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TRANSFORMING THREE-WAY ARRAYS TO MAXIMAL SIMPLICITY

ROBERTO ROCCI

UNIVERSITY OF MOLISE

JOS M.F. TEN BERGE

UNIVERSITY OF GRONINGEN

Transforming the core array in Tucker three-way component analysis to simplicity is an intriguing way of revealing structures in between standard Tucker three-way PCA, where the core array is unconstrained, and CANDECOMP/PARAFAC, where the core array has a generalized diagonal form. For certain classes of arrays, transformations to simplicity, that is, transformations that produce a large number of zeros, can be obtained explicitly by solving sets of linear equations. The present paper extends these results. First, a method is offered to simplify $J \times J \times 2$ arrays. Next, it is shown that the transformation that simplifies an $I \times J \times K$ array can be used to also simplify the (complementary) arrays of order $(JK - I) \times J \times K$, of order $I \times (IK - J) \times K$ and of order $I \times J \times (IJ - K)$. Finally, the question of what constitutes the maximal simplicity for arrays (the maximal number of zero elements) will be considered. It is shown that cases of extreme simplicity, considered in the past, are, in fact, cases of maximal simplicity.

Key words: three-way PCA, core array, simplicity.

Tucker 3-analysis (Tucker, 1966) is a three-way generalisation of PCA based on the following approximate factorisation of the data array

$$x_{ijk} \approx \sum_{p=1}^{P} \sum_{q=1}^{Q} \sum_{r=1}^{R} a_{ip} b_{jq} c_{kr} g_{pqr},$$

where x_{ijk} is the value of unit i on variable j at occasion k, a_{ip} is an element of an $I \times P$ component matrix **A** for individuals, b_{jq} is an element of a $J \times Q$ component matrix **B** for variables, c_{kr} an element of a $K \times R$ component matrix **C** for occasions, and g_{pqr} is an element of a so-called three-way *core* array $\underline{\mathbf{G}}$ of order $P \times Q \times R$, containing weights for the joint impact of any triple of components from **A**, **B** and **C**. The parameters are usually estimated by minimising the sum of squared residuals for fixed numbers of components in each mode (Kroonenberg & de Leeuw, 1980).

It is well-known that the parameters of the Tucker-3 model are not uniquely determined. In particular, the core array can be transformed in three directions. For instance, a $3 \times 3 \times 2$ core array containing two slabs or slices $\mathbf{G}_1$ and $\mathbf{G}_2$ can be replaced by an array with slices $\mathbf{SG}_1\mathbf{T}$ and $\mathbf{SG}_2\mathbf{T}$, respectively, for any pair of nonsingular 3×3 matrices **S** and **T**. In addition, there is the possibility of transforming the array in the third direction by so-called slabmixing. That is, when **U** is any nonsingular 2×2 matrix, we may also transform $\mathbf{SG}_1\mathbf{T}$ and $\mathbf{SG}_2\mathbf{T}$ into $\mathbf{G}_1^* = u_{11}\mathbf{SG}_1\mathbf{T} + u_{21}\mathbf{SG}_2\mathbf{T}$ and $\mathbf{G}_2^* = u_{12}\mathbf{SG}_1\mathbf{T} + u_{22}\mathbf{SG}_2\mathbf{T}$, respectively. In general, the slabs $\mathbf{G}_1, \ldots, \mathbf{G}_R$, of any core array can be transformed to $\mathbf{G}_1^*, \ldots, \mathbf{G}_R^*$ by means of the *Tucker transformation*

Requests for reprints should be sent to Jos M.F. ten Berge, Heÿmans Institute of Psychological Research, University of Groningen, Grote Kruisstraat 2/1, 9712 TS Groningen, THE NETHERLANDS. E-Mail: j.m.f.ten.berge@ppsw.rug.nl

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$$\mathbf{G}_l^* = \mathbf{S}\left(\sum_{m=1}^{R} u_{ml}\mathbf{G}_m\right)\mathbf{T}, l = 1, \ldots, R,$$

where **S**, **T** and **U** are nonsingular.

The Tucker-3 model fit is not affected by such transformations provided that the component matrices are counter-transformed by the inverse matrices $\mathbf{S}^{-1}$, $(\mathbf{T}')^{-1}$, and $(\mathbf{U}')^{-1}$. In fact, rewriting the model in matrix notation as

$$\mathbf{X}_k \approx \mathbf{A}\left(\sum_{r=1}^{R} c_{kr}\mathbf{G}_r\right)\mathbf{B}', \quad k = 1, 2, \ldots, K,$$

we have

$$\begin{aligned}\mathbf{A}\left(\sum_{r=1}^{R} c_{kr}\mathbf{G}_r\right)\mathbf{B}' &= \mathbf{AS}^{-1}\mathbf{S}\left[\sum_{r=1}^{R} c_{kr}\sum_{l=1}^{R} u_{lr}^*\sum_{m=1}^{R} u_{ml}\mathbf{G}_m\right]\mathbf{TT}^{-1}\mathbf{B}' \\ &= \left(\mathbf{AS}^{-1}\right)\left[\sum_{l=1}^{R}\left(\sum_{r=1}^{R} c_{kr}u_{lr}^*\right)\mathbf{S}\left(\sum_{m=1}^{R} u_{ml}\mathbf{G}_m\right)\mathbf{T}\right]\left(\mathbf{T}^{-1}\mathbf{B}'\right) \\ &= \mathbf{A}^*\left(\sum_{l=1}^{R} c_{kl}^*\mathbf{G}_l^*\right)\mathbf{B}^{*\prime}, \quad k = 1, 2, \ldots, K\end{aligned}$$

where u_{lr}^* indicates an element of $\mathbf{U}^{-1}$, $\mathbf{A}^* = \mathbf{AS}^{-1}$, $\mathbf{B}^* = \mathbf{B}(\mathbf{T}')^{-1}$ and $\mathbf{C}^* = \mathbf{C}\left(\mathbf{U}'\right)^{-1}$, also see Tucker (1966).

The interpretation of a Tucker-3 analysis can be rather difficult because we have to evaluate the impact of each triple of components to explain the data. To reduce this difficulty, we can use the transformational freedom of the model to attain a "simple" core, that is, a core with a large majority of zero elements. In this way the interpretation of the results should be easier because many triples of components appear to have no impact, see Kiers (1998a, 1998b) for a discussion. This approach is supported by previous studies on transformations to simplicity which have shown that many elements of the core array can be zeroed without any loss of fit (see Murakami, ten Berge, & Kiers, 1998; Rocci, 2001; ten Berge & Kiers, 1999). For instance, it will be shown below that the slabs of a $3 \times 3 \times 2$ array can generally be simplified to

$$\mathbf{G}_1^* = \begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix} \quad \mathbf{G}_2^* = \begin{bmatrix}0 & 0 & 0\\ 0 & 0 & x\\ 0 & y & 0\end{bmatrix}, \tag{1}$$

where x and y stand for nonzero elements.

The question of how a core array in Tucker-3 analysis can be transformed to simplicity (a large number of zeros) will be studied here from a more general point of view. That is, we shall deal with the general question of how any (real valued) three-way array can be transformed by (real valued) nonsingular transformations in three directions, to have as many zeros as possible. The answer will have various implications for three-way analysis.

1. In the context of CANDECOMP/PARAFAC (Carroll & Chang, 1970; Harshman, 1970), maximal simplicity has direct implications for the rank (the smallest number of components sufficient to fully decompose the array in CANDECOMP/PARAFAC) of a three-way array. For instance, if a $3 \times 3 \times 2$ array can be transformed to the form (1), we know at once that the rank of the original array will not be above 5, because the number of nonzero elements in a three-way array is a universal upper bound to the rank, and the transformations used to attain (1) are rank-preserving.

2. As indicated above, simplifying a Tucker-3 core array may simplify the interpretation because many triples of components appear to have no impact. However, it should be pointed out that Murakami (1999) has given an example where the components tend to collinearity when the core is transformed to extreme simplicity. In his particular example, the simplicity transformation happened to be unique. Conceivably, the collinearity problem at hand can be avoided when the transformation involved is not unique.
3. Simplicity results seem particularly interesting for three-way methods in between CANDECOMP/PARAFAC and Tucker-3. For example, Kiers, ten Berge and Rocci (1997) have described a model based on 9 nonzero elements in a $3 \times 3 \times 3$ Tucker-3 core array, and have proven that it is unique. It would be interesting to know whether or not the simple core array they specified can always be obtained by choosing a certain simplicity transformation, to distinguish mathematical artifacts from empirical results.

Another example can be found in Gurden, Westerhuis, Bijlsma and Smilde (2001), who fitted a Tucker-3 model with the core array, of order $5 \times 5 \times 3$, constrained to have only 5 nonzero elements in specified places. It is relevant to know whether or not this simple core can always be attained by transformations (as it happens, it cannot). Again, it is important to know where artifacts begin, because that is where meaningful empirical research comes to an end.

The search for simplicity transformations is a fairly recent endeavor. It started with iterative procedures, designed to obtain a large number of zeros in Tucker-3 core arrays. For instance, Kiers (1998b), also see Kiers (1992), has developed methods to attain small numbers of nonzero elements directly. However, simplicity can also be obtained indirectly, as a by-product of iterative orthonormalizing transformations (ten Berge, Kiers, Murakami & van der Heijden, 2000).

These numerical procedures gave rise to certain hypotheses about feasible simple forms that were subsequently dealt with from a purely algebraic point of view, to obtain closed-form solutions for the required transformations. So far, this has led to only a couple of results of some generality. Murakami, ten Berge and Kiers (1998) have shown how $I \times J \times K$ arrays, when $K = IJ - 1$ and $J \geq I$, can be transformed to have only $I + K - 1$ nonzero elements. Ten Berge and Kiers (1999) have described transformations to extreme simplicity for $I \times J \times 2$ arrays, when $I \neq J$. Both results will be reviewed in the next section.

The present paper goes beyond these results, in three respects. Firstly, we provide simplicity transformations for $2 \times 2 \times 2$ and $3 \times 3 \times 2$ arrays and, in fact, for $J \times J \times 2$ arrays in general (see the Appendix). Secondly, it will be shown that simplicity transformations for any array of a particular order $I \times J \times K$ can be used to simplify *complementary arrays*, defined as arrays of order $(JK - I) \times J \times K$, $I \times (IK - J) \times K$ and $I \times J \times (IJ - K)$, at once, which considerably broadens the class of arrays for which explicit simplicity transformations are available.

Thirdly, we will enhance the practical value of existing simplicity results by taking up the very issue of *maximal* simplicity. So far, all available transformations to simplicity yield "extreme simplicity," without knowledge on what constitutes maximal simplicity, defined as the maximum number of zero elements that can be attained. It will be proven that extreme simplicity resulting from various explicit transformation methods are, in fact, maximal simplicity results, which implies that it is not possible to obtain more zeros by any other Tucker transformation. We start by considering previous simplicity results.

Previous Simplicity Results

Murakami, ten Berge and Kiers (1998) have shown that $I \times J \times K$ arrays can be transformed to have only $I + K - 1$ nonzero elements when $K = IJ - 1$ and $J \geq I$. In addition, these nonzero elements can be set to any specified value, such as 1. For example, a $2 \times 3 \times 5$ array can be transformed into an array with slabs

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

with all but 6 elements zero. Similarly, $3 \times 3 \times 8$ arrays can be transformed to

$$\begin{bmatrix}1&0&0\\0&0&0\\0&0&1\end{bmatrix}\begin{bmatrix}0&0&0\\0&1&0\\0&0&1\end{bmatrix}\begin{bmatrix}0&1&0\\0&0&0\\0&0&0\end{bmatrix}\begin{bmatrix}0&0&1\\0&0&0\\0&0&0\end{bmatrix}\begin{bmatrix}0&0&0\\0&0&1\\0&0&0\end{bmatrix}\begin{bmatrix}0&0&0\\1&0&0\\0&0&0\end{bmatrix}\begin{bmatrix}0&0&0\\0&0&0\\1&0&0\end{bmatrix}\begin{bmatrix}0&0&0\\0&0&0\\0&1&0\end{bmatrix}$$

with only 10 elements nonzero. In general, we obtain $I(J-1)$ slabs with only one nonzero element and $I-1$ slices with only two nonzero elements.

Ten Berge and Kiers (1999) have shown that, for almost all $I \times J \times 2$ arrays with $I > J$, we can attain the identity submatrix form

$$\begin{bmatrix}\mathbf{I}_J\\ \hline \mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{0}\\ \hline \mathbf{I}_J\end{bmatrix},$$

which has the identity matrix $\mathbf{I}_J$ on top in the first slab, and zeros below, and vice versa for the second slab. For example, $4 \times 3 \times 2$ arrays can be simplified to

$$\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\\0&0&0\end{bmatrix}\begin{bmatrix}0&0&0\\1&0&0\\0&1&0\\0&0&1\end{bmatrix}. \tag{2}$$

Both the Murakami form (when$K = IJ-1$) and the ten Berge & Kiers form (when $K = 2$) can be attained by transforming the array in only two of the three possible directions. The present paper goes beyond these results, by using all three of these. The first class of problems that will be considered is concerned with the $I \times J \times K$ case where $K = 2$, but with I and J equal. This is the part of the $K = 2$ class that was not treated by ten Berge and Kiers (1999).

Simplifying the $J \times J \times 2$ Arrays

A $J \times J \times 2$ array $\underline{\mathbf{X}}$ consists of two slices (slabs) $\mathbf{X}_1$ and $\mathbf{X}_2$ of order $J \times J$. We exclusively consider cases where there exists at least one invertible matrix which is a slabmix of $\mathbf{X}_1$ and $\mathbf{X}_2$, whence, without loss of generality, we suppose that $\mathbf{X}_1$ is nonsingular. We also suppose that $\mathbf{X}_1^{-1}\mathbf{X}_2$ is diagonalizable, that is, it can be written as $\mathbf{K}\mathbf{\Lambda}\mathbf{K}^{-1}$, with $\mathbf{\Lambda}$ diagonal, where some elements of $\mathbf{\Lambda}$ or $\mathbf{K}$ may be complex. Other cases do in theory exist but never seem to arise in practice.

When $\mathbf{X}_1^{-1}\mathbf{X}_2$ has a real eigendecomposition $\mathbf{X}_1^{-1}\mathbf{X}_2 = \mathbf{K}\mathbf{\Lambda}\mathbf{K}^{-1}$, that is, $\mathbf{\Lambda}$ and $\mathbf{K}$ do not have complex elements, the eigenvectors can be used to diagonalize the matrices simultaneously, for example, ten Berge (1991). Specifically, we can replace $\mathbf{X}_1$ and $\mathbf{X}_2$ by the diagonal matrices $\mathbf{S}\mathbf{X}_1\mathbf{T} = \mathbf{I}_J$ and $\mathbf{S}\mathbf{X}_2\mathbf{T} = \mathbf{\Lambda}$, using $\mathbf{S} = \mathbf{K}^{-1}\mathbf{X}_1^{-1}$ and $\mathbf{T} = \mathbf{K}$. A slabmix will also set two of the diagonal elements to zero, reducing the number of nonzero elements to $2J-2$. Let λ_j, $j = 1, \ldots, J$, be the eigenvalues in $\mathbf{\Lambda}$. Then, for $J = 2$, we can attain the simplified form

$$\begin{bmatrix}\lambda_2-\lambda_1 & 0\\ 0 & 0\end{bmatrix}, \begin{bmatrix}0 & 0\\ 0 & \lambda_2-\lambda_1\end{bmatrix}.$$

For $J = 3$, we can attain a simplified array of the form

$$\begin{bmatrix}\lambda_2-\lambda_1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & \lambda_2-\lambda_3\end{bmatrix}, \begin{bmatrix}0 & 0 & 0\\ 0 & \lambda_2-\lambda_1 & 0\\ 0 & 0 & \lambda_3-\lambda_1\end{bmatrix}, \tag{3}$$

and so on.

When some elements of $\mathbf{\Lambda}$ and $\mathbf{K}$ are complex, simultaneous diagonality is not possible. Still, we can find a very simple form. At this point, it is important to note that $(\mathbf{S}\mathbf{X}_1\mathbf{T})^{-1}\mathbf{S}\mathbf{X}_2\mathbf{T}$

has the same eigenvalues as $\mathbf{X}_1^{-1}\mathbf{X}_2$. The only way to change the eigenvalues of "the inverse of one slab times the other slab" rests in the slabmix. It is worth pinpointing this influence in detail. Suppose we mix the slabs by a nonsingular matrix $\mathbf{U}$, of the form

$$\mathbf{U} = \begin{bmatrix} 1 & u_{12} \\ u_{21} & 1 \end{bmatrix}.$$

We thus create mixed slabs $\mathbf{Y}_1 = \mathbf{X}_1 + u_{21}\mathbf{X}_2$, and $\mathbf{Y}_2 = u_{12}\mathbf{X}_1 + \mathbf{X}_2$. The question is how the eigenvalues of $\mathbf{Y}_1^{-1}\mathbf{Y}_2$ can be manipulated by $\mathbf{U}$. Without loss of generality, we set $\mathbf{X}_1 = \mathbf{I}$, and define $\mathbf{\Lambda} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_J)$ as the matrix of eigenvalues of $\mathbf{X}_2$, so $\mathbf{X}_2 = \mathbf{K\Lambda K}^{-1}$, with $\mathbf{K}$ and $\mathbf{\Lambda}$ complex. Now, requiring that $u_{21} \neq -1/\lambda_h$ if $\text{IM}(\lambda_h) = 0$, we can write

$$\mathbf{Y}_1^{-1}\mathbf{Y}_2 = (\mathbf{KK}^{-1} + u_{21}\mathbf{K\Lambda K}^{-1})^{-1}(u_{12}\mathbf{KK}^{-1} + \mathbf{K\Lambda K}^{-1}) = \mathbf{K}(\mathbf{I} + u_{21}\mathbf{\Lambda})^{-1}(u_{12}\mathbf{I} + \mathbf{\Lambda})\mathbf{K}^{-1}.$$

Because $\mathbf{\Gamma} \equiv (\mathbf{I} + u_{21}\mathbf{\Lambda})^{-1}(u_{12}\mathbf{I} + \mathbf{\Lambda})$ is diagonal, each eigenvalue λ_h of $\mathbf{X}_2$ is transformed to an eigenvalue γ_h of $\mathbf{Y}_1^{-1}\mathbf{Y}_2$ by the rule

$$\gamma_h = (u_{12} + \lambda_h)/(1 + u_{21}\lambda_h),$$

or, letting $\gamma_h = \eta + i\mu$, $\lambda_h = \alpha + i\beta$, and using the real coding of complex numbers,

$$\eta + i\mu = \frac{1}{(1 + u_{21}\alpha)^2 + (u_{21}\beta)^2}\left\{(1 + u_{21}\alpha)(u_{12} + \alpha) + u_{21}\beta^2 + i\beta(1 - u_{21}u_{12})\right\}. \quad (4)$$

This expression is at the basis of

Result 1. The slabmix permits producing complex eigenvalues with real part zero.

Proof. It is immediate from (4) that the real part of γ_h, that is, η, vanishes if and only if

$$(1 + u_{21}\alpha)(u_{12} + \alpha) + u_{21}\beta^2 = 0. \quad (5)$$

□

Note that, because $\mathbf{U}$ is nonsingular, the h-th eigenvalue γ_h after the slabmix is real if and only if the h-th eigenvalue λ_h before the slabmix is real. This shows that the slabmix cannot change the *number* of complex eigenvalues. Result 1 does show, however, that solving (5) allows us to change the *nature* of the complex eigenvalues, to the effect that at least one pair of them will be purely complex (i.e., with real part zero).

When $J = 2$, any solution for $\mathbf{U}$ which satisfies (5) will produce a pair of purely complex eigenvalues $i\mu$ and $-i\mu$ for $\mathbf{Y}_1^{-1}\mathbf{Y}_2$. We have ample freedom to do this. For instance, we may solve (5) with $u_{21} = 0$ or with $u_{12} = 0$, or we may solve (5) subject to $u_{21} = -u_{12}$, which renders $\mathbf{U}$ proportional to an orthonormal matrix. We shall now demonstrate how purely complex eigenvalues can be used to obtain simplicity, when $J = 2$.

It is clear that $\mathbf{Y}_1^{-1}\mathbf{Y}_2 = \mathbf{K\Gamma K}^{-1}$, with $\mathbf{\Gamma} = \text{diag}(i\mu, -i\mu)$. Define $\mathbf{A} = \mathbf{Y}_1^{-1}\mathbf{Y}_2$. Then $\mathbf{A}^2$ has two equal real eigenvalues $-\mu^2$. Let $\mathbf{t}_1$ be a real eigenvector of $\mathbf{A}^2$, so $\mathbf{A}^2\mathbf{t}_1 = -\mu^2\mathbf{t}_1$. Define $\mathbf{t}_2 = -\mathbf{A}\mathbf{t}_1/\mu$, and let $\mathbf{T} = [\mathbf{t}_1|\mathbf{t}_2]$, and $\mathbf{S} = \mathbf{T}^{-1}\mathbf{Y}_1^{-1}$. Then we have already $\mathbf{SY}_1\mathbf{T} = \mathbf{I}_2$. Next, we note that $\mathbf{At}_1 = -\mu\mathbf{t}_2$, so $\mathbf{A}^2\mathbf{t}_1 = -\mu\mathbf{At}_2 = -\mu^2\mathbf{t}_1$. Hence $\mathbf{At}_1 = -\mu\mathbf{t}_2$ and $\mathbf{At}_2 = \mu\mathbf{t}_1$, which means that

$$\mathbf{AT} = [-\mu\mathbf{t}_2 \mid \mu\mathbf{t}_1] = \mathbf{T}\begin{bmatrix} 0 & \mu \\ -\mu & 0 \end{bmatrix}.$$

It follows that $\mathbf{Y}_1^{-1}\mathbf{Y}_2\mathbf{T} = \mathbf{T}\begin{bmatrix} 0 & \mu \\ -\mu & 0 \end{bmatrix}$, so $\mathbf{Y}_2\mathbf{T} = \mathbf{Y}_1\mathbf{T}\begin{bmatrix} 0 & \mu \\ -\mu & 0 \end{bmatrix}$, hence $\mathbf{S}\mathbf{Y}_2\mathbf{T} = \begin{bmatrix} 0 & \mu \\ -\mu & 0 \end{bmatrix}$. Note that $\mathbf{T}$ must be invertible, otherwise, if $\mathbf{t}_1$ is proportional to $\mathbf{t}_2$, $\mathbf{t}_1$ would be an eigenvetor associated with a real eigenvalue of $\mathbf{A}$.

We have thus simplified the $2 \times 2 \times 2$ array to the form

$$\mathbf{S}\mathbf{Y}_1\mathbf{T} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \mathbf{S}\mathbf{Y}_2\mathbf{T} = \begin{bmatrix} 0 & \mu \\ -\mu & 0 \end{bmatrix}. \tag{6}$$

When $J = 3$, and two eigenvalues are complex, we may obtain one eigenvalue zero by taking $u_{12} = -\lambda_1$, where λ_1 is the real eigenvalue of $\mathbf{X}_1^{-1}\mathbf{X}_2$. The associated eigenvector will also be real, and is the first column of $\mathbf{T}$. We solve (5) for u_{21}, which amounts to evaluating $u_{21} = \frac{\lambda_1-\alpha}{\alpha^2-\alpha\lambda_1+\beta^2}$. Using an eigenvector of $\mathbf{A}^2$, associated with a nonzero eigenvalue, and applying the method used in the $J = 2$ case, yields the other two columns of $\mathbf{T}$. Finally, upon setting $\mathbf{S} = \mathbf{T}^{-1}\mathbf{Y}_1^{-1}$, we find simplicity in the form

$$\mathbf{S}\mathbf{Y}_1\mathbf{T} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \mathbf{S}\mathbf{Y}_2\mathbf{T} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \mu \\ 0 & -\mu & 0 \end{bmatrix}. \tag{7}$$

It can be shown that, if the eigenvalues are real, we also can obtain (7), but without the minus sign in $\mathbf{S}\mathbf{Y}_2\mathbf{T}$. Since this form is less simple than (3), in the sense that it has more nonzero elements, it will be ignored.

Simplicity for $J \times J \times 2$ arrays with $J > 3$ will be treated in the Appendix. We continue with the orthogonal complement method.

The Orthogonal Complement Algorithm

So far we have been concerned with Tucker transformations to simplicity for arrays with $K = 2$ (ten Berge & Kiers, 1999, and the previous section). For arrays with $K = IJ - 1$ we can use the results of Murakami, ten Berge & Kiers (1998). The "smallest" array in the Murakami class, which is not in the $K = 2$ class, is the $3 \times 3 \times 8$ array. So we can simplify the $3 \times 3 \times 8$ array and the $3 \times 3 \times 2$ array (previous section), but nothing in between. We shall now show how to simplify, for instance, a $3 \times 3 \times 7$ array introducing the *orthogonal complement* algorithm which is an algorithm to simplify an array "indirectly." Before illustrating the algorithm in detail, we have to introduce the concept of *orthogonal complementary array* and its main properties.

Below, we shall often use the (row) vectorised version of a matrix, where the rows of a matrix $\mathbf{W}$ are stacked one below the other into a column vector denoted by $\text{vec}(\mathbf{W})$. We shall use also a matrix version of an $I \times J \times K$ array, where the I rows of each slice are stacked column-wise into a $IJ \times K$ matrix. This $IJ \times K$ matrix will be referred to as the mvec form of the array. Specifically, $\text{mvec}(\underline{\mathbf{X}}) = [\text{vec}(\mathbf{X}_1)| \cdots |\text{vec}(\mathbf{X}_K)]$.

For example, a $3 \times 3 \times 7$ array can be rewritten in mvec form as a 9×7 matrix. Clearly, there exists a 9×2 matrix which completes that matrix to a square 9×9 matrix. The latter 9×2 matrix, in turn, can be thought of as the mvec form of a $3 \times 3 \times 2$ array. In this sense, we shall say that the $3 \times 3 \times 7$ and the $3 \times 3 \times 2$ arrays are of complementary sizes.

In general, arrays of size $I \times J \times K$ are complementary to arrays of size $(JK - I) \times J \times K$, of size $I \times (IK - J) \times K$, and of size $I \times J \times (IJ - K)$. For instance, $5 \times 4 \times 3$ arrays are complementary to $7 \times 4 \times 3$ arrays, to $5 \times 11 \times 3$ arrays, and to $5 \times 4 \times 17$ arrays. However, for the sake of brevity and without loss of generality, in what follows we will refer only to arrays which are of complementary sizes along the third way, that is $I \times J \times K$ and $I \times J \times (IJ - K)$. We will also ignore the case where an array has linearly dependent slices in one of the three directions.

Two arrays of complementary sizes may be also *orthogonal* in the following sense:

Definition 1. An orthogonal complement to an $I \times J \times K$ array $\underline{\mathbf{X}}$ is an $I \times J \times (IJ-K)$ array $\underline{\mathbf{X}}_c$ such that the columns of its mvec form $\mathbf{X}_c$ span the space orthogonal to the column space of $\mathbf{X}$, the mvec form of $\underline{\mathbf{X}}$, and completes $\mathbf{X}$ to a square nonsingular matrix. That is, $[\mathbf{X} \mid \mathbf{X}_c]$ is nonsingular and $\mathbf{X}'\mathbf{X}_c = 0$. Note that it is not required that the columns within $\mathbf{X}$ or within $\mathbf{X}_c$ are orthogonal. The following result is immediate:

Result 2. If $\mathbf{X}_c$ is an orthogonal complement to $\mathbf{X}$ then every other orthogonal complementary matrix can be written in the form $\mathbf{X}_c\mathbf{V}$, for some nonsingular $\mathbf{V}$.

We are interested in orthogonal complementary arrays because it can be easily verified that every array in simple form has an orthogonal complementary array which is also in simple form. For example, suppose we have a $3 \times 3 \times 2$ array $\underline{\mathbf{X}}$ having the following simple mvec form

$$\mathbf{X}'_{9,2} = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \mu & 0 & -\mu & 0 \end{bmatrix}$$

which is the mvec form of (7). A simple orthogonal complement is given by

$$\mathbf{X}_{9,7} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 \end{bmatrix}. \tag{8}$$

It is readily seen that $\mathbf{X}_{9,7}$ is of rank 7, and that its columns are orthogonal to those of $\mathbf{X}_{9,2}$.

The simplicity transformations considered in the present paper typically entail simplicity for the orthogonal complementary arrays also. This is because the mvec forms involved can be permuted into direct sum form, and finding an orthogonal complement to a direct sum amounts to finding orthogonal complements for the nonzero blocks in the direct sum. An example may clarify this:

The mvec form $\mathbf{X}_{9,2}$ given above can be permuted row-wise into the direct sum form

$$\begin{bmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{B} \\ \mathbf{0} & \mathbf{0} \end{bmatrix},$$

where $\mathbf{A} = [1\,1\,1]'$, and $\mathbf{B} = [\mu - \mu]'$. Finding a simple orthogonal complement can be done by taking the direct sum of a 3×2 matrix $\mathbf{A}^*$ orthogonal to $\mathbf{A}$, a simple 2×1 matrix $\mathbf{B}^*$ orthogonal to $\mathbf{B}$, and 4 columns of the identity matrix. So the orthogonal complement has the form

$$\begin{bmatrix} \mathbf{A}^* & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{B}^* & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_4 \end{bmatrix}.$$

Permuting the rows back to the original order gives $\mathbf{X}_{9,7}$ given above.

It can be proven generally that the structure of optimal simplicity for the orthogonal complement of a direct sum is another direct sum. What remains is to find optimal block-wise simplicity. The possibilities are completely determined by the order of the complementary blocks. When, for instance, the block $\mathbf{A}$ has p rows and q columns, $\mathbf{A}^*$ is of order $p \times (p-q)$. It can be shown that $\mathbf{A}^*$ can be taken in banded form where each column has only $q+1$ nonzero elements (proofs are available from the authors).

The last property we have to establish is the link between the orthogonal complement of an array and the orthogonal complement of its Tucker transformation.

It is well-known that, for any three matrices **A**, **B**, and **C**, $\text{vec}(\mathbf{ABC}) = (\mathbf{A} \otimes \mathbf{C}')\text{vec}(\mathbf{B})$, with $\otimes$ the (right hand) Kronecker product. Given an $I \times J \times K$ array $\underline{\mathbf{X}}$ we consider its mvec form $\mathbf{X}_{IJ,K} = [\text{vec}(\mathbf{X}_1)| \cdots |\text{vec}(\mathbf{X}_K)]$ and the Tucker transformation

$$\begin{aligned}\mathbf{H}_{IJ,K} &= [\text{vec}(\mathbf{H}_1)| \cdots |\text{vec}(\mathbf{H}_K)] \\ &= [\text{vec}(\mathbf{S}(u_{11}\mathbf{X}_1 + \cdots + u_{K1}\mathbf{X}_K)\mathbf{T})| \cdots |\text{vec}(\mathbf{S}(u_{1K}\mathbf{X}_1 + \cdots + u_{KK}\mathbf{X}_K)\mathbf{T})],\end{aligned}$$

also see Kiers (2000). Because

$$\text{vec}(\mathbf{H}_k) = (\mathbf{S} \otimes \mathbf{T}')\text{vec}(u_{1k}\mathbf{X}_1 + \cdots + u_{Kk}\mathbf{X}_K),$$

we can write

$$\begin{aligned}\mathbf{H}_{IJ,K} &= [\text{vec}(\mathbf{H}_1)| \cdots |\text{vec}(\mathbf{H}_K)] \\ &= (\mathbf{S} \otimes \mathbf{T}')\mathbf{X}_{IJ,K}\mathbf{U}.\end{aligned}$$

In this notation, it is quite easy to see how **S** and **T** play a key role in linking the orthogonal complement of $\mathbf{X}_{IJ,K}$ to that of $\mathbf{H}_{IJ,K}$.

Result 3. If the mvec form $\mathbf{X}_{IJ,K}$ of an $I \times J \times K$ array $\underline{\mathbf{X}}$ is Tucker-transformed to $\mathbf{H}_{IJ,K} = (\mathbf{S} \otimes \mathbf{T}')\mathbf{X}_{IJ,K}\mathbf{U}$ and $\mathbf{H}_{IJ,(IJ-K)}$ is an orthogonal complement of $\mathbf{H}_{IJ,K}$, then every orthogonal complement of $\mathbf{X}_{IJ,K}$ can be written as $\mathbf{X}_{IJ,(IJ-K)} = (\mathbf{S}' \otimes \mathbf{T})\mathbf{H}_{IJ,(IJ-K)}\mathbf{V}$, where **V** is some nonsingular matrix.

Proof. Let $\mathbf{W} = (\mathbf{S}' \otimes \mathbf{T})\mathbf{H}_{IJ,(IJ-K)}$. Noting that $\mathbf{X}_{IJ,K} = (\mathbf{S} \otimes \mathbf{T}')^{-1}\mathbf{H}_{IJ,K}\mathbf{U}^{-1}$, it is easy to verify that the columns of **W** are orthogonal to those of $\mathbf{X}_{IJ,K}$, and that rank of **W** is the same as that of $\mathbf{H}_{IJ,(IJ-K)}$. The statement follows because by Result 2 we know that every orthogonal complement of $\mathbf{X}_{IJ,K}$ can be written as $\mathbf{X}_{IJ,(IJ-K)} = \mathbf{WV} = (\mathbf{S}' \otimes \mathbf{T})\mathbf{H}_{IJ,(IJ-K)}\mathbf{V}$, for some nonsingular matrix **V**. □

At this point, we can introduce the orthogonal complement algorithm to simplify an array indirectly by using the simplifying solution for an orthogonal complement.

The orthogonal complement algorithm:

1. Given the array $\mathbf{X}_{IJ,K}$ compute an orthogonal complement $\mathbf{X}_{IJ,(IJ-K)}$;
2. Compute $\mathbf{H}_{IJ,(IJ-K)} = (\mathbf{S} \otimes \mathbf{T}')\mathbf{X}_{IJ,(IJ-K)}\mathbf{U}$ in such a way that $\mathbf{H}_{IJ,(IJ-K)}$ is in simple form;
3. Find the orthogonal complement of $\mathbf{H}_{IJ,(IJ-K)}$ in simple form, say $\mathbf{H}_{IJ,K}$;
4. Find the matrix **V** such that $\mathbf{X}_{IJ,K} = (\mathbf{S}' \otimes \mathbf{T})^{-1}\mathbf{H}_{IJ,K}\mathbf{V}$ (see Result 3).

As an example, let us apply the algorithm to a $3 \times 3 \times 7$ array $\underline{\mathbf{X}}$. First, we compute an orthogonal complement $\underline{\mathbf{X}}_c$ which is a $3 \times 3 \times 2$ array. From the previous section, we know that there exist three matrices **S**, **T** and **U** such that this kind of array can be simplified in either the form (7) or the form (3). In the former case, we can take (8) as orthogonal complement, in mvec form. In the latter case, we can take the matrix

$$\mathbf{H}_{9,7} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \lambda_3 - \lambda_2 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda_1 - \lambda_3 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda_2 - \lambda_1 \end{bmatrix}.$$

Finally, it is straightforward to compute the matrix $\mathbf{V}$ such that $\mathbf{X}_{9,7} = (\mathbf{S}' \otimes \mathbf{T})^{-1}\mathbf{H}_{9,7}\mathbf{V}$.

The orthogonal complement method was inspired by the method of Murakami, ten Berge and Kiers (1998). They simplified, for instance, the $3 \times 3 \times 8$ array by using the singular value decomposition of a certain 3×3 matrix. The $3 \times 3 \times 1$ mvec form representing that matrix happened to be an orthogonal complement of the original $3 \times 3 \times 8$ array. We have now generalized this by simplifying, for instance, a $3 \times 3 \times 7$ array by simplifying the orthogonal complementary $3 \times 3 \times 2$ array. Similarly, once we know how to simplify the $3 \times 3 \times 3$ array we can simplify the $3 \times 3 \times 6$ array, and simplifying the $3 \times 3 \times 4$ array will amount to simplifying the $3 \times 3 \times 5$ array.

The method of finding a complementary array size can be used repeatedly. For instance, the $3 \times 3 \times 2$ array has the $3 \times 3 \times 7$ array as its complement, which in turn has the $7 \times 18 \times 3$ array as a complement, which has the $47 \times 18 \times 3$ array as a complement, and so on, ad infinitum. Solving one simplicity transformation problem thus solves the simplicity problem for a whole chain of arrays of complementary sizes.

Maximal Simplicity

In the previous sections we faced the problem of finding, directly or indirectly, the Tucker transformation to simplicity of an array. Now we move on to the issue of optimal simplicity. Whenever we apply a particular transformation to simplicity, the question arises whether or not this simplification is optimal. In other words, it is important to know if it is possible to find a different transformation which produces a larger number of zeros or, equivalently, a smaller number of nonzero elements. In this section we will show that the Tucker transformation proposed by ten Berge & Kiers (1999) and the one proposed by Murakami, ten Berge and Kiers are indeed optimal in the sense that they produce the maximum number of zeros, see Results 4 and 5. We also give Result 6, dealing with optimal simplicity when $I > J$ and $K = IJ - 2$. We start with the result of ten Berge and Kiers.

Result 4. When an array $\underline{\mathbf{X}}$ of order $I \times J \times 2$, with $I > J$, can be transformed to the simple form

$$\mathbf{A}\mathbf{X}_1\mathbf{B} = \mathbf{G}_1 = \begin{bmatrix} \mathbf{I}_J \\ \hline \mathbf{0} \end{bmatrix}, \mathbf{A}\mathbf{X}_2\mathbf{B} = \mathbf{G}_2 = \begin{bmatrix} \mathbf{0} \\ \hline \mathbf{I}_J \end{bmatrix}$$

by nonsingular matrices $\mathbf{A}$ and $\mathbf{B}$, then the smallest possible number of nonzero elements that can be attained by Tucker transformations is $2J$.

Proof. Suppose there exist three nonsingular matrices $\mathbf{S}$, $\mathbf{T}$ and

$$\mathbf{U} = \begin{bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{bmatrix}$$

such that the total number of nonzero elements of

$$\mathbf{H}_1 = \mathbf{S}(u_{11}\mathbf{X}_1 + u_{21}\mathbf{X}_2)\mathbf{T}$$
$$\mathbf{H}_2 = \mathbf{S}(u_{12}\mathbf{X}_1 + u_{22}\mathbf{X}_2)\mathbf{T}$$

is strictly less than $2J$. This implies that $\mathbf{H}_1$ and/or $\mathbf{H}_2$ have a rank strictly less than J. However, we note that

$$\text{rank}(\mathbf{H}_i) = \text{rank}(u_{1i}\mathbf{X}_1 + u_{2i}\mathbf{X}_2) = \text{rank}(u_{1i}\mathbf{G}_1 + u_{2i}\mathbf{G}_2) = \text{rank}\left(u_{1i}\begin{bmatrix}\mathbf{I}_J \\ \hline \mathbf{0}\end{bmatrix} + u_{2i}\begin{bmatrix}\mathbf{0} \\ \hline \mathbf{I}_J\end{bmatrix}\right).$$

It follows that $\text{rank}(\mathbf{H}_i)$ is strictly less than J if and only if $u_{1i} = u_{2i} = 0$. In other words, it is not possible to have less than $2J$ nonzero elements unless $\mathbf{U}$ is singular. □

Next, we show that Murakami's transformation is optimal. This transformation yields as few as $I + K - 1$ nonzero elements, when $K = IJ - 1$ and $I \leq J$. It will now be shown that this is the smallest possible number of nonzero elements.

Result 5. Let $\underline{\mathbf{X}}$ be an array of order $I \times J \times K$, where $K = IJ - 1$, having the slices along the third direction linearly independent. The minimal number of nonzero elements for a Tucker transformation of $\underline{\mathbf{X}}$ is $K + r - 1$, where r is the rank of the orthogonal complementary array.

Proof. Let $\underline{\mathbf{H}}$ be a Tucker transformation of $\underline{\mathbf{X}}$, having z nonzero elements. First, we note that if m is the number of slices in the third direction of $\underline{\mathbf{H}}$ having only one nonzero element then

$$\begin{aligned} z &= m + (\text{number of nonzero elements in the remaining } K - m \text{ slices}) \\ &\geq m + 2(K - m) = 2K - m, \end{aligned} \tag{9}$$

because we cannot have zero slices in $\underline{\mathbf{H}}$ when the slices of $\underline{\mathbf{X}}$ are linearly independent. Let $\underline{\mathbf{X}}_c$ be the $I \times J \times 1$ orthogonal complement array to $\underline{\mathbf{X}}$, and let $\underline{\mathbf{H}}_c$ be a $I \times J \times 1$ orthogonal complement array to $\mathbf{H}$. Then we note that

(a) $\text{rank}(\mathbf{X}_c) = \text{rank}(\mathbf{H}_c)$ because it is clear from Result 3 that one is a Tucker transformation of the other;
(b) if the slice $\mathbf{H}_j$ of $\mathbf{H}$ has only one nonzero element in the (k, l) position then the matrix $\mathbf{H}_c$ must have a zero in the same position;
(c) if the slice $\mathbf{H}_j$ of $\underline{\mathbf{H}}$ has only one nonzero element in the (k, l) position and the slice $\mathbf{H}_{j'}$ has only one nonzero element in the (k', l') position then $(k, l) \neq (k', l')$ otherwise the slabs of $\underline{\mathbf{H}}$, as well as the slabs of $\underline{\mathbf{X}}$, would not be linearly independent.

From (b) and (c) we deduce that $\underline{\mathbf{H}}_c$ must have m elements equal to zero. However, we know by (a) that $\text{rank}(\underline{\mathbf{H}}_c) = \text{rank}(\underline{\mathbf{X}}_c) = r$ which implies

$$m \leq IJ - r \tag{10}$$

Combining (9) and (10) we have

$$z \geq 2K - m \geq 2K - IJ + r = K + r - 1.$$ □

To link this result to the Murakami transformation, note that, in the present case $\underline{\mathbf{H}}_c$ is just an $I \times J$ matrix, typically of rank I.

We end this section with a result about the maximal simplicity of arrays of order $I \times J \times K$, where $K = IJ - 2$ and $I > J$.

Result 6. Let $\underline{\mathbf{X}}$ be an array of order $I \times J \times K$, where $K = IJ - 2$ and $I > J$, having the slices along the third direction linearly independent. If its complementary array is a Tucker transformation of an $I \times J \times 2$ array $\underline{\mathbf{G}}$ of the form

$$\mathbf{G}_1 = \begin{bmatrix} \mathbf{I}_J \\ \hline \mathbf{0} \end{bmatrix}, \mathbf{G}_2 = \begin{bmatrix} \mathbf{0} \\ \hline \mathbf{I}_J \end{bmatrix},$$

then the minimum number of nonzero elements that a Tucker transformation can produce is $IJ + 2J - 4$.

Proof. The proof is analogous to that of the previous result. Let $\underline{\mathbf{H}}$ be a Tucker transformation of $\underline{\mathbf{X}}$, we note that if m is the number of slices in the third direction of $\underline{\mathbf{H}}$ having only one nonzero element then

$$z \geq 2K - m, \tag{11}$$

because the slices of $\underline{\mathbf{X}}$ are linearly independent. If $\underline{\mathbf{X}}_c$ is a $I \times J \times 2$ array orthogonal complement of $\underline{\mathbf{X}}$ and $\underline{\mathbf{H}}_c$ is a $I \times J \times 2$ array orthogonal complement of $\underline{\mathbf{H}}$, then we note that

(a) if the slice $\mathbf{H}_j$ of $\underline{\mathbf{H}}$ has only one nonzero element in the (k, l) position then the two $I \times J$ slices of $\underline{\mathbf{H}}_c$ must have a zero in the same position;
(b) if the slice $\mathbf{H}_j$ of $\underline{\mathbf{H}}$ has only one nonzero element in the (k, l) position and the slice $\mathbf{H}_{j'}$ has only one nonzero element in the (k', l') position then $(k, l) \neq (k', l')$ because otherwise the slabs of $\underline{\mathbf{H}}$, as well as the slabs of $\underline{\mathbf{X}}$, would be linearly dependent.

From (a) and (b) it follows that both slices of $\underline{\mathbf{H}}_c$ must have at least m elements equal to zero in the same position. This implies

$$m \leq J(I - 2) \tag{12}$$

provided that it is not possible to find a complementary array of $\underline{\mathbf{H}}$ having the same column with only one nonzero element in both the slices at the same position. To show that the latter condition is met, first we note that every $\underline{\mathbf{H}}_c$ is a Tucker transformation of $\underline{\mathbf{X}}_c$ which is a Tucker transformation of $\underline{\mathbf{G}}$. This implies that every $\underline{\mathbf{H}}_c$ is a Tucker transformation of $\underline{\mathbf{G}}$, say

$$\mathbf{H}_{c;1} = \mathbf{S}(u_{11}\mathbf{G}_1 + u_{21}\mathbf{G}_2)\mathbf{T}$$
$$\mathbf{H}_{c;2} = \mathbf{S}(u_{12}\mathbf{G}_1 + u_{22}\mathbf{G}_2)\mathbf{T}$$

where **S**, **T** and **U** are nonsingular. If the two slabs of $\underline{\mathbf{H}}_c$ would have the same column with only one nonzero element then there would exist a linear combination of them with rank less than J. However,

$$\begin{aligned} \text{rank}(v_1\mathbf{H}_{c,1} + v_2\mathbf{H}_{c,2}) &= \text{rank}(v_1(u_{11}\mathbf{G}_1 + u_{21}\mathbf{G}_2) + v_2(u_{12}\mathbf{G}_1 + u_{22}\mathbf{G}_2)) \\ &= \text{rank}((v_1u_{11} + v_2u_{12})\mathbf{G}_1 + (v_1u_{21} + v_2u_{22})\mathbf{G}_2) = J, \end{aligned}$$

unless $(v_1u_{11} + v_2u_{12}) = (v_1u_{21} + v_2u_{22}) = 0$, which holds if and only if $v_1 = v_2 = 0$ because **U** is nonsingular. Combining (11) and (12) we obtain

$$z \geq 2K - m \geq 2K - J(I - 2) = IJ + 2J - 4. \qquad \square$$

The question that remains is whether or not the lower bound of $IJ+2J-4$ nonzero elements can be attained by a Tucker transformation. The answer is positive and relies on the orthogonal complement algorithm. We demonstrate this for an example.

Let $\underline{\mathbf{X}}$ be a $4 \times 3 \times 10$ array. We compute an orthogonal complement $\underline{\mathbf{X}}_c$ which is a $4 \times 3 \times 2$ array. From ten Berge and Kiers (1999) we know that there exist three matrices $\mathbf{S}$, $\mathbf{T}$ and $\mathbf{U} = \mathbf{I}$ such that this kind of array can be simplified in the form (2). As an orthogonal complement, in mvec form, we can take the matrix

$$\mathbf{H}_{12,10} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}.$$

The last step is to compute the matrix $\mathbf{V}$ such that $\mathbf{X}_{12,10} = (\mathbf{S}' \otimes \mathbf{T})^{-1}\mathbf{H}_{12,10}\mathbf{V}$.

Discussion

In the derivation of simplicity transformations, we have ignored cases that arise with probability zero. For instance, the ten Berge and Kiers (1999) transformation for two-slab arrays (like the $4 \times 3 \times 2$ array) works almost surely (with probability one), which means that simplicity for the complementary arrays (like the $4 \times 3 \times 10$ array) also can be attained almost surely. A similar statement can be made for the Murakami transformation (when $K = IJ - 1$). Also for the $J \times J \times 2$ arrays, we have ignored certain cases of zero probability. It seems, therefore, that the transformations of this paper generally work. However, in view of one particular realm of application, a word of caution is in order. The probability results assume random sampling from a continuous distribution. The core matrix of Tucker-3 analysis, however, is not randomly sampled, but arises at convergence of an iterative algorithm. This means that we cannot infer that simplicity transformations which work almost surely for random arrays will also work for Tucker-3 core arrays. Fortunately, all Tucker-3 core arrays encountered so far do seem to behave as if randomly sampled from a continuous distribution, and do allow the transformations to simplicity that we have considered. Still, a formal proof for this is lacking.

The proofs of maximum simplicity derived in this paper seem particularly relevant for core-constrained Tucker-3 analysis. When a Tucker-3 core is constrained to have more zeros than would be possible for arrays of that size, then this part of the analysis becomes non-trivial rather than a tautology based on an inactive constraint. On the other hand, when fewer core elements are constrained to be zero than the maximal number, we cannot infer triviality at once: It may still happen that, even when a given number of zero elements is trivially attainable, the particular *pattern* (location) of the hypothesized zeros involved represents an active constraint for arrays of that size.

Appendix

Simplifying the $2 \times J \times J$ *Array with Complex Eigenvalues When* $J > 3$

For $2 \times 2 \times 2$ arrays and $2 \times 3 \times 3$ arrays, there was ample freedom to remove the real part from the pair of complex eigenvalues involved. When a $2 \times 4 \times 4$ array, with slices $\mathbf{X}_1$ and $\mathbf{X}_2$ of order 4×4, has only two eigenvalues of $\mathbf{X}_1^{-1}\mathbf{X}_2$ complex, we are in a situation similar to the $2 \times 3 \times 3$ case with complex eigenvalues. There is again freedom to render one real eigenvalue zero, and, using essentially the same method, we arrive at the simple form

$$\mathbf{SY}_1\mathbf{T} = \mathbf{I}_4, \mathbf{SY}_2\mathbf{T} = \begin{bmatrix} \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu \\ 0 & 0 & -\mu & 0 \end{bmatrix}.$$

In general, when two out of J eigenvalues are complex, for $J > 3$, we can use the slabmix to remove the real part from these eigenvalues, and have freedom left to set one real eigenvalue to zero. This leaves us with J nonzero elements in $\mathbf{SY}_1\mathbf{T} = \mathbf{I}$, and $J-1$ nonzero elements in $\mathbf{SY}_2\mathbf{T}$. We now turn to the situation where we have two or more pairs of complex eigenvalues. We shall use the following matrix result:

Result 7. For each $J \times J$ matrix $\mathbf{A}$ with distinct real eigenvalues $\lambda_1, \ldots, \lambda_m$ and distinct complex eigenvalues $\alpha_1 \pm i\beta_1, \ldots, \alpha_n \pm i\beta_n$ such that $m + 2n = J$, there exists a real-valued matrix $\mathbf{K}$ such that

$$\mathbf{K}^{-1}\mathbf{AK} = \begin{bmatrix} \lambda_1 & & & & & \\ & \ddots & & & & \\ & & \lambda_m & & & \\ & & & \Gamma_1 & & \\ & & & & \ddots & \\ & & & & & \Gamma_n \end{bmatrix} \tag{A1}$$

where

$$\Gamma_j = \begin{bmatrix} \alpha_j & \beta_j \\ -\beta_j & \alpha_j \end{bmatrix}.$$

The decomposition is well-known and can be found, for example, in Horn and Johnson (1993, chapter 3) or Lutkepohl (1996, p. 89). When the eigenvalues are not all distinct the decomposition can fail. However, this exception, which arises with probability zero, will be ignored. We shall now apply this decomposition to simplify $J \times J \times 2$ arrays with four or more complex eigenvalues.

We have shown (see (5)) how to find a slabmix that guarantees two purely complex eigenvalues for $\mathbf{Y}_1^{-1}\mathbf{Y}_2$. We also have seen that there is freedom left. It will now be shown how to use this freedom for removing the real parts from four complex eigenvalues simultaneously. All it takes is to solve two equations of the form (5), to obtain that $\mathbf{A} = \mathbf{Y}_1^{-1}\mathbf{Y}_2$ has four purely complex eigenvalues. Let four complex eigenvalues of $\mathbf{X}_1^{-1}\mathbf{X}_2$ be $\alpha_1 + i\beta_1$, $\alpha_1 - i\beta_1$, $\alpha_2 + i\beta_2$, and $\alpha_2 - i\beta_2$. Then we need to solve

$$-u_{21}\beta_1^2 = (u_{12} + \alpha_1)(1 + u_{21}\alpha_1) \tag{A2}$$

and

$$-u_{21}\beta_2^2 = (u_{12} + \alpha_2)(1 + u_{21}\alpha_2). \tag{A3}$$

Write (A2) as

$$u_{12} = (-u_{21}\beta_1^2 - \alpha_1 - u_{21}\alpha_1^2)/(1 + u_{21}\alpha_1)$$

and (A3) as

$$u_{12} = (-u_{21}\beta_2^2 - \alpha_2 - u_{21}\alpha_2^2)/(1 + u_{21}\alpha_2).$$

Then $(-u_{21}\beta_1^2 - \alpha_1 - u_{21}\alpha_1^2)/(1 + u_{21}\alpha_1) = (-u_{21}\beta_2^2 - \alpha_2 - u_{21}\alpha_2^2)/(1 + u_{21}\alpha_2)$, a quadratic equation in u_{21}. The two solutions for u_{21} are

$$u_{21} = \frac{\alpha_2^2 + \beta_2^2 - \alpha_1^2 - \beta_1^2 \pm ((\alpha_1 - \alpha_2)^4 + (\beta_1^2 - \beta_2^2)^2 + 2(\beta_1^2 + \beta_2^2)(\alpha_1 - \alpha_2)^2)^{1/2}}{2\alpha_2(\alpha_1^2 + \beta_1^2) - 2\alpha_1(\alpha_2^2 + \beta_2^2)}. \quad \text{(A4)}$$

The solutions yield the same columns of $\mathbf{U}$, but in a different order.

If we apply (A4) to mix the slabs first, and then use the transformation given in (A1), we obtain zero diagonals for $\mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_2$, or any other pair of $\mathbf{\Gamma}_i$ and $\mathbf{\Gamma}_j$. Once we have this form, solving for $\mathbf{S}$ and $\mathbf{T}$ is easy, using the same method as was used to arrive at (6). The resulting array has one slab $\mathbf{I}_J$ and the other of the form (A1), with four real parts of complex eigenvalues set to zero. For example, if we have a $9 \times 9 \times 2$ array with 8 complex eigenvalues, we arrive at a transformed array with one slab $\mathbf{SY}_1\mathbf{T} = \mathbf{I}_9$, and the other of the form

$$\mathbf{SY}_2\mathbf{T} = \begin{bmatrix} \lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \beta_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\beta_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \beta_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\beta_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \alpha_3 & \beta_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\beta_3 & \alpha_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha_4 & \beta_4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\beta_4 & \alpha_4 \end{bmatrix}. \quad \text{(A5)}$$

It should be noted that there is still room for further simplification of $\mathbf{\Gamma}_3$ and $\mathbf{\Gamma}_4$. When these submatrices are postmultiplied by $\mathbf{L}_i = \begin{bmatrix} 1 & -\alpha_i/\beta_i \\ 0 & 1 \end{bmatrix}$ and premultiplied with $\mathbf{L}_i^{-1} = \begin{bmatrix} 1 & \alpha_i/\beta_i \\ 0 & 1 \end{bmatrix}$, $i = 3, 4$, respectively, only three nonzero elements remain. By absorbing these multiplications in $\mathbf{S}$ and $\mathbf{T}$, any $\mathbf{L}^{-1}\mathbf{\Gamma}_i\mathbf{L}$ can be guaranteed to have at least one zero element. Applying this final step to the example (A5), we end up with 9 nonzero elements in the first slab, and 11 in the second slab.

In general, when $\mathbf{X}_1^{-1}\mathbf{X}_2$ is diagonalizable and has m real and $2n$ complex eigenvalues and $m + 2n = J > 2$, the transformation yields a simplified array having only $2(J-1) + n$ nonzero elements. The optimality of this transformation, in the sense that no Tucker transformation could yield more zeros, can be proven when at most four complex eigenvalues are involved. For cases with more than four complex values it is our conjecture that the transformation described above is optimal. A formal proof has eluded the authors.

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