Candecomp/Parafac

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CANDECOMP/PARAFAC: FROM DIVERGING COMPONENTS TO A DECOMPOSITION IN BLOCK TERMS*

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Abstract. Fitting an R-component Candecomp/Parafac (CP) decomposition to a multiway array or higher-order tensor $\mathcal{Z}$ is equivalent to finding a best rank-R approximation of $\mathcal{Z}$. Such a best rank-R approximation may not exist due to the fact that the set of multiway arrays with rank at most R is not closed. In this case, trying to compute the approximation results in diverging CP components. We present an approach to avoid diverging components for real $I \times J \times K$ arrays with $R \leq \min(I, J, K)$. We show that a CP decomposition $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ featuring diverging components can be rewritten as a decomposition in block terms, where each block term corresponds to a group of diverging components. Moreover, we show that if the diverging components occur in groups of two or three, then the limiting boundary point $\mathcal{X}$ (i.e., the limit of the sequence of CP updates) can be obtained by fitting an appropriate constrained Tucker3 model to $\mathcal{Z}$, using the block term decomposition of $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ as initial values. Our results are demonstrated by means of numerical experiments.

Key words. tensor decomposition, low-rank approximation, Candecomp, Parafac, Schur decomposition, block decomposition, diverging components

AMS subject classifications. 15A18, 15A22, 15A69, 49M27, 62H25

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1. Introduction.

Tensors of order n are defined on the outer product of n linear spaces, S_ℓ, $1 \leq \ell \leq n$. Once bases of spaces S_ℓ are fixed, they can be represented by n-way arrays. For simplicity, tensors are usually assimilated with their array representation. Note that a two-way array is a matrix.

For $n \geq 3$, a generalized rank and related decomposition of an n-way array was introduced in 1927 [22], [23]. Around 1970, the same decomposition was reintroduced in psychometrics [4] and phonetics [19] for component analysis of n-way data arrays. It was then named Candecomp and Parafac, respectively. We denote the three-way Candecomp/Parafac (CP) model, i.e., the decomposition with a residual term, as

$$\mathcal{Z} = \sum_{r=1}^{R} \omega_r \, (\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r) + \mathcal{E} \,, \tag{1.1}$$

where $\mathcal{Z}$ is an $I \times J \times K$ data array, ω_r is the weight of term r, $\circ$ denotes the outer product, and $\|\mathbf{a}_r\| = \|\mathbf{b}_r\| = \|\mathbf{c}_r\| = 1$ for $r = 1, \ldots, R$, with $\|\cdot\|$ denoting the Frobenius norm (i.e., the square root of the sum-of-squares). To find the R terms $\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$ and the weights ω_r, an iterative algorithm is used which minimizes the Frobenius norm of the residual array $\mathcal{E}$. The most well-known algorithm is Alternating Least Squares. For an overview and comparison of CP algorithms, see [24], [59], [6].

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For later use, we mention that the CP model (1.1) is a special case of the Tucker3 model [60]. The latter is defined as

$$\mathcal{Z} = \sum_{r=1}^{R}\sum_{p=1}^{P}\sum_{q=1}^{Q} g_{rpq}\,(\mathbf{a}_r \circ \mathbf{b}_p \circ \mathbf{c}_q) + \mathcal{E}\,. \tag{1.2}$$

Clearly, the case with $R = P = Q$ and $g_{rpq} = 0$ if $(r,p,q) \neq (r,r,r)$ yields (1.1). The $R \times P \times Q$ array $\mathcal{G}$ with entries g_{rpq} is referred to as the core array. The matrices $\mathbf{A} = [\mathbf{a}_1|\ldots|\mathbf{a}_R]$, $\mathbf{B} = [\mathbf{b}_1|\ldots|\mathbf{b}_P]$ and $\mathbf{C} = [\mathbf{c}_1|\ldots|\mathbf{c}_Q]$ are called the component matrices.

A matrix form of the CP model (1.1) is

$$\mathbf{Z}_k = \mathbf{A}\,\mathbf{C}_k\,\mathbf{B}^T + \mathbf{E}_k\,, \qquad k = 1,\ldots,K\,, \tag{1.3}$$

where $\mathbf{Z}_k$ and $\mathbf{E}_k$ are the kth $I \times J$ frontal slices of $\mathcal{Z}$ and $\mathcal{E}$, respectively, and $\mathbf{C}_k$ is the diagonal matrix with row k of $\mathbf{C}$ as its diagonal. In (1.3), the weights ω_r are absorbed into $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$.

We use the notation $\mathcal{X} = (\mathbf{S},\mathbf{T},\mathbf{U}) \cdot \mathcal{Y}$ to denote the multilinear matrix multiplication of an array $\mathcal{Y} \in \mathbb{R}^{I\times J\times K}$ with matrices $\mathbf{S}$ $(I_2 \times I)$, $\mathbf{T}$ $(J_2 \times J)$, and $\mathbf{U}$ $(K_2 \times K)$. The result of the multiplication is an $I_2 \times J_2 \times K_2$ array $\mathcal{X}$ with entries

$$x_{ijk} = \sum_{r=1}^{I}\sum_{p=1}^{J}\sum_{q=1}^{K} s_{ir}\,t_{jp}\,u_{kq}\,y_{rpq}\,, \tag{1.4}$$

where s_{ir}, t_{jp}, and u_{kq} are entries of $\mathbf{S}$, $\mathbf{T}$, and $\mathbf{U}$, respectively. Using this notation, the Tucker3 model (1.2) can be written as $\mathcal{Z} = (\mathbf{A},\mathbf{B},\mathbf{C}) \cdot \mathcal{G} + \mathcal{E}$.

CP and Tucker3 can be seen as generalizations of principal components analysis or factor analysis for matrices. They can be used for exploratory component analysis of three-way data. Such (real-valued) applications of CP and Tucker3 occur in psychology [33], [29] and chemometrics [46]. Complex-valued CP is used in, e.g., signal processing and telecommunications research [44], [45], [15]. Here, the decompositions are mostly used to separate signal sources from an observed mixture of signals. Four-way CP describes the basic structure of fourth-order cumulants of multivariate data on which many algebraic methods for Independent Component Analysis (ICA) are based [5], [13], [12], [7]. A general overview of applications of CP and Tucker3 can be found in [30], [1].

The most attractive feature of CP is that, for fixed residuals, the vectors $\mathbf{a}_r$, $\mathbf{b}_r$, and $\mathbf{c}_r$ and the weights ω_r are unique up to sign changes and a reordering of the summands in (1.1) under mild conditions [34], [53], [40], [43], [27], [8], [51].

In this paper, we consider the real-valued three-way CP model (1.1). The application of CP may be hampered by nonexistence of a best fitting CP solution in (1.1). As a consequence, diverging components occur in the sequence of CP updates resulting from an iterative CP algorithm. We propose a method for dealing with such situations when $R \leq \min(I,J,K)$. But first, we discuss the problem of nonexistence of a best fitting CP solution.

The rank (over the real field) of $\mathcal{Z}$ is defined in the usual way, i.e., the smallest number of (real) rank-1 arrays whose sum equals $\mathcal{Z}$. A three-way array has rank 1 if it is the outer product of three vectors, i.e., $\mathbf{a} \circ \mathbf{b} \circ \mathbf{c}$. We denote tensor rank as $\operatorname{rank}(\mathcal{Z})$. Let

$$S_R(I,J,K) = \{\mathcal{Y} \in \mathbb{R}^{I\times J\times K} \mid \operatorname{rank}(\mathcal{Y}) \leq R\}\,. \tag{1.5}$$

Since the CP model (1.1) constitutes a sum of R rank-1 arrays, fitting the CP model to $\mathcal{Z}$ boils down to solving the following minimization problem:

$$\text{Minimize } ||\mathcal{Z} - \mathcal{Y}|| \qquad \text{subject to} \qquad \mathcal{Y} \in S_R(I, J, K)\,. \tag{1.6}$$

Hence, we are looking for a best rank-R approximation to $\mathcal{Z}$. Assuming $\text{rank}(\mathcal{Z}) > R$, an optimal solution of (1.6) will be a boundary point of the set $S_R(I, J, K)$. However, the set $S_R(I, J, K)$ is not closed for $R \geq 2$, and the CP problem (1.6) may not have an optimal solution because of this fact [16]. Nonexistence of an optimal solution results in diverging rank-1 arrays when an attempt is made to compute a best rank-R approximation to $\mathcal{Z}$. This was conjectured by [35] and recently proven by [32]. We refer to this phenomenon as *diverging CP components*, but it is also known as CP "degeneracy" [20, 50]. In such cases, while running a CP algorithm, the decrease of $||\mathcal{Z} - \mathcal{Y}||$ becomes very slow, and some (groups of) columns of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ become nearly linearly dependent, while the corresponding weights ω_r become large in magnitude. However, the sum of the corresponding rank-1 terms remains small and contributes to a better CP fit. More formally, a group of diverging components corresponds to an index set $D \subseteq \{1, \ldots, R\}$ such that

$$|\omega_r^{(n)}| \to \infty \qquad \text{for all } r \in D\,, \tag{1.7}$$

$$\text{while} \quad \left\| \sum_{r \in D} \omega_r^{(n)} \, (\mathbf{a}_r^{(n)} \circ \mathbf{b}_r^{(n)} \circ \mathbf{c}_r^{(n)}) \right\| \quad \text{is bounded}\,, \tag{1.8}$$

where the superscript (n) denotes the nth CP update of the iterative CP algorithm. In practice and in simulation studies with random data $\mathcal{Z}$, groups of diverging components are such that the corresponding columns of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ become nearly identical up to sign. Other forms of linear dependency are possible but exceptional [56].

More than one group of diverging components may exist. In that case (1.7)–(1.8) hold for the corresponding disjoint index sets. The slow convergence of the CP objective function value is also referred to as being stuck in a "swamp" [38]. A numerical example of diverging components is as follows. For a random $6 \times 6 \times 6$ array $\mathcal{Z}$ and $R = 6$, a CP algorithm terminates with

$$\mathbf{A} = \begin{bmatrix} 0.1879 & 0.2128 & 0.7316 & 0.7093 & 0.7150 & 0.5485 \\ 0.0211 & 0.0349 & 0.1253 & 0.1583 & 0.1504 & 0.2090 \\ -0.4753 & -0.4874 & -0.2498 & -0.2604 & -0.2582 & 0.4797 \\ -0.3848 & -0.3535 & -0.1035 & -0.1466 & -0.1360 & -0.6106 \\ -0.7682 & -0.7687 & -0.5828 & -0.5784 & -0.5797 & 0.1383 \\ -0.0133 & 0.0034 & -0.1908 & -0.2191 & -0.2119 & 0.1826 \end{bmatrix}, \tag{1.9}$$

$$\mathbf{B} = \begin{bmatrix} 0.1556 & -0.1605 & -0.3042 & -0.3089 & 0.3077 & -0.6768 \\ 0.1043 & -0.1188 & -0.0284 & -0.0466 & 0.0423 & 0.5075 \\ -0.7401 & 0.7325 & 0.2446 & 0.2798 & -0.2716 & -0.2670 \\ 0.0657 & -0.0775 & 0.3483 & 0.3707 & -0.3649 & -0.0148 \\ 0.6414 & -0.6416 & -0.2735 & -0.2742 & 0.2741 & 0.3239 \\ -0.0380 & 0.0766 & 0.8067 & 0.7820 & -0.7883 & -0.3285 \end{bmatrix}, \tag{1.10}$$

$$\text{(1.11)}\quad \mathbf{C} = \begin{bmatrix} -0.4598 & -0.4478 & -0.6200 & -0.6267 & -0.6251 & -0.5416 \\ -0.3797 & -0.3738 & -0.1736 & -0.1695 & -0.1709 & 0.6200 \\ 0.6055 & 0.6078 & 0.0237 & 0.0117 & 0.0150 & 0.1191 \\ -0.0096 & 0.0234 & 0.4039 & 0.3636 & 0.3736 & 0.2102 \\ -0.5263 & -0.5381 & -0.6454 & -0.6638 & -0.6593 & 0.1737 \\ -0.0269 & -0.0150 & -0.0724 & -0.0744 & -0.0739 & -0.4834 \end{bmatrix},$$

and corresponding weights $\omega_1 = 130.22$, $\omega_2 = 133.47$, $\omega_3 = 2083.3$, $\omega_4 = 6386.1$, $\omega_5 = 8466.6$, and $\omega_6 = 4.44$. Hence, in this example we have one group of two diverging components (1 and 2), one group of three diverging components (3, 4, and 5), and one nondiverging component (6).

Diverging components cannot be interpreted and may thus be a serious problem in the practical use of CP. In simulation studies involving randomly sampled data $\mathcal{Z}$, diverging components occur very often, with percentages of up to 50, 60, or even 100 [47], [49], [48]. Also, it has been shown that all $2 \times 2 \times 2$ arrays of rank 3 (a set of positive volume in $\mathbb{R}^{2\times2\times2}$) have no optimal CP solution for $R = 2$ [16].

In practice, diverging components due to nonexistence of an optimal CP solution are often avoided by imposing constraints in CP. For example, imposing orthogonality constraints on the components matrices guarantees an optimal CP solution [32], and an optimal CP solution exists for nonnegative $\mathcal{Z}$ under the restriction of nonnegative component matrices [36]. Also, [37] shows that constraining the magnitude of the inner products between pairs of columns of component matrices guarantees an optimal CP solution. However, these constraints are not suitable for all applications of CP.

A different approach to deal with diverging components is as follows. In order to guarantee the existence of an optimal solution, it has been proposed to consider the following minimization problem instead [16]:

$$\text{(1.12)}\qquad \text{Minimize } ||\mathcal{Z} - \mathcal{Y}|| \qquad \text{subject to} \qquad \mathcal{Y} \in \overline{S}_R(I,J,K)\,,$$

where $\overline{S}_R(I,J,K)$ denotes the closure of $S_R(I,J,K)$, i.e., the union of the set itself and its boundary points in $\mathbb{R}^{I\times J\times K}$. Naturally, (1.12) has an optimal solution. If (1.6) has an optimal solution, then it is also an optimal solution of (1.12). If (1.6) does not have an optimal solution, then the sequence of CP updates will converge (assuming the CP algorithm minimizes $||\mathcal{Z} - \mathcal{Y}||$) to an optimal solution of problem (1.12). This optimal solution is a boundary point of $S_R(I,J,K)$ with rank larger than R, and the sequence of CP updates converging to it will feature diverging components [32].

To solve (1.12), we need to characterize the boundary points of $S_R(I,J,K)$ and we need an algorithm to find an optimal boundary point. For $R = 2$, the boundary points of $S_2(I,J,K)$ are determined by [16], and [41] show that (1.12) can be solved by fitting a Tucker3 model with columnwise orthonormal component matrices and a constrained $2 \times 2 \times 2$ core array. For $K = 2$, the boundary points of $S_R(I,J,2)$ are characterized by [47], [49], [52], and [54] show that (1.12) can be solved for $I \times J \times 2$ arrays by fitting a Generalized Schur Decomposition (GSD), which has the matrix form

$$\text{(1.13)}\qquad \mathbf{Z}_k = \mathbf{Q}_a\,\mathbf{R}_k\,\mathbf{Q}_b^T + \mathbf{E}_k\,, \qquad k = 1,2\,,$$

where $\mathbf{Q}_a$ $(I \times R)$ and $\mathbf{Q}_b$ $(J \times R)$ are columnwise orthonormal, and $\mathbf{R}_k$ are $R \times R$ upper triangular. The set of arrays satisfying the GSD with perfect fit is identical to $\overline{S}_R(I,J,2)$ [52]. Note that $R \leq \min(I,J)$ must hold in the GSD. However, for

$R > \min(I, J)$ the problem of diverging CP components does not seem to occur [49]. For a detailed discussion of the relations between CP and GSD, and a GSD algorithm, we refer to [54].

In this paper, we propose a new constructive method to find an optimal boundary point of (1.12) for general $I \times J \times K$ arrays with $R \leq \min(I, J, K)$. We first try to solve the CP problem (1.6). If the CP algorithm that is used terminates with a CP decomposition $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ featuring diverging components, and we are convinced that the CP problem does not have an optimal solution, then we proceed as follows. We reorder the R rank-1 terms such that $\mathbf{A} = [\mathbf{A}_1 \,|\, \ldots \,|\, \mathbf{A}_m]$, $\mathbf{B} = [\mathbf{B}_1 \,|\, \ldots \,|\, \mathbf{B}_m]$, $\mathbf{C} = [\mathbf{C}_1 \,|\, \ldots \,|\, \mathbf{C}_m]$, with $\mathbf{A}_j$, $\mathbf{B}_j$, $\mathbf{C}_j$ having d_j columns and defining a group of d_j diverging components if $d_j \geq 2$, and a nondiverging component if $d_j = 1$, $j = 1, \ldots, m$. We have $R = \sum_{j=1}^{m} d_j$. Let $\mathcal{Y}_j$ be the $I \times J \times K$ array defined by the d_j components in $(\mathbf{A}_j, \mathbf{B}_j, \mathbf{C}_j)$. Then $\text{rank}(\mathcal{Y}_j) = d_j$, and $\mathcal{Y} = \sum_{j=1}^{m} \mathcal{Y}_j$ is the array defined by the CP decomposition $(\mathbf{A}, \mathbf{B}, \mathbf{C})$. We assume that for $d_j \geq 2$, the array $\mathcal{Y}_j$ converges to some $\mathcal{X}_j$ with $\text{rank}(\mathcal{X}_j) > d_j$. We show that for $d_j \in \{2, 3\}$, such a limit $\mathcal{X}_j$ has a Tucker3 decomposition $\mathcal{X}_j = (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ with a sparse $d_j \times d_j \times d_j$ core array $\mathcal{G}_j$ in canonical form and with $\text{rank}(\mathcal{G}_j) = \text{rank}(\mathcal{X}_j) > d_j$. The $d_j = 2$ canonical form follows from [16], and the $d_j = 3$ canonical form is proven in this paper. A nondiverging component, i.e., $\mathcal{Y}_j$ with $d_j = 1$, has a rank-1 limit $\mathcal{X}_j = (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ with core $\mathcal{G}_j$ of size $1 \times 1 \times 1$. Hence, for $\max(d_j) \leq 3$ the sequence of CP updates $\mathcal{Y} = \sum_{j=1}^{m} \mathcal{Y}_j$ converges to a limit point $\mathcal{X} = \sum_{j=1}^{m} \mathcal{X}_j$ that has a Tucker3 decomposition with an $R \times R \times R$ block-diagonal core array $\mathcal{G} = \text{blockdiag}(\mathcal{G}_1, \ldots, \mathcal{G}_m)$, i.e., $\mathcal{X} = (\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \mathcal{G} = \sum_{j=1}^{m} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$, with $\mathbf{S} = [\mathbf{S}_1 \,|\, \ldots \,|\, \mathbf{S}_m]$, $\mathbf{T} = [\mathbf{T}_1 \,|\, \ldots \,|\, \mathbf{T}_m]$, and $\mathbf{U} = [\mathbf{U}_1 \,|\, \ldots \,|\, \mathbf{U}_m]$. The limit process is visualized below:

$$\begin{array}{ccccccccc} \mathcal{Y} & = & (\mathbf{A}_1, \mathbf{B}_1, \mathbf{C}_1) & + & (\mathbf{A}_2, \mathbf{B}_2, \mathbf{C}_2) & + \cdots + & (\mathbf{A}_m, \mathbf{B}_m, \mathbf{C}_m) \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ \mathcal{X} & = & (\mathbf{S}_1, \mathbf{T}_1, \mathbf{U}_1) \cdot \mathcal{G}_1 & + & (\mathbf{S}_2, \mathbf{T}_2, \mathbf{U}_2) \cdot \mathcal{G}_2 & + \cdots + & (\mathbf{S}_m, \mathbf{T}_m, \mathbf{U}_m) \cdot \mathcal{G}_m \end{array}$$

The decomposition of $\mathcal{X}$ is an example of a decomposition into block terms, introduced in [9], [10], [11], where the block terms are $(\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$. We show that $\mathcal{X}$ is a boundary point of $S_R(I, J, K)$ with $\text{rank}(\mathcal{X}) > R$. If the error sum-of-squares corresponding to the sequence of CP updates is converging to the infimum of the CP problem (1.6), then $\mathcal{X}$ is an optimal boundary point of problem (1.12). To obtain $\mathcal{X}$ and its decomposition $\sum_{j=1}^{m} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ from the CP decomposition $(\mathbf{A}, \mathbf{B}, \mathbf{C})$, we fit the decomposition $\sum_{j=1}^{m} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ with blocks $\mathcal{G}_j$ in canonical form to the data array $\mathcal{Z}$, using initial values obtained from $(\mathbf{A}, \mathbf{B}, \mathbf{C})$.

A brief illustration of our method for the CP solution (1.9)–(1.11) is as follows. We have one group of two diverging components, one group of three diverging components, and one nondiverging component. We set $m = 3$, $d_1 = 2$, $d_2 = 3$, and $d_3 = 1$. After obtaining the limit point $\mathcal{X}$ and its decomposition into block terms, $\sum_{j=1}^{3} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$, the component matrices $[\mathbf{S}_1 \,|\, \mathbf{S}_2 \,|\, \mathbf{S}_3]$, $[\mathbf{T}_1 \,|\, \mathbf{T}_2 \,|\, \mathbf{T}_3]$, and $[\mathbf{U}_1 \,|\, \mathbf{U}_2 \,|\, \mathbf{U}_3]$ have condition numbers 21.8, 6.3, and 61.0, respectively. The core blocks $\mathcal{G}_j$ are in sparse canonical form and do not contain large numbers. Hence, the problems of diverging CP components have vanished. The error sum-of-squares of the CP decomposition (1.9)–(1.11) equals $||\mathcal{Z} - \mathcal{Y}||^2 = 54.5370$. For the limit point $\mathcal{X}$ we have $||\mathcal{Z} - \mathcal{X}||^2 = 54.5336$, which shows that the boundary point $\mathcal{X}$ is indeed a little closer to $\mathcal{Z}$ than $\mathcal{Y}$.

Compared to the previously considered cases of $R = 2$ in [41] and $K = 2$ in [54], our method is much less restrictive by assuming only $R \leq \min(I, J, K)$. However,

diverging components do also occur for $R > \min(I, J, K)$; see [48]. Our restriction to $\max(d_j) \leq 3$ is due to the difficulty of proving canonical forms for $d_j \geq 4$. However, groups of more than three diverging components (cases with $d_j \geq 4$) occur much less often than groups of two or three diverging components. This can be seen in our simulation study in section 5, and in [47]. Groups of more than three diverging components can be handled when proofs of canonical forms for $d_j \geq 4$ become available.

Our procedure eliminates the nearly identical components and the large component weights that occur when the CP problem does not have an optimal solution. When imposing constraints in CP to guarantee an optimal solution is not suitable, obtaining a decomposition of the limiting boundary point $\mathcal{X}$ may be a good alternative. A discussion of potential applications of our procedure is provided in section 6.

The CP decomposition is a Tucker3 decomposition with a diagonal core array. Trying to compute a best-fitting CP decomposition of an $R \times R \times R$ array can be seen as an approximate diagonalization of the array. As an anonymous reviewer observed, in this case the idea of packing groups of diverging CP components together in a Tucker3 decomposition with block-diagonal core has an analogy with the problem of matrix diagonalization. Indeed, suppose the $R \times R$ matrix $\mathbf{Y}$ has eigendecomposition $\mathbf{A}\,\mathbf{C}\,\mathbf{A}^{-1}$, with $\mathbf{C}$ diagonal. If $\mathbf{A}$ is ill-conditioned, there will be large numbers in $\mathbf{A}^{-1}$. In particular, if two eigenvectors in $\mathbf{A}$ are nearly identical up to sign, and the corresponding eigenvalues are nearly identical, then the corresponding rank-1 terms in $\mathbf{A}\,\mathbf{C}\,\mathbf{A}^{-1}$ feature large numbers and nearly cancel each other. In such a case, a block-diagonal $\mathbf{C}$ may be computed in which the two nearly identical eigenvalues are packed together in a 2×2 diagonal block, and the corresponding columns of $\mathbf{A}$ are well conditioned. See [17, section 7.6] for more details. In the above, it is assumed that matrix $\mathbf{Y}$ is diagonalizable, which is analogous to array $\mathcal{Y}$ having a CP decomposition. The full analogy with diverging CP components, however, would be to try to compute a diagonalizable $\mathbf{Y}$ that minimizes $||\mathbf{Z} - \mathbf{Y}||$, where $\mathbf{Z}$ is not diagonalizable.

This paper is organized as follows. In section 2, we present the details of our approach to deal with diverging components. We use several results on decompositions of arrays in $\overline{S}_R(I, J, K)$ and decompositions in block terms. For ease of presentation, these results are postponed until section 3. In section 4, we illustrate our approach by means of examples. In section 5, we demonstrate our method in a simulation study. Finally, section 6 contains a discussion of our findings.

We denote vectors as $\mathbf{x}$, matrices as $\mathbf{X}$, and three-way arrays as $\mathcal{X}$. Entry x_{ijk} of $\mathcal{X}$ is in row i, column j, and frontal slice k. We use $\otimes$ to denote the Kronecker product, and $\odot$ denotes the (columnwise) Khatri–Rao product, i.e., for matrices $\mathbf{X}$ and $\mathbf{Y}$ with R columns, $\mathbf{X} \odot \mathbf{Y} = [\mathbf{x}_1 \otimes \mathbf{y}_1 | \ldots | \mathbf{x}_R \otimes \mathbf{y}_R]$. The transpose of $\mathbf{X}$ is denoted as $\mathbf{X}^T$. We refer to an $I \times J$ matrix as having *full column rank* if its rank equals J, and as having *full row rank* if its rank equals I. We refer to the multilinear matrix multiplication $(\mathbf{I}_I, \mathbf{I}_J, \mathbf{U}) \cdot \mathcal{X}$ with $\mathbf{U}$ nonsingular as a *slicemix* of $\mathcal{X}$. A block-diagonal three-way array is denoted as $\mathcal{X} = \text{blockdiag}(\mathcal{X}_1, \ldots, \mathcal{X}_m)$, where the $\mathcal{X}_j$ have size $d_j \times d_j \times d_j$, and the diagonal $(x_{iii},\ i = 1, \ldots, n)$ of $\mathcal{X}$ consists of the diagonals of the blocks.

2. From diverging CP components to a decomposition in block terms of the limiting boundary point. Here, we give a detailed presentation of our approach to deal with diverging CP components. Below, we sometimes refer to theoretical results that can be found in section 3. A detailed understanding of these results is,

however, not necessary to follow the exposition of our method.

We assume $R \leq \min(I, J, K)$ and start with a CP decomposition $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ featuring (groups of) diverging components. The CP decomposition has been obtained as the output of a CP algorithm designed to solve the CP problem (1.6). Let

$$\mathcal{Y} = \sum_{r=1}^{R} \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r \tag{2.1}$$

be the array in $S_R(I, J, K)$ defined by the CP decomposition $(\mathbf{A}, \mathbf{B}, \mathbf{C})$. In this section, the weights ω_r have been absorbed in the vectors $\mathbf{a}_r$, $\mathbf{b}_r$, $\mathbf{c}_r$. We assume the CP problem (1.6) does not have an optimal solution, and the diverging components result from $\mathcal{Y}$ converging to a boundary point $\mathcal{X}$ of $S_R(I, J, K)$ with $\text{rank}(\mathcal{X}) > R$. If the error sum-of-squares corresponding to the sequence of CP updates is converging to the infimum of the CP problem (1.6), then the limit array $\mathcal{X}$ is an optimal boundary point of problem (1.12).

From $(\mathbf{A}, \mathbf{B}, \mathbf{C})$, we obtain the groups of diverging components as follows. Recall that in a group of diverging components, the corresponding columns of $\mathbf{A}, \mathbf{B}, \mathbf{C}$, when normed to length 1, are nearly identical up to sign. Other forms of linear dependency are possible but exceptional [56]. We put components s and t in the same group of diverging components if

$$\left| \left(\frac{\mathbf{a}_s^T \mathbf{a}_t}{\sqrt{\mathbf{a}_s^T \mathbf{a}_s}\sqrt{\mathbf{a}_t^T \mathbf{a}_t}} \right) \left(\frac{\mathbf{b}_s^T \mathbf{b}_t}{\sqrt{\mathbf{b}_s^T \mathbf{b}_s}\sqrt{\mathbf{b}_t^T \mathbf{b}_t}} \right) \left(\frac{\mathbf{c}_s^T \mathbf{c}_t}{\sqrt{\mathbf{c}_s^T \mathbf{c}_s}\sqrt{\mathbf{c}_t^T \mathbf{c}_t}} \right) \right| > 0.95\,. \tag{2.2}$$

The left-hand side of (2.2), without absolute value, is known as the "triple cosine" and is equal to the product of the cosines of the angles between each pair of vectors s and t. Clearly, this approaches ± 1 if and only if all three pairs of vectors s and t become nearly proportional. The triple cosine is commonly used as an indicator of nearly proportional CP components; see, e.g., Krijnen [31] or Rocci and Giordani [41]. The triple cosine is equal to the cosine of the angle between the vectorized rank-1 terms s and t, where the latter are $\mathbf{f}_s = \mathbf{a}_s \otimes \mathbf{b}_s \otimes \mathbf{c}_s$ and $\mathbf{f}_t = \mathbf{a}_t \otimes \mathbf{b}_t \otimes \mathbf{c}_t$, respectively. Indeed, the expression $|\, (\mathbf{f}_s^T \mathbf{f}_t)/(\sqrt{\mathbf{f}_s^T \mathbf{f}_s}\,\sqrt{\mathbf{f}_t^T \mathbf{f}_t}) \,|$ is equal to the left-hand side of (2.2).

For the practical use of criterion (2.2), one should realize that as the CP algorithm runs longer (i.e., when a smaller convergence criterion is used) the triple cosine of two diverging components in the same group will be closer to -1. Hence, if the CP algorithm runs longer, the critical value 0.95 in (2.2) can be chosen larger. However, it is our experience that a critical value of 0.95 captures all (and only) diverging components when the convergence criterion is `1e-9` in the CP ALS (CP Alternating Least Squares) algorithm; see the simulation study in section 5.

Let the R components of $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ be ordered such that $\mathbf{A} = [\mathbf{A}_1 \,|\, \ldots \,|\, \mathbf{A}_m]$, $\mathbf{B} = [\mathbf{B}_1 \,|\, \ldots \,|\, \mathbf{B}_m]$, $\mathbf{C} = [\mathbf{C}_1 \,|\, \ldots \,|\, \mathbf{C}_m]$, with $\mathbf{A}_j$, $\mathbf{B}_j$, $\mathbf{C}_j$ having d_j columns and defining a group of d_j diverging components if $d_j \geq 2$, and a nondiverging component if $d_j = 1$. Let $\mathcal{Y}_j$ be the $I \times J \times K$ array defined by the d_j CP components in $(\mathbf{A}_j, \mathbf{B}_j, \mathbf{C}_j)$. Hence, $\mathcal{Y}_j \in S_{d_j}(I, J, K)$ and $\mathcal{Y} = \sum_{j=1}^{m} \mathcal{Y}_j$. Regarding the convergence of $\mathcal{Y}_j$, we assume the following.

Assumption I. Each array $\mathcal{Y}_j$, defined by a group of d_j diverging components, converges to an array $\mathcal{X}_j$ with $\text{rank}(\mathcal{X}_j) > d_j$.

It follows that the limit $\mathcal{X}_j$ of $\mathcal{Y}_j$ can be approximated arbitrarily well by rank-d_j arrays. Hence, $\mathcal{X}_j \in \overline{S}_{d_j}(I, J, K)$.

From Assumption I and Lemma 3.2 (b), it follows that $\mathcal{Y}_j$ with $d_j \geq 2$ has a limit of the form $\mathcal{X}_j = (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ with $\mathbf{S}_j$, $\mathbf{T}_j$, $\mathbf{U}_j$ columnwise orthonormal, and $\mathcal{G}_j \in \overline{S}_{d_j}(d_j, d_j, d_j)$ with $\text{rank}(\mathcal{G}_j) > d_j$, and all frontal slices of $\mathcal{G}_j$ upper triangular. For a nondiverging component the array $\mathcal{G}_j$ is a scalar instead.

Next, we consider canonical forms of a $d_j \times d_j \times d_j$ array $\mathcal{G}_j \in \overline{S}_{d_j}(d_j, d_j, d_j)$ with $\text{rank}(\mathcal{G}_j) > d_j$. It has been shown in [16] that if $\mathcal{G}_j \in \overline{S}_2(2, 2, 2)$ has rank larger than 2, then it has rank 3, border rank 2, and there exist nonsingular $\mathbf{L}$, $\mathbf{M}$, $\mathbf{N}$ such that $(\mathbf{L}, \mathbf{M}, \mathbf{N}) \cdot \mathcal{G}_j$ equals

$$\left[\begin{array}{cc|cc} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{array}\right]. \tag{2.3}$$

Here, we denote the $2 \times 2 \times 2$ array $\mathcal{G}_j$ with 2×2 slabs $\mathbf{G}_1$ and $\mathbf{G}_2$ as $[\mathbf{G}_1 \,|\, \mathbf{G}_2]$. We refer to (2.3) as the *canonical form* of a boundary array of $S_2(2, 2, 2)$ with rank larger than 2.

For $\mathcal{G}_j \in \overline{S}_3(3, 3, 3)$ with rank larger than 3, we have the following result.

LEMMA 2.1. *Let $\mathcal{G}_j \in \overline{S}_3(3, 3, 3)$ have multilinear rank $(3, 3, 3)$ and rank larger than 3. If there exists a rank-3 sequence converging to $\mathcal{G}_j$ with three diverging components, then for almost all $\mathcal{G}_j$ there exist nonsingular $\mathbf{L}$, $\mathbf{M}$, $\mathbf{N}$ such that $(\mathbf{L}, \mathbf{M}, \mathbf{N}) \cdot \mathcal{G}_j$ equals*

$$\left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & d & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & e & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right]. \tag{2.4}$$

It holds that $\text{rank}(\mathcal{G}_j) = 5$.

Proof. See the appendix for the proof. ∎

Under the conditions of Lemma 2.1, the limiting array $\mathcal{G}_j$ necessarily has rank 5. When the assumption of multilinear rank $(3, 3, 3)$ is dropped, a limit of rank 4 is also possible. The multilinear rank is defined in section 3.

For a group of $d_j = 2$ diverging components, the limit of $\mathcal{Y}_j$ can be written as $\mathcal{X}_j = (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ with $\mathbf{S}_j$, $\mathbf{T}_j$, $\mathbf{U}_j$ of rank 2, and $\mathcal{G}_j$ equal to the canonical form (2.3). For the limit of a group of $d_j = 3$ diverging components, we assume the following.

Assumption II. The limit $\mathcal{X}_j$ of an array $\mathcal{Y}_j$, defined by a group of $d_j = 3$ diverging components, can be written as $\mathcal{X}_j = (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ with $\mathbf{S}_j$, $\mathbf{T}_j$, $\mathbf{U}_j$ of rank 3, and $\mathcal{G}_j$ equal to the canonical form (2.4).

From the above, it follows that the limiting boundary point $\mathcal{X} = \sum_{j=1}^{m} \mathcal{X}_j$ of $\mathcal{Y} = \sum_{j=1}^{m} \mathcal{Y}_j$ satisfies a decomposition in block terms $\mathcal{X} = \sum_{j=1}^{m} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$, where $\mathcal{G}_j$ is a scalar for $d_j = 1$, has canonical form (2.3) for $d_j = 2$, and canonical form (2.4) for $d_j = 3$. We need the following assumption on this decomposition of $\mathcal{X}$.

Assumption III. In the decomposition $\mathcal{X} = \sum_{j=1}^{m} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ of the limiting boundary point $\mathcal{X}$, the matrices $\mathbf{S} = [\mathbf{S}_1 \,|\, \ldots \,|\, \mathbf{S}_m]$, $\mathbf{T} = [\mathbf{T}_1 \,|\, \ldots \,|\, \mathbf{T}_m]$, $\mathbf{U} = [\mathbf{U}_1 \,|\, \ldots \,|\, \mathbf{U}_m]$ have rank R.

The following lemma states that we may assume that if $d_j = 1$, then $\mathcal{G}_j$ is nonzero in the decomposition of $\mathcal{X}$. Otherwise, arrays close to $\mathcal{X}$ exist that are closer to the data array $\mathcal{Z}$.

LEMMA 2.2. *Let $\mathcal{Z} \in \mathbb{R}^{I \times J \times K}$ with $\mathcal{Z} \notin \overline{S}_R(I, J, K)$. Let $\mathcal{X}$ be as in Assumption* III*, where $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ have rank R, and arrays $\mathcal{G}_j \in \overline{S}_{d_j}(d_j, d_j, d_j)$ have* $\text{rank}(\mathcal{G}_j) > d_j$

if $d_j \geq 2$. If for some j, $d_j = 1$ and $\mathcal{G}_j = 0$, then an array $\tilde{\mathcal{X}}$ exists with $||\mathcal{Z} - \tilde{\mathcal{X}}|| < ||\mathcal{Z} - \mathcal{X}||$. Moreover, $\tilde{\mathcal{X}}$ has a decomposition in block terms of the same form as $\mathcal{X}$.

Proof. The proof is analogous to [16, Lemma 8.2]. At least one entry of $\mathcal{Z} - \mathcal{X}$ is nonzero, say entry (i, j, k) is equal to $\delta \neq 0$. Let $\tilde{\mathcal{X}} = \mathcal{X} + \mathbf{a} \circ \mathbf{b} \circ \mathbf{c}$ such that $\mathbf{a} \circ \mathbf{b} \circ \mathbf{c}$ is zero except for entry (i, j, k) which equals δ. This completes the proof. ∎

Assumption III, Lemma 2.2, and Lemma 3.4 (b) imply that $\mathcal{X}$ is indeed a boundary point of $S_R(I, J, K)$ with rank larger than R, if at most one group of three or more diverging components is present (i.e., $d_j \geq 3$ for at most one j). If only groups of two diverging components are present (i.e., $\max(d_j) = 2$), then Lemma 3.5 describes the ambiguities in the decomposition $\mathcal{X} = \sum_{j=1}^{m} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$. That is, the limits $\mathcal{X}_j = (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ of the groups of diverging components form unique block terms in the decomposition, as do the limits of the nondiverging components.

If $\max(d_j) \leq 3$, then the number of rank-1 terms in the decomposition of $\mathcal{X}$ can be obtained from the canonical forms (2.3) and (2.4). Namely, each nonzero core entry contributes one rank-1 term to the decomposition. Hence, each $2 \times 2 \times 2$ core block contributes three rank-1 terms, and each $3 \times 3 \times 3$ core block contributes six rank-1 terms. Obviously, each $1 \times 1 \times 1$ core block contributes one rank-1 term. Since the canonical form (2.3) has rank 3, it follows from Lemma 3.3 that the number of rank-1 terms in the decomposition of $\mathcal{X}$ is equal to $\text{rank}(\mathcal{X})$ when $\max(d_j) = 2$.

In the remaining part of this section, we explain how the limiting boundary point $\mathcal{X}$ and its decomposition $\mathcal{X} = \sum_{j=1}^{m} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ can be obtained, starting with the CP decomposition $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ featuring diverging components. In section 2.1, we show how to obtain a block Simultaneous GSD (SGSD) of $\mathcal{Y}$ from its CP decomposition $(\mathbf{A}, \mathbf{B}, \mathbf{C})$. The block SGSD has the form

$$\mathcal{Y} = \sum_{j=1}^{m} \mathcal{Y}_j = \sum_{j=1}^{m} (\tilde{\mathbf{S}}_j, \tilde{\mathbf{T}}_j, \tilde{\mathbf{U}}_j) \cdot \tilde{\mathcal{G}}_j \,, \tag{2.5}$$

where $\tilde{\mathbf{S}}_j$, $\tilde{\mathbf{T}}_j$, $\tilde{\mathbf{U}}_j$ are columnwise orthogonal, and $\tilde{\mathcal{G}}_j \in S_{d_j}(d_j, d_j, d_j)$ has all frontal slices upper triangular. In section 2.2, we use the block SGSD (2.5) to compute initial values for the decomposition $\sum_{j=1}^{m} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$, which we then fit to the data array $\mathcal{Z}$ to yield the decomposition of $\mathcal{X}$. The analysis in section 2.2 holds for $\max(d_j) \leq 3$ only. Below, we summarize the steps of our method, where the detailed computations can be found in sections 2.1 and 2.2.

FROM CP WITH DIVERGING COMPONENTS TO A DECOMPOSITION IN BLOCK TERMS

Input: Data array $\mathcal{Z} \in \mathbb{R}^{I \times J \times K}$, and CP decomposition $\mathcal{Y} = (\mathbf{A}, \mathbf{B}, \mathbf{C})$ with groups of two or three diverging components, obtained from an algorithm for solving the CP problem (1.6). The number of components R satisfies $R \leq \min(I, J, K)$.

Output: Decomposition in block terms $\mathcal{X} = (\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \mathcal{G} = \sum_{j=1}^{m} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$, where $\mathcal{X}$ is the limit point of $\mathcal{Y}$ and an optimal solution of (1.12).

1. Identify the groups of diverging components in $\mathbf{A}, \mathbf{B}, \mathbf{C}$. For automatic identification, the criterion (2.2) may be used.
2. Simultaneously reorder the columns of $\mathbf{A}, \mathbf{B}, \mathbf{C}$ such that $\mathbf{A} = [\mathbf{A}_1 \,|\, \ldots \,|\, \mathbf{A}_m]$, $\mathbf{B} = [\mathbf{B}_1 \,|\, \ldots \,|\, \mathbf{B}_m]$, $\mathbf{C} = [\mathbf{C}_1 \,|\, \ldots \,|\, \mathbf{C}_m]$, with $\mathbf{A}_j$, $\mathbf{B}_j$, $\mathbf{C}_j$ having d_j columns and corresponding to a group of d_j diverging components if $d_j \geq 2$, and a nondiverging component if $d_j = 1$. We have $\sum_{j=1}^{m} d_j = R$.
3. (Block SGSD: section 2.1). For each $\mathcal{Y}_j = (\mathbf{A}_j, \mathbf{B}_j, \mathbf{C}_j)$, compute $\mathcal{Y}_j = (\tilde{\mathbf{S}}_j, \tilde{\mathbf{T}}_j, \tilde{\mathbf{U}}_j) \cdot \tilde{\mathcal{G}}_j$ in (2.5) as follows. If $d_j = 1$, then $\tilde{\mathbf{S}}_j = \mathbf{A}_j$, $\tilde{\mathbf{T}}_j = \mathbf{B}_j$,

$\tilde{\mathbf{U}}_j = \mathbf{C}_j$, and $\tilde{\mathcal{G}}_j = 1$. If $d_j \geq 2$, then compute $\mathbf{A}_j = \tilde{\mathbf{S}}_j \mathbf{R}_a^{(j)}$ (QR-decomp), and $\mathbf{B}_j = \tilde{\mathbf{T}}_j \mathbf{L}_b^{(j)}$ (QL-decomp), and set $\mathbf{R}_k^{(j)} = \mathbf{R}_a^{(j)} \mathbf{C}_k^{(j)} (\mathbf{L}_b^{(j)})^T$, $k = 1, \ldots, K$. For $\mathbf{H}_j$ given by (2.7), compute the singular value decomposition $\mathbf{H}_j = \mathbf{Q}_1 \mathbf{D} \mathbf{Q}_2^T$. Set $\tilde{\mathbf{U}}_j = (\mathbf{Q}_2^\dagger)^T$.

4. (Initial values: section 2.2). From the block SGSD (2.5), we obtain initial values $\mathbf{S}_j^{(0)}$, $\mathbf{T}_j^{(0)}$, $\mathbf{U}_j^{(0)}$, $\mathcal{G}_j^{(0)}$, $j = 1, \ldots, m$, for fitting the decomposition $\sum_{j=1}^m (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$. For $d_j = 1$, set $\mathbf{S}_j^{(0)} = \mathbf{A}_j$, $\mathbf{T}_j^{(0)} = \mathbf{B}_j$, $\mathbf{U}_j^{(0)} = \mathbf{C}_j$, and $\mathcal{G}_j^{(0)} = 1$. For $d_j \in \{2, 3\}$, set $\mathbf{S}_j^{(0)} = \tilde{\mathbf{S}}_j \tilde{\mathbf{G}}_1^{(j)}$ and $\mathbf{T}_j^{(0)} = \tilde{\mathbf{T}}_j$. For $d_j = 2$, set $\mathbf{U}_j^{(0)}$ equal to (2.9), and $\mathcal{G}_j^{(0)}$ equal to (2.8) with $a = b = 0$. For $d_j = 3$, set $\mathbf{U}_j^{(0)}$ equal to (2.11), and $\mathcal{G}_j^{(0)}$ equal to (2.10) with $a = b = c = f = \alpha = \beta = \gamma = \delta = \epsilon = 0$.
5. Using the initial values and the Alternating Least Squares algorithm of [28], fit the (constrained Tucker3) decomposition $(\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \mathcal{G} = \sum_{j=1}^m (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ to $\mathcal{Z}$ with

$$\mathcal{G}_j = \begin{cases} 1 & \text{if } d_j = 1\,, \\ \text{canonical form (2.3)} & \text{if } d_j = 2\,, \\ \text{canonical form (2.4)} & \text{if } d_j = 3\,, \end{cases}$$

   where $\mathbf{S}, \mathbf{T}, \mathbf{U}$ and the nonzero entries of core $\mathcal{G} = \text{blockdiag}(\mathcal{G}_1, \ldots, \mathcal{G}_m)$ are free parameters.
6. Normalize (most of) the nonzero core entries of each $\mathcal{G}_j$ to one. For $d_j \in \{2, 3\}$, premultiply the core slices by $(\mathbf{G}_1^{(j)})^{-1}$, and normalize the resulting second and third slices. Postmultiply $\mathbf{S}_j$ by $\mathbf{G}_1^{(j)}$, and $\mathbf{U}_j$ by the inverse slice normalization(s). For $d_j = 3$, only one of d and e in (2.4) can be normalized to one when both are nonzero.

2.1. From diverging CP components to a block SGSD. Here, we show how to obtain the block SGSD (2.5), i.e., $\mathcal{Y} = \sum_{j=1}^m \mathcal{Y}_j = \sum_{j=1}^m (\tilde{\mathbf{S}}_j, \tilde{\mathbf{T}}_j, \tilde{\mathbf{U}}_j) \cdot \tilde{\mathcal{G}}_j$, where $\tilde{\mathbf{S}}_j$, $\tilde{\mathbf{T}}_j$, $\tilde{\mathbf{U}}_j$ are columnwise orthogonal, and $\tilde{\mathcal{G}}_j \in S_{d_j}(d_j, d_j, d_j)$ has all frontal slices upper triangular. Existence of the block SGSD follows from the fact that each group of d_j diverging components defines an array $\mathcal{Y}_j \in S_{d_j}(I, J, K)$, and Lemma 3.2 (b) applied to each $\mathcal{Y}_j$. Next, we show how to obtain $\mathcal{Y}_j = (\tilde{\mathbf{S}}_j, \tilde{\mathbf{T}}_j, \tilde{\mathbf{U}}_j) \cdot \tilde{\mathcal{G}}_j$.

If $d_j = 1$, then we set $\tilde{\mathbf{S}}_j = \mathbf{A}_j$, $\tilde{\mathbf{T}}_j = \mathbf{B}_j$, $\tilde{\mathbf{U}}_j = \mathbf{C}_j$, and $\tilde{\mathcal{G}}_j = 1$. Next, suppose $d_j \geq 2$. Let $\mathbf{A}_j = \tilde{\mathbf{S}}_j \mathbf{R}_a^{(j)}$ be a QR-decomposition of $\mathbf{A}_j$, with $\tilde{\mathbf{S}}_j$ $(I \times d_j)$ columnwise orthonormal, and $\mathbf{R}_a^{(j)}$ $(d_j \times d_j)$ upper triangular. Let $\mathbf{B}_j = \tilde{\mathbf{T}}_j \mathbf{L}_b^{(j)}$ be a QL-decomposition of $\mathbf{B}_j$, with $\tilde{\mathbf{T}}_j$ $(J \times d_j)$ columnwise orthonormal, and $\mathbf{L}_b^{(j)}$ $(d_j \times d_j)$ lower triangular. Then the matrix form (1.3) of the CP decomposition of $\mathcal{Y}_j$ can be written as

$$\mathbf{A}_j \mathbf{C}_k^{(j)} \mathbf{B}_j^T = \tilde{\mathbf{S}}_j (\mathbf{R}_a^{(j)} \mathbf{C}_k^{(j)} (\mathbf{L}_b^{(j)})^T) \tilde{\mathbf{T}}_j^T = \tilde{\mathbf{S}}_j \mathbf{R}_k^{(j)} \tilde{\mathbf{T}}_j^T\,, \qquad k = 1, \ldots, K\,, \tag{2.6}$$

where $\mathbf{C}_k^{(j)}$ denotes the $d_j \times d_j$ diagonal matrix with row k of $\mathbf{C}_j$ as its diagonal. The right-hand side of (2.6) defines an SGSD of $\mathcal{Y}_j$. Hence, $\mathcal{Y}_j = (\tilde{\mathbf{S}}_j, \tilde{\mathbf{T}}_j, \mathbf{I}_K) \cdot \mathcal{R}_j$, where $\mathcal{R}_j$ is the $d_j \times d_j \times K$ array with upper triangular frontal slices $\mathbf{R}_k^{(j)}$.

As in the proof of Lemma 3.2 (b), it follows that there exists $\tilde{\mathbf{U}}_j$ $(K \times d_j)$ columnwise orthonormal such that $\mathcal{R}_j = (\mathbf{I}_{d_j}, \mathbf{I}_{d_j}, \tilde{\mathbf{U}}_j) \cdot \tilde{\mathcal{G}}_j$, with $\tilde{\mathcal{G}}_j \in S_{d_j}(d_j, d_j, d_j)$. The

matrix $\tilde{\mathbf{U}}_j$ can be obtained as follows. For a $d \times d$ upper triangular matrix $\mathbf{R}$, let vech($\mathbf{R}$) denote the $d(d+1)/2 \times 1$ vector obtained by stacking the entries in the upper triangular part of $\mathbf{R}$ above each other. Let

$$\mathbf{H}_j = [\text{vech}(\mathbf{R}_1^{(j)}) \mid \ldots \mid \text{vech}(\mathbf{R}_K^{(j)})]\,. \tag{2.7}$$

If the singular value decomposition of $\mathbf{H}_j$ is given by $\mathbf{H}_j = \mathbf{Q}_1\,\mathbf{D}\,\mathbf{Q}_2^T$, where the $d_j \times d_j$ diagonal matrix $\mathbf{D}$ contains the singular values, then we may take $\tilde{\mathbf{U}}_j = (\mathbf{Q}_2^\dagger)^T$, where $\mathbf{Q}_2^\dagger$ is the pseudoinverse of $\mathbf{Q}_2$. Note that the rank of $\mathbf{H}_j$ is equal to the mode-3 rank of $\mathcal{R}_j$, and is less than or equal to d_j by $\mathcal{R}_j = (\mathbf{I}_{d_j}, \mathbf{I}_{d_j}, \tilde{\mathbf{U}}_j) \cdot \tilde{\mathcal{G}}_j$.

Hence, it follows that $\mathcal{Y}_j = (\tilde{\mathbf{S}}_j, \tilde{\mathbf{T}}_j, \tilde{\mathbf{U}}_j) \cdot \tilde{\mathcal{G}}_j$.

2.2. From a block SGSD to the limiting boundary point. If $\max(d_j) \leq 3$, then we may obtain the limiting boundary point $\mathcal{X}$ and its block term decomposition as follows. As stated above, $\mathcal{X}$ satisfies the block term decomposition $\mathcal{X} = (\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \mathcal{G} = \sum_{j=1}^m (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$, with $\mathbf{S}_j$, $\mathbf{T}_j$, $\mathbf{U}_j$ of rank d_j, and core blocks $\mathcal{G}_j$ having canonical form (2.3) for $d_j = 2$, and (2.4) for $d_j = 3$. This decomposition of $\mathcal{X}$ can be obtained by fitting it as a constrained Tucker3 model to the data array $\mathcal{Z}$. The constraints in this Tucker3 model are the core entries of $\mathcal{G} = \text{blockdiag}(\mathcal{G}_1, \ldots, \mathcal{G}_m)$ that are equal to zero. The nonzero core entries of each $\mathcal{G}_j$ and the component matrices $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ are treated as free parameters. An Alternating Least Squares algorithm for fitting this constrained Tucker3 model can be found in [28]. Below, we explain how initial values for this algorithm can be obtained from the block SGSD of $\mathcal{Y}$ in (2.5).

We denote the initial values of $\sum_{j=1}^m (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$ as $\mathbf{S}_j^{(0)}$, $\mathbf{T}_j^{(0)}$, $\mathbf{U}_j^{(0)}$, and $\mathcal{G}_j^{(0)}$. For $d_j = 1$, we set $\mathbf{S}_j^{(0)} = \mathbf{A}_j$, $\mathbf{T}_j^{(0)} = \mathbf{B}_j$, $\mathbf{U}_j^{(0)} = \mathbf{C}_j$, and $\mathcal{G}_j^{(0)} = 1$. For $d_j \in \{2, 3\}$, we do the following. We may assume that $\mathcal{Y}_j = (\tilde{\mathbf{S}}_j, \tilde{\mathbf{T}}_j, \tilde{\mathbf{U}}_j) \cdot \tilde{\mathcal{G}}_j$ is close to its limit point $\mathcal{X}_j$. Hence, $\tilde{\mathcal{G}}_j$ is close to a $d_j \times d_j \times d_j$ array that can be transformed to either canonical form (2.3) or to canonical form (2.4).

In the case $d_j = 2$, we write $\tilde{\mathcal{G}}_j = [\tilde{\mathbf{G}}_1^{(j)} \mid \tilde{\mathbf{G}}_2^{(j)}]$. Let $\mathbf{T}_j^{(0)} = \tilde{\mathbf{T}}_j$. Next, we premultiply the slices of $\tilde{\mathcal{G}}_j$ by $(\tilde{\mathbf{G}}_1^{(j)})^{-1}$, and postmultiply $\tilde{\mathbf{S}}_j$ by $\tilde{\mathbf{G}}_1^{(j)}$. The latter gives $\mathbf{S}_j^{(0)} = \tilde{\mathbf{S}}_j \tilde{\mathbf{G}}_1^{(j)}$. We obtain

$$\tilde{\mathcal{G}}_j = \left[\begin{array}{cc|cc} 1 & 0 & a & c \\ 0 & 1 & 0 & b \end{array}\right]. \tag{2.8}$$

By assumption, $a \approx b$. Next, we subtract $(a+b)/2$ times $\tilde{\mathbf{G}}_1^{(j)}$ from $\tilde{\mathbf{G}}_2^{(j)}$, and postmultiply $\tilde{\mathbf{U}}_j$ by the inverse of this slicemix. The latter yields

$$\mathbf{U}_j^{(0)} = \tilde{\mathbf{U}}_j \begin{bmatrix} 1 & 0 \\ -u & 1 \end{bmatrix}^{-1} = \tilde{\mathbf{U}}_j \begin{bmatrix} 1 & 0 \\ u & 1 \end{bmatrix}, \tag{2.9}$$

with $u = (a+b)/2$. Finally, we take $\mathcal{G}_j^{(0)}$ as in (2.8) with $a = b = 0$.

In the case $d_j = 3$, we write $\tilde{\mathcal{G}}_j = [\tilde{\mathbf{G}}_1^{(j)} \mid \tilde{\mathbf{G}}_2^{(j)} \mid \tilde{\mathbf{G}}_3^{(j)}]$. Let $\mathbf{T}_j^{(0)} = \tilde{\mathbf{T}}_j$. Next, we premultiply the slices of $\tilde{\mathcal{G}}_j$ by $(\tilde{\mathbf{G}}_1^{(j)})^{-1}$, and postmultiply $\tilde{\mathbf{S}}_j$ by $\tilde{\mathbf{G}}_1^{(j)}$. The latter gives $\mathbf{S}_j^{(0)} = \tilde{\mathbf{S}}_j \tilde{\mathbf{G}}_1^{(j)}$. We obtain

$$\tilde{\mathcal{G}}_j = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & a & d & f & \alpha & \delta & \nu \\ 0 & 1 & 0 & 0 & b & e & 0 & \beta & \epsilon \\ 0 & 0 & 1 & 0 & 0 & c & 0 & 0 & \gamma \end{array}\right]. \tag{2.10}$$

By assumption, $a \approx b \approx c$ and $\alpha \approx \beta \approx \gamma$ (see the proof of Lemma 2.1 in the appendix). Next, we subtract $(a+b+c)/3$ times $\tilde{\mathbf{G}}_1^{(j)}$ from $\tilde{\mathbf{G}}_2^{(j)}$, and $(\alpha+\beta+\gamma)/3$ times $\tilde{\mathbf{G}}_1^{(j)}$ from $\tilde{\mathbf{G}}_3^{(j)}$, and postmultiply $\tilde{\mathbf{U}}_j$ by the inverse of this slicemix. In $\tilde{\mathcal{G}}_j$, we set $a=b=c=0$ and $\alpha=\beta=\gamma=0$.

By assumption, $\delta e \approx \epsilon d$ (see the proof of Lemma 2.1 in the appendix). We subtract $(\delta/d+\epsilon/e)/2$ times $\tilde{\mathbf{G}}_2^{(j)}$ from $\tilde{\mathbf{G}}_3^{(j)}$, and postmultiply $\tilde{\mathbf{U}}_j$ by the inverse of this slicemix. In $\tilde{\mathcal{G}}_j$, we set $\delta=\epsilon=0$. Finally, we subtract f/ν times $\tilde{\mathbf{G}}_3^{(j)}$ from $\tilde{\mathbf{G}}_2^{(j)}$, and postmultiply $\tilde{\mathbf{U}}_j$ by the inverse of this slicemix. In $\tilde{\mathcal{G}}_j$, we set $f=0$. We take $\mathcal{G}_j^{(0)}$ equal to (2.10) with $a=b=c=f=\alpha=\beta=\gamma=\delta=\epsilon=0$. It follows that the matrix $\mathbf{U}_j^{(0)}$ is obtained as

$$\begin{aligned}\mathbf{U}_j^{(0)} &= \tilde{\mathbf{U}}_j \begin{bmatrix} 1 & 0 & 0 \\ -u & 1 & 0 \\ -w & 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -x & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -y \\ 0 & 0 & 1 \end{bmatrix}^{-1} \\ &= \tilde{\mathbf{U}}_j \begin{bmatrix} 1 & 0 & 0 \\ u & 1 & y \\ w & x & xy+1 \end{bmatrix},\end{aligned} \tag{2.11}$$

with $u=(a+b+c)/3$, $w=(\alpha+\beta+\gamma)/3$, $x=(\delta/d+\epsilon/e)/2$, and $y=f/\nu$.

3. Theoretical results. In this section, we present results on decompositions for arrays in $\overline{S}_R(I,J,K)$ and decompositions in block terms. These results are referred to in section 2, where the details of our method are discussed. For ease of presentation we postpone the results until the current section.

First, however, we introduce some definitions. A mode-j vector of an $I \times J \times K$ array is defined as a vector that is obtained by varying the jth index and keeping the other two indices fixed. Hence, a mode-2 vector has size $J \times 1$. The mode-j rank of the array is the rank of the set of mode-j vectors. The *multilinear rank* is defined as the triplet (mode-1 rank, mode-2 rank, mode-3 rank). The *border rank* of an array $\mathcal{Y}$, which we denote by brank($\mathcal{Y}$), is defined as [3] [16]:

$$\text{brank}(\mathcal{Y}) = \min\{R : \ \mathcal{Y} \text{ can be approximated arbitrarily well by arrays of rank } R\}. \tag{3.1}$$

Hence, if brank($\mathcal{Y}$) $= R$, then $\mathcal{Y} \in \overline{S}_R(I,J,K)$ but $\mathcal{Y} \notin \overline{S}_{R-1}(I,J,K)$.

We denote the set of arrays satisfying the R-component SGSD [61] [14] with perfect fit as $P_R(I,J,K)$, i.e.,

$$P_R(I,J,K) = \{\mathcal{Y} \in \mathbb{R}^{I\times J\times K} \mid \mathbf{Y}_k = \mathbf{Q}_a \mathbf{R}_k \mathbf{Q}_b^T, \ k=1,\ldots,K\}, \tag{3.2}$$

where $\mathbf{Y}_k$ denotes the kth frontal slice ($I \times J$) of $\mathcal{Y}$, matrices $\mathbf{Q}_a$ ($I \times R$) and $\mathbf{Q}_b$ ($J \times R$) are columnwise orthonormal and $\mathbf{R}_k$ are $R \times R$ upper triangular.

3.1. Results on decompositions of arrays in $\overline{S}_R(I,J,K)$. We need the following lemma.

LEMMA 3.1. *Let $R \leq \min(I,J,K)$, and $\mathcal{Y} = (\mathbf{S},\mathbf{T},\mathbf{U}) \cdot \mathcal{G}$ with columnwise orthonormal $\mathbf{S}$ ($I \times R$), $\mathbf{T}$ ($J \times R$), and $\mathbf{U}$ ($K \times R$). Then $\mathcal{Y} \in \overline{S}_R(I,J,K)$ if and only if $\mathcal{G} \in \overline{S}_R(R,R,R)$, and $\mathcal{Y} \in S_R(I,J,K)$ if and only if $\mathcal{G} \in S_R(R,R,R)$. Moreover, the representation exists for any $\mathcal{Y} \in \overline{S}_R(I,J,K)$ and any $\mathcal{Y} \in S_R(I,J,K)$, and we may take $\mathbf{S} = \mathbf{I}_R$ if $R = I$, $\mathbf{T} = \mathbf{I}_R$ if $R = J$, and $\mathbf{U} = \mathbf{I}_R$ if $R = K$.*

Proof. See [16, Theorem 5.2] for the proof. ∎

Lemma 3.1 implies that any array in $\overline{S}_R(I,J,K)$ has a Tucker3 representation $(\mathbf{S},\mathbf{T},\mathbf{U})\cdot\mathcal{G}$ with columnwise orthonormal component matrices and a core array of size $R\times R\times R$. Moreover, the array is an interior (boundary) point if and only if its core array $\mathcal{G}$ is an interior (boundary) point of $S_R(I,J,K)$.

The following result states that arrays in $\overline{S}_R(I,J,K)$ have a perfect-fitting SGSD for $R\leq\min(I,J)$. Moreover, for $R\leq\min(I,J,K)$ they have a Tucker3 representation $(\mathbf{S},\mathbf{T},\mathbf{U})\cdot\mathcal{G}$ with columnwise orthonormal component matrices and an $R\times R\times R$ core array $\mathcal{G}$ with all frontal slices upper triangular.

LEMMA 3.2.

(a) *For $R\leq\min(I,J)$ it holds that $\overline{S}_R(I,J,K)\subseteq P_R(I,J,K)$.*

(b) *For $R\leq\min(I,J,K)$ and $\mathcal{Y}\in\overline{S}_R(I,J,K)$, it holds that $\mathcal{Y}=(\mathbf{S},\mathbf{T},\mathbf{U})\cdot\mathcal{G}$ for some $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ columnwise orthonormal, and some $\mathcal{G}\in\overline{S}_R(R,R,R)$ with all frontal slices upper triangular. Moreover, $\mathcal{Y}\in S_R(I,J,K)$ if and only if $\mathcal{G}\in S_R(R,R,R)$.*

Proof. We know from [14] that $S_R(I,J,K)\subset P_R(I,J,K)$. Let $\mathcal{Z}$ be a boundary point of $S_R(I,J,K)$ with rank larger than R. Then $\mathcal{Z}$ can be approximated arbitrarily closely from $S_R(I,J,K)$ and, hence, the best-fitting SGSD problem for $\mathcal{Z}$ yields an infimum of zero. Since the SGSD problem always has an optimal solution [54], it follows that this infimum must be attained, and that $\mathcal{Z}\in P_R(I,J,K)$. This proves (a).

The proof of (b) is as follows. Statement (a) implies that $\mathcal{Y}=(\mathbf{S},\mathbf{T},\mathbf{I}_K)\cdot\mathcal{R}$ for some $\mathbf{S}$ and $\mathbf{T}$ columnwise orthonormal, and some $\mathcal{R}\in\mathbb{R}^{R\times R\times K}$ with all frontal slices upper triangular. Analogous to Lemma 3.1 we have that $\mathcal{R}\in\overline{S}_R(R,R,K)$, and that $\mathcal{Y}\in S_R(I,J,K)$ if and only if $\mathcal{R}\in S_R(R,R,K)$. Moreover, Lemma 3.1 yields that $\mathcal{R}=(\mathbf{I}_R,\mathbf{I}_R,\mathbf{U})\cdot\mathcal{G}$ for some $\mathbf{U}$ columnwise orthonormal, and $\mathcal{G}\in\overline{S}_R(R,R,R)$. Also, $\mathcal{R}\in S_R(R,R,K)$ if and only if $\mathcal{G}\in S_R(R,R,R)$. It holds that $\mathcal{G}=(\mathbf{I}_R,\mathbf{I}_R,\mathbf{U}^T)\cdot\mathcal{R}$, which shows that $\mathcal{G}$ has all frontal slices upper triangular. The proof is complete by observing that $\mathcal{Y}=(\mathbf{S},\mathbf{T},\mathbf{I}_K)\cdot(\mathbf{I}_R,\mathbf{I}_R,\mathbf{U})\cdot\mathcal{G}=(\mathbf{S},\mathbf{T},\mathbf{U})\cdot\mathcal{G}$. ∎

3.2. Results on decompositions in block terms. Here, we consider a decomposition in block terms, as introduced in [9], [10], [11]. Let a Tucker3 decomposition $\mathcal{X}=(\mathbf{S},\mathbf{T},\mathbf{U})\cdot\mathcal{G}$ satisfy $\mathcal{G}=\text{blockdiag}(\mathcal{G}_1,\ldots,\mathcal{G}_m)$, $\mathbf{S}=[\mathbf{S}_1\,|\,\ldots\,|\,\mathbf{S}_m]$, $\mathbf{T}=[\mathbf{T}_1\,|\,\ldots\,|\,\mathbf{T}_m]$, and $\mathbf{U}=[\mathbf{U}_1\,|\,\ldots\,|\,\mathbf{U}_m]$, where $\mathcal{G}_j$ has size $d_j\times d_j\times d_j$ and parts $\mathbf{S}_j$, $\mathbf{T}_j$, $\mathbf{K}_j$ have d_j columns. The core blocks $\mathcal{G}_j$ are assumed to have multilinear rank (d_j,d_j,d_j). The decomposition in block terms can be written as

$$\mathcal{X}=(\mathbf{S},\mathbf{T},\mathbf{U})\cdot\mathcal{G}=\sum_{j=1}^{m}(\mathbf{S}_j,\mathbf{T}_j,\mathbf{U}_j)\cdot\mathcal{G}_j\,. \tag{3.3}$$

We set $R=\sum_{j=1}^{m}d_j$ and assume $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ have rank R, which implies $\text{rank}(\mathcal{X})=\text{rank}(\mathcal{G})$. The block-diagonal $\mathcal{G}$ is also called the direct sum of $\mathcal{G}_1,\ldots,\mathcal{G}_m$. As stated in [16], it is conjectured [57] that $\text{rank}(\mathcal{G})$ equals the sum of $\text{rank}(\mathcal{G}_j)$, $j=1,\ldots,m$. However, only in the following case a proof of this is known.

LEMMA 3.3. *Let $\mathcal{G}=\text{blockdiag}(\mathcal{G}_1,\ldots,\mathcal{G}_m)$, with $\mathcal{G}_j$ of size $d_j\times d_j\times d_j$. If $d_j\geq 3$ for at most one j, then*

$$\text{rank}(\mathcal{G})=\sum_{j=1}^{m}\text{rank}(\mathcal{G}_j)\,. \tag{3.4}$$

Proof. See [26] for the proof. ∎

The following result states that under the condition of Lemma 3.3, array $\mathcal{X}$ in (3.3) is a boundary point of $S_R(I,J,K)$ with rank larger than R if each $\mathcal{G}_j$ is a boundary point of $S_{d_j}(d_j,d_j,d_j)$ with rank larger than d_j (for $d_j \geq 2$).

LEMMA 3.4. *Let $\mathcal{X}$ be as in* (3.3)*, where* $\mathbf{S}$*,* $\mathbf{T}$*,* $\mathbf{U}$ *have rank R,* $\max(d_j) \geq 2$*, arrays $\mathcal{G}_j \in \overline{S}_{d_j}(d_j,d_j,d_j)$ have multilinear rank (d_j,d_j,d_j),* $\operatorname{rank}(\mathcal{G}_j) > d_j$ *if $d_j \geq 2$, and* $\operatorname{rank}(\mathcal{G}_j) = 1$ *if $d_j = 1$, $j = 1,\ldots,m$.*

(a) *It holds that $\mathcal{X} \in \overline{S}_R(I,J,K)$ and* $\operatorname{brank}(\mathcal{X}) = R$.

(b) *If $d_j \geq 3$ for at most one j, then $\mathcal{X}$ is a boundary point of $S_R(I,J,K)$ with* $\operatorname{rank}(\mathcal{X}) = \sum_{j=1}^{m} \operatorname{rank}(\mathcal{G}_j) > R$.

Proof. Since $\mathcal{G}_j \in \overline{S}_{d_j}(d_j,d_j,d_j)$, each term $(\mathbf{S}_j,\mathbf{T}_j,\mathbf{U}_j)\cdot\mathcal{G}_j$ in (3.3) can be approximated arbitrarily closely by rank-d_j arrays. Adding the approximating sequences for $j = 1,\ldots,m$ yields an arbitrarily close approximation of $\mathcal{X}$ from $S_R(I,J,K)$. This implies $\mathcal{X} \in \overline{S}_R(I,J,K)$ and $\operatorname{brank}(\mathcal{X}) \leq R$. It is shown in [49, Proposition 1.1] that $\operatorname{brank}(\mathcal{X})$ is at least equal to the mode-j rank of $\mathcal{X}$, for $j = 1,2,3$. Since each $\mathcal{G}_j$ has multilinear rank (d_j,d_j,d_j), it follows that $\mathcal{G}$ has multilinear rank (R,R,R). The matrices $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ having rank R implies that $\mathcal{X}$ also has multilinear rank (R,R,R). Hence, by [49], $\operatorname{brank}(\mathcal{X}) \geq R$. Together with $\operatorname{brank}(\mathcal{X}) \leq R$, this completes the proof of (a).

Next, we prove (b). Since $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ have rank R, we have $\operatorname{rank}(\mathcal{X}) = \operatorname{rank}(\mathcal{G})$. The condition of (b), together with Lemma 3.3, implies that $\operatorname{rank}(\mathcal{X}) = \sum_{j=1}^{m} \operatorname{rank}(\mathcal{G}_j)$. The assumptions on $\operatorname{rank}(\mathcal{G}_j)$ complete the proof. ∎

3.3. Uniqueness of a decomposition in block terms. The decomposition in block terms (3.3) is called *essentially unique* if any alternative decomposition $\mathcal{X} = \sum_{j=1}^{m}(\bar{\mathbf{S}}_j,\bar{\mathbf{T}}_j,\bar{\mathbf{U}}_j)\cdot\mathcal{H}_j$ satisfies $\bar{\mathbf{S}}_j = \mathbf{S}_{\pi(j)}\mathbf{L}_{\pi(j)}$, $\bar{\mathbf{T}}_j = \mathbf{T}_{\pi(j)}\mathbf{M}_{\pi(j)}$, $\bar{\mathbf{U}}_j = \mathbf{U}_{\pi(j)}\mathbf{N}_{\pi(j)}$, and $\mathcal{H}_j = (\mathbf{L}_{\pi(j)}^{-1},\mathbf{M}_{\pi(j)}^{-1},\mathbf{N}_{\pi(j)}^{-1})\cdot\mathcal{G}_{\pi(j)}$, for nonsingular matrices $\mathbf{L}_{\pi(j)}$, $\mathbf{M}_{\pi(j)}$, $\mathbf{N}_{\pi(j)}$, and a permutation π of $(1,\ldots,m)$. Hence, the only existing ambiguities are nonsingular transformations between the matrices $\mathbf{S}_j$, $\mathbf{T}_j$, $\mathbf{U}_j$ and the core blocks $\mathcal{G}_j$, and a permutation of the summands in (3.3).

Let the decomposition of $\mathcal{X}$ satisfy the assumptions of Lemma 3.4 and let $\max(d_j) = 2$. For $d_j = 2$ and $\mathcal{G}_j$ equal to (2.3), we have $(\mathbf{L},\mathbf{M},\mathbf{N})\cdot\mathcal{G}_j = \mathcal{G}_j$, with

$$\mathbf{L} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix}, \qquad \mathbf{M} = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}, \qquad \mathbf{N} = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix}. \tag{3.5}$$

Since any $\mathcal{G}_j \in \overline{S}_2(2,2,2)$ with $\operatorname{rank}(\mathcal{G}_j) > 2$ can be transformed to (2.3), it follows that the decomposition in block terms is not essentially unique. However, the following result states that such nonsingular transformations of single $2\times2\times2$ core blocks are the only other ambiguities in the decomposition. This implies that the block terms $(\mathbf{S}_j,\mathbf{T}_j,\mathbf{U}_j)\cdot\mathcal{G}_j$ in the decomposition remain separated in alternative decompositions.

LEMMA 3.5. *Let $\mathcal{X}$ be as in* (3.3)*, where* $\mathbf{S}$*,* $\mathbf{T}$*,* $\mathbf{U}$ *have rank R,* $\max(d_j) = 2$*, and arrays $\mathcal{G}_j \in \overline{S}_{d_j}(d_j,d_j,d_j)$ have* $\operatorname{rank}(\mathcal{G}_j) > 2$ *if $d_j = 2$, and* $\operatorname{rank}(\mathcal{G}_j) = 1$ *if $d_j = 1$, $j = 1,\ldots,m$. Then the ambiguities in the decomposition in block terms* (3.3) *are those under essential uniqueness, and nonsingular transformations of the form $(\mathbf{L},\mathbf{M},\mathbf{N})\cdot\mathcal{G}_j = \mathcal{G}_j$, for $d_j = 2$.*

Proof. See the appendix for the proof. ∎

4. Some examples. Here, we illustrate the method outlined in section 2.

Example I. We generate a random $5\times5\times5$ array $\mathcal{Z}$ and set $R = 3$. For random initial values and a convergence criterion of `1e-9`, the CP ALS algorithm terminates

after 11100 iterations with diverging components and objective value $||\mathcal{Z} - \mathcal{Y}||^2 = 61.9711$. Nearly the same result is obtained for many other random initial values, which is evidence that the CP problem does not have an optimal solution. The obtained component matrices are

$$\mathbf{A} = \begin{bmatrix} 0.1307 & 0.4772 & -0.4756 \\ 0.3896 & 0.8494 & -0.8545 \\ 0.8207 & 0.1133 & -0.1140 \\ -0.3238 & -0.1421 & 0.1308 \\ 0.2295 & -0.1332 & 0.1164 \end{bmatrix}, \qquad \mathbf{B} = \begin{bmatrix} 0.0617 & -0.1033 & 0.0971 \\ -0.3512 & -0.5379 & 0.5368 \\ -0.4254 & 0.7695 & -0.7717 \\ -0.1941 & -0.0181 & 0.0015 \\ 0.8089 & -0.3279 & 0.3269 \end{bmatrix}, \tag{4.1}$$

$$\mathbf{C} = \begin{bmatrix} 0.7150 & -0.2729 & 0.2792 \\ -0.1566 & 0.6723 & -0.6654 \\ 0.0509 & -0.4897 & 0.5039 \\ 0.3136 & -0.4824 & 0.4743 \\ -0.6027 & -0.0335 & 0.0187 \end{bmatrix}, \tag{4.2}$$

with corresponding weights $\omega_1 = 5.22$, $\omega_2 = 188.27$, and $\omega_3 = 188.95$. Clearly, components 2 and 3 form a group of diverging components, while component 1 is nondiverging. Hence, we set $m = 2$, $d_1 = 1$, and $d_2 = 2$.

Next, we compute the block SGSD of $\mathcal{Y}$ in (2.5), as indicated in section 2.1. We get $\tilde{\mathcal{G}}_1 = 1$ and

$$\tilde{\mathcal{G}}_2 = [\tilde{\mathbf{G}}_1^{(2)} \,|\, \tilde{\mathbf{G}}_2^{(2)}] = \left[\begin{array}{cc|cc} -3.1467 & -2.2131 & -1.2184 & 3.9918 \\ 0 & -3.7274 & 0 & -1.3416 \end{array}\right]. \tag{4.3}$$

Next, we compute the initial values of the decomposition in block terms $\sum_{j=1}^{m} (\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$, as indicated in section 2.2. After premultiplying both slices of (4.3) by $(\tilde{\mathbf{G}}_1^{(2)})^{-1}$, we obtain the array

$$\left[\begin{array}{cc|cc} 1 & 0 & 0.3872 & -1.5217 \\ 0 & 1 & 0 & 0.3599 \end{array}\right]. \tag{4.4}$$

Hence, we have $a \approx b$ in (2.8) indeed. After computing the initial values of the decomposition in block terms, we fit it as a constrained Tucker3 decomposition to $\mathcal{Z}$ using the ALS algorithm of [28] with convergence criterion `1e-12`. After only 38 iterations, the algorithm terminates with $\mathcal{X} = (\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \mathcal{G}$ with

$$\mathcal{G} = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{array}\right]. \tag{4.5}$$

The component matrices $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ have condition numbers 5.66, 1.62, and 7.18, respectively, which proves that the problems of diverging components have vanished. We have $||\mathcal{Z} - \mathcal{X}||^2 = 61.9705$, which shows that the limiting boundary point $\mathcal{X}$ is indeed a little closer to $\mathcal{Z}$ than $\mathcal{Y}$.

Example II. A brief discussion of this example is contained in section 1. We generate a random $6 \times 6 \times 6$ array $\mathcal{Z}$ and set $R = 6$. For random initial values and a convergence criterion of `1e-9`, the CP ALS algorithm terminates after 19645 iterations with diverging components and objective value $||\mathcal{Z} - \mathcal{Y}||^2 = 54.5370$. Nearly

the same result is obtained for many other random initial values, which is evidence that the CP problem does not have an optimal solution. The obtained component matrices are given by (1.9)–(1.11) with corresponding weights $\omega_1 = 130.22$, $\omega_2 = 133.47$, $\omega_3 = 2083.3$, $\omega_4 = 6386.1$, $\omega_5 = 8466.6$, and $\omega_6 = 4.44$. Hence, we have one group of two diverging components, one group of three diverging components, and one nondiverging component. We set $m = 3$, $d_1 = 2$, $d_2 = 3$, and $d_3 = 1$.

Next, we compute the block SGSD of $\mathcal{Y}$ in (2.5), as indicated in section 2.1. We report only the computations for the group of three diverging components. The results for the group of two diverging components are analogous to Example I. We get $\tilde{\mathcal{G}}_2 = [\tilde{\mathbf{G}}_1^{(2)} \,|\, \tilde{\mathbf{G}}_2^{(2)} \,|\, \tilde{\mathbf{G}}_3^{(2)}]$ equal to

$$\left[\begin{array}{rrr|rrr|rrr} -4.6523 & 2.3364 & -5.6641 & 1.3904 & 3.1486 & -0.8284 & 1.0044 & -0.9592 & -2.7747 \\ 0 & -4.9265 & -1.5300 & 0 & 1.7271 & -4.6452 & 0 & 1.0335 & 0.7191 \\ 0 & 0 & 3.5192 & 0 & 0 & -1.1872 & 0 & 0 & -0.7418 \end{array}\right]. \tag{4.6}$$

Next, we compute the initial values of the decomposition in block terms $\sum_{j=1}^{m}(\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$, as indicated in section 2.2. Again, we report only the results for the group of three diverging components. After premultiplying the slices of (4.6) by $(\tilde{\mathbf{G}}_1^{(2)})^{-1}$, we obtain the array

$$\left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & -0.2989 & -0.8528 & 1.1149 & -0.2159 & 0.1008 & 0.8126 \\ 0 & 1 & 0 & 0 & -0.3506 & 1.0477 & 0 & -0.2098 & -0.0805 \\ 0 & 0 & 1 & 0 & 0 & -0.3374 & 0 & 0 & -0.2108 \end{array}\right]. \tag{4.7}$$

Hence, we have $a \approx b \approx c$ and $\alpha \approx \beta \approx \gamma$ in (2.10) indeed. Also, $\delta e = 0.1056 \approx \epsilon d = 0.0687$. After computing the initial values of the decomposition in block terms, we fit it as a constrained Tucker3 decomposition to $\mathcal{Z}$ using the ALS algorithm of [28] with convergence criterion `1e-12`. After 137 iterations, the algorithm terminates with $\mathcal{X} = (\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \mathcal{G}$. The core array is given by $\mathcal{G} = \text{blockdiag}(\mathcal{G}_1, \mathcal{G}_2, \mathcal{G}_3)$, with $\mathcal{G}_1$ equal to (2.3), $\mathcal{G}_3 = 1$, and

$$\mathcal{G}_2 = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & -1.2265 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right]. \tag{4.8}$$

The component matrices $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ have condition numbers 21.8, 6.3, and 61.0, respectively. We have $||\mathcal{Z} - \mathcal{X}||^2 = 54.5336$, which shows that the limiting boundary point $\mathcal{X}$ is indeed a little closer to $\mathcal{Z}$ than $\mathcal{Y}$.

5. Simulation study. Here, we demonstrate the method presented in section 2 in a simulation study. For sizes $10 \times 10 \times 10$, $20 \times 10 \times 10$, and $100 \times 15 \times 10$, we generate 100 random arrays $\mathcal{Z}$ and use the CP ALS algorithm to try to solve the CP problem (1.6). For the $10 \times 10 \times 10$ arrays we consider both $R = 5$ and $R = 6$. For the $20 \times 10 \times 10$ and $100 \times 15 \times 10$ arrays we use $R = 6$. For each array, we run CP ALS 10 times with random starting values, and keep the solution $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ with smallest error $||\mathcal{Z} - \mathcal{Y}||^2$. We use convergence criterion `1e-9` in CP ALS. If $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ features diverging components in groups of no more than three components, then we apply our method to obtain the optimal boundary point $\mathcal{X}$ and its decomposition in block terms $\mathcal{X} = \sum_{j=1}^{m}(\mathbf{S}_j, \mathbf{T}_j, \mathbf{U}_j) \cdot \mathcal{G}_j$. We fit this decomposition to $\mathcal{Z}$ as a constrained Tucker3 decomposition by using the ALS algorithm of [28] with convergence criterion `1e-9`. The groups of diverging components are identified by criterion (2.2).

In Table 1 we report the frequencies of solutions with and without diverging components, and also the sizes of the groups of diverging components. As can be seen, diverging components occur for 70, 79, 74, and 62 percent of the arrays. Also, larger groups of diverging components occur much less often than smaller groups, with one group of two diverging components making up more than 45 percent of all cases with diverging components. Of the $10 \times 10 \times 10$ arrays, 65 had diverging components for both $R = 5$ and $R = 6$. Only 5 had diverging components for $R = 5$ but not for $R = 6$. The converse is true for 14 arrays. Finally, 16 arrays did not have diverging components for both $R = 5$ and $R = 6$.

TABLE 1

Frequencies of CP solutions with and without diverging components. The column 2 contains cases with one group of two diverging components and $R - 2$ nondiverging components; the column $2 + 2$ contains cases with two groups of two diverging components and $R - (2 + 2)$ nondiverging components; et cetera.

$I \times J \times K$	R	No div. comp.	2	$2+2$	$2+2+2$	3	$3+2$	4	$4+2$	5	Total cases
$10 \times 10 \times 10$	5	30	43	6	0	14	3	4	0	0	100
$10 \times 10 \times 10$	6	21	38	16	1	14	5	3	1	1	100
$20 \times 10 \times 10$	6	26	43	12	0	13	6	0	0	0	100
$100 \times 15 \times 10$	6	38	39	10	0	12	1	0	0	0	100

In Table 2 we give a summary of the application of our method to all cases of diverging components except those with a group of four or five diverging components. We report the maximal number of iterations needed by the ALS algorithm to fit the constrained Tucker3 decomposition. As can be seen, the algorithm does not need many iterations. The value of 1695 for $10 \times 10 \times 10$ is an outlier, with all other iteration counts for these arrays being less than or equal to 430. Next, we compare the error term $||\mathcal{Z} - \mathcal{Y}||^2$ (from fitting CP) to $||\mathcal{Z} - \mathcal{X}||^2$ (from fitting the constrained Tucker3 model). We report the minimal and maximal percentage of relative error decrease

$$100 \left(\frac{||\mathcal{Z} - \mathcal{Y}||^2 - ||\mathcal{Z} - \mathcal{X}||^2}{||\mathcal{Z} - \mathcal{Y}||^2} \right). \tag{5.1}$$

In all cases, the boundary point $\mathcal{X}$ is closer to $\mathcal{Z}$ than $\mathcal{Y}$, which suggests that $\mathcal{X}$ is indeed an optimal boundary point. Also, the percentage of relative error decrease is very small in all cases. Hence, the CP solution array $\mathcal{Y}$ is very close to the optimal boundary point $\mathcal{X}$.

The results of the simulation study demonstrate that our method works fine for arrays of large sizes, and is robust with respect to the size $I \times J \times K$, the number of components R, and the number of groups of diverging components. Also, the results validate our Assumptions I and II in section 2, at least for random data.

6. Discussion. In this paper, we have proposed, analyzed, and demonstrated a novel method to deal with diverging CP components due to the nonexistence of an optimal solution to the CP problem for $I \times J \times K$ arrays with $R \leq \min(I, J, K)$. Contrary to $K = 2$ treated in [54] and $R = 2$ treated in [41], we have no known decomposition yielding the closure of the rank-R set. Also, contrary to the case $R = 2$, the number of diverging components (if they occur) is not known in advance. Because of these issues, we propose to first try solving the CP problem. When this results in

TABLE 2

Results of applying the method in section 2 to the cases of diverging components in Table 1 with groups of no more than three diverging components. The columns contain the maximal number of iterations needed for fitting the block term decomposition, and the minimal and maximal percentage of relative error decrease.

$I \times J \times K$	R	max(iters)	minimal (5.1)	maximal (5.1)	Total cases
$10 \times 10 \times 10$	5	1695	0.0005	0.0015	66
$10 \times 10 \times 10$	6	373	0.0002	0.0021	74
$20 \times 10 \times 10$	6	261	0.0002	0.0014	74
$100 \times 15 \times 10$	6	196	0.0001	0.0006	62

diverging components, and we are convinced that the CP problem does not have an optimal solution, then we fit a particular decomposition in block terms (interpreted as Tucker3 with a constrained block-diagonal core) with initial values obtained from the final CP update. When only groups of two or three diverging components are present, we have shown that this results in a decomposition in block terms of the limiting boundary point $\mathcal{X}$. Each block term has a $d_j \times d_j \times d_j$ core array in canonical form and, for $d_j = 2, 3$, it is the limit of a group of d_j diverging components. For $d_j = 1$, the block term is the rank-1 limit of a nondiverging component.

The decomposition of $\mathcal{X}$ does not feature nearly identical vectors or large weights, and may still be interpretable to the researcher. When imposing orthogonality or nonnegativity constraints in CP (to guarantee an optimal solution) is not suitable, obtaining a decomposition of the limiting boundary point $\mathcal{X}$ may be a good alternative. Since the decomposition of $\mathcal{X}$ is not of CP form (but Tucker3 with only few nonzero core entries), the application must allow this. Various such applications in the social and behavioral sciences can be found in [33]. Chemometric applications are only suitable if the CP structure does not represent some chemical "law" underlying the data; see [46, Chapter 10] for an overview. If the aim is to speed up computations on the data by doing them on a simple-structure decomposition close to the data array $\mathcal{Z}$ rather than on $\mathcal{Z}$ itself, then our method may be of use as well. Such applications can be found in scientific computing, for example the approximation on a grid of a function $f(x, y, z)$ by triple products of one-dimensional functions; see [2] and [18].

As in the case $K = 2$, convergence to identical eigenvalues with only one associated eigenvector is the underlying cause of a group of diverging components (see the proof of Lemma 2.1 in the appendix).

Our method does not involve advanced algorithms, but uses CP ALS and a constrained Tucker3 ALS algorithm instead. Although we need to run a CP algorithm resulting in diverging components first, the fitting of the constrained Tucker3 decomposition requires very little time.

The result of diverging CP components having a limit in the form of a particular Tucker3 decomposition is in line with [21] who explains diverging CP components as "Parafac trying to model Tucker variation." See also [39].

Some questions that remain unanswered are as follows. Diverging CP components also occur for $R > \min(I, J, K)$; see, e.g., [48]. More research is needed to determine whether such cases can also be treated by fitting a suitable decomposition in block terms. Another extension of our method would be to prove canonical forms such as (2.3) and (2.4) for sizes $d_j \times d_j \times d_j$ with $d_j \geq 4$. Also this will be the subject of

future research.

Another open problem is the uniqueness of the decomposition in block terms. In Lemma 3.5 we have shown that although the decomposition of $\mathcal{X}$ in block terms is not essentially unique, the block terms remain separated in any alternative decomposition. This result was obtained for groups of two diverging components only. In the proof (see the appendix) we use the knowledge of the canonical forms of $2 \times 2 \times 2$ arrays of rank 3. For an analogous proof when one group of three diverging components is present, more results on canonical forms of $3 \times 3 \times 3$ arrays of rank 5 are needed. Alternatively, the analogue of Lemma 3.3 for the border rank may be of help. However, particular counterexamples to the additivity of border rank are shown by [42]. One property that is the same for $2 \times 2 \times 2$ core blocks and $3 \times 3 \times 3$ core blocks is the following. For $\mathcal{G}_j$ equal to (2.4) we have $(\mathbf{L}, \mathbf{M}, \mathbf{N}) \cdot \mathcal{G}_j = \mathcal{G}_j$, with

$$\text{(6.1)}\quad \mathbf{L} = \begin{bmatrix} 1 & -d & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{M} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -e & 1 \end{bmatrix}, \qquad \mathbf{N} = \begin{bmatrix} 1 & 1 & de \\ 0 & 1 & 2de \\ 0 & 0 & 1 \end{bmatrix}.$$

Hence, also here the decomposition in block terms is not essentially unique, but the block terms themselves may still be unique.

Appendix. Proofs. *Proof of Lemma* 2.1. By Lemma 3.2 (b), there exist orthonormal $\mathbf{L}$, $\mathbf{M}$, $\mathbf{N}$ such that $(\mathbf{L}, \mathbf{M}, \mathbf{N}) \cdot \mathcal{G}_j$ has all frontal slices upper triangular. By assumption, $\mathcal{G}_j$ has multilinear rank $(3, 3, 3)$. We also assume that $\mathcal{G}_j$ has a nonsingular slicemix, i.e., $(\mathbf{I}_3, \mathbf{I}_3, \mathbf{U}) \cdot \mathcal{G}_j$ has a nonsingular frontal slice for some nonsingular $\mathbf{U}$. This is true for almost all $\mathcal{G}_j$. In fact, if $\mathcal{G}_j$ does not have a nonsingular slicemix, then its upper triangular slices have a zero on their diagonals in the same position. We apply a slicemix to $\mathcal{G}_j$ such that its first slice is nonsingular. Next, we premultiply the slices of $\mathcal{G}_j$ by the inverse of its first slice. Then $\mathcal{G}_j$ is of the form

$$\text{(A.1)}\qquad \mathcal{G}_j = [\mathbf{G}_1^{(j)} \mid \mathbf{G}_2^{(j)} \mid \mathbf{G}_3^{(j)}] = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & a & d & f & \alpha & \delta & \nu \\ 0 & 1 & 0 & 0 & b & e & 0 & \beta & \epsilon \\ 0 & 0 & 1 & 0 & 0 & c & 0 & 0 & \gamma \end{array}\right].$$

By assumption, there exists a sequence $\mathcal{Y}^{(n)}$ in $S_3(3, 3, 3)$ converging to $\mathcal{G}_j$, and $\operatorname{rank}(\mathcal{G}_j) > 3$.

Since a matrix cannot be approximated arbitrarily well by a matrix of lower rank, it follows that the approximating sequence $\mathcal{Y}^{(n)}$ in $S_3(3, 3, 3)$ has multilinear rank $(3, 3, 3)$ and a nonsingular slicemix for n large enough. Moreover, by Lemma 3.2 we may assume without loss of generality that $\mathcal{Y}^{(n)}$ has the form (A.1). We denote the entries of $\mathcal{Y}^{(n)}$ with subscript n, i.e., $a_n, \ldots, f_n$ and $\alpha_n, \ldots, \nu_n$. Hence,

$$\text{(A.2)}\quad \mathcal{Y}^{(n)} = [\mathbf{Y}_1^{(n)} \mid \mathbf{Y}_2^{(n)} \mid \mathbf{Y}_3^{(n)}] = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & a_n & d_n & f_n & \alpha_n & \delta_n & \nu_n \\ 0 & 1 & 0 & 0 & b_n & e_n & 0 & \beta_n & \epsilon_n \\ 0 & 0 & 1 & 0 & 0 & c_n & 0 & 0 & \gamma_n \end{array}\right].$$

Next, we consider the rank-3 decomposition $(\mathbf{A}^{(n)}, \mathbf{B}^{(n)}, \mathbf{C}^{(n)})$ of $\mathcal{Y}^{(n)}$, which can be written as $\mathbf{Y}_k^{(n)} = \mathbf{A}^{(n)}\, \mathbf{C}_k^{(n)}\, (\mathbf{B}^{(n)})^T$, where diagonal matrix $\mathbf{C}_k^{(n)}$ has row k of $\mathbf{C}^{(n)}$ as its diagonal, $k = 1, 2, 3$. Since $\mathbf{Y}_1^{(n)} = \mathbf{I}_3$, matrices $\mathbf{A}^{(n)}$ and $\mathbf{B}^{(n)}$ are nonsingular. Without loss of generality, we set $\mathbf{C}_1^{(n)} = \mathbf{I}_3$. Then $(\mathbf{A}^{(n)})^{-1} = (\mathbf{B}^{(n)})^T$ and $\mathbf{Y}_k^{(n)} = \mathbf{A}^{(n)}\, \mathbf{C}_k^{(n)}\, (\mathbf{A}^{(n)})^{-1}$ for $k = 2, 3$. Hence, slices $\mathbf{Y}_2^{(n)}$ and $\mathbf{Y}_3^{(n)}$ have the same eigenvectors. Moreover, their three eigenvectors are linearly independent, and

their eigenvalues are on the diagonals of $\mathbf{C}_2^{(n)}$ and $\mathbf{C}_3^{(n)}$, respectively. Since $\mathbf{Y}_2^{(n)}$ and $\mathbf{Y}_3^{(n)}$ have eigenvalues a_n, b_n, c_n and $\alpha_n, \beta_n, \gamma_n$, respectively, we obtain

$$\mathbf{C}^{(n)} = \begin{bmatrix} 1 & 1 & 1 \\ a_n & b_n & c_n \\ \alpha_n & \beta_n & \gamma_n \end{bmatrix}. \tag{A.3}$$

Next, we show that in the limit $a = b = c$ and $\alpha = \beta = \gamma$. From Krijnen, Dijkstra, and Stegeman [32] we know that $\mathbf{A}^{(n)}$, $\mathbf{B}^{(n)}$, and $\mathbf{C}^{(n)}$ converge to matrices with ranks less than 3. The eigendecomposition $\mathbf{Y}_k^{(n)} = \mathbf{A}^{(n)}\,\mathbf{C}_k^{(n)}\,(\mathbf{A}^{(n)})^{-1}$ converges to frontal slice $\mathbf{G}_k$ of $\mathcal{G}$, $k = 2, 3$. Hence, the eigenvectors in $\mathbf{A}^{(n)}$ converge to those of $\mathbf{G}_k$, $k = 2, 3$. Suppose $\mathbf{A}^{(n)}$ has a rank-1 limit. Then $\mathbf{G}_k$ has only one eigenvector and three identical eigenvalues, $k = 2, 3$. Hence, $a = b = c$ and $\alpha = \beta = \gamma$. Suppose $\mathbf{A}^{(n)}$ has a rank-2 limit $[\mathbf{a}_1\ \mathbf{a}_2\ \mathbf{a}_3]$. Without loss of generality, let $\mathbf{a}_1$ and $\mathbf{a}_2$ be linearly independent. If $\mathbf{a}_3$ is proportional to either $\mathbf{a}_1$ or $\mathbf{a}_2$, then $\mathbf{B}^{(n)} = (\mathbf{A}^{(n)})^{-T}$ has large numbers in only two columns. This violates the assumption of three diverging components; see (1.7). Hence, $\mathbf{a}_3$ is in the linear span of $\{\mathbf{a}_1, \mathbf{a}_2\}$ and not proportional to $\mathbf{a}_1$ or to $\mathbf{a}_2$. Recall that these are eigenvectors of $\mathbf{G}_k$, $k = 2, 3$. For an eigenvalue λ of $\mathbf{G}_k$, we define the eigenspace

$$E_k(\lambda) = \{\mathbf{x} \in \mathbb{R}^3 :\ \mathbf{G}_k\mathbf{x} = \lambda\,\mathbf{x}\}, \qquad k = 2, 3. \tag{A.4}$$

It holds that $\lambda_1 \neq \lambda_2$ implies $E_k(\lambda_1) \cap E_k(\lambda_2) = \{\mathbf{0}\}$. If a, b, c are distinct, then $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ would be linearly independent, which is not the case. Without loss of generality, let $a = b$. Then $\mathbf{a}_3 \in E_2(a) \cap E_2(c)$, which is impossible if $a \neq c$. Hence, it follows that $a = b = c$. The proof of $\alpha = \beta = \gamma$ is analogous.

As $\mathcal{Y}^{(n)} \to \mathcal{G}_j$, we first assume that the eigenvalues a_n, b_n, c_n are distinct and the eigenvalues $\alpha_n, \beta_n, \gamma_n$ are distinct. It can be verified that the eigenvectors of $\mathbf{Y}_2^{(n)}$ associated with eigenvalues a_n, b_n, c_n are, respectively,

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} \frac{d_n}{b_n - a_n} \\ 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} \frac{d_n e_n + f_n(c_n - b_n)}{(c_n - a_n)(c_n - b_n)} \\ \frac{e_n}{c_n - b_n} \\ 1 \end{pmatrix}. \tag{A.5}$$

Since the eigenvectors of $\mathbf{Y}_2^{(n)}$ and $\mathbf{Y}_3^{(n)}$ (in terms of $\alpha_n, \ldots, \nu_n$) are equal, we have

$$\begin{aligned} \frac{d_n}{b_n - a_n} &= \frac{\delta_n}{\beta_n - \alpha_n}, \qquad \frac{e_n}{c_n - b_n} = \frac{\epsilon_n}{\gamma_n - \beta_n}, \\ \frac{d_n e_n + f_n(c_n - b_n)}{(c_n - a_n)(c_n - b_n)} &= \frac{\delta_n \epsilon_n + \nu_n(\gamma_n - \beta_n)}{(\gamma_n - \alpha_n)(\gamma_n - \beta_n)}. \end{aligned} \tag{A.6}$$

We assume that $\mathcal{G}_j$ has $d \neq 0$, $e \neq 0$, $f \neq 0$, $\delta \neq 0$, $\epsilon \neq 0$, and $\nu \neq 0$. This holds for almost all $\mathcal{G}_j$. Next, we show that this implies $\delta e = \epsilon d$. Let $g(n) = b_n - a_n \to 0$ and $h(n) = c_n - b_n \to 0$. From (A.6) we get $\beta_n - \alpha_n = (\delta_n/d_n)\,g(n) \to 0$ and $\gamma_n - \beta_n = (\epsilon_n/e_n)\,h(n) \to 0$. Obviously, also $c_n - a_n$ and $\gamma_n - \alpha_n$ converge to zero. Substituting these expressions into the third equation of (A.6) yields

$$\frac{d_n e_n + f_n\,h(n)}{(g(n) + h(n))\,h(n)} = \frac{\delta_n \epsilon_n + \nu_n\,(\epsilon_n/e_n)\,h(n)}{((\delta_n/d_n)\,g(n) + (\epsilon_n/e_n)\,h(n))\,(\epsilon_n/e_n)\,h(n)}. \tag{A.7}$$

Without loss of generality, let $l = \lim_{n\to\infty}(g(n)/h(n))$ be finite. Cancelling $h(n)^{-1}$ on both sides of (A.7) and rewriting gives

$$d_n e_n + f_n\, h(n) = \left(\frac{g(n)+h(n)}{(\delta_n/d_n)\, g(n) + (\epsilon_n/e_n)\, h(n)}\right) \frac{e_n}{\epsilon_n} \left(\delta_n \epsilon_n + \nu_n\, (\epsilon_n/e_n)\, h(n)\right). \tag{A.8}$$

Letting $n \to \infty$ on both sides yields

$$de = \left(\frac{l+1}{(\delta/d)\, l + (\epsilon/e)}\right) \frac{e}{\epsilon}\, \delta\epsilon\,. \tag{A.9}$$

Simplifying gives $\delta e = \epsilon d$.

Hence, we have $\mathcal{G}_j$ equal to (A.1) with $a = b = c$, $\alpha = \beta = \gamma$, and $\delta e = \epsilon d$. Subtracting a times $\mathbf{G}_1^{(j)}$ from $\mathbf{G}_2^{(j)}$ and α times $\mathbf{G}_1^{(j)}$ from $\mathbf{G}_3^{(j)}$ is a nonsingular transformation that sets the diagonals of $\mathbf{G}_2^{(j)}$ and $\mathbf{G}_3^{(j)}$ to zero. Next, we subtract δ/d times $\mathbf{G}_2^{(j)}$ from $\mathbf{G}_3^{(j)}$, and f/ν times $\mathbf{G}_3^{(j)}$ from $\mathbf{G}_2^{(j)}$. This transformation is nonsingular unless $f\delta = d\nu$, which implies that $\mathcal{G}_j$ has mode-3 rank 2. After multiplying $\mathbf{G}_3^{(j)}$ by ν^{-1}, we obtain canonical form (2.4).

In our analysis above, we assumed that $d, e, f, \delta, \epsilon, \nu$ are nonzero. Next, we consider some of the other possibilities. Note that this is not necessary to prove Lemma 2.1, since these cases are exceptions to almost all $\mathcal{G}_j$. From the above, it follows that $\delta_n\, e_n \sim \epsilon_n\, d_n$. Suppose $d = 0$. Then $\delta e = 0$. Taking into account that $\mathcal{G}_j$ has mode-3 rank 3, this yields three possibilities. If $e = 0$ and $\delta \neq 0$, then $f \neq 0$. If $\delta = 0$ and $e \neq 0$, then $f\epsilon \neq e\nu$. If $\delta = e = 0$, then $\epsilon \neq 0$ and $f \neq 0$. It can be verified that in all three cases, we get canonical form (2.4) after mixing and normalizing $\mathbf{G}_2^{(j)}$ and $\mathbf{G}_3^{(j)}$. Note that in some cases, slice $\mathbf{G}_2^{(j)}$ of the canonical form has only one nonzero entry. The situations where we suppose that $e = 0$ or $\delta = 0$ or $\epsilon = 0$ can be dealt with analogously. The canonical form (2.4) with $d = 0$ and $e = 1$ was first discovered in [39, sect. 7].

It remains to consider the cases where the eigenvalues a_n, b_n, c_n and $\alpha_n, \beta_n, \gamma_n$ are not all distinct. Below, we show that such cases can be left out of consideration. We only consider cases where some of a_n, b_n, c_n are identical. Cases where some of α, β, γ are identical can be treated analogously. If $a_n = b_n \neq c_n$ for n large enough, then we must have $d_n = 0$ to obtain three linearly independent eigenvectors of $\mathbf{Y}_2^{(n)}$. This is due to the upper triangular form of $\mathbf{Y}_2^{(n)}$ in (A.2). This implies that $d = 0$ in the limit, which does not hold for almost all $\mathcal{G}_j$.

The case $a_n \neq b_n = c_n$ can be dealt with analogously. Here, we must have $e_n = 0$ to obtain three linearly independent eigenvectors of $\mathbf{Y}_2^{(n)}$ in (A.2). This implies that $e = 0$ in the limit, which does not hold for almost all $\mathcal{G}_j$.

Next, suppose $a_n = c_n \neq b_n$ for n large enough. To obtain three linearly independent eigenvectors of $\mathbf{Y}_2^{(n)}$ in (A.2), we must have $d_n e_n + f_n(c_n - b_n) = 0$. Since $c_n - b_n \to c - b = 0$, this implies that $de = 0$ in the limit, which does not hold for almost all $\mathcal{G}_j$.

Finally, we consider the case $a_n = b_n = c_n$ for n large enough. To obtain three linearly independent eigenvectors of $\mathbf{Y}_2^{(n)}$ in (A.2), we must have $d_n = e_n = f_n = 0$. This implies that $d = e = f = 0$ in the limit, which does not hold for almost all $\mathcal{G}_j$.

Finally, we prove that $\text{rank}(\mathcal{G}_j) = 5$ when $\mathcal{G}_j$ equals (2.4) with at least one of d and e nonzero. First, note that $\text{rank}(\mathcal{G}_j) \leq 5$ follows from the maximal rank of $3\times3\times2$ arrays (slices $\mathbf{G}_1^{(j)}$ and $\mathbf{G}_2^{(j)}$) being 4 [25], and the fact that slice $\mathbf{G}_3^{(j)}$ requires one

additional rank-1 term. Next, we show that $\text{rank}(\mathcal{G}_j) \geq 5$. As in [39], we use [34, Corollary 1', p.108], which implies

$$\text{rank}(\mathcal{G}_j) \geq \min_{u \neq 0} (\text{rank}(u\,\mathbf{G}_1^{(j)} + v\,\mathbf{G}_2^{(j)} + w\,\mathbf{G}_3^{(j)})) + \text{rank}_3(\mathcal{G}_j) - 1\,, \tag{A.10}$$

with $\text{rank}_3(\mathcal{G}_j)$ denoting the mode-3 rank of $\mathcal{G}_j$. Using (2.4) yields $\text{rank}(\mathcal{G}_j) \geq 3+3-1 = 5$. ∎

Proof of Lemma 3.5. Without loss of generality, we set $\mathcal{G}_j = 1$ if $d_j = 1$ and $\mathcal{G}_j$ equal to canonical form (2.3) if $d_j = 2$. Premultiplying $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ by nonsingular matrices does not change the uniqueness properties of the decomposition. We premultiply by matrices that transform each of $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$ to $\left[\begin{smallmatrix}\mathbf{I}_R \\ \mathbf{O}\end{smallmatrix}\right]$. The uniqueness properties of the decomposition do not depend on the all-zero rows of the component matrices [58, p. 401], [55, Lemma 3.4]. Hence, without loss of generality, we consider the decomposition (3.3) with $\mathcal{X} = (\mathbf{I}_R, \mathbf{I}_R, \mathbf{I}_R) \cdot \mathcal{G}$. We denote an alternative decomposition as $(\bar{\mathbf{S}}, \bar{\mathbf{T}}, \bar{\mathbf{U}}) \cdot \mathcal{H}$, with $\bar{\mathbf{S}}$, $\bar{\mathbf{T}}$, and $\bar{\mathbf{U}}$ nonsingular $R \times R$ matrices. The nonsingularity of $\bar{\mathbf{S}}$, $\bar{\mathbf{T}}$, $\bar{\mathbf{U}}$ follows from [55, Proposition 3.3].

The multilinear rank of $\mathcal{H}$ must be equal to that of $\mathcal{G}$, which equals (R, R, R). This implies that each $2 \times 2 \times 2$ core block of $\mathcal{H}$ has multilinear rank $(2, 2, 2)$, and each $1 \times 1 \times 1$ core block is nonzero. Moreover, Lemma 3.3 implies that each $2 \times 2 \times 2$ core block of $\mathcal{H}$ must have rank 3. The $2 \times 2 \times 2$ core blocks of $\mathcal{H}$ either have canonical form (2.3) or canonical form

$$\left[\begin{array}{cc|cc} 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \end{array}\right], \tag{A.11}$$

where (2.3) has border rank 2 and (A.11) has border rank 3 [16, sect. 7]. As we will see below, the $2 \times 2 \times 2$ core blocks of $\mathcal{H}$ must have canonical form (2.3).

A Kruskal-type essential uniqueness condition for a decomposition (3.3) with $2 \times 2 \times 2$ core blocks having canonical form (A.11) has been proven in [10, Theorem 5.6]. In our case, we may have scalar core blocks as well, and the $2 \times 2 \times 2$ core blocks have canonical form (2.3). Since the techniques of [10] do not seem to be of use in our case, we focus on equating the decomposition to its alternative.

First, we consider the case where only one $2 \times 2 \times 2$ core block is present. In particular, we set $R = 3$, $m = 2$, $d_1 = 1$, and $d_2 = 2$. Hence, the core $\mathcal{G}$ is as in (4.5). Let $\mathcal{H} = \text{blockdiag}(\mathcal{H}_1, \mathcal{H}_2)$, where $\mathcal{H}_2$ has 2×2 slices $\mathbf{H}_{21}$ and $\mathbf{H}_{22}$, and $\mathcal{H}_1 = 1$ without loss of generality. We equate the two decompositions as $(\bar{\mathbf{S}}^{-1}, \bar{\mathbf{T}}^{-1}, \mathbf{I}_R) \cdot \mathcal{G} = (\mathbf{I}_R, \mathbf{I}_R, \bar{\mathbf{U}}) \cdot \mathcal{H}$. We set $\bar{\mathbf{S}}^{-1} = [\mathbf{s}_1\ \mathbf{s}_2\ \mathbf{s}_3]$ and $\bar{\mathbf{T}}^{-1} = [\mathbf{t}_1\ \mathbf{t}_2\ \mathbf{t}_3]$. The equations for the three slices of the decomposition are as follows:

$$\mathbf{s}_1\,\mathbf{t}_1^T = \begin{bmatrix} u_{11} & \mathbf{0} \\ \mathbf{0}^T & u_{12}\,\mathbf{H}_{21} + u_{13}\,\mathbf{H}_{22} \end{bmatrix}, \quad \mathbf{s}_2\,\mathbf{t}_2^T + \mathbf{s}_3\,\mathbf{t}_3^T = \begin{bmatrix} u_{21} & \mathbf{0} \\ \mathbf{0}^T & u_{22}\,\mathbf{H}_{21} + u_{23}\,\mathbf{H}_{22} \end{bmatrix}, \tag{A.12}$$

$$\mathbf{s}_2\,\mathbf{t}_3^T = \begin{bmatrix} u_{31} & \mathbf{0} \\ \mathbf{0}^T & u_{32}\,\mathbf{H}_{21} + u_{33}\,\mathbf{H}_{22} \end{bmatrix}, \tag{A.13}$$

where u_{ji} denote the entries of $\bar{\mathbf{U}}$.

If $u_{j1} \neq 0$, then $u_{j2}\,\mathbf{H}_{21} + u_{j3}\,\mathbf{H}_{22} = \mathbf{O}$, $j = 1, 3$. Since $\mathcal{H}_2$ has multilinear rank $(2, 2, 2)$, the latter implies $u_{j2} = u_{j3} = 0$. If $u_{11} \neq 0$ and $u_{31} \neq 0$, then rows 1 and 3 of $\bar{\mathbf{U}}$ are proportional. Hence, at least one of u_{11} and u_{31} must be zero. If $u_{j1} = 0$, then $u_{j2}\,\mathbf{H}_{21} + u_{j3}\,\mathbf{H}_{22}$ must have rank 1, $j = 1, 3$. However, this is not possible for

real u_{j2} and u_{j3} when $\mathcal{H}_2$ has canonical form (A.11). Hence, we have shown that $\mathcal{H}_2$ must have canonical form (2.3).

Without loss of generality, we assume that $\mathcal{H}_2$ is equal to its canonical form. The equations (A.12)–(A.13) become

$$\mathbf{s}_1\,\mathbf{t}_1^T = \begin{bmatrix} u_{11} & 0 & 0 \\ 0 & u_{12} & u_{13} \\ 0 & 0 & u_{12} \end{bmatrix}, \qquad \mathbf{s}_2\,\mathbf{t}_2^T + \mathbf{s}_3\,\mathbf{t}_3^T = \begin{bmatrix} u_{21} & 0 & 0 \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{22} \end{bmatrix}, \tag{A.14}$$

$$\mathbf{s}_2\,\mathbf{t}_3^T = \begin{bmatrix} u_{31} & 0 & 0 \\ 0 & u_{32} & u_{33} \\ 0 & 0 & u_{32} \end{bmatrix}. \tag{A.15}$$

If $u_{11} = u_{31} = 0$, then $u_{12} = u_{32} = 0$ and rows 1 and 3 of $\bar{\mathbf{U}}$ are proportional. Combined with the above, this leaves two possibilities only: either $u_{11} \neq 0$ and $u_{31} = 0$, or $u_{11} = 0$ and $u_{31} \neq 0$. In the first case, it follows from (A.14)–(A.15) that $\bar{\mathbf{S}}^{-1}$, $\bar{\mathbf{T}}^{-1}$, and $\bar{\mathbf{U}}$ have the following form:

$$\bar{\mathbf{S}}^{-1} = \begin{bmatrix} * & 0 & 0 \\ 0 & * & * \\ 0 & * & * \end{bmatrix}, \qquad \bar{\mathbf{T}}^{-1} = \begin{bmatrix} * & 0 & 0 \\ 0 & * & * \\ 0 & * & * \end{bmatrix}, \qquad \bar{\mathbf{U}} = \begin{bmatrix} * & 0 & 0 \\ 0 & * & * \\ 0 & 0 & * \end{bmatrix}. \tag{A.16}$$

Since $\bar{\mathbf{S}}$ and $\bar{\mathbf{T}}$ have the same structure as $\bar{\mathbf{S}}^{-1}$, $\bar{\mathbf{T}}^{-1}$, it follows that the alternative decomposition $(\bar{\mathbf{S}}, \bar{\mathbf{T}}, \bar{\mathbf{U}}) \cdot \mathcal{H}$ falls within the ambiguities stated in Lemma 3.5. In the case $u_{11} = 0$ and $u_{31} \neq 0$ the same is true, but the ordering of the two blocks has been reversed.

When only one $2 \times 2 \times 2$ core block is present, together with several scalar blocks (and not just one), an analogous approach as above can be used. We conclude this proof by considering the case of two $2 \times 2 \times 2$ core blocks. Together with the proof above, this should convince the reader that Lemma 3.5 is true for any combination of $2 \times 2 \times 2$ and $1 \times 1 \times 1$ core blocks.

Let $R = 4$, $m = 2$, and $d_1 = d_2 = 2$. Analogous to (A.12)–(A.13), we have

$$\mathbf{s}_j\,\mathbf{t}_j^T + \mathbf{s}_{j+1}\,\mathbf{t}_{j+1}^T = \begin{bmatrix} u_{j1}\,\mathbf{H}_{11} + u_{j2}\,\mathbf{H}_{12} & \mathbf{O} \\ \mathbf{O} & u_{j3}\,\mathbf{H}_{21} + u_{j4}\,\mathbf{H}_{22} \end{bmatrix}, \qquad j = 1, 3, \tag{A.17}$$

$$\mathbf{s}_{j-1}\,\mathbf{t}_j^T = \begin{bmatrix} u_{j1}\,\mathbf{H}_{11} + u_{j2}\,\mathbf{H}_{12} & \mathbf{O} \\ \mathbf{O} & u_{j3}\,\mathbf{H}_{21} + u_{j4}\,\mathbf{H}_{22} \end{bmatrix}, \qquad j = 2, 4, \tag{A.18}$$

with $\mathbf{H}_{ki}$ the slices of $\mathcal{H}_k$. It follows from (A.18) that either $u_{j1}\,\mathbf{H}_{11} + u_{j2}\,\mathbf{H}_{12}$ has rank 1 or $u_{j3}\,\mathbf{H}_{21} + u_{j4}\,\mathbf{H}_{22}$ has rank 1, $j = 2, 4$. As observed above, this is impossible when $\mathcal{H}_1$ and $\mathcal{H}_2$ both have canonical form (A.11). Suppose $\mathcal{H}_1$ has canonical form (2.4) and $\mathcal{H}_2$ has canonical form (A.11). Then (A.18) implies that $u_{j1}\,\mathbf{H}_{11} + u_{j2}\,\mathbf{H}_{12}$ has rank 1 for $j = 2, 4$. Since $\mathcal{H}_1$ has canonical form (2.4), we get $(u_{21}\ u_{22})$ proportional to $(u_{41}\ u_{42})$. Since $\mathcal{H}_2$ has multilinear rank $(2, 2, 2)$, it follows from (A.18) that $u_{23} = u_{24} = u_{43} = u_{44} = 0$. But then rows 2 and 4 of $\bar{\mathbf{U}}$ are proportional. We conclude that both $\mathcal{H}_1$ and $\mathcal{H}_2$ must have canonical form (2.4).

Without loss of generality, we assume that $\mathcal{H}_1$ and $\mathcal{H}_2$ are equal to their canonical form. The equations (A.17)–(A.18) become

$$\mathbf{s}_j\,\mathbf{t}_j^T + \mathbf{s}_{j+1}\,\mathbf{t}_{j+1}^T = \begin{bmatrix} u_{j1} & u_{j2} & 0 & 0 \\ 0 & u_{j1} & 0 & 0 \\ 0 & 0 & u_{j3} & u_{j4} \\ 0 & 0 & 0 & u_{j3} \end{bmatrix}, \qquad j = 1, 3\,, \tag{A.19}$$

$$\mathbf{s}_{j-1}\,\mathbf{t}_j^T = \begin{bmatrix} u_{j1} & u_{j2} & 0 & 0 \\ 0 & u_{j1} & 0 & 0 \\ 0 & 0 & u_{j3} & u_{j4} \\ 0 & 0 & 0 & u_{j3} \end{bmatrix}, \qquad j = 2, 4\,. \tag{A.20}$$

From (A.20), it follows that $u_{21} = u_{23} = u_{41} = u_{43} = 0$. Also, exactly one of u_{22} and u_{24} is nonzero, and exactly one of u_{42} and u_{44} is nonzero. Suppose $u_{22} \neq 0$. To avoid rows 2 and 4 of $\bar{\mathbf{U}}$ being proportional, this implies $u_{24} = 0$, $u_{42} = 0$, and $u_{44} \neq 0$. From the form of the rank-1 matrices in (A.20), we obtain that $\mathbf{s}_1 = (*\ 0\ 0\ 0)^T$, $\mathbf{t}_2 = (0\ *\ 0\ 0)^T$, $\mathbf{s}_3 = (0\ 0\ *\ 0)^T$, and $\mathbf{t}_4 = (0\ 0\ 0\ *)^T$. Together with the form of the matrices in (A.19), this implies that $\mathbf{t}_1 = (*\ *\ 0\ 0)^T$, $\mathbf{s}_2 = (*\ *\ 0\ 0)^T$, $\mathbf{t}_3 = (0\ 0\ *\ *)^T$, and $\mathbf{s}_4 = (0\ 0\ *\ *)^T$. Moreover, $u_{13} = u_{14} = 0$ and $u_{31} = u_{32} = 0$. From the forms of $\bar{\mathbf{S}}^{-1}$, $\bar{\mathbf{T}}^{-1}$, and $\bar{\mathbf{U}}$ we conclude that the alternative decomposition $(\bar{\mathbf{S}}, \bar{\mathbf{T}}, \bar{\mathbf{U}}) \cdot \mathcal{H}$ falls within the ambiguities stated in Lemma 3.5. The same is true if we suppose that $u_{24} \neq 0$ and $u_{22} = 0$, but then the ordering of the two blocks has been reversed. ∎

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