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DEGENERACY IN CANDECOMP/PARAFAC EXPLAINED FOR $p \times p \times 2$ ARRAYS OF RANK $p + 1$ OR HIGHER

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The Candecomp/Parafac (CP) model decomposes a three-way array into a prespecified number R of rank-1 arrays and a residual array, in which the sum of squares of the residual array is minimized. The practical use of CP is sometimes complicated by the occurrence of so-called degenerate solutions, in which some components are highly correlated in all three modes and the elements of these components become arbitrarily large. We consider the real-valued CP model in which $p \times p \times 2$ arrays of rank $p + 1$ or higher are decomposed into p rank-1 arrays and a residual array. It is shown that the CP objective function does not have a minimum in these cases, but an infimum. Moreover, any sequence of CP approximations, of which the objective value approaches the infimum, will become degenerate. This result extends Ten Berge, Kiers, & De Leeuw (1988), who consider a particular $2 \times 2 \times 2$ array of rank 3.

Key words: Candecomp, Parafac, three-way arrays, degenerate solutions.

Introduction

Carroll & Chang (1970) and Harshman (1970) have independently proposed the same method for component analysis of three-way arrays, and named it Candecomp and Parafac, respectively. For a given three-way array $\underline{\mathbf{X}}$ of order $I \times J \times K$ and a fixed number of R components, Candecomp/Parafac (CP) yields component matrices $\mathbf{A}$ ($I \times R$), $\mathbf{B}$ ($J \times R$), and $\mathbf{C}$ ($K \times R$) such that $\sum_{k=1}^{K} \text{tr}(\mathbf{E}_k^T \mathbf{E}_k)$is minimized in the model

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

where $\mathbf{X}_k$ denotes the kth slice of order $I \times J$ R and $\mathbf{C}_k$ is the diagonal matrix containing the elements of the kth row of $\mathbf{C}$. We consider the real-valued CP model, i.e., we assume the array $\underline{\mathbf{X}}$ and the component matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ to be real-valued. The real-valued CP model is used in a majority of applications in psychology and chemistry (see Kroonenberg, 1983; Smilde, Bro, & Geladi, 2004). Complex-valued applications of CP occur in, e.g., signal processing and telecommunications research (see Sidiropoulos, 2004).

Notice that (1) can also be written as

$$\underline{\mathbf{X}} = \sum_{r=1}^{R} \underline{\mathbf{Y}}^{(r)} + \underline{\mathbf{E}}, \qquad \text{with} \quad \underline{\mathbf{Y}}^{(r)} = \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r, \tag{2}$$

where $\mathbf{a}_r$, $\mathbf{b}_r$, $\mathbf{c}_r$ are the rth columns of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$, respectively, $\circ$ denotes the outer vector product, and $\underline{\mathbf{E}}$ is the residual array with slices $\mathbf{E}_k$, $k = 1, 2, \ldots, K$. Hence, CP decomposes $\underline{\mathbf{X}}$ into

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R rank-1 arrays $\underline{\mathbf{Y}}^{(r)}$ and a residual array $\underline{\mathbf{E}}$.The three-way rank of $\underline{\mathbf{X}}$ over the real field is defined as the smallest number of real-valued rank-1 arrays whose sum equals $\underline{\mathbf{X}}$. Hence, the smallest number R for which $\underline{\mathbf{X}}$ satisfies the (real-valued) CP model with perfect fit (i.e., $\underline{\mathbf{E}} = \underline{\mathbf{O}}$) is by definition equal to the three-way rank (over the real field) of $\underline{\mathbf{X}}$. In the sequel, the rank of any array is assumed to be the *rank* over the real field.

To any set of component matrices ($\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$) corresponds a fitted model array $\hat{\underline{\mathbf{X}}} = \sum_{r=1}^{R} \underline{\mathbf{Y}}^{(r)}$, see (2). We will refer to a set ($\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$) and the corresponding $\hat{\underline{\mathbf{X}}}$, which minimizes the sum of squares of $\underline{\mathbf{E}}$ in (2), as *a best rank-R approximation of* $\underline{\mathbf{X}}$ or as *an optimal CP solution*. A set ($\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$) and the corresponding $\hat{\underline{\mathbf{X}}}$, for which the sum of squares of $\underline{\mathbf{E}}$ is not minimal, will be referred to as *a rank-R approximation of* $\underline{\mathbf{X}}$ or as *a CP solution*.

CP is a special case of the Tucker3 model, which was introduced by Tucker (1966). For a three-way array $\underline{\mathbf{X}}$ of order $I \times J \times K$, the Tucker3 model is given by

$$\underline{\mathbf{X}} = \sum_{r=1}^{R} \sum_{p=1}^{P} \sum_{q=1}^{Q} g_{rpq} (\mathbf{s}_r \circ \mathbf{t}_p \circ \mathbf{u}_q) + \underline{\mathbf{E}}, \tag{3}$$

where $\underline{\mathbf{E}}$ is the residual array, R, P, and Q are the numbers of components in the three modes, $\mathbf{S}$ ($I \times R$), $\mathbf{T}$ ($J \times P$), and $\mathbf{U}$ ($K \times Q$) are the component matrices with columns $\mathbf{s}_r, \mathbf{t}_p, \mathbf{u}_q$, respectively, and $\underline{\mathbf{G}}$ is an $R \times P \times Q$ core array with elements g_{rpq}. It can be seen that (2) and (3) are equivalent if $R = P = Q$ and the core array $\underline{\mathbf{G}}$ satisfies $g_{rrr} = 1$ and $g_{rpq} = 0$ if r, p, and q are not all identical.

One of the most attractive features of CP is its uniqueness property. The uniqueness of a CP solution is usually studied for a given fitted model array $\hat{\underline{\mathbf{X}}}$. It can be seen that the component matrices ($\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$) corresponding to $\hat{\underline{\mathbf{X}}}$ can only be unique up to rescaling and jointly permuting columns of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$. Indeed, the fitted model array $\hat{\underline{\mathbf{X}}}$ will be the same for the solution given by $\bar{\mathbf{A}} = \mathbf{A}\mathbf{P}\mathbf{T}_a$, $\bar{\mathbf{B}} = \mathbf{B}\mathbf{P}\mathbf{T}_b$, and $\bar{\mathbf{C}} = \mathbf{C}\mathbf{P}\mathbf{T}_c$, for a permutation matrix $\mathbf{P}$ and diagonal matrices $\mathbf{T}_a$, $\mathbf{T}_b$, and $\mathbf{T}_c$ with $\mathbf{T}_a\mathbf{T}_b\mathbf{T}_c = \mathbf{I}_R$. Usually, these are the only transformational indeterminacies in CP. When, for a given model array $\hat{\underline{\mathbf{X}}}$, the matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are unique up to these indeterminacies, the CP solution ($\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$) is called *essentially unique*. To avoid the scaling indeterminacy the columns of two component matrices can be normed at unit length (in this way, the diagonal elements of $\mathbf{T}_a$ and $\mathbf{T}_b$ are only allowed to be -1 or 1). In the sequel, we will implicitly assume these restrictions have been imposed, and label each component matrix as either *restricted* (of which there are two) or *unrestricted* (of which there is one).

Kruskal (1977) has shown that (essential) uniqueness holds under relatively mild conditions. Kruskal's condition relies on a particular concept of matrix rank that he introduced, which has been named k-rank (Kruskal rank) after him. Specifically, the k-rank of a matrix is the largest number x such that every subset of x columns of the matrix is linearly independent. We denote the k-rank of a matrix $\mathbf{A}$ as k_A. Kruskal (1977) proved that the following condition is sufficient for essential uniqueness in CP:

$$2R + 2 \leq k_{\mathrm{A}} + k_{\mathrm{B}} + k_{\mathrm{C}}. \tag{4}$$

The practical use of CP has sometimes been complicated by the occurrence of so-called *degenerate solutions*. In such cases, convergence of the CP solution is extremely slow and some components are highly correlated in at least two modes. Degenerate CP solutions were first reported in Harshman & Lundy (1984). In the majority of such cases, exactly two factors, say $\underline{\mathbf{Y}}^{(s)}$ and $\underline{\mathbf{Y}}^{(t)}$, of the solution display the following pattern:

- In all three component matrices, the columns s and t are almost exactly equal up to a sign change, the product of these sign changes tending toward -1.
- The magnitudes of the elements of columns s and t in the unrestricted component matrix become arbitrarily large.

This pattern is called a *two-factor degeneracy* (see Kruskal, Harshman, & Lundy, 1989). The contributions of $\underline{\mathbf{Y}}^{(s)}$ and $\underline{\mathbf{Y}}^{(t)}$ diverge in nearly opposite directions. However, their sum $\underline{\mathbf{Y}}^{(s)} + \underline{\mathbf{Y}}^{(t)}$ still contributes to a better fit of the decomposed array. Degenerate CP solutions can be avoided by imposing constraints on the component matrices, such as orthogonality or nonnegativity (see Harshman & Lundy, 1984; Lim, 2005). Of course, this will come with some loss of fit of the fitted CP model.

Kruskal et al. (1989) have argued that degenerate solutions occur due to the fact that the CP objective function has no minimum, but an infimum. They reason that every sequence of CP solutions of which the CP objective value approaches the infimum must fail to converge and displays the pattern of degeneracy as stated above. In particular, Kruskal et al. (1989) consider rank-2 approximations of $2 \times 2 \times 2$ arrays of rank 3. Kruskal (1989) shows that the eight-dimensional space of $2 \times 2 \times 2$ arrays is divided into a set of rank-2 arrays, a set of rank-3 arrays (both of which have positive volume, i.e., dimensionality 8), and a seven-dimensional boundary between those two sets. On this boundary, arrays may have rank 0, 1, 2, or 3. Kruskal et al. (1989) use this framework and state that a sequence of rank-2 approximations to a rank-3 array becomes degenerate because it approaches a rank-3 array on the boundary between the sets of rank-2 and rank-3 arrays. This boundary array can be approximated arbitrarily closely from the set of rank-2 arrays.

Paatero (2000) provides a characterization of the rank-3 arrays on the boundary and constructs sequences of rank-2 arrays which have a rank-3 boundary array as limit point and tend toward a two-factor degeneracy. Paatero (2000) shows that these sequences of rank-2 arrays satisfy a particular Tucker3 model (3) with a $2 \times 2 \times 2$ core array. This is in line with the idea of Harshman & Lundy (1984), who conjecture that degenerate CP solutions occur when CP tries to model "Tucker variation" (see also Kruskal et al., 1989; Harshman, 2004).

Mitchell & Burdick (1994) have introduced the term *swamp* for a situation where the alternating least squares (ALS) algorithm used to fit a CP model advances very slowly. They have fitted a four-component CP model to simulated data arrays of order $40 \times 40 \times 4$ and found that if the ALS algorithm is going through a swamp, the CP solution becomes a two-factor degeneracy. Sometimes the ALS algorithm terminates inside a swamp and yields a CP solution with a two-factor degeneracy, but on other occasions the ALS algorithm is temporarily stuck in a swamp and terminates with a nondegenerate CP solution. The relation between swamps and two-factor degeneracies was used by Rayens & Mitchell (1997) to construct a modified CP algorithm, especially designed to avoid swamps. In the case of rank-2 approximations to $2 \times 2 \times 2$ arrays, Paatero (2000) conducts numerical experiments which show that swamps occur near the boundary between the sets of rank-2 and rank-3 arrays. If the target array $\underline{\mathbf{X}}$ has rank 2 and is close to the boundary, the CP algorithm may pass through a temporary swamp and end in $\underline{\mathbf{X}}$ itself. However, Paatero (2000) also presents an example where the starting point of the CP algorithm is chosen such that the CP algorithm cannot get around a curve in the boundary between the starting point and $\underline{\mathbf{X}}$. In this case, the CP algorithm terminates close to the boundary with a two-factor degeneracy.

Apart from two-factor degeneracies, also degeneracies involving more than two components can occur. Paatero (2000) has constructed a sequence of rank-3 arrays which has a $3 \times 3 \times 3$ array of rank 5 as limit point and tends toward a *three-factor degeneracy*, in which the three factors $\underline{\mathbf{Y}}^{(s)}$, $\underline{\mathbf{Y}}^{(t)}$, and $\underline{\mathbf{Y}}^{(u)}$ display the following pattern:

- In two-component matrices, the columns s, t, and u are almost exactly equal up to a sign change. In the third component matrix, the sum of the three columns (up to a sign change) is close to zero.
- In the unrestricted component matrix, the magnitudes of the elements of columns s, t, and u become arbitrarily large.

The sign changes are such that the contributions of two of the factors nearly cancel the contribution of the other factor, while the sum $\underline{\mathbf{Y}}^{(s)} + \underline{\mathbf{Y}}^{(t)} + \underline{\mathbf{Y}}^{(u)}$ still contributes to a better fit of the decomposed array.

Another example of a three-factor degeneracy as above is when the three-component CP model is fitted to the $3 \times 3 \times 2$ array with slices

$$\mathbf{X}_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{X}_2 = \begin{bmatrix} 1 & 0 & -1 \\ 2 & 1 & 3 \\ 0 & -4 & 2 \end{bmatrix}. \tag{5}$$

With **A** and **B** restricted and **C** unrestricted, we obtain the following solution:

$$\mathbf{A} = \begin{bmatrix} 0.4864 & 0.4616 & -0.4738 \\ -0.6649 & -0.6535 & 0.6599 \\ -0.5671 & -0.5999 & 0.5835 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 0.7236 & -0.6933 & 0.7086 \\ 0.6068 & -0.6507 & 0.6290 \\ 0.3291 & -0.3098 & 0.3203 \end{bmatrix},$$
$$\mathbf{C} = \begin{bmatrix} 653.4 & -625.3 & 1277.9 \\ 2162.1 & -2238.9 & 4397.9 \end{bmatrix}, \tag{6}$$

which is a three-factor degeneracy.

Paatero (2000) has also constructed a degeneracy involving four factors, by means of a superposition of two two-factor degeneracies. Below, we will see that *four-factor degeneracies* and *five-factor degeneracies*, analogous to the three-factor degeneracy above, can also be encountered.

In the present paper we will use the framework of Kruskal et al. (1989) to explain the occurrence of degenerate solutions for rank-2 approximations to $2 \times 2 \times 2$ arrays of rank 3. We will analyze the more general setting of rank-p approximations of $p \times p \times 2$ arrays which have rank $p + 1$ or higher. Analogous to the eight-dimensional space of real-valued $2 \times 2 \times 2$ arrays, the $2p^2$-dimensional space of real-valued $p \times p \times 2$ arrays consists of a set of rank-p arrays, a set of rank-$(p + 1)$ arrays (both of which have positive volume, see ten Berge & Kiers, 1999) and a lower-dimensional boundary between those two sets. On this boundary, arrays may have all rank values from 0 up to the maximal rank for real-valued $p \times p \times 2$ arrays, which is equal to $p + \text{floor}(p/2)$ (see Ja' Ja', 1979; Kruskal, 1989). In our analysis, we only consider arrays in the following set:

$$R_p = \{\, \gamma \text{ is a real-valued } p \times p \times 2 \text{ array with } \mathbf{Y}_1 \text{ invertible}\}.$$

All arrays in R_p have at least rank p and the boundary between the rank-p and rank-$(p + 1)$ arrays, intersected with R_p, contains virtually only arrays of rank $p + 1$ or higher. Our main result is the following.

Theorem 1. *Let $\underline{\mathbf{X}}$ be a real-valued $p \times p \times 2$ array with $p \times p$ slices $\mathbf{X}_1$ and $\mathbf{X}_2$. Suppose that $\mathbf{X}_1^{-1}$ exists. If the rank of $\underline{\mathbf{X}}$ is $p + 1$ or higher, then:*

(i) *the CP objective function of the best approximation of $\underline{\mathbf{X}}$ by rank-p arrays in R_p does not have a minimum, but an infimum; and*
(ii) *any sequence of rank-p arrays in R_p of which the CP objective value approaches the infimum, will become degenerate.*

To prove (i) we proceed as follows. By D_p we denote the set of rank-p arrays in R_p. Since $\underline{\mathbf{X}}$ does not lie in D_p, any interior point of D_p can be improved by "moving toward the boundary of D_p." Hence, an optimal CP solution will be a boundary point of D_p. However, virtually all

boundary points of D_p have rank $p+1$ or higher and, hence, do not lie in D_p itself. The boundary points of D_p which have rank p constitute a lower-dimensional set and play no role in practice. Hence, the interior of D_p is virtually equal to D_p itself (this is equivalent to D_p being an open set), and this implies that the CP objective function does not have a minimum but an infimum. To prove (ii) we show that any sequence in (ii) has a limit point on the boundary. This limit point will have rank $p+1$ or higher and is approximated arbitrarily closely by the rank-p sequence in (ii). When this sequence gets close to the limit point, it necessarily becomes degenerate. This shows that our result extends and proves the statements made by Kruskal et al. (1989) for the $2 \times 2 \times 2$ case.

In the proof of Theorem 1 we will make use of Ten Berge (1991), who developed a rank criterion for a real-valued $p \times p \times 2$ array $\underline{\mathbf{X}}$ based on the eigendecomposition of $\mathbf{X}_2\mathbf{X}_1^{-1}$. We illustrate our result by using a CP algorithm to calculate rank-p approximations of random $p \times p \times 2$ arrays of rank $p+1$ for $p = 2, 3, 4, 5$.

Before we prove Theorem 1, we will examine a particular $2 \times 2 \times 2$ array of rank 3, which is the only array so far for which it has been proven that the CP objective function does not have a minimum. We will refer to this array as the K3 array (Kruskal rank-3 array), since it was introduced in Kruskal (1989). The K3 array has slices

$$\mathbf{X}_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \qquad \text{and} \qquad \mathbf{X}_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{7}$$

Ten Berge, Kiers, and De Leeuw (1988) show that when the K3 array is approximated by rank-2 arrays, the CP objective function does not have a minimum but an infimum of 1. Below we will show that all CP solutions, of which the CP objective value approaches the infimum, will become degenerate. Moreover, it will be shown that a boundary point $\tilde{\underline{\mathbf{X}}}$ of the set of rank-3 arrays exists, which can be approximated arbitrarily closely from the set of rank-2 arrays, and for which $\left\|\tilde{\underline{\mathbf{X}}} - \underline{\mathbf{X}}\right\|^2 = 1$, where $\underline{\mathbf{X}}$ is the K3 array and $\|\cdot\|$ denotes the Frobenius norm.

First, however, we discuss the eigendecomposition of a real-valued square matrix and a link between simultaneous diagonalization of two square matrices and the rank of $p \times p \times 2$ arrays. Both concepts are used heavily throughout the paper, and for ease of presentation we summarize all relevant results and properties below.

The Eigendecomposition of a Real-Valued Square Matrix

Let $\mathbf{X}$ be a real-valued $p \times p$ matrix. If, for some nonzero column vector $\mathbf{k}$ and some scalar λ, there holds

$$\mathbf{X}\mathbf{k} = \lambda\mathbf{k}. \tag{8}$$

then λ is called an *eigenvalue* of $\mathbf{X}$ and $\mathbf{k}$ is called an *eigenvector* of $\mathbf{X}$, associated with eigenvalue λ. It is well known that the eigenvalues of $\mathbf{X}$ are the solutions of the characteristic equation $\det(\mathbf{X} - \lambda\mathbf{I}_p) = 0$. Since $q(\lambda) = \det(\mathbf{X} - \lambda\mathbf{I}_p)$ is a pth degree polynomial in λ, it follows that $\mathbf{X}$ has exactly p eigenvalues, which are the p roots of $q(\lambda) = 0$. Once the eigenvalues of $\mathbf{X}$ are known, the associated eigenvectors may be determined from (8). For each eigenvalue, there exists at least one associated eigenvector. Note that eigenvectors are determined up to scalar multiplication (i.e., if $\mathbf{k}$ is an eigenvector associated with λ, then so is $c\mathbf{k}$, for any nonzero scalar c).

For a real-valued matrix, an eigenvector associated with a real eigenvalue can always be chosen real-valued, while an eigenvector associated with a complex eigenvalue is necessarily complex-valued. An example of a real-valued matrix with complex eigenvalues is the following. The matrix $\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$ has eigenvalues i and $-i$, and eigenvectors $\begin{pmatrix} i \\ 1 \end{pmatrix}$ (associated with eigenvalue i) and $\begin{pmatrix} -i \\ 1 \end{pmatrix}$ (associated with eigenvalue $-i$).

It can be seen from (8) that if the real-valued matrix $\mathbf{X}$ has a complex eigenvalue λ and an associated (necessarily complex) eigenvector $\mathbf{k}$, then the complex conjugate $\bar{\lambda}$ is also an eigenvalue of $\mathbf{X}$ and the complex conjugated vector $\bar{\mathbf{k}}$ is an eigenvector associated with $\bar{\lambda}$. Hence, complex eigenvalues always occur in pairs when $\mathbf{X}$ is real-valued.

Next, we define the following concepts. The *algebraic multiplicity* $a(\lambda)$ of an eigenvalue λ is defined as the multiplicity of λ as a root of the characteristic equation $q(\lambda) = 0$. The *geometric multiplicity* $g(\lambda)$ of an eigenvalue λ is defined as the maximum number of linearly independent eigenvectors associated with λ. Finally, the *eigenspace* $E(\lambda)$ of λ is defined as the subspace spanned by all eigenvectors associated with λ. It follows that the geometric multiplicity of λ is equal to the dimensionality of $E(\lambda)$. Note that any nonzero vector in $E(\lambda)$ is an eigenvector associated with λ.

The following facts are well known. Let $\mathbf{X}$ have M (and no more than M) distinct eigenvalues $\lambda_1, \cdots, \lambda_M$. Then there holds:

(a) $1 \leq g(\lambda_m) \leq a(\lambda_m), m = 1, \ldots, M$;
(b) $\sum_{m=1}^{M} a(\lambda_m) = p$;
(c) $\sum_{m=1}^{m} g(\lambda_m) \leq p$;
(d) any set of eigenvectors $\mathbf{k}_1, \cdots, \mathbf{k}_M$ associated with $\lambda_1, \cdots, \lambda_M$, respectively, is linearly independent.

If $\mathbf{X}$ has p distinct eigenvalues (i.e., $M = p$), then (a) implies that the sum of all geometric multiplicities in (c) is equal to p. Some examples of algebraic and geometric multiplicities are the following. The identity matrix $\left[\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right]$ has an eigenvalue 1 with algebraic and geometric multiplicity equal to 2, since $\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$ and $\left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$ are eigenvectors associated with eigenvalue 1. The matrix $\left[\begin{smallmatrix} 1 & 0 \\ 1 & 1 \end{smallmatrix}\right]$ also has an eigenvalue 1 with algebraic multiplicity 2, but now the geometric multiplicity equals 1. The only eigenvector (up to scalar multiplication) associated with the eigenvalue 1 is $\left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$.

Suppose the sum of all geometric multiplicities in (c) is equal to p, i.e., for all distinct eigenvalues the algebraic and geometric multiplicities are equal. Then $\mathbf{X}$ has p (and no more than p) linearly independent eigenvectors. Let these eigenvectors be the columns of the $p \times p$ matrix $\mathbf{K}$. Let the diagonal matrix $\mathbf{\Lambda}$ contain the associated eigenvalues on its diagonal, in the same order as the eigenvectors appear as columns of $\mathbf{K}$. From (8) it follows that there holds $\mathbf{XK} = \mathbf{K\Lambda}$. Since $\mathbf{K}$ is nonsingular we may write

$$\mathbf{X} = \mathbf{K\Lambda K}^{-1}, \tag{9}$$

which is called the *eigendecomposition* of $\mathbf{X}$. The matrices $\mathbf{K}$ and $\mathbf{\Lambda}$ are not uniquely determined. Indeed, the ordering of the eigenvectors and associated eigenvalues may be changed. Also, the eigenvectors in $\mathbf{K}$ are determined up to scalar multiplication (they are usually normed to length 1, which determines them up to sign). And, finally, for an eigenvalue λ with algebraic multiplicity $a(\lambda)$ larger than 1, we may include in $\mathbf{K}$ any $a(\lambda)$ eigenvectors spanning the eigenspace $E(\lambda)$.

The eigendecomposition (9) exists if and only if the sum of all geometric multiplicities in (c) is equal to p. In this case, the matrix $\mathbf{X}$ is said to be *diagonalizable*, since there exists a nonsingular matrix $\mathbf{K}$ such that $\mathbf{K}^{-1}\mathbf{XK}$ is a diagonal matrix. For more information, see, e.g., Apostol (1969, chaps. 4 and 5).

Simultaneous Diagonalization of Two Square Matrices and the Rank of $p \times p \times 2$ Arrays

Here, we discuss a link between the simultaneous diagonalization of two square matrices and the rank of $p \times p \times 2$ arrays. This provides the tools for our analysis.

Let $\underline{\mathbf{X}}$ be a real-valued $p \times p \times 2$ array with $p \times p$ slices $\mathbf{X}_1$ and $\mathbf{X}_2$. If $\mathbf{X}_1^{-1}$ exists, Ten Berge (1991) has shown that a sufficient condition for $\underline{\mathbf{X}}$ to have rank p is that $\mathbf{X}_2\mathbf{X}_1^{-1}$

has p distinct real eigenvalues. A rank-p decomposition can then be obtained through the eigendecomposition

$$\mathbf{X}_2\mathbf{X}_1^{-1} = \mathbf{K}\mathbf{\Lambda}\mathbf{K}^{-1}, \tag{10}$$

where $\mathbf{\Lambda}$ is the $p \times p$ diagonal matrix of eigenvalues and $\mathbf{K}$ contains the associated eigenvectors. Taking

$$\mathbf{A} = \mathbf{K}, \qquad \mathrm{B}^T = \mathbf{K}^{-1}\mathbf{X}_1, \qquad \mathbf{C}_1 = \mathbf{I}_p, \qquad \mathbf{C}_2 = \Lambda, \tag{11}$$

yields a full real-valued rank-p decomposition of $\underline{\mathbf{X}}$ (as in (1) with $\mathbf{E}_k = \mathbf{O}$). Note that (11) defines a simultaneous diagonalization of $\mathbf{X}_1$ and $\mathbf{X}_2$, since we have nonsingular matrices $\mathbf{A}$ and $\mathbf{B}$ and diagonal matrices $\mathbf{C}_1$ and $\mathbf{C}_2$ such that $\mathbf{A}^{-1}\mathbf{X}_1\mathbf{B}^{-T} = \mathbf{C}_1$ and $\mathbf{A}^{-1}\mathbf{X}_2\mathbf{B}^{-T} = \mathbf{C}_2$. The following lemma gives rank conditions for real-valued $p \times p \times 2$ arrays. It is equivalent to Ja' Ja' (1979, Lemma 3.1) and sharpens the condition of Ten Berge (1991).

Lemma 1. *Let $\underline{\mathbf{X}}$ be a real-valued $p \times p \times 2$ array with $p \times p$ slices $\mathbf{X}_1$ and $\mathbf{X}_2$. Suppose $\mathbf{X}_1^{-1}$ exists. The following statements hold:*

(i) If $\mathbf{X}_2\mathbf{X}_1^{-1}$ *has p real eigenvalues and is diagonalizable, then* $\mathrm{rank}(\underline{\mathbf{X}}) = p$.
(ii) If $\mathbf{X}_2\mathbf{X}_1^{-1}$ *has at least one pair of complex eigenvalues, then* $\mathrm{rank}(\underline{\mathbf{X}}) \geq p + 1$.
(iii) If $\mathbf{X}_2\mathbf{X}_1^{-1}$ *has p real eigenvalues but is not diagonalizable, then* $\mathrm{rank}(\underline{\mathbf{X}}) \geq p + 1$.

Proof. Recall that a $p \times p$ matrix is diagonalizable if it has p linearly independent eigenvectors. Statement (i) follows from the use of the rank-p decomposition (11) above. Note that since $\mathbf{X}_1^{-1}$ exists, the array $\underline{\mathbf{X}}$ has at least rank p. The proof of (ii) and (iii) is as follows. Suppose $\mathbf{X}_2\mathbf{X}_1^{-1}$ has at least one pair of complex eigenvalues or that it has p real eigenvalues but is not diagonalizable. If $\mathrm{rank}(\underline{\mathbf{X}}) = p$, then there exist $p \times p$ matrices $\mathbf{A}$ and $\mathbf{B}$ and diagonal matrices $\mathbf{C}_1$ and $\mathbf{C}_2$ such that $\mathbf{X}_1 = \mathbf{A}\mathbf{C}_1\mathbf{B}^T$ and $\mathbf{X}_2 = \mathbf{A}\mathbf{C}_2\mathbf{B}^T$. Since $\mathbf{X}_1^{-1}$ exists, we have $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}_1$ non-singular. But then $\mathbf{X}_2\mathbf{X}_1^{-1} = \mathbf{C}\mathbf{A} = \mathbf{C}_1^{-1}\mathbf{A}^{-1}$ is an eigendecomposition with p real eigenvalues and p linearly independent eigenvectors, which contradicts our assumption. Hence, the rank of $\underline{\mathbf{X}}$ has to be larger than or equal to $p + 1$. □

Statement (i) states that $\mathbf{X}_2\mathbf{X}_1^{-1}$ must have p real eigenvalues for $\underline{\mathbf{X}}$ to have rank p. If these p are not only real but also distinct, then the rank-p decomposition of $\underline{\mathbf{X}}$ in (11) is essentially unique. We can use Kruskal's uniqueness condition (4) to see this. The component matrices $\mathbf{A}$ and $\mathbf{B}$ are both nonsingular, which implies $k_A = p$ and $k_B = p$. For $\mathbf{C}$, there holds $k_C = 2$ if all eigenvalues of $\mathbf{X}_2\mathbf{X}_1^{-1}$ are distinct and $k_\mathbf{C} = 1$ otherwise. If $k_\mathbf{C} = 2$, then Kruskal's condition (4) is satisfied (with $R = p$) and, hence, the rank-p decomposition of $\underline{\mathbf{X}}$ is essentially unique. If the rank-p decomposition of $\underline{\mathbf{X}}$ is not unique, i.e., when $\mathbf{X}_2\mathbf{X}_1^{-1}$ has (at least) one eigenvalue λ with algebraic multiplicity larger than 1, then the only way to construct alternative decompositions is by taking different eigenvectors of λ as the columns of $\mathbf{A} = \mathbf{K}$ (see also Ten Berge, 2004).

The K3 Array Revisited

Let $R = 2$ and let $\underline{\mathbf{X}}$ be the K3 array in (7). Ten Berge et al. (1988) show that if $\underline{\mathbf{X}}$ is approximated by rank-2 arrays, then the CP objective function does not have a minimum but an infimum of 1. Below we will show that all CP solutions approaching the infimum become degenerate. Moreover, it will be shown that a boundary point $\tilde{\underline{\mathbf{X}}}$ of the set of rank-3 arrays exists, which can be approximated arbitrarily closely from the set of rank-2 arrays, and for which $\left\|\tilde{\underline{\mathbf{X}}} - \underline{\mathbf{X}}\right\|^2 = 1$.

The component matrices **A** and **B** will be restricted to have columns of length 1. Hence, we may write

$$\mathbf{A} = \begin{bmatrix} \sin\alpha & \sin\beta \\ \cos\alpha & \cos\beta \end{bmatrix} \qquad \text{and} \qquad \mathbf{B} = \begin{bmatrix} \sin\gamma & \sin\delta \\ \cos\gamma & \cos\delta \end{bmatrix}, \tag{12}$$

for some α, β, γ, and δ. Ten Berge et al. (1988) show that, for the K3 array $\underline{\mathbf{X}}$, it follows that

$$\mathbf{C} = \frac{1}{1-\mu^2} \begin{bmatrix} -\cos(\alpha+\gamma) + \mu\cos(\beta+\delta) & \mu\cos(\alpha+\gamma) - \cos(\beta+\delta) \\ \sin(\alpha+\gamma) - \mu\sin(\beta+\delta) & -\mu\sin(\alpha+\gamma) + \sin(\beta+\delta) \end{bmatrix}, \tag{13}$$

where $\mu = \cos(\alpha-\beta)\ \cos(\gamma-\delta)$. The CP objective function is thus a function of the four parameters α, β, γ, and δ. Ten Berge et al. (1988) show that it has the form

$$f(\alpha,\beta,\gamma,\delta) = 2 - \frac{2\mu\lambda}{1-\mu^2}, \tag{14}$$

where $\lambda = \sin(\alpha-\beta)\ \sin(\gamma-\delta)$. Since f in (14) has an infimum of 1, it is clear that any path to the infimum should satisfy

$$\frac{2\mu\lambda}{1-\mu^2} \to 1. \tag{15}$$

We will assume that **A** and **B** are nonsingular, which is equivalent to $\mu^2 < 1$. From the fact that $(\mu+\lambda)^2 = \cos^2(\alpha-\beta+\delta-\gamma) \leq 1$, we know that

$$\frac{2\mu\lambda}{1-\mu^2} + \frac{\lambda^2}{1-\mu^2} \leq 1. \tag{16}$$

Combining (15) and (16), we see that $\lambda \to 0$. From (15), it follows that $(1-\mu^2)/2\mu = (2\mu)^{-1} - \mu/2 \to 0$. Since $\mu \in [-1, 1]$ this implies either $\mu \to 1$ or $\mu \to -1$. Therefore, only the following four limit regimes are appropriate:

$$\alpha-\beta \to 0, \quad \gamma-\delta \to 0 \quad \Rightarrow \quad \lambda \to 0, \quad \mu \to 1, \tag{17}$$

$$\alpha-\beta \to 0, \quad \gamma-\delta \to \pi \quad \Rightarrow \quad \lambda \to 0, \quad \mu \to -1, \tag{18}$$

$$\alpha-\beta \to \pi, \quad \gamma-\delta \to 0 \quad \Rightarrow \quad \lambda \to 0, \quad \mu \to -1, \tag{19}$$

$$\alpha-\beta \to \pi, \quad \gamma-\delta \to \pi \quad \Rightarrow \quad \lambda \to 0, \quad \mu \to 1. \tag{20}$$

Notice that in (17)–(20) the values of α and γ are arbitrary. This implies that a sequence of rank-2 approximations $\underline{\mathbf{Y}}^{(n)}$ of $\underline{\mathbf{X}}$, where for each n the fitted model array $\underline{\mathbf{Y}}^{(n)}$ is constructed from the component matrices $(\mathbf{A}^{(n)}, \mathbf{B}^{(n)}, \mathbf{C}^{(n)})$, has infinitely many limiting points $\tilde{\underline{\mathbf{X}}}$ such that $\left\|\underline{\mathbf{Y}}^{(n)} - \underline{\mathbf{X}}\right\|^2$ converges to the infimum if $\underline{\mathbf{Y}}^{(n)}$ converges to $\tilde{\underline{\mathbf{X}}}$. Next, we consider the component matrices **A**, **B**, and **C** in each of the limit regimes in (17)–(20). It can be seen that all elements of $(1-\mu^2)\mathbf{C}$ converge to zero, see (13). However, using the fact that $\mu^2 \to 1$ and the observation that by (15) the rates of convergence of $\alpha-\beta$ and $\gamma-\delta$ must be asymptotically equal (otherwise, the limit in (15) would be zero), it can be verified that all elements in **C** converge to either infinity or minus infinity. Furthermore, if $\mu \to 1$, then the columns in **C** will become the negative of each other, while if $\mu \to -1$ they will become more and more alike. We may now conclude the following:

- For (17), the columns in **A** and **B** become more and more alike, while those in **C** become the negative of each other.
- For (18), the columns in **A** and **C** become more and more alike, while those in **B** become the negative of each other.

- For (19), the columns in **B** and **C** become more and more alike, while those in **A** become the negative of each other.
- For (20), the columns in **A**, **B**, and **C** become the negative of each other.

Hence, for each of the four limit regimes in (17)–(20) a two-factor degeneracy will be obtained. In other words, a two-factor degeneracy is obtained for each sequence of CP solutions of which the CP objective value approaches the infimum of 1.

Next, we show that a boundary point $\underline{\tilde{\mathbf{X}}}$ of the set of rank-3 arrays exists, which can be approximated arbitrarily closely from the set of rank-2 arrays, and for which $\left\|\underline{\tilde{\mathbf{X}}} - \underline{\mathbf{X}}\right\|^2 = 1$. That is, $\underline{\tilde{\mathbf{X}}}$ is a limiting point for a sequence of rank-2 approximations of $\underline{\mathbf{X}}$, for which the CP objective value converges to the infimum. Consider the following $2 \times 2 \times 2$ array $\underline{\tilde{\mathbf{X}}}$ with slices

$$\tilde{\mathbf{X}}_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \qquad \text{and} \qquad \tilde{\mathbf{X}}_2 = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}. \tag{21}$$

It is clear that $\left\|\underline{\tilde{\mathbf{X}}} - \underline{\mathbf{X}}\right\|^2 = 1$. Since $\tilde{\mathbf{X}}_1^{-1}$ exists, a necessary and sufficient condition for $\underline{\tilde{\mathbf{X}}}$ to have rank 2 is that $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ has two real eigenvalues and is diagonalizable; see Lemma 1. We have

$$\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1} = \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix}, \tag{22}$$

which has an eigenvalue 0 with algebraic multiplicity 2 and geometric multiplicity 1; the only eigenvector is $\binom{0}{1}$ (up to scalar multiplication). Hence, $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ is not diagonalizable and the array $\underline{\tilde{\mathbf{X}}}$ has rank 3. However, the array $\underline{\tilde{\mathbf{X}}}$ can be approximated arbitrarily closely by rank-2 arrays. For example, we may choose $\underline{\mathbf{Y}}$ such that $\mathbf{Y}_2\mathbf{Y}_1^{-1} = \begin{bmatrix} \varepsilon & 0 \\ -1 & -\varepsilon \end{bmatrix}$ and $\underline{\mathbf{Y}} \to \underline{\tilde{\mathbf{X}}}$ as $\varepsilon \downarrow 0$. For $\varepsilon > 0$, the matrix $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ has two real eigenvalues (ε and $-\varepsilon$) and is diagonalizable. Hence, it follows from Lemma 1 that $\underline{\mathbf{Y}}$ has rank 2 for all $\varepsilon > 0$. This implies that $\underline{\tilde{\mathbf{X}}}$ is a boundary point of the set of rank-3 arrays and the CP objective function (with $R = 2$) for $\underline{\tilde{\mathbf{X}}}$ has an infimum of zero. Since the CP objective function for $\underline{\mathbf{X}}$ has an infimum of 1, there do not exist boundary points $\underline{\mathbf{Z}}$ of the set of rank-3 arrays for which $\left\|\underline{\mathbf{Z}} - \underline{\mathbf{X}}\right\|^2 < 1$. There is only one limiting point for a sequence of rank-2 approximations of $\underline{\tilde{\mathbf{X}}}$ for which the CP objective value converges to the infimum of zero. Namely, this limiting point is $\underline{\tilde{\mathbf{X}}}$ itself. In this limiting regime, the CP solution (**A**, **B**, **C**) becomes a two-factor degeneracy. As shown above, there are infinitely many such limiting points for rank-2 approximations of the K3 array $\underline{\mathbf{X}}$. This implies that there are infinitely many boundary points $\underline{\mathbf{Z}}$ of the set of rank-3 arrays with $\left\|\underline{\mathbf{Z}} - \underline{\mathbf{X}}\right\|^2 = 1$. Each such boundary point $\underline{\mathbf{Z}}$ is a limiting point for a sequence of rank-2 approximations of $\underline{\mathbf{X}}$ for which the CP objective value converges to the infimum. Recall the statement by Kruskal et al. (1989) that, for $2 \times 2 \times 2$ arrays of rank 3 and $R = 2$, degeneracy occurs when the sequence of CP solutions approaches a boundary point of the set of rank-3 arrays, which can be approximated arbitrarily closely from the set of rank-2 arrays. This statement is valid indeed when the K3 array is considered.

For any CP solution approaching the infimum of 1 for $\underline{\mathbf{X}}$, we have $k_A = k_B = k_C = 2$ (if either **A** or **B** is singular, i.e., either $\alpha = \beta$ or $\gamma = \delta$, then $\lambda = 0$ and the CP objective value equals 2, see (14); if both **A** and **B** are singular, then the CP objective function has a minimum of 3 (see Ten Berge et al., 1988, Lemma 1). Hence, Kruskal's condition (4) holds (with $R = 2$) and the CP solution (**A**, **B**, **C**) is essentially unique. Note that this does not contradict the fact that there are infinitely many limiting points $\underline{\tilde{\mathbf{X}}}$. Indeed, Kruskal's condition guarantees the absence of transformational freedom of the CP solution (besides the intrinsic transformational indeterminacies of CP mentioned above) for a fixed fitted model array. The fitted model arrays, however, are different for each iteration of the CP algorithm.

Degeneracy for $p \times p \times 2$ Arrays of Rank $p+1$ or Higher

Here, we extend the analysis above to $p \times p \times 2$ arrays of rank $p+1$ or higher. Our main result is Theorem 1 (see the Introduction), which states that if the CP model with $R = p$ components is fitted to such an array, then the CP objective function has no minimum but an infimum, and any sequence of CP solutions of which the objective value approaches the infimum will become degenerate. As mentioned in the Introduction, we only consider arrays in the following set:

$$R_p = \{\underline{\mathbf{Y}} \text{ is a real-valued } p \times p \times 2 \text{ array with } \mathbf{Y}_1 \text{invertible}\}.$$

Note that the restriction to arrays in the set R_p is only virtual. This can be seen as follows. The set of $p \times p \times 2$ arrays which do not lie in R_p has dimensionality lower than $2p^2$. This implies that when $\underline{\mathbf{Y}}$ is randomly sampled from a $2p^2$-dimensional continuous distribution, it lies in R_p with probability 1. Also, any array not in R_p can be approximated arbitrarily closely by arrays in R_p. Although we cannot consider any CP algorithm as a generator of random arrays, we can safely assume, based on these observations and the results from our simulations below, that CP solutions not lying in the set R_p will not be encountered in practice.

The remaining part of this section is devoted to proving Theorem 1. We define the following subsets of R_p. Let

$$\begin{aligned} S_p &= \{\underline{\mathbf{Y}} \in R_p \ : \mathbf{Y}_2 \ \mathbf{Y}_1^{-1} \text{ has } p \text{ real eigenvalues}\}, \\ D_p &= \{\underline{\mathbf{Y}} \in R_p \ : \mathbf{Y}_2 \ \mathbf{Y}_1^{-1} \text{ has } p \text{ real eigenvalues and is diagonalizable}\}. \end{aligned}$$

It can be seen that $D_p \subset S_p \subset R_p$. By Lemma 1, all arrays in D_p have rank p and all arrays in $S_p \setminus D_p$, where

$$S_p \setminus D_p = \{\underline{\mathbf{Y}} \in R_p \ : \mathbf{Y}_2 \ \mathbf{Y}_1^{-1} \text{has } p \text{ real eigenvalues and is not diagonalizable}\},$$

have rank $p+1$ or higher. Moreover, D_p contains all rank-p arrays in R_p. Hence, for $\underline{\mathbf{X}}$ as in Theorem 1, fitting the rank-p CP model yields the following optimization problem:

$$\begin{array}{ll} \text{Minimize} & \left\|\underline{\mathbf{X}} - \underline{\mathbf{Y}}\right\|^2 \\ \text{subject to} & \underline{\mathbf{Y}} \in D_p. \end{array} \tag{23}$$

For later use, we also define the problem

$$\begin{array}{ll} \text{Minimize} & \left\|\underline{\mathbf{X}} - \underline{\mathbf{Y}}\right\|^2 \\ \text{subject to} & \underline{\mathbf{Y}} \in S_p. \end{array} \tag{24}$$

In Table 1 below, we have summarized the defintions of the sets D_p and S_p. Also the rank values of arrays in these sets (as proven in Lemma 1) are given. Note that

$$R_p \setminus S_p = \{\underline{\mathbf{Y}} \in R_p : \mathbf{Y}_2\mathbf{Y}_1^{-1} \text{ has at least one pair of complex eigenvalues}\}.$$

We need the following result, the proof of which is postponed until the end of this section.

Lemma 2.

(i). *The boundary points of D_p (which lie in R_p) are the arrays $\underline{\mathbf{Y}}$ for which $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ has p real eigenvalues which are not all distinct.*

TABLE 1.
Definitions and volumes of the sets D_p, $S_p \backslash D_p$ and $R_p \backslash S_p$. The rank values of the arrays in these sets are proven in Lemma 1. The volumes follow from Corollary 1 below.

$\mathbf{Y}_2\mathbf{Y}_1^{-1}$	p real eigenvalues	Some complex eigenvalues
Diagonalizable	$\text{rank}(\underline{\mathbf{Y}}) = p$ $\mathbf{Y} \in D_p \subset S_p$ positive volume	$\text{rank}(\underline{\mathbf{Y}}) \geq p+1$ $\mathbf{Y} \in R_p \backslash S_p$ positive volume
Not diagonalizable	$\text{rank}(\underline{\mathbf{Y}}) \geq p+1$ $\underline{\mathbf{Y}} \in S_p \backslash D_p$ zero volume	$\text{rank}(\underline{\mathbf{Y}}) \geq p+1$ $\underline{\mathbf{Y}} \in R_p \backslash S_p$ zero volume

(ii). *Virtually all boundary points* $\underline{\mathbf{Y}}$ *of* D_p *(which lie in* R_p*) have* rank $p+1$ *or higher and lie in the set* $S_p \backslash D_p$*, i.e., for these arrays* $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ *is not diagonalizable.*

(iii). *The set* S_p *is a closed subset of* R_p *and has the same boundary points as* D_p*.*

Next, we use the statements of Lemma 2 to prove Theorem 1. Let $\underline{\mathbf{X}}$ be as in Theorem 1. Since $\mathbf{X}_1^{-1}$ exists, the array $\underline{\mathbf{X}}$ satisfies either (ii) or (iii) of Lemma 1. Below, we will treat these cases separately.

Suppose $\mathbf{X}_2\mathbf{X}_1^{-1}$ *Has at Least One Pair of Complex Eigenvalues*

Consider the problem (24). Since $\underline{\mathbf{X}}$ does not lie in the set S_p and the set S_p is closed (see Lemma 2), it follows that the objective function in (24) has a minimum and an optimal solution $\underline{\tilde{\mathbf{X}}}$ exists. Moreover, since the objective function in (24) is strictly decreasing in any direction toward $\underline{\mathbf{X}}$, any optimal solution $\underline{\tilde{\mathbf{X}}}$ of (24) will be a boundary point of S_p. Indeed, a line can be drawn from any interior point $\underline{\mathbf{Y}}$ of S_p to $\underline{\mathbf{X}}$. This line will intersect with the boundary of S_p. The boundary point at the intersection is closer to $\underline{\mathbf{X}}$ and, hence, has a lower objective value than the interior point $\underline{\mathbf{Y}}$ of S_p we started with. In this way, the objective value of any interior point $\underline{\mathbf{Y}}$ of S_p can be decreased by "moving toward the boundary of S_p." From Lemma 2, it follows that virtually any optimal solution $\underline{\tilde{\mathbf{X}}}$ of problem (24) lies in the set $S_p \backslash D_p$.

Since in (24) the objective value of any interior point of S_p can be decreased, it follows that in (23) the objective value of any interior point $\underline{\mathbf{Y}} \in D_p$ can be decreased by "moving toward the boundary of D_p." However, from Lemma 2 it follows that the boundary of D_p consists almost entirely of rank-$(p+1)$ arrays. Since these arrays do not lie in D_p, the set D_p is virtually open and the objective function in (23) has no minimum, but an infimum. In practice, boundary points of rank p do not occur as optimal solutions of (23) since these arrays lie in a lower-dimensional subset of the boundary of D_p. This proves (i) of Theorem 1. Note that the value of the infimum is equal to $\left\|\underline{\tilde{\mathbf{X}}} - \underline{\mathbf{X}}\right\|^2 > 0$, where $\underline{\tilde{\mathbf{X}}}$ is an optimal solution of problem (24).

Next, we will show that any sequence of CP solutions $\underline{\mathbf{Y}}^{(n)}$ of (23), for which $\left\|\underline{\mathbf{Y}}^{(n)} - \underline{\mathbf{X}}\right\|^2$ converges to the infimum, yields a sequence $(\mathbf{A}^{(n)}, \mathbf{B}^{(n)}, \mathbf{C}^{(n)})$ which becomes degenerate. This will prove (ii) of Theorem 1. From the proof of (i) above, we know that $\underline{\mathbf{Y}}^{(n)}$ converges to some $\underline{\tilde{\mathbf{X}}} \in S_p \backslash D_p$. Since $\underline{\tilde{\mathbf{X}}} \in S_p \backslash D_p$, we have that $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ has p real eigenvalues but is not diagonalizable.

Let $\underline{\mathbf{Y}} \in D_p$. Then the matrix $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ has a real-valued eigendecomposition $\mathbf{K}\Lambda\mathbf{K}^{-1}$ and a rank-p decomposition can be obtained with $\mathbf{A} = \mathbf{K}$, $\mathbf{B}^T = \mathbf{K}^{-1}\mathbf{Y}_1$, $\mathbf{C}_1 = \mathbf{I}_p$, and $\mathbf{C}_2 = \Lambda$; see (11). If all eigenvalues of $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ are distinct, then this rank-p decomposition of $\underline{\mathbf{Y}}$ is essentially unique; see the discussion below Lemma 1.

Consider a sequence $\underline{\mathbf{Y}}^{(n)} \in D_p$ which converges to some $\underline{\tilde{\mathbf{X}}} \in S_p \backslash D_p$ as $n \to \infty$, and for which the rank-p decomposition is essentially unique for all n. We denote the component matrices of the rank-p decomposition of $\underline{\mathbf{Y}}^{(n)}$ by $(\mathbf{A}^{(n)}, \mathbf{B}^{(n)}, \mathbf{C}^{(n)})$ and assume that $\mathbf{A}^{(n)}$ and $\mathbf{C}^{(n)}$ are restricted to have columns of length 1. Note that $\mathbf{Y}_2^{(n)}(\mathbf{Y}_1^{(n)})^{-1}$ will converge to $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ as $n \to \infty$, and $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ does not have p linearly independent eigenvectors. The matrix $\mathbf{A}^{(n)}$ contains the eigenvectors of $\mathbf{Y}_2^{(n)}(\mathbf{Y}_1^{(n)})^{-1}$ and will converge to a matrix containing the eigenvectors of $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$. Hence, $\mathbf{A}^{(n)}$ will converge to a matrix with at least two linearly dependent columns. The eigenvalues corresponding to these linearly dependent eigenvectors of $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ are necessarily identical. Hence, in the matrix $\mathbf{C}^{(n)}$ these columns will become identical (up to a sign change). In the matrix $\mathbf{B}^{(n)}$, the magnitude of the elements of these columns will become arbitrarily large. Hence, the rank-p decomposition of $\underline{\mathbf{Y}}^{(n)}$ will become degenerate as $\underline{\mathbf{Y}}^{(n)}$ approaches $\underline{\tilde{\mathbf{X}}}$.

If the rank-p decomposition of $\underline{\mathbf{Y}} \in D_p$ is not unique, i.e., when $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ has (at least) one eigenvalue λ with algebraic multiplicity larger than 1, then the only way to construct alternative decompositions is by taking different eigenvectors of λ as the columns of $\mathbf{A} = \mathbf{K}$; see the discussion below Lemma 1. Hence, the reasoning above also applies to these arrays. This means that we have shown that all rank-p decompositions of any sequence $\underline{\mathbf{Y}}^{(n)} \in D_p$ converging to $\underline{\tilde{\mathbf{X}}}$, will become degenerate for large n. This completes the proof of (ii) of Theorem 1.

An illustration of the case where $\mathbf{X}_2\mathbf{X}_1^{-1}$ has at least one pair of complex eigenvalues can be found in Fig. 1.

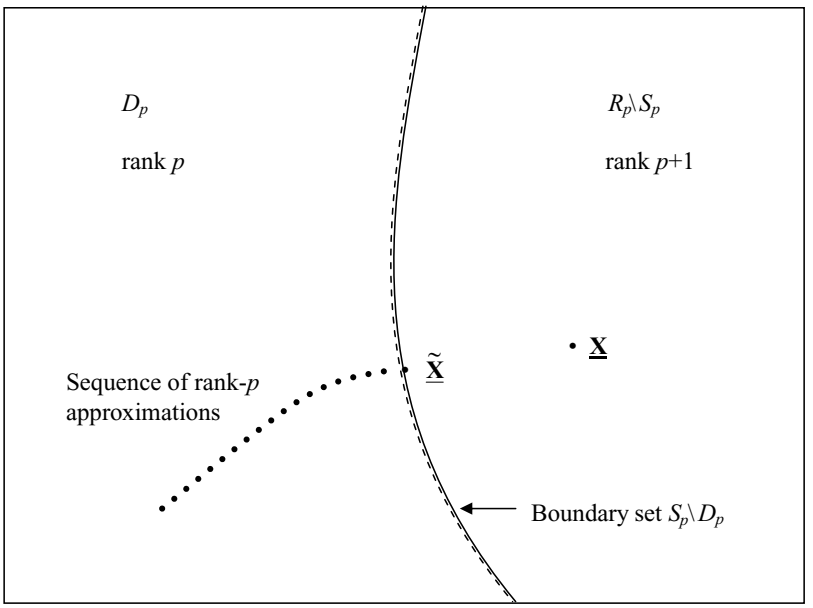

FIGURE 1.
Illustration of the case where $\mathbf{X}_2\mathbf{X}_1^{-1}$ has at least one pair of complex eigenvalues, i.e., $\underline{\mathbf{X}} \in R_p \backslash S_p$. The sets D_p and $R_p \backslash S_p$ both have positive volume in the space of real-valued $p \times p \times 2$ arrays, while the boundary set $S_p \backslash D_p$ has zero volume; see Table 1. The set D_p is virtually open, which is indicated by the dotted boundary line. The continuous boundary line represents the boundary of S_p, which is a closed set. The boundary point $\underline{\tilde{\mathbf{X}}} \in S_p \backslash D_p$ is the optimal solution of problem (24) and is approximated arbitrarily closely by the sequence of rank-p solutions. Note that this figure is similar to the illustration in Kruskal et al. (1989) for the $2 \times 2 \times 2$ case.

Suppose $\mathbf{X}_2\mathbf{X}_1^{-1}$ *Has p Real Eigenvalues but Is not Diagonalizable*

In this case $\mathbf{X} \in S_p \backslash D_p$ and $\underline{\mathbf{X}}$ can be approximated arbitrarily closely by arrays in D_p. Hence, the value of the infimum in (23) is zero and $\underline{\mathbf{X}}$ itself plays the role of $\tilde{\underline{\mathbf{X}}}$ above. We can use the proof above to show that also in this case there holds that any sequence of CP solutions of (23), of which the objective value converges to the infimum, will become degenerate.

Remark on the Type of Degeneracy in $(\mathbf{A}^{(n)}, \mathbf{B}^{(n)}, \mathbf{C}^{(n)})$

Assume that $\mathbf{A}^{(n)}$ and $\mathbf{C}^{(n)}$ are restricted to have columns of length 1 and $(\mathbf{A}^{(n)}, \mathbf{B}^{(n)}, \mathbf{C}^{(n)})$ is of the form (11) as above. From the algebraic and geometric multiplicities of the eigenvalues of $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ the number of components of $(\mathbf{A}^{(n)}, \mathbf{B}^{(n)}, \mathbf{C}^{(n)})$ involved in the degeneracy can be determined. For example, suppose that $p = 5$ and $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ has three eigenvalues with geometric multiplicity 1 and algebraic multiplicities 1, 1, and 3. Then, for the eigenvalue with algebraic multiplicity 3, the matrix $\mathbf{A}^{(n)}$ contains three nearly identical columns (up to a sign change), which are approximately equal to the eigenvector of $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ associated with this eigenvalue. The same three columns in $\mathbf{C}^{(n)}$ are nearly identical (up to a sign change), as explained above. The elements of these columns in $\mathbf{B}^{(n)}$ will become arbitrarily large. Moreover, it can be shown that their sum will remain small. This is exactly a three-factor degeneracy as introduced in the Introduction and presented in (6).

Next, consider the following example. Suppose that $p = 3$ and $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ has one eigenvalue with geometric multiplicity 2 and algebraic multiplicity 3. In this case, the matrix $\mathbf{A}^{(n)}$ contains three columns which are approximately equal to an eigenvector of $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$, and which are nearly linearly dependent. The columns in $\mathbf{A}^{(n)}$ do not have to be nearly identical (up to a sign change), since there exist two linearly independent eigenvectors of $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$. In $\mathbf{C}^{(n)}$ the columns are again nearly identical (up to a sign change) and in $\mathbf{B}^{(n)}$ we have arbitrarily large elements in all three columns. Moreover, there will be a linear combination of the columns of $\mathbf{B}^{(n)}$ which remains small. This linear combination depends on the form of linear dependence of the columns of $\mathbf{A}^{(n)}$. Hence, if the columns of $\mathbf{A}^{(n)}$ are not nearly identical up to a sign change, then we have a degeneracy involving three factors which is different from the three-factor degeneracy in (6). This example can be extended to any eigenvalue λ of $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ with $a(\lambda) > g(\lambda) \geq 2$, in which case we have a degeneracy involving $a(\lambda)$ factors, and the corresponding columns of $\mathbf{A}^{(n)}$ have at most rank $g(\lambda)$ in the limit. Remarkably, the cases where more than two factors form a degeneracy, but the corresponding columns of $\mathbf{A}^{(n)}$ are not nearly identical up to a sign change, did not occur in our simulations below. However, such degeneracies can be obtained by approximating an array $\tilde{\underline{\mathbf{X}}} \in S_p \backslash D_p$ for which $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ has an eigenvalue λ as above, and choosing a suitable starting point for the CP algorithm.

Note that if $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$ has several distinct eigenvalues for which the geometric multiplicity is smaller than the algebraic multiplicity, then there will be a group of degenerate factors for each such eigenvalue.

Proof of Lemma 2

First, we prove (i). By definition, the boundary points of D_p can be approximated arbitrarily closely by arrays in D_p and by arrays in $R_p \backslash D_p$. Let $\underline{\mathbf{Y}}$ be an array for which $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ has p real eigenvalues which are not all distinct. Since the eigenvalues of $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ depend continuously on the elements of $\underline{\mathbf{Y}}$, it follows that $\underline{\mathbf{Y}}$ can be approximated arbitrarily closely by arrays in D_p. Indeed, a sequence of arrays $\underline{\mathbf{U}}^{(\varepsilon,)}$, with $\underline{\mathbf{U}}^{(\varepsilon)} \to \underline{\mathbf{Y}}$ as $\varepsilon \downarrow 0$, can be constructed such that $\mathbf{U}_2^{(\varepsilon)}(\mathbf{U}_2^{(\varepsilon)})^{-1}$ has p real and distinct eigenvalues, i.e., $\underline{\mathbf{U}}^{(\varepsilon)} \in D_p$ for all $\varepsilon > 0$.

Next, we show that $\underline{\mathbf{Y}}$ can be approximated arbitrarily closely by arrays in $R_p \backslash D_p$. Suppose $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ has a double real eigenvalue λ with only one eigenvector $\mathbf{x}$, i.e., $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ is not diago-

nalizable. Let $^{(\varepsilon,)}$ be a sequence of arrays such that $\mathbf{Z}_2^{(\varepsilon,)}(\mathbf{Z}_1^{(\varepsilon,)})^{-1}$ has the same eigenvalues and eigenvectors as $\mathbf{Y}_2\mathbf{Y}_1^{-1}$, except that the double eigenvalue λ is replaced by the complex-valued pair $\lambda \pm i\varepsilon$, and the corresponding eigenvectors are $\mathbf{x} \pm i\,\varepsilon\,\mathbf{y}$, where $\mathbf{y}$ is linearly independent from the other eigenvectors of $Z_2^{(\varepsilon,)}(Z_1^{(\varepsilon,)})^{-1}$. Clearly, the arrays $\underline{\mathbf{Z}}^{(\varepsilon,)}$ lie in $R_p \backslash D_p$ and we can choose the sequence such that $\underline{\mathbf{Z}}^{(\varepsilon)} \rightarrow \underline{\mathbf{Y}}$ as $\varepsilon \downarrow 0$. This shows that $\underline{\mathbf{Y}}$ is a boundary point of D_p. Next, suppose $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ is diagonalizable and has a double real eigenvalue λ with two linearly independent eigenvectors $\mathbf{x}$ and $\mathbf{y}$. Then the complex-valued vectors $\mathbf{x} \pm i\mathbf{y}$ are also eigenvectors of $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ corresponding to the eigenvalue λ. Let the sequence of arrays $^{(\varepsilon,)}$ be such that $Z_2^{(\varepsilon,)}(Z_1^{(\varepsilon,)})^{-1}$ has the same eigenvalues and eigenvectors as $\underline{\mathbf{Y}}$, except that the double eigenvalue λ is replaced by the complex-valued pair $\lambda \pm i\varepsilon$, and the corresponding eigenvectors are $\mathbf{x} \pm i\,\mathbf{y}$. Then $^{(\varepsilon,)}$ lies in $R_p \backslash D_p$ for all $\varepsilon > 0$ and converges to $\underline{\mathbf{Y}}$ as $\varepsilon \downarrow 0$. Hence, $\underline{\mathbf{Y}}$ is a boundary point of D_p.

It remains to show if $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ has some complex eigenvalues or if it has p real and distinct eigenvalues, then $\underline{\mathbf{Y}}$ is not a boundary point of D_p. Suppose first that $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ has some complex eigenvalues. The eigenvalues of $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ depend continuously on the elements of $\underline{\mathbf{Y}}$. This implies that the array $\underline{\mathbf{Y}}$ cannot be approximated arbitrarily closely by a sequence of arrays $\underline{\mathbf{U}}^{(\varepsilon)}$ in D_p, since $\mathbf{U}_2^{(\varepsilon,)}\left(\mathbf{U}_1^{(\varepsilon,)}\right)^{-1}$ will have p real eigenvalues for all $\varepsilon > 0$. Hence, $\underline{\mathbf{Y}}$ is not a boundary point of D_p. Next, suppose $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ has p real and distinct eigenvalues. Complex-valued eigenvalues of real-valued matrices occur only in complex-conjugated pairs $\lambda \pm i\mu$. Hence, if a sequence of real-valued matrices with complex eigenvalues converges to a real-valued matrix with only real eigenvalues, then the latter matrix necessarily has some identical real eigenvalues. This implies that $\underline{\mathbf{Y}}$ cannot be approximated arbitrarily closely by a sequence of arrays $^{(\varepsilon,)}$ such that $Z_2^{(\varepsilon,)}(Z_1^{(\varepsilon,)})^{-1}$ has some complex eigenvalues for all $\varepsilon > 0$. Hence, $\underline{\mathbf{Y}}$ is not a boundary point of D_p. This completes the proof of (i).

Next, we prove (ii) by showing that the set of boundary points of D_p for which $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ is diagonalizable has lower dimensionality than the set of boundary points for which $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ is not diagonalizable. This implies that virtually all boundary points $\underline{\mathbf{Y}}$ of D_p have $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ not diagonalizable and, hence, lie in the set $S_p \backslash D_p$. Our proof is as follows. For a real-valued square matrix with real eigenvalues to have two identical eigenvalues, requires a deterministic relation between the elements of the matrix. The matrix then automatically has one eigenvector corresponding to the pair of identical eigenvalues. However, to have two linearly independent eigenvectors corresponding to the pair of identical eigenvalues, requires an *additional* deterministic relation between the elements of the matrix. Hence, the matrices which are diagonalizable lie in a set of lower dimensionality than the matrices which are not diagonalizable. Analogously, the set of boundary arrays $\underline{\mathbf{Y}}$ for which $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ is diagonalizable has lower dimensionality than the set of boundary arrays for which $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ is not diagonalizable. This completes the proof of (ii).

Next, we prove (iii). We need to show that the set S_p is closed. We do this by proving that all boundary points of S_p are included in S_p itself. By definition, the boundary points of S_p can be approximated arbitrarily closely by arrays in S_p and by arrays in $R_p \backslash S_p$. From the definition of the set S_p and the proof of (i) above, it follows that the boundary points of S_p are the same as the boundary points of D_p. Hence, for a boundary point $\underline{\mathbf{Y}}$ of S_p the matrix $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ has p real eigenvalues which are not all distinct. Since $\underline{\mathbf{Y}}$ lies in S_p this completes the proof of Lemma 2.

A Numerical Example for $p = 3$

As an illustration of a sequence of CP solutions converging to a boundary point $\tilde{\underline{\mathbf{X}}}$ of S_p, we will consider the $3 \times 3 \times 2$ array $\underline{\mathbf{X}}$ in (5). Since $\mathbf{X}_2\mathbf{X}_1^{-1}$ has two complex eigenvalues and the maximal rank of real-valued $3 \times 3 \times 2$ arrays equals 4, it follows from
Lemma 1 that $\underline{\mathbf{X}}$ has

rank 4. When the CP model with three components is fitted to $\underline{\mathbf{X}}$, we obtain the solution (6), which is a three-factor degeneracy. For this solution, the CP objective value is 0.4871. Since almost the same solution (up to sign changes and jointly permuting columns of **A**, **B,** and **C**) is obtained for a variety of different (random) starting values for **A**, **B,** and **C**, it is reasonable to assume that the solution is unique, i.e., there is a unique optimal solution $\tilde{\underline{\mathbf{X}}}$ of problem (24), which is approximated arbitrarily closely (depending on the stopping criterion of the CP algorithm) by arrays $\underline{\mathbf{Y}}$ in D_p. From the solution in (6), the approximating array $\underline{\mathbf{Y}}$ can be obtained as $\mathbf{Y}_1 = \mathbf{A}\mathbf{C}_1\mathbf{B}'$ and $\mathbf{Y}_2 = \mathbf{A}\mathbf{C}_2\mathbf{B}'$. The matrices **K** and $\mathbf{\Lambda}$ of the eigendecomposition $\mathbf{K}\mathbf{\Lambda}\mathbf{K}^{-1}$ of $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ then approximate the matrices of eigenvectors and eigenvalues, respectively, of $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$. From (6), we obtain the following for **K** and $\mathbf{\Lambda}$, where the columns of **K** have length 1:

$$\mathbf{K} = \begin{bmatrix} -0.4864 & -0.4737 & -0.4615 \\ 0.6648 & 0.6598 & 0.6535 \\ 0.5670 & 0.5834 & 0.5999 \end{bmatrix}, \qquad \mathbf{\Lambda} = \begin{bmatrix} 3.3092 & 0 & 0 \\ 0 & 3.4416 & 0 \\ 0 & 0 & 3.5804 \end{bmatrix}. \tag{25}$$

Notice that **K** is determined up to a sign change for each column. From (25) it can be seen that $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ is close to having one eigenvalue with algebraic multiplicity 3 and geometric multiplicity 1. This will hold exactly for $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$, which shows that $\tilde{\underline{\mathbf{X}}}$ is a boundary point of S_3; see Lemma 2.

Next, we sharpen the stopping criterion of the CP algorithm. As a consequence, the algorithm runs longer, the solution array $\underline{\mathbf{Y}}$ is closer to the boundary point $\tilde{\underline{\mathbf{X}}}$, and the CP objective value is closer to the value of the infimum. The new CP solution was computed using the same starting values as for (6) and reads as

$$\mathbf{A} = \begin{bmatrix} 0.4814 & 0.4663 & -0.4738 \\ -0.6627 & -0.6558 & 0.6595 \\ -0.5737 & -0.5938 & 0.5837 \end{bmatrix}, \qquad \mathbf{B} = \begin{bmatrix} 0.7178 & -0.6993 & 0.7086 \\ 0.6153 & -0.6422 & 0.6288 \\ 0.3258 & -0.3140 & 0.3202 \end{bmatrix},$$

$$\mathbf{C} = \begin{bmatrix} 1742.3 & -1689.7 & 3431.0 \\ 5853.1 & 5956.0 & 1180.5 \end{bmatrix}, \tag{26}$$

which is again a three-factor degeneracy. The CP objective value is now 0.4867. Compared with the previous solution (6), there are no big changes in the elements of **A** and **B**, but the elements of **C** have increased in magnitude. For this new solution, the eigendecomposition $\mathbf{K}\mathbf{\Lambda}\mathbf{K}^{-1}$ of $\mathbf{Y}_2\mathbf{Y}_1^{-1}$ satisfies:

$$\mathbf{K} = \begin{bmatrix} -0.4814 & -0.4737 & -0.4663 \\ 0.6627 & 0.6595 & 0.6558 \\ 0.5737 & 0.5837 & 0.5938 \end{bmatrix}, \qquad \Lambda = \begin{bmatrix} 3.3595 & 0 & 0 \\ 0 & 3.4409 & 0 \\ 0 & 0 & 3.5249 \end{bmatrix}. \tag{27}$$

Comparing (25) and (27), we see that the columns of **K** have become more alike and the three eigenvalues in $\mathbf{\Lambda}$ are closer to each other. This illustrates the convergence to $\tilde{\mathbf{X}}_2\tilde{\mathbf{X}}_1^{-1}$, which has one eigenvalue with algebraic multiplicity 3 and geometric multiplicity 1.

Approximating a Random $p \times p \times 2$ Array of Rank $p + 1$

In the remaining part of this paper, we consider a $p \times p \times 2$ array $\underline{\mathbf{X}}$ of which the elements are drawn from a $2p^2$-dimensional continuous distribution F. Ten Berge & Kiers (1999) have shown that, with probability 1, the rank of $\underline{\mathbf{X}}$ is either p or $p + 1$, where both rank values occur with positive probability. Hence, the *typical rank* of real-valued $p \times p \times 2$ arrays equals $\{p,$

$p + 1\}$. Note that, for a set A of real-valued $p \times p \times 2$ arrays, the statement "A occurs with positive probability," i.e., $F(A) > 0$, is equivalent to the statement "A has positive volume," i.e., the dimensionality of A equals $2p^2$.

Note that $\mathbf{X}_1^{-1}$ exists with probability 1 and $\mathbf{X}_2\mathbf{X}_1^{-1}$ has p distinct eigenvalues, i.e., is diagonalizable, with probability 1. Therefore, we have the following corollary of Lemma 1. This also shows that the sets D_p and $R_p \backslash S_p$ have positive volume, while the set $S_p \backslash D_p$ has zero volume; see Table 1.

Corollary 1. *Let $\underline{\mathbf{X}}$ be a real-valued $p \times p \times 2$ array with $p \times p$ slices $\mathbf{X}_1$ and $\mathbf{X}_2$. If the elements of $\underline{\mathbf{X}}$ are drawn from a $2p^2$-dimensional continuous distribution, then the following statements hold with probability 1:*

(i). If $\mathbf{X}_2\mathbf{X}_1^{-1}$ has p real eigenvalues, then rank($\underline{\mathbf{X}}$) = p.
(ii). If $\mathbf{X}_2\mathbf{X}_1^{-1}$ has at least one pair of complex eigenvalues, then rank($\underline{\mathbf{X}}$) = p + 1.

Simulation Results

Theorem 1 states that when the CP model is fitted to a random $p \times p \times 2$ array $\underline{\mathbf{X}}$ of rank $p + 1$, and the number of components equals p, then the CP objective function has no minimum but an infimum and all CP solutions approaching the infimum will become degenerate. To investigate which patterns of degeneracies tend to occur in the CP solutions, we have conducted a simulation study. For values of p from 2 up to 5, we have generated random $p \times p \times 2$ arrays $\underline{\mathbf{X}}$. If the rank of $\underline{\mathbf{X}}$ is $p + 1$, i.e., when $\mathbf{X}_2\mathbf{X}_1^{-1}$ has at least one pair of complex eigenvalues, we have fitted the rank-p CP model to $\underline{\mathbf{X}}$. For this, we used the Multilinear Engine program (Paatero, 1999), which was kindly provided to us by Pentti Paatero.

We have considered six categories of arrays $\underline{\mathbf{X}}$, namely $2 \times 2 \times 2$ arrays where $\mathbf{X}_2\mathbf{X}_1^{-1}$ has two complex eigenvalues, $3 \times 3 \times 2$ arrays where $\mathbf{X}_2\mathbf{X}_1^{-1}$ has two complex eigenvalues, $4 \times 4 \times 2$ arrays where $\mathbf{X}_2\mathbf{X}_1^{-1}$ has one pair of complex eigenvalues, $4 \times 4 \times 2$ arrays where $\mathbf{X}_2\mathbf{X}_1^{-1}$ has two pairs of complex eigenvalues, $5 \times 5 \times 2$ arrays where $\mathbf{X}_2\mathbf{X}_1^{-1}$ has one pair of complex eigenvalues, and $5 \times 5 \times 2$ arrays where $\mathbf{X}_2\mathbf{X}_1^{-1}$ has two pairs of complex eigenvalues. We have calculated the rank-p approximation of 10 arrays of each category. For each array we used 10 different (random) starting values for the component matrices **A**, **B,** and **C**. We have restricted **A** and **B** to have columns of unit length. In a vast majority of cases (581 out of 600) all 10 runs for one array yielded almost the same solution (up to sign changes and a joint permutation of the columns of **A**, **B,** and **C**). In the other 19 cases the algorithm terminated with a suboptimal solution. We discarded the outcomes of these 19 runs and will speak of *the* CP solution for a certain array $\underline{\mathbf{X}}$ from now on. Notice that this indicates that usually there is a unique boundary point $\tilde{\underline{\mathbf{X}}}$ of S_p, which is the optimal solution of problem (24). This boundary point is then approximated arbitrarily closely (depending on the stopping criterion of the CP algorithm) by the rank-p arrays in D_p. Note that for the K3 array, which we discussed above, there are infinitely many such boundary points $\tilde{\underline{\mathbf{X}}}$. In this sense, the K3 array is an exception.

As we expected, all solution arrays lie in the set R_p, i.e., their first slice is invertible. The types of degenerate solutions obtained for the arrays of the six categories can be found in Table 2 below. The notation x-fd denotes a degeneracy involving x factors. The notation 2-fd + 2-fd indicates that two different pairs of factors in the solution each form a two-factor degeneracy. The notation of 2-fd + 3-fd is used analogously. Remarkably, each time an x-fd is obtained for $x \geq 3$, the x columns are nearly identical (up to a sign change) in two of the component matrices and their sum (up to a sign change) is close to zero in the third component matrix. Hence, the 4-fd and 5-fd cases we obtained are generalizations of the three-factor degeneracy in the Introduction. It should

TABLE 2.
Frequencies of different degenerate CP solutions resulting from rank-p approximations of random $p \times p \times 2$ arrays $\underline{\mathbf{X}}$ of rank $p + 1$. Of each category, 10 different arrays are considered

Category	2-fd	2-fd + 2-fd	3-fd	2-fd + 3-fd	4-fd	5-fd
$p = 2$	10	—	—	—	—	—
$p = 3$	9	—	1	—	—	—
$p = 4$[a]	4	0	5	—	1	—
$p = 4$[b]	0	7	1	—	2	—
$p = 5$[c]	7	0	1	0	2	0
$p = 5$[d]	0	3	1	4	1	1

[a]Two complex eigen values.
[b]Four complex eigen values.
[c]Two complex eigen values.
[d]Four complex eigen values.

be noted, however, that especially for $p = 4$ and $p = 5$ the convergence of the CP algorithm was very slow and the type of degeneracy was obtained by extrapolating the CP solution. Therefore, the numbers in Table 2 should be regarded with some reservation.

It can be seen from Table 2 that for $p > 3$, several different types of degenerate CP solutions are obtained for different random arrays. It is tempting to search for general rules which predict, based on the eigenvalues of $\mathbf{X}_2\mathbf{X}_1^{-1}$, the type of degenerate solution that will be obtained. However, we have not found any indications of the existence of such rules.

Discussion

We have shown that if the p-component CP model is fitted to a real-valued $p \times p \times 2$ array of rank $p + 1$ or higher, then the CP objective function does not have a minimum but an infimum. Moreover, any sequence of CP solutions of which the objective value converges to the infimum, will converge to a limit point on the boundary between the sets of rank-p and rank-$(p + 1)$ arrays. This limit point has rank $p + 1$ or higher. When the rank-p sequence gets close to the limit point, it necessarily becomes degenerate. This result extends and proves the statements made by Kruskal et al. (1989) for the $2 \times 2 \times 2$ case.

The result of Theorem 1 can be extended in the following ways.

- All norms on the finite-dimensional vector space are equivalent and induce the same (i.e., the Euclidean) topology. Therefore, the result of Theorem 1 still holds if the Frobenius norm in the CP objective function is replaced by any other norm, e.g. weighted least squares or Gaussian maximum likelihood.
- Let $\underline{\mathbf{X}}$ be an $I \times J \times K$ array, with $I \geq J \geq p$, and suppose $\underline{\mathbf{X}}$ satisfies the Tucker3 model (3) with perfect fit, and with a $p \times p \times 2$ core array $\underline{\mathbf{G}}$ of rank $p + 1$ or higher. If rank($\underline{\mathbf{X}}$) = rank($\underline{\mathbf{G}}$), slice $\mathbf{G}_1$ is invertible and $\underline{\mathbf{X}}$ is approximated by rank-p arrays, then it can be shown (analogous to the proof of Theorem 1) that the CP objective function has no minimum but an infimum and all CP solutions of which the objective value approaches the infimum will become degenerate.
- For real-valued $p \times q \times 2$ arrays, sometimes (with positive probability for certain combinations of p, q, and R) degenerate CP solutions are encountered. In Stegeman (2005a) it is explained how this happens, using the result of Theorem 1.

- For $5 \times 3 \times 3$ arrays, Ten Berge (2004) has developed a rank criterion similar to Lemma 1. A seventh degree polynomial is constructed, the coefficients of which depend on the elements of the array. If the polynomial has real and distinct roots, the $5 \times 3 \times 3$ array has rank 5. If some roots are complex, the array has rank 6 or higher. Using this result, and the (partial) uniqueness of the rank-5 decomposition of $5 \times 3 \times 3$ arrays of rank 5, Stegeman (2005b) explains why degenerate CP solutions occur when $5 \times 3 \times 3$ arrays of rank 6 are approximated by rank-5 arrays.

Note that the type of degeneracy described in this paper and in Stegeman (2005a, 2005b) does not occur in the complex-valued CP model. In the latter case, it does not matter whether our polynomial (in Lemma 1 or in Ten Berge, 2004) has real or complex roots, and the rank of the array over the complex field is equal to the rank over the real field in the case of only real roots. The degeneracies in the real-valued CP model, described here and in Stegeman (2005a, 2005b), occur due to a two-valued typical rank and (partial) uniqueness of the rank-R decomposition. Whether this is the case for all degeneracies in the real-valued CP model is still an open problem.

Analogous to Paatero (2000), we may consider swamps as areas of the space of real-valued $p \times p \times 2$ arrays where the sequence of rank-p approximations, generated by the CP algorithm, advances very slowly. It follows from Theorem 1 that if the target array $\underline{\mathbf{X}}$ has rank $p+1$ or higher, the swamps occur near the boundary between the sets of rank-p and rank-$(p+1)$ arrays. In this case, the CP algorithm necessarily terminates in the swamp and modifications to the CP algorithm cannot prevent this. The only way to avoid degeneracies is to include additional restrictions on the component matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$.

We may also consider the case where $\underline{\mathbf{X}}$ has rank p, but is located inside or near a swamp. Such arrays are easy to construct by taking $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ as in (11), with $\mathbf{A}$ and $\mathbf{B}$ (or also $\mathbf{C}$) nearly rank-deficient. Note that it follows from (11) that a nearly rank-deficient $\mathbf{A}$ implies a nearly rank-deficient $\mathbf{B}$ and vice versa. Since this rank-p decomposition is unique, any rank-p sequence converging to $\underline{\mathbf{X}}$ will become as degenerate as the $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ used to construct $\underline{\mathbf{X}}$. For the $2 \times 2 \times 2$ case, such examples can be found in Paatero (2000). We conjecture that also the example in Paatero (2000), again for the $2 \times 2 \times 2$ case, where the starting point of the CP algorithm is chosen such that the rank-2 sequence cannot get around a curve in the boundary between the starting point and the rank-2 target array $\underline{\mathbf{X}}$, can be generalized to the setting of $p \times p \times 2$ arrays, although it may be difficult to visualize. In the case where a rank-p array $\underline{\mathbf{X}}$ is located inside or near a swamp, modifications of the CP algorithm may speed up the convergence to $\underline{\mathbf{X}}$.

Zijlstra & Kiers (2002) observed that two-factor degeneracies occur not only in CP but also in other variants of factor analysis. They show that two- and three-way factor analysis models which yield degenerate solutions, necessarily have rotationally unique components. It would be interesting to consider these factor analysis models and try to explain the occurrence of degenerate solutions by using the same framework and tools as in the proof of Theorem 1.

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