L}$ is always allowed, provided that the inverse of $\mathbf{L}$ is accounted for elsewhere. For instance, when slice $\mathbf{X}_k$ is decomposed as $\mathbf{X}_k = \mathbf{AC}_k\mathbf{B}' + \mathbf{E}_k$, the fitted part $\mathbf{AC}_k\mathbf{B}'$ can equivalently be expressed as $\mathbf{AC}_k\mathbf{B}' = \mathbf{ALL}^{-1}\mathbf{C}_k\mathbf{B}' = \mathbf{ALC}_k\mathbf{L}^{-1}\mathbf{B}' = (\mathbf{AL})\mathbf{C}_k(\mathbf{BL}^{-1})'$, showing that $\mathbf{AL}$ may replace $\mathbf{A}$ when $\mathbf{BL}^{-1}$ replaces $\mathbf{B}$. Also, simultaneous permutations of columns of $\mathbf{A}$ and $\mathbf{B}$ and diagonal elements of $\mathbf{C}_k$, $k = 1, \ldots, K$, are allowed. However, apart from rescaling and permuting columns of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$, there is usually no transformational freedom in CP.

Although CP uniqueness is not the topic of this paper, a brief digression may be in order. The first uniqueness proofs of CP date back to Jennrich (quoted in Reference [2]), Harshman [3] and Kruskal [4], who showed that CP has *essential uniqueness*, as explained above, under mild *sufficient* conditions. After decades of silence the topic of CP uniqueness has recently been revived. Sidiropoulos and Bro [5] have given a short-cut proof for Kruskal's sufficient condition and generalized it to n-way arrays ($n > 3$). Ten Berge and Sidiropoulos [6] have shown that Kruskal's *sufficient* conditions are *necessary* for $r = 2$ or 3 but, surprisingly, not for $r > 3$.

CP has acquired great popularity from its application to arrays with symmetric slices. The scalar product version of

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the INDSCAL method of Carroll and Chang [1] relies on CP, hoping that, upon convergence, CP will yield **A** and **B** equal. In practice, this always seems to work. Then each (symmetric) slice is decomposed as

$$\mathbf{X}_k = \mathbf{A}\mathbf{C}_k\mathbf{A}' + \mathbf{E}_k \quad (2)$$

$\mathbf{C}_k$ diagonal, $k=1,\ldots,K$, in the least squares sense. Again, INDSCAL has *essential uniqueness* under mild conditions.

3. TUCKER THREE-WAY PCA

Tucker three-way PCA (3PCA) has been proposed by Tucker [7]. Kroonenberg and De Leeuw [8] have offered an alternating least squares algorithm. It yields matrices **A**, **B** and **C**, with P, Q and R columns respectively, and a $P \times Q \times R$ core array $\underline{\mathbf{G}}$ such that the sum of squares of elements of $\underline{\mathbf{E}}$ is minimized in the decomposition

$$\underline{\mathbf{X}} = \sum_{p=1}^{P}\sum_{q=1}^{Q}\sum_{r=1}^{R} g_{pqr}(\mathbf{a}_p \circ \mathbf{b}_q \circ \mathbf{c}_r) + \underline{\mathbf{E}} \quad (3)$$

where $\mathbf{a}_p \circ \mathbf{b}_q \circ \mathbf{c}_r$ is the so-called outer product of three vectors. It is the three-way array holding slices $\mathbf{a}_p\mathbf{b}_q'$, each multiplied by an element of $\mathbf{c}_r$.

It is important to note that CP is a constrained version of 3PCA, where $P=Q=R$ and the core array is unit superdiagonal: $g_{pqr}=0$ unless $p=q=r$, in which case $g_{pqr}=1$. Hence the ith frontal slice of $\underline{\mathbf{G}}$ is $\mathbf{e}_i\mathbf{e}_i'$, where $\mathbf{e}_i$ is column i of **I**. In 3PCA there are no uniqueness properties like we have for CP. This can be seen from the matrix form of 3PCA, where $\mathbf{X} = [\mathbf{X}_1|\ldots|\mathbf{X}_K]$ is decomposed as

$$\mathbf{X} = [\mathbf{X}_1|\ldots|\mathbf{X}_K] = \mathbf{A}\mathbf{G}(\mathbf{C}' \otimes \mathbf{B}') + [\mathbf{E}_1|\ldots|\mathbf{E}_K] \quad (4)$$

with $\mathbf{G} = [\mathbf{G}_1|\ldots|\mathbf{G}_R]$ the matricized core array. If **S**, **T** and **U** are non-singular matrices, we may equivalently write the fitted part $\mathbf{A}\mathbf{G}(\mathbf{C}' \otimes \mathbf{B}')$ as

$$\begin{aligned}\mathbf{A}\mathbf{G}(\mathbf{C}' \otimes \mathbf{B}') &= \mathbf{A}(\mathbf{S}')^{-1}\mathbf{S}'\mathbf{G}(\mathbf{U}\otimes\mathbf{T})(\mathbf{U}^{-1}\otimes\mathbf{T}^{-1})(\mathbf{C}'\otimes\mathbf{B}') \\ &= \mathbf{A}(\mathbf{S}')^{-1}\mathbf{S}'\mathbf{G}(\mathbf{U}\otimes\mathbf{T})(\mathbf{U}^{-1}\mathbf{C}'\otimes\mathbf{T}^{-1}\mathbf{B}')\end{aligned} \quad (5)$$

Clearly, we may switch to new component matrices $\mathbf{A}(\mathbf{S}')^{-1}$, $\mathbf{B}(\mathbf{T}')^{-1}$ and $\mathbf{C}(\mathbf{U}')^{-1}$ associated with a new core array $\mathbf{S}'\mathbf{G}(\mathbf{U}\otimes\mathbf{T})$. This invariance property implies that there is no uniqueness in 3PCA. Without loss of fit we may pre-multiply all frontal slices of **G** by $\mathbf{S}'$, post-multiply them by **T** and 'mix' them (take linear combinations) by **U**. These transformations are called *Tucker transformations* [9].

4. HYBRID MODELS IN BETWEEN 3PCA AND CP

To introduce the concept of hybrid models, an example will be instructive. Consider a $3\times3\times3$ core array $\underline{\mathbf{G}}$ of 3PCA in matrix form. All its elements, denoted by ?, are unconstrained:

$$\mathbf{G} = \left[\begin{array}{ccc|ccc|ccc} ? & ? & ? & ? & ? & ? & ? & ? & ? \\ ? & ? & ? & ? & ? & ? & ? & ? & ? \\ ? & ? & ? & ? & ? & ? & ? & ? & ? \end{array}\right] \quad (6)$$

In CP, on the other hand, the ith frontal slice of the core is $\mathbf{e}_i\mathbf{e}_i'$, which gives the fully constrained core

$$\mathbf{G} = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \quad (7)$$

Hybrid models have partially constrained cores. For instance, we have six free parameters in

$$\mathbf{G} = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & ? & 0 & ? & 0 \\ 0 & 0 & ? & 0 & 1 & 0 & ? & 0 & 0 \\ 0 & ? & 0 & ? & 0 & 0 & 0 & 0 & 1 \end{array}\right] \quad (8)$$

When dealing with such partially constrained models in between CP and 3PCA, two questions are of interest. First, there is the *question of (non-)triviality*: do Tucker transformations of an unconstrained solution exist which satisfy the constraints? If so, we can run 3PCA first and instil the constraints afterwards, using the freedom of transformation. Secondly, there is the *question of uniqueness*: are Tucker transformations possible (other than trivial transformations such as rescaling or permuting columns of **A** and rows of **G** simultaneously) that preserve the pattern of zeros? If not, there is no transformational freedom left and the solution is unique. Obviously, both non-triviality and uniqueness are desirable characteristics of a constrained core. In the particular hybrid core of (8) the model seems to be trivial with positive probability, and it is essentially unique, just like CP [10]. A discussion of the hybrid core (8) in the context of log–linear modeling can be found in Reference [11].

An even better understood case of constrained cores is that of order $3\times3\times2$. When the two slices can be diagonalized simultaneously, it is possible to arrive at the form

$$\left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & x & 0 & 0 & y & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \quad (9)$$

However, it is generally possible to transform the array to the form

$$\left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & x \\ 0 & 0 & 1 & 0 & y & 0 \end{array}\right] \quad (10)$$

with $x^2=y^2$. Hence cores of the form (10) are trivial. They have been proven partly unique [9].

A practical example that arose in chemometrics is the flow injection analysis system with UV diode array detection of Nørgaard and Ridder [12]. Kiers and Smilde [13] have proven partial uniqueness for the implied core array, constrained to have slices

$$\mathbf{G}_1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \qquad \mathbf{G}_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (11)$$

Although it may seem intuitively obvious that such a constrained core, containing a zero row in each slice, is nontrivial, a formal proof for this has not been given. This will be done below.

Another example from chemometrics arose in Gurden *et al.* [14], who used a hybrid core of the form

$$\mathbf{G} = \left[\begin{array}{ccc|ccc|ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \tag{12}$$

Non-triviality and uniqueness of this core have been discussed by ten Berge and Smilde [15]. We shall revisit their approach to the non-triviality issue below.

Although answers to questions of non-triviality and uniqueness can sometimes be given on an *ad hoc* basis, general rules to decide about triviality and uniqueness are to be preferred. Some rules can be obtained from maximal simplicity results and some from typical rank results. The next sections will be devoted to such rules.

5. TUCKER TRANSFORMATIONS TO MAXIMAL SIMPLICITY

The search for methods to simplify three-way core arrays started with numerical approaches. For instance, Kiers [16] derived three-way Simplimax, an iterative rotation method aimed at finding a core with a specified (small) number of non-zero elements. However, iterative orthonormalization [17] has also been successful in a variety of cases.

The results from these iterative procedures led to a search for direct algebraic solutions for simplicity transformations. In some cases, direct solutions are straightforward. For instance, consider a core of order $5 \times 2 \times 2$. It is trivial to find $\mathbf{S}$ such that

$$\mathbf{S}'\mathbf{G}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}, \qquad \mathbf{S}'\mathbf{G}_2 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{13}$$

All it takes is constructing a 5×5 matrix by putting an extra random column in between $\mathbf{G}_1$ and $\mathbf{G}_2$ and taking $\mathbf{S}'$ as the inverse of that matrix. In this case there is no need to invoke $\mathbf{T}$ or $\mathbf{U}$. However, cases like this, with $P > QR$, do not arise in 3PCA, because they would represent a case of overfactoring (see Reference [7], p. 288).

A more complicated class of cases arises when the array has two slices, with $2Q > P > Q$. Ten Berge and Kiers [18] have shown how to find transformation matrices $\mathbf{S}$ and $\mathbf{T}$ such that

$$\mathbf{S}'\mathbf{G}_1\mathbf{T} = \left[\begin{array}{c} \mathbf{I}_Q \\ \hline \mathbf{O} \end{array}\right], \qquad \mathbf{S}'\mathbf{G}_2\mathbf{T} = \left[\begin{array}{c} \mathbf{O} \\ \hline \mathbf{I}_Q \end{array}\right] \tag{14}$$

Again the solution is non-unique, because $\mathbf{U}$ has not been invoked. Further explicit simplicity results have been given by Rocci and ten Berge [9]. More importantly, they have considered the question of what constitutes *maximal simplicity*. For instance, they proved that $P \times Q \times 2$ arrays with $2Q > P > Q$ cannot have fewer than $2Q$ non-zero elements, as in (14). This is a powerful result, because *all hybrid cores involving more than maximal simplicity are non-trivial*. Unfortunately, except for two-slice arrays and cases where $P = QR - 1$ [19], little has been achieved in the way of maximal simplicity results.

There is an alternative: we may also use typical rank results. Before considering those, however, we revisit the constrained core of (11). The number of six non-zero elements by itself does not imply non-triviality, because it is generically possible to attain a simple form (14), which gives, in this case,

$$\mathbf{H}_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \qquad \mathbf{H}_2 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{15}$$

also having only six non-zero elements. However, the very proof that six non-zero elements is the smallest possible number for an array of this format can be invoked to show that the form (11) is non-trivial; see the proof of Result 4 in Reference [9]. Specifically, if we first transform the array to the simple form (15) and then seek further transformations to obtain slices of rank 2, like we have in (11), we arrive at a contradiction. Starting with the slices given in (15), any transformation will yield slices of the form $\mathbf{S}'(u_{1j}\mathbf{H}_1 + u_{2j}\mathbf{H}_2)\mathbf{T}$, $j = 1{,}2$, with $\mathbf{S}$ and $\mathbf{T}$ non-singular, u_{1j} and u_{2j} being the elements of column j of $\mathbf{U}$, also non-singular. Because multiplying by $\mathbf{S}$ or $\mathbf{T}$ preserves the rank, a transformed slice can have rank less than 3 only if $u_{1j}\mathbf{H}_1 + u_{2j}\mathbf{H}_2$ has rank less than 3, which requires that $u_{1j} = u_{2j} = 0$, rendering column j of the (non-singular) transformation matrix $\mathbf{U}$ zero. The contradiction implies that the core (11) of Nørgaard and Ridder [12] is non-trivial.

6. TYPICAL RANK OF THREE-WAY ARRAYS

Each pair of vectors $\{\mathbf{a},\mathbf{b}\}$ defines a rank-1 matrix $\mathbf{ab}'$, and *vice versa*. A rank-1 matrix has proportional rows and proportional columns. The rank of a matrix $\mathbf{X}$ is the smallest number of rank-1 matrices generating $\mathbf{X}$ as their sum. These matrix concepts immediately transfer to three-way arrays. Specifically, each triplet of vectors $\{\mathbf{a},\mathbf{b},\mathbf{c}\}$ defines a three-way array of rank 1, and *vice versa*. That is, the outer product $\mathbf{a} \circ \mathbf{b} \circ \mathbf{c}$ is the three-way array which has all slices proportional to the rank-1 matrix $\mathbf{ab}'$, the constants of proportionality being the elements of $\mathbf{c}$. A rank-1 array has proportional slices in each direction. Parallel to the definition of matrix rank, the rank of three-way array $\underline{\mathbf{X}}$ is defined as the smallest number of rank-1 arrays generating $\underline{\mathbf{X}}$ as their sum [4,20] (also J. B. Kruskal, unpublished manuscript, 1983). For example, the $3 \times 3 \times 2$ array $\underline{\mathbf{X}}$ with matricized form

$$[\mathbf{X}_1|\mathbf{X}_2] = \left[\begin{array}{ccc|ccc} 2 & 3 & 1 & 1 & 3 & -1 \\ 3 & 5 & 1 & 3 & 7 & -1 \\ 4 & 7 & 1 & 5 & 11 & -1 \end{array}\right] \tag{16}$$

has rank 2 because it can be written as the sum of two non-proportional rank-1 arrays

$$\left[\begin{array}{ccc|ccc} 1 & 2 & 0 & 2 & 4 & 0 \\ 2 & 4 & 0 & 4 & 8 & 0 \\ 3 & 6 & 0 & 6 & 12 & 0 \end{array}\right] + \left[\begin{array}{ccc|ccc} 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \end{array}\right] \tag{17}$$

The rank of a three-way array has a direct link to CP: it is the smallest number of components that is enough for a full CP decomposition.

Usually, *matrices* have the maximal rank they can have, given their order. For instance, a randomly generated 7×5 matrix has rank 5 almost surely. This does not hold for three-way arrays. There is a gap between *typical* rank (the rank an array format has with positive probability under random sampling from a continuous distribution) and *maximal* rank (J. B. Kruskal, unpublished manuscript, 1983). For instance, a $4 \times 4 \times 2$ array has maximal rank 6 and typical rank 4.5. Kruskal [20] has given a general expression for the maximal rank of $P \times Q \times 2$ arrays. In the present context we focus on typical rank, which is more relevant from a practical point of view.

The first results on typical rank go back to J. B. Kruskal (unpublished manuscript, 1983). Recently, a few general principles have been obtained. Because Tucker transformations leave the rank of an array unaffected, transformations to simplicity have proven very helpful in the study of typical rank. Tables I and II demonstrate some of the results. Table I is based on ten Berge and Kiers [18], who solved the typical rank issue for all $P \times Q \times 2$ arrays. Table II gives some values for $P \times Q \times 3$ arrays from ten Berge [21], with the addition that the typical rank of $5 \times 3 \times 3$ arrays has recently been shown to be {5,6}, [22]. The bold face entry in Table II for the typical rank of $5 \times 5 \times 3$ arrays is based on ten Berge and Smilde [15], who applied it to the array (12). This array is the sum of five linearly independent rank-1 arrays, hence its rank is 5. Because arrays of format $5 \times 5 \times 3$ have almost surely rank 6 or higher, the array (12) is non-trivial. This demonstrates how typical rank results can settle questions of non-triviality of hybrid core arrays in between 3PCA and CP.

7. DISCUSSION

Although recently some advances have been made both in simplicity results and in typical rank results, much remains to be done. As far as simplicity is concerned, the two-slice arrays have been settled, but for three-slice arrays only the $3 \times 3 \times 2$, $3 \times 3 \times 7$ and $3 \times 3 \times 8$ cases have been solved [9]. Yet numerical approaches often reveal extreme simplicity as in (8) for $3 \times 3 \times 3$ arrays. A closed-form solution for this form of simplicity is still sorely wanted.

As far as typical rank is concerned, more cases have been solved. Still, general recipes as exist for typical rank over the complex field are absent for the real field. The solutions that do exist often rely on solving up to fourth-degree polynomials. The prospects for extending these results by dealing with higher order polynomials seem remote.

Table I. Typical rank of $P \times Q \times 2$ arrays

	$Q=2$	$Q=3$	$Q=4$
$P=2$	{2,3}	3	4
$P=3$	3	{3,4}	4
$P=4$	4	4	{4,5}
$P=5$	4	5	5
$P=6$	4	6	6
$P=7$	4	6	7
$P=8$	4	6	8
$P=9$	4	6	8

Table II. Typical rank of $P \times Q \times 3$ arrays

	$Q=3$	$Q=4$	$Q=5$
$P=5$	{5,6}	?	$\geqslant$ **6**
$P=6$	6	?	?
$P=7$	7	?	?
$P=8$	8	{8,9}	?
$P=9$	9	9	?
$P=10$	9	10	10
$P=11$	9	11	11
$P=12$	9	12	12

The typical rank results discussed in this paper do not apply to arrays of symmetric slices. In general, it seems that symmetry often entails a lower typical rank, which means that we need fewer components for a full INDSCAL decomposition of symmetric slices than for CP of non-symmetric slices of the same order. However, in a number of cases the typical rank of symmetric arrays is as high as that of their non-symmetric counterparts. Further details can be found in Reference [23].

Just like CP is a constrained version of 3PCA, INDSCAL is a constrained version of three-mode scaling (see Reference [24], p. 49), a variant of 3PCA applied to arrays of symmetric slices. It has $\mathbf{A} = \mathbf{B}$, and the core consists of symmetric slices also. The typical rank results for symmetric arrays might apply here, to scrutinize a constrained simple core array for possible triviality. However, we are not aware of any recent applications of three-mode scaling.

Acknowledgements

The author is obliged to an anonymous referee and Alwin Stegeman for helpful comments on a previous draft.

REFERENCES

1. Carroll JD, Chang JJ. Analysis of individual differences in multidimensional scaling via an *N*-way generalization of Eckart–Young decomposition. *Psychometrika* 1970; **35**: 283–319.
2. Harshman RA. Foundations of the PARAFAC procedure: models and conditions for an 'explanatory' multi-mode factor analysis. *UCLA Working Papers Phonet*. 1970; **16**: 1–84.
3. Harshman RA. Determination and proof of minimum uniqueness conditions for PARAFAC1. *UCLA Working Papers Phonet*. 1972; **22**: 111–117.
4. Kruskal JB. Three-way arrays: rank and uniqueness of trilinear decompositions, with applications to arithmetic complexity and statistics. *Linear Algebra Appl*. 1977; **18**: 95–138.
5. Sidiropoulos ND, Bro R. On the uniqueness of multilinear decomposition of *N*-way arrays. *J. Chemometrics* 2000; **14**: 229–239.
6. Ten Berge JMF, Sidiropoulos ND. On uniqueness in CANDECOMP/PARAFAC. *Psychometrika* 2002; **67**: 399–409.
7. Tucker LR. Some mathematical notes on three-mode factor analysis. *Psychometrika* 1966; **31**: 279–311.
8. Kroonenberg PM, De Leeuw J. Principal component analysis of three-mode data by means of alternating least-squares. *Psychometrika* 1980; **45**: 69–97.

9. Rocci R, ten Berge JMF. Transforming three-way arrays to maximal simplicity. *Psychometrika* 2002; **67**: 351–365.
10. Kiers HAL, ten Berge JMF, Rocci R. Uniqueness of three-mode factor models with sparse cores: the $3 \times 3 \times 3$ case. *Psychometrika* 1997; **62**: 349–374.
11. Wong RS-K. Multidimensional association models. A multilinear approach. *Sociol Methods Res* 2001; **30**: 197–240.
12. Nørgaard L, Ridder C. *Chemometrics Intell. Lab. Syst.* 1994; **23**: 107–114.
13. Kiers HAL, Smilde AK. Constrained three-mode factor analysis as a tool for parameter estimation with second-order instrumental data. *J. Chemometrics* 1998; **12**: 125–147.
14. Gurden SP, Westerhuis JA, Bijlsma S, Smilde A. Modeling of spectroscopic batch process data using grey models to incorporate external information. *J. Chemometrics* 2001; **15**: 101–121.
15. Ten Berge JMF, Smilde AK. Non-triviality and identification of a constrained Tucker3 analysis. *J. Chemometrics* 2002; **16**: 609–612.
16. Kiers HAL. Three-way SIMPLIMAX for oblique rotation of the three-mode factor analysis core to simple structure. *Comput. Statist. Data Anal.* 1998; **28**: 307–324.
17. Ten Berge JMF, Kiers HAL, Murakami T, Van der Heijden R. Transforming three-way arrays to multiple orthonormality. *J. Chemometrics* 2000; **14**: 275–284.
18. Ten Berge JMF, Kiers HAL. Simplicity of core arrays in three-way principal component analysis and the typical rank of $P \times Q \times 2$ arrays. *Linear Algebra Appl.* 1999; **294**: 169–179.
19. Murakami T, ten Berge JMF, Kiers HAL. A case of extreme simplicity of the core matrix in three-mode principal components analysis. *Psychometrika* 1998; **63**: 255–261.
20. Kruskal JB. Rank, decomposition, and uniqueness for 3-way and *N*-way arrays. In *Multiway Data Analysis*, Coppi R, Bolasco S (eds). Elsevier: Amsterdam, 1989; 7–18.
21. Ten Berge JMF. The typical rank of tall three-way arrays. *Psychometrika* 2000; **65**: 525–532.
22. Ten Berge JMF. Partial uniqueness in CANDECOMP/PARAFAC. *J. Chemometrics* 2004; **18**: 12–16.
23. Ten Berge JMF, Sidiropoulos ND, Rocci R. Typical rank and INDSCAL dimensionality for symmetric arrays of order $I \times 2 \times 2$ or $I \times 3 \times 3$. *Linear Algebra Appl* (in press).
24. Kroonenberg PM. *Three-mode Principal Component Analysis*. DSWO: Leiden, 1983.

