

A METHOD TO AVOID DIVERGING COMPONENTS IN THE CANDECOMP/PARAFAC MODEL FOR GENERIC $I \times J \times 2$ ARRAYS*

ALWIN STEGEMAN[†] AND LIEVEN DE LATHAUWER[‡]

Abstract. Computing the Candecomp/Parafac (CP) solution of R components (i.e., the best rank- R approximation) for a generic $I \times J \times 2$ array may result in diverging components, also known as “degeneracy.” In such a case, several components are highly correlated in all three modes, and their component weights become arbitrarily large. Evidence exists that this is caused by the nonexistence of an optimal CP solution. Instead of using CP, we propose to compute the best approximation by means of a generalized Schur decomposition (GSD), which always exists. The obtained GSD solution is the limit point of the sequence of CP updates (whether it features diverging components or not) and can be separated into a nondiverging CP part and a sparse Tucker3 part or into a nondiverging CP part and a smaller GSD part. We show how to obtain both representations and illustrate our results with numerical experiments.

Key words. canonical decomposition, parallel factors analysis, low-rank tensor approximations, degenerate Parafac solutions, diverging components

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1. Introduction. Hitchcock [16, 17] introduced a generalized rank and related decomposition of a multiway array or tensor. The same decomposition was proposed independently by Carroll and Chang [3] and Harshman [13] for component analysis of three-way data arrays. They named it Candecomp and Parafac, respectively. We denote the Candecomp/Parafac (CP) model, i.e., the decomposition with a residual term, as

$$(1.1) \quad \mathbf{Z} = \sum_{h=1}^R \omega_h (\mathbf{a}_h \otimes \mathbf{b}_h \otimes \mathbf{c}_h) + \mathbf{E},$$

where \mathbf{Z} is an $I \times J \times K$ data array, ω_h is the weight of component h , \otimes denotes the outer product, and $\|\mathbf{a}_h\| = \|\mathbf{b}_h\| = \|\mathbf{c}_h\| = 1$ for $h = 1, \dots, R$, with $\|\cdot\|$ denoting the Frobenius norm. To find the R components $\mathbf{a}_h \otimes \mathbf{b}_h \otimes \mathbf{c}_h$ and the weights ω_h , an iterative algorithm is used which minimizes the Frobenius norm of the residual

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[†]Corresponding author. Heymans Institute for Psychological Research, University of Groningen, Grote Kruisstraat 2/1, 9712 TS Groningen, The Netherlands (a.w.stegeman@rug.nl, <http://www.gmw.rug.nl/~stegeman>). This author’s research was supported by the Dutch Organization for Scientific Research (NWO), VENI grant 451-04-102.

[‡]Subfaculty Science and Technology, Katholieke Universiteit Leuven, Campus Kortrijk, E. Sabbe-
laan 53, 8500 Kortrijk, Belgium (Lieven.DeLathauwer@kuleuven-kortrijk.be) and Research Division
SCD, Department of Electrical Engineering (ESAT), Katholieke Universiteit Leuven, Kasteelpark
Arenberg 10, B-3001 Leuven, Belgium (Lieven.DeLathauwer@esat.kuleuven.be, <http://homes.esat.kuleuven.be/~delathau/home.html>). This author’s research was supported by (1) Research Council K.U.Leuven: GOA-Ambiorics, CoE EF/05/006 Optimization in Engineering (OPTEC), CIF1, STRT1/08/23; (2) F.W.O. (a) project G.0321.06; (b) Research Communities ICCoS, ANMMM, and MLDM; (3) the Belgian Federal Science Policy Office IUAP P6/04 (DYSCO, “Dynamical systems, control, and optimization,” 2007–2011); (4) EU: ERNSI. A large part of this research was carried out when the author was with the French Centre National de la Recherche Scientifique (C.N.R.S.).

array $\underline{\mathbf{E}}$. For an overview and comparison of CP algorithms, see Hopke et al. [18] and Tomasi and Bro [45].

The rank of a three-way array $\underline{\mathbf{Z}}$ is defined in the usual way, i.e., the smallest number of rank-1 arrays whose sum equals $\underline{\mathbf{Z}}$. A three-way array has rank 1 if it is the outer product of three vectors, i.e., $\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}$. We denote three-way rank as $\text{rank}_{\otimes}(\underline{\mathbf{Z}})$. It follows that the CP model tries to find a best rank- R approximation to the three-way array $\underline{\mathbf{Z}}$.

The real-valued CP model, i.e., where $\underline{\mathbf{Z}}$ and the model parameters are real-valued, was introduced in psychometrics (Carroll and Chang [3]) and phonetics (Harshman [13]). Later on, it was also applied in chemometrics and the food industry (Bro [1] and Smilde, Bro, and Geladi [37]). For other applications of CP in psychometrics, see Kroonenberg [25]. Complex-valued applications of CP occur in signal processing, especially wireless telecommunications; see Sidiropoulos, Giannakis, and Bro [35], Sidiropoulos, Bro, and Giannakis [36], and De Lathauwer and Castaing [9]. Also, CP describes the basic structure of fourth-order cumulants of multivariate data on which a lot of algebraic methods for independent component analysis are based (Comon [4], De Lathauwer, De Moor, and Vandewalle [5], and Hyvärinen, Karhunen, and Oja [20]). In this paper, we consider the real-valued CP model. All occurrences of three-way rank are assumed to be over the real field.

For later use, we mention that the CP model (1.1) is a special case of the Tucker3 model of Tucker [46]. The latter is defined as

$$(1.2) \quad \underline{\mathbf{Z}} = \sum_{h=1}^R \sum_{i=1}^P \sum_{j=1}^Q g_{hij} (\mathbf{a}_h \otimes \mathbf{b}_i \otimes \mathbf{c}_j) + \underline{\mathbf{E}}.$$

Clearly, the case with $R = P = Q$ and $g_{hij} = 0$ if $(h, i, j) \neq (h, h, h)$ yields (1.1). The $R \times P \times Q$ array $\underline{\mathbf{G}}$ with entries g_{hij} is referred to as the core array. The matrices $[\mathbf{a}_1 | \dots | \mathbf{a}_R]$, $[\mathbf{b}_1 | \dots | \mathbf{b}_P]$, and $[\mathbf{c}_1 | \dots | \mathbf{c}_Q]$ are called the component matrices.

A matrix notation of the CP model (1.1) is as follows. Let \mathbf{Z}_k ($I \times J$) and \mathbf{E}_k ($I \times J$) denote the k th slices of $\underline{\mathbf{Z}}$ and $\underline{\mathbf{E}}$, respectively. Then (1.1) can be written as

$$(1.3) \quad \mathbf{Z}_k = \mathbf{A} \mathbf{C}_k \mathbf{B}^T + \mathbf{E}_k, \quad k = 1, \dots, K,$$

where the component matrices \mathbf{A} ($I \times R$) and \mathbf{B} ($J \times R$) have the vectors \mathbf{a}_h and \mathbf{b}_h as columns, respectively, and \mathbf{C}_k ($R \times R$) is the diagonal matrix with the k th elements of the vectors $\omega_h \mathbf{c}_h$ on its diagonal. The model part of the CP model is characterized by $(\mathbf{A}, \mathbf{B}, \mathbf{C})$, where component matrix \mathbf{C} ($K \times R$) has the vectors \mathbf{c}_h as columns. Hence, it is assumed that the weights ω_h are absorbed by the matrix \mathbf{C} .

The most attractive feature of CP is its uniqueness property. Kruskal [26] has shown that, for fixed residuals $\underline{\mathbf{E}}$, the vectors \mathbf{a}_h , \mathbf{b}_h , and \mathbf{c}_h and the weights ω_h are unique up to sign changes and a reordering of the summands in (1.1) if

$$(1.4) \quad k_{\mathbf{A}} + k_{\mathbf{B}} + k_{\mathbf{C}} \geq 2R + 2,$$

where $k_{\mathbf{A}}$, $k_{\mathbf{B}}$, $k_{\mathbf{C}}$ denote the k-ranks of the component matrices. The k-rank of a matrix is the largest number x such that every subset of x columns of the matrix is linearly independent. If a CP solution is unique up to these indeterminacies, it is called *essentially unique*. Two CP solutions which are identical up to the essential uniqueness indeterminacies will be called *equivalent*.

In case one of the component matrices \mathbf{A} , \mathbf{B} , and \mathbf{C} has full column rank, a weaker uniqueness condition than (1.4) has been derived by Jiang and Sidiropoulos [22] and De Lathauwer [7]. See also Stegeman, Ten Berge, and De Lathauwer [41].

The practical use of CP has been hampered by the occurrence of diverging CP components, also known as “degeneracy.” In such cases, convergence of a CP algorithm is extremely slow, and some components display the following pattern. Let the model parameters of the n th update of a CP algorithm be denoted by a superscript (n) . For the diverging components, the weights $\omega_h^{(n)}$ become arbitrarily large in magnitude, and the corresponding columns in $\mathbf{A}^{(n)}$, $\mathbf{B}^{(n)}$, and $\mathbf{C}^{(n)}$ become nearly linearly dependent. Although the individual diverging components may diverge in nearly opposite directions, their sum still contributes to a better fit of the CP model. Diverging CP components are a problem to the analysis of three-way arrays, since the obtained CP solution is hardly interpretable. The occurrence of diverging components can be avoided by imposing orthogonality constraints on the components matrices; see Krijnen, Dijkstra and Stegeman [24], but this will come with some loss of fit. Lim [29] shows that diverging components do not occur for nonnegative $\underline{\mathbf{Z}}$ under the restriction of nonnegative component matrices.

The first case of diverging CP components was reported in Harshman and Lundy [14]. Contrived examples are given by Ten Berge, Kiers, and De Leeuw [43] and Paatero [33]. Kruskal, Harshman, and Lundy [27] have argued that diverging CP components occur due to the fact that the array $\underline{\mathbf{Z}}$ has no best rank- R approximation, i.e., CP has no optimal solution. They reason that every sequence of CP updates, of which the objective value is approaching the infimum of the CP objective function, must fail to converge and displays a pattern of a diverging CP components. This has recently been proven by Krijnen, Dijkstra, and Stegeman [24].

De Silva and Lim [10] give results on the existence of a best rank- R approximation of N -way arrays with $N \geq 3$. For the three-way CP model, [10] shows that for $R = 1$, an optimal CP solution always exists, while for any $I, J, K \geq 2$ and any $R \in \{2, \dots, \min(I, J, K)\}$, a rank- $(R + 1)$ array $\underline{\mathbf{Z}}$ exists which has no optimal CP solution. Also, [10] shows that all $2 \times 2 \times 2$ arrays of rank 3 (a set of positive volume in $\mathbb{R}^{2 \times 2 \times 2}$) have no optimal CP solution for $R = 2$ and that, for any $I, J, K \geq 2$, the set of arrays in $\mathbb{R}^{I \times J \times K}$, which have no optimal CP solution for $R = 2$ has positive volume.

Stegeman [38, 40] has mathematically analyzed diverging CP components occurring for generic $I \times J \times 2$ arrays $\underline{\mathbf{Z}}$ and all values of R . In these cases, diverging components occur if the sequence of CP updates converges to a limit point $\underline{\mathbf{X}}$, which has rank larger than R . Formally, these occurrences of diverging components can be described as follows. There exist disjoint index sets $D_1, \dots, D_r \subset \{1, \dots, R\}$ such that

$$(1.5) \quad |\omega_h^{(n)}| \rightarrow \infty, \quad \text{for all } h \in D_j, \quad j = 1, \dots, r,$$

$$(1.6) \quad \text{while } \left\| \sum_{h \in D_j} \omega_h^{(n)} (\mathbf{a}_h^{(n)} \otimes \mathbf{b}_h^{(n)} \otimes \mathbf{c}_h^{(n)}) \right\| \text{ is bounded, } j = 1, \dots, r.$$

Stegeman [38, 40] gives a complete characterization of the diverging components (1.5)–(1.6) in terms of properties of the limit point of the sequence of CP updates. Also, [40] provides a link between diverging CP components and results from the theory of matrix pencils and algebraic complexity theory.

The only mathematically analyzed cases of diverging CP components so far are the contrived examples in Ten Berge, Kiers, and De Leeuw [43] and Paatero [33], generic $I \times J \times 2$ arrays in Stegeman [38, 40], and generic $5 \times 3 \times 3$ and $8 \times 4 \times 3$ arrays, and generic $3 \times 3 \times 4$ and $3 \times 3 \times 5$ arrays with symmetric slices in Stegeman [39].

A numerical example of diverging CP components is the following. Let $\underline{\mathbf{Z}}$ be a $4 \times 4 \times 2$ array with slices

$$(1.7) \quad \mathbf{Z}_1 = \begin{bmatrix} -0.5 & -1.2 & 0.3 & -0.6 \\ -1.7 & 1.1 & 0.1 & 2.1 \\ 0.1 & 1.1 & -0.2 & -0.2 \\ 0.2 & -0.1 & 0.7 & 0.1 \end{bmatrix} \quad \text{and} \quad \mathbf{Z}_2 = \begin{bmatrix} 0.8 & 1.1 & -1.7 & -0.9 \\ 0.7 & -1.3 & 0.2 & 0.5 \\ 1.2 & -0.1 & -1.1 & 0.2 \\ 0.6 & -0.2 & 1.4 & -1.0 \end{bmatrix}.$$

This array was randomly generated such that $\text{rank}_{\otimes}(\underline{\mathbf{Z}}) = 5$. Next, we try to fit the CP model with $R = 4$ components using the multilinear engine of Paatero [32]. For a convergence criterion of $1\text{e-}15$, the algorithm terminates after 162055 iterations with an objective value of 0.051204 and final CP update

$$(1.8) \quad \mathbf{A} = \begin{bmatrix} 0.6787 & 0.1278 & 0.6767 & -0.6778 \\ -0.6642 & -0.7946 & -0.6735 & 0.6693 \\ -0.1189 & -0.5895 & -0.1464 & 0.1320 \\ -0.2898 & 0.0690 & -0.2590 & 0.2746 \end{bmatrix},$$

$$(1.9) \quad \mathbf{B} = \begin{bmatrix} -0.6870 & -0.8259 & -0.6919 & -0.6895 \\ -0.2365 & -0.0386 & -0.2609 & -0.2481 \\ -0.0509 & 0.4005 & -0.0080 & -0.0298 \\ 0.6852 & 0.3949 & 0.6732 & 0.6800 \end{bmatrix},$$

$$(1.10) \quad \mathbf{C} = \begin{bmatrix} 1454 & -2.8913 & 1443 & 2895 \\ 789 & 4.4617 & 634 & 1426 \end{bmatrix},$$

where the columns of \mathbf{A} and \mathbf{B} are normalized to length 1. It can be seen that columns 1, 3, and 4 in \mathbf{A} and \mathbf{B} are nearly identical up to a sign change. Also, these columns have large magnitudes in \mathbf{C} . Hence, CP components 1, 3, and 4 appear to be diverging. The multilinear engine terminates with nearly the same CP update for all tried random starting values. The alternating least squares CP algorithm gives the same results.

Since diverging CP components cannot be interpreted, one may wonder whether they can be avoided. However, the discussion above shows that for some array sizes and some values of R , there is no best rank- R approximation and, hence, trying to fit the CP model results in diverging components. To ensure the existence of a best rank- R approximation, De Silva and Lim [10] propose to consider the closure of the set of arrays with at most rank R instead. For each array size and value of R , this involves characterizing the boundary arrays of this set. These are the limit points of the sequences of CP updates featuring diverging CP components. De Silva and Lim [10] show that for $R = 2$, these limit points have rank 3 with the following decomposition into rank-1 terms:

$$(1.11) \quad \underline{\mathbf{X}} = \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3.$$

In this paper, we apply the idea of De Silva and Lim [10] to the CP model for generic $I \times J \times 2$ arrays $\underline{\mathbf{Z}}$. Apart from the results in Stegeman [39], this is the only class of arrays for which the analysis of diverging components is nearly complete. Instead of fitting the CP model, we propose to find the best approximation of $\underline{\mathbf{Z}}$ in terms of the generalized Schur decomposition (GSD), which was considered in De Lathauwer, De Moor, and Vandewalle [6]. The GSD model is the same as (1.3) except that \mathbf{A} and

\mathbf{B} are columnwise orthonormal and \mathbf{C}_k are upper triangular $k = 1, 2$. We show that an optimal solution to the GSD model always exists. Moreover, for $I \times J \times 2$ arrays, the set of feasible GSD solutions equals the closure of the set of feasible CP solutions. Hence, the optimal GSD solution, if it is unique, is the limit point of the sequence of CP updates, whether the latter features diverging components or not.

Next, we show how to write the obtained GSD solution in several alternative forms. First, using the Jordan normal form, the GSD solution may be written as the sum of the nondiverging CP components and a sparse Tucker3 part. Here, each of the m sets of diverging CP components in (1.5)–(1.6) forms one block in the Tucker3 part. We call this the CP+Jordan form. Although this is not a decomposition into rank-1 terms, it is an essentially unique decomposition, and its blocks may be interpretable to the researcher. Second, the obtained GSD solution may be written as the sum of the nondiverging CP components and a smaller GSD part. We call this the CP+GSD form. If one is only interested in obtaining the nondiverging CP components, this is a fast way to get them. Third, using the CP+Jordan form, the GSD solution may also be written as a sum of rank-1 terms where the number of terms equals the rank of the solution array. However, this rank-revealing decomposition is not essentially unique. During the computation of the GSD solution, the problems of diverging CP components do not arise, neither during the computation of the mentioned alternative forms for the GSD solution.

As explained above, the analyzed cases of diverging CP components most likely occur because the CP model has no optimal solution. Hence, modified CP algorithms designed to avoid diverging components (e.g., Rayens and Mitchell [34], Cao et al. [2]) are no remedy here. With our method for $I \times J \times 2$ arrays, the problems of diverging CP components are avoided without imposing additional constraints.

Note that the occurrences of diverging CP components we consider do not include cases where $\text{rank}_{\otimes}(\mathbf{Z}) \leq R$ and either its full CP decomposition resembles a case of diverging components or where diverging components occur due to an unlucky choice of the starting position of the CP algorithm. Examples of these cases can be found in Mitchell and Burdick [30] and Paatero [33]. We will assume instead that $\text{rank}_{\otimes}(\mathbf{Z}) > R$.

This paper is organized as follows. We discuss the analysis of diverging CP components for typical $I \times I \times 2$ arrays \mathbf{Z} of rank $I + 1$ and $R = I$ in section 3. For this, we need results on the rank of $I \times I \times 2$ arrays. These are presented in section 2. In section 4 we discuss the simultaneous GSD model. In section 5, we consider the GSD model for $I \times I \times 2$ arrays and show how it is related to the CP model. In section 6, we show how to obtain the CP+Jordan and CP+GSD representations of the GSD solution. In section 7, we discuss the extension of our analysis for $I \times I \times 2$ arrays and $R = I$ to $I \times J \times 2$ arrays and general R . Section 8 contains numerical experiments which illustrate our results. Finally, section 9 provides a discussion.

2. The rank of $I \times I \times 2$ arrays. For an array $\mathbf{Y} \in \mathbb{R}^{I \times I \times 2}$, we denote its $I \times I$ frontal slices by \mathbf{Y}_k , $k = 1, 2$. Let

$$(2.1) \quad \mathcal{R}_I = \{\mathbf{Y} \in \mathbb{R}^{I \times I \times 2} : \det(\mathbf{Y}_k) \neq 0, k = 1, 2\}.$$

The following result on the rank of arrays in \mathcal{R}_I is due to Ja' Ja' [21]. For later use, we also give its proof as formulated in Stegeman [38].

LEMMA 2.1. *For $\mathbf{X} \in \mathcal{R}_I$, the following statements hold:*

- (i) *If $\mathbf{X}_2 \mathbf{X}_1^{-1}$ has I real eigenvalues and is diagonalizable, then \mathbf{X} has rank I .*

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

Proof. If (i) holds, then $\mathbf{X}_2\mathbf{X}_1^{-1}$ has an eigendecomposition $\mathbf{K}\mathbf{\Lambda}\mathbf{K}^{-1}$, where $\mathbf{\Lambda}$ is the $I \times I$ diagonal matrix of eigenvalues and \mathbf{K} contains the associated eigenvectors. Taking

$$(2.2) \quad \mathbf{A} = \mathbf{K}, \quad \mathbf{B}^T = \mathbf{K}^{-1}\mathbf{X}_1, \quad \mathbf{C}_1 = \mathbf{I}_I, \quad \mathbf{C}_2 = \mathbf{\Lambda},$$

yields a full rank- I decomposition of $\underline{\mathbf{X}}$ as in (1.3).

The proof of (ii)–(iii) is as follows. Since its $I \times I$ slices are nonsingular, it follows that $\underline{\mathbf{X}}$ has at least rank I . Suppose $\underline{\mathbf{X}}$ has rank I . Then there exist nonsingular matrices \mathbf{A} and \mathbf{B} and nonsingular diagonal matrices \mathbf{C}_1 and \mathbf{C}_2 such that $\mathbf{X}_k = \mathbf{A}\mathbf{C}_k\mathbf{B}^T$, $k = 1, 2$. But then $\mathbf{X}_2\mathbf{X}_1^{-1} = \mathbf{A}\mathbf{C}_2\mathbf{C}_1^{-1}\mathbf{A}^{-1}$ is an eigendecomposition with I real eigenvalues and I linearly independent eigenvectors, which contradicts (ii)–(iii). Hence, the rank of $\underline{\mathbf{X}}$ is at least $I + 1$. \square

If $\underline{\mathbf{X}}$ satisfies (iii) of Lemma 2.1, the rank of $\underline{\mathbf{X}}$ can be deduced from the Jordan normal form of $\mathbf{X}_2\mathbf{X}_1^{-1}$. This is stated in the following result, also due to Ja’ Ja’ [21].

LEMMA 2.2. *Let $\underline{\mathbf{X}} \in \mathcal{R}_I$ and suppose $\mathbf{X}_2\mathbf{X}_1^{-1}$ has I real eigenvalues. Let the Jordan normal form of $\mathbf{X}_2\mathbf{X}_1^{-1}$ be given by $\text{diag}(\lambda_1, \dots, \lambda_p, \mathbf{J}_{m_1}(\mu_1), \dots, \mathbf{J}_{m_r}(\mu_r))$, where $\mathbf{J}_{m_j}(\mu_j)$ denotes an $m_j \times m_j$ Jordan block with diagonal elements equal to μ_j and $m_j \geq 2$. Then*

$$(2.3) \quad \text{rank}_{\otimes}(\underline{\mathbf{X}}) = I + r.$$

For an eigenvalue λ_j of an $I \times I$ matrix \mathbf{G} , we define the *algebraic multiplicity* of λ_j as the multiplicity of λ_j as root of the characteristic polynomial $\det(\mathbf{G} - \lambda\mathbf{I}_I)$, and the *geometric multiplicity* of λ_j as the maximum number of linearly independent eigenvectors of \mathbf{G} associated with λ_j (i.e., the dimensionality of the eigenspace of λ_j). Let $\mathbf{G} = \text{diag}(\lambda_1, \dots, \lambda_p, \mathbf{J}_{m_1}(\mu_1), \dots, \mathbf{J}_{m_r}(\mu_r))$, with $m_j \geq 2$ for $j = 1, \dots, r$. Then the eigenvalues of \mathbf{G} are $\lambda_1, \dots, \lambda_p, \mu_1, \dots, \mu_r$ (not necessarily distinct), and each Jordan block $\mathbf{J}_{m_j}(\mu_j)$ adds m_j to the algebraic multiplicity of μ_j and 1 to the geometric multiplicity of μ_j . This establishes a relation between the eigenvalues of $\mathbf{X}_2\mathbf{X}_1^{-1}$ and the rank of the array $\underline{\mathbf{X}}$ in Lemma 2.2. In particular, if $\mathbf{X}_2\mathbf{X}_1^{-1}$ has I real eigenvalues and is diagonalizable, then $\underline{\mathbf{X}}$ has rank I , which is case (i) of Lemma 2.1.

When $I \times I \times 2$ arrays are randomly drawn from a continuous distribution, they have rank I or $I + 1$, both with positive probability; see Ten Berge and Kiers [44]. Their *typical rank* is said to be $\{I, I + 1\}$. A typical array $\underline{\mathbf{X}}$ of rank I satisfies (i) of Lemma 2.1, and $\mathbf{X}_2\mathbf{X}_1^{-1}$ has I distinct real eigenvalues. A typical array $\underline{\mathbf{X}}$ of rank $I + 1$ satisfies (ii) of Lemma 2.1, and the eigenvalues of $\mathbf{X}_2\mathbf{X}_1^{-1}$ are again distinct.

If a three-way array of size $I \times J \times K$ has a one-valued typical rank, this is called its *generic rank*. In this case, a generic $I \times J \times K$ array has rank equal to its generic rank.

3. Diverging CP components for $I \times I \times 2$ arrays of rank $I + 1$ and $R = I$. Here, we discuss the analysis of Stegeman [38] that shows how diverging CP components occur for typical $I \times I \times 2$ arrays of rank $I + 1$ and $R = I$. Let

$$(3.1) \quad \mathcal{S}_I = \{\underline{\mathbf{Y}} \in \mathcal{R}_I : \underline{\mathbf{Y}} \text{ has rank at most } I\}.$$

Hence, the set \mathcal{S}_I consists of the arrays in \mathcal{R}_I which satisfy (i) of Lemma 2.1. Note that \mathcal{S}_I contains only arrays of rank I , and not less than I , due to its restriction to \mathcal{R}_I .

Let $\underline{\mathbf{Z}} \in \mathcal{R}_I$ be typical and have rank $I + 1$. Then $\underline{\mathbf{Z}}$ satisfies (ii) of Lemma 2.1. We consider the following CP problem:

$$(3.2) \quad \begin{aligned} & \text{Minimize } \|\underline{\mathbf{Z}} - \underline{\mathbf{Y}}\|^2 \\ & \text{subject to } \underline{\mathbf{Y}} \in \mathcal{S}_I. \end{aligned}$$

If problem (3.2) has an optimal solution $\underline{\mathbf{X}}$, then $\underline{\mathbf{X}}$ is a boundary point of \mathcal{S}_I . The following result defines the interior points and boundary points of \mathcal{S}_I in \mathcal{R}_I and is due to Stegeman [38].

LEMMA 3.1. *For $\underline{\mathbf{X}} \in \mathcal{R}_I$, the following statements hold:*

- (a) $\underline{\mathbf{X}}$ is an interior point of \mathcal{S}_I if and only if $\mathbf{X}_2\mathbf{X}_1^{-1}$ has I distinct real eigenvalues.
- (b) $\underline{\mathbf{X}}$ is a boundary point of \mathcal{S}_I in \mathcal{R}_I if and only if $\mathbf{X}_2\mathbf{X}_1^{-1}$ has I real eigenvalues but not all distinct.

The boundary points in (b) can have rank I or rank $\geq I + 1$, depending on whether $\mathbf{X}_2\mathbf{X}_1^{-1}$ is diagonalizable (type I) or not (type II); see Lemma 2.1. Hence, the set \mathcal{S}_I is not a closed subset of \mathcal{R}_I , and the existence of an optimal solution for problem (3.2) is not guaranteed. If problem (3.2) has an optimal solution $\underline{\mathbf{X}}$, then it is a boundary point of type I.

Remark 3.2. For a typical $\underline{\mathbf{Z}}$ of rank $I + 1$, problem (3.2) does not seem to have an optimal solution in practice. We conjecture the following explanation for this. For $m \geq 2$, define the sets of matrices

$$\begin{aligned} \mathcal{B}(\lambda_0, m) &= \{\mathbf{Y} \in \mathbb{R}^{I \times I} : \mathbf{Y} \text{ has eigenvalue } \lambda_0 \text{ with algebraic multiplicity } m\} \\ &= \mathcal{B}_1(\lambda_0, m) \cup \cdots \cup \mathcal{B}_m(\lambda_0, m), \end{aligned}$$

with

$$\mathcal{B}_l(\lambda_0, m) = \{\mathbf{Y} \in \mathcal{B}(\lambda_0, m) : \text{rank}(\mathbf{Y} - \lambda_0 \mathbf{I}_I) = I - l\}, \quad l = 1, \dots, m.$$

Due to the upper-semicontinuity of matrix rank, the set $\mathcal{B}_l(\lambda_0, m)$ lies dense in $\mathcal{B}_l(\lambda_0, m) \cup \cdots \cup \mathcal{B}_m(\lambda_0, m)$. For a boundary point $\underline{\mathbf{X}}$ of \mathcal{S}_I , all eigenvalues of $\mathbf{X}_2\mathbf{X}_1^{-1}$ are real and $\mathbf{X}_2\mathbf{X}_1^{-1} \in \mathcal{B}(\lambda_0, m)$ for some eigenvalue λ_0 and $m \geq 2$ (see Lemma 3.1 (b)). For a boundary point of type I (with rank I), it holds that $\mathbf{X}_2\mathbf{X}_1^{-1} \in \mathcal{B}_m(\lambda_0, m)$ for all multiple eigenvalues λ_0 of $\mathbf{X}_2\mathbf{X}_1^{-1}$. For a boundary point of type II (with rank at least $I + 1$), it holds that $\mathbf{X}_2\mathbf{X}_1^{-1} \in \mathcal{B}_l(\lambda_0, m)$, with $l < m$ for some multiple eigenvalue λ_0 of $\mathbf{X}_2\mathbf{X}_1^{-1}$. From these observations, it follows that the set of boundary points of type II lies dense on the boundary of the set \mathcal{S}_I . As stated above, if problem (3.2) has an optimal solution, then it is a boundary point of type I. We conjecture that this implies that, for a typical array $\underline{\mathbf{Z}}$ of rank $I + 1$, problem (3.2) has no optimal solution.

If problem (3.2) does not have an optimal solution, then the sequence of CP updates $\underline{\mathbf{Y}}^{(n)}$ converges to a boundary point $\underline{\mathbf{X}}$ of type II (i.e., with $\mathbf{X}_2\mathbf{X}_1^{-1}$ having I real eigenvalues and not diagonalizable) such that $\|\underline{\mathbf{Z}} - \underline{\mathbf{X}}\|^2$ equals the infimum of $\|\underline{\mathbf{Z}} - \underline{\mathbf{Y}}\|^2$ over \mathcal{S}_I . Stegeman [38] shows that when $\underline{\mathbf{Y}}^{(n)}$ converges to $\underline{\mathbf{X}}$, the sequence $\underline{\mathbf{Y}}^{(n)}$ features diverging components. This can be seen as follows. The boundary point $\underline{\mathbf{X}}$ satisfies (iii) of Lemma 2.1, and its rank, which is at least $I + 1$, is given by Lemma 2.2. We assume $\underline{\mathbf{Y}}^{(n)}$ to be interior points of \mathcal{S}_I , i.e., $\mathbf{Y}_2^{(n)}(\mathbf{Y}_1^{(n)})^{-1}$ has I distinct real eigenvalues. Then $\underline{\mathbf{Y}}^{(n)}$ has a rank- I decomposition of the form (2.2). Moreover, for the k-ranks we have $k_{\mathbf{A}^{(n)}} = k_{\mathbf{B}^{(n)}} = I$ and $k_{\mathbf{C}^{(n)}} = 2$, and

Kruskal’s condition (1.4) yields that the decomposition is essentially unique. By continuity, $\mathbf{Y}_2^{(n)}(\mathbf{Y}_1^{(n)})^{-1}$ converges to $\mathbf{X}_2\mathbf{X}_1^{-1}$. Denote the eigendecomposition of $\mathbf{Y}_2^{(n)}(\mathbf{Y}_1^{(n)})^{-1}$ by $\mathbf{K}^{(n)}\mathbf{\Lambda}^{(n)}(\mathbf{K}^{(n)})^{-1}$. The matrix $\mathbf{X}_2\mathbf{X}_1^{-1}$ has I real eigenvalues but is not diagonalizable, and we have $\mathbf{A}^{(n)} = \mathbf{K}^{(n)}$, $\mathbf{B}^{(n)} = ((\mathbf{K}^{(n)})^{-1}\mathbf{Y}_1^{(n)})^T$, $\mathbf{C}_1^{(n)} = \mathbf{I}_I$, and $\mathbf{C}_2^{(n)} = \mathbf{\Lambda}^{(n)}$. Let λ be an eigenvalue of $\mathbf{X}_2\mathbf{X}_1^{-1}$ with algebraic multiplicity strictly larger than its geometric multiplicity, and associated Jordan block of size $m \times m$. Then m columns of $\mathbf{A}^{(n)}$ converge to the same eigenvector (up to a sign change) of λ , the corresponding m columns of $\mathbf{B}^{(n)}$ tend to linear dependency and large magnitudes, and the m corresponding columns of $\mathbf{C}^{(n)}$ become nearly identical to $(1 \ \lambda)^T$. The pattern of the m CP components is such that their sum does not blow up. Clearly, this is a case of diverging CP components as defined by (1.5)–(1.6).

The diverging CP components are related to the Jordan form of $\mathbf{X}_2\mathbf{X}_1^{-1}$ in the way described above. Hence, based on Lemma 2.2, one may conclude that the number of groups of diverging CP components equals the rank of the boundary array $\underline{\mathbf{X}}$ minus I .

To illustrate the phenomenon of diverging CP components as described above, we return to the example in (1.7). For this randomly sampled $4 \times 4 \times 2$ array $\underline{\mathbf{Z}}$, the matrix $\mathbf{Z}_2\mathbf{Z}_1^{-1}$ has one pair of complex eigenvalues. Hence, $\underline{\mathbf{Z}}$ is a typical $4 \times 4 \times 2$ array of rank 5. Trying to fit the CP model with $R = 4$, results in three diverging components, as shown in (1.8)–(1.10). Next, we compute the array $\underline{\mathbf{Y}}$ corresponding to the final CP update, i.e., $\mathbf{Y}_k = \mathbf{A} \mathbf{C}_k \mathbf{B}^T$ for $k = 1, 2$. This $\underline{\mathbf{Y}}$ is an approximation of the optimal boundary array $\underline{\mathbf{X}}$. For the eigenvalues of $\mathbf{Y}_2\mathbf{Y}_1^{-1}$, we get

$$(3.3) \quad -1.5431, \quad 0.4395, \quad 0.4925, \quad 0.5427.$$

Hence, three eigenvalues are close together. This corresponds to the three diverging components in (1.8)–(1.10) as discussed above.

4. A simultaneous GSD. Here, we introduce the simultaneous GSD (SGSD) model for $I \times I \times K$ arrays and show that it always has an optimal solution. We also discuss a relation between the CP model and the SGSD model as presented in De Lathauwer, De Moor, and Vandewalle [6]. In matrix notation, the SGSD model for an array $\underline{\mathbf{Z}}$ is

$$(4.1) \quad \mathbf{Z}_k = \mathbf{Q}_a \mathbf{R}_k \mathbf{Q}_b^T + \mathbf{E}_k, \quad k = 1, \dots, K,$$

where \mathbf{Q}_a and \mathbf{Q}_b are $I \times I$ orthonormal and \mathbf{R}_k are $I \times I$ upper triangular $k = 1, \dots, K$. The matrices \mathbf{Q}_a , \mathbf{Q}_b , and \mathbf{R}_k are determined by minimizing the sum-of-squares of the residuals \mathbf{E}_k , $k = 1, \dots, K$. For this purpose, a Jacobi-type algorithm is presented in [6], and Van der Veen and Paulraj [47] developed an extended QZ algorithm. Like the CP model, we consider the real-valued SGSD model.

Next, we show that the SGSD model, contrary to the CP model, always has an optimal solution. Our approach is analogous to Krijnen [23]. We make use of the following lemma, which can be found in Ortega and Rheinboldt [31, p. 104].

LEMMA 4.1. *Let $g : D \subset \mathbb{R}^q \rightarrow \mathbb{R}$, where D is unbounded. Then all level sets of g are bounded if and only if $g(\boldsymbol{\theta}_n) \rightarrow \infty$ whenever $\{\boldsymbol{\theta}_n\} \subset D$ and $\|\boldsymbol{\theta}_n\| \rightarrow \infty$.*

We define the parameter vector of the SGSD model as

$$\boldsymbol{\theta} = \text{vec}(\text{vec}(\mathbf{Q}_a), \text{vec}(\mathbf{Q}_b), \text{vec}(\mathbf{R}_1), \dots, \text{vec}(\mathbf{R}_K)).$$

Let $f(\boldsymbol{\theta})$ be the sum-of-squares of the residuals of the SGSD model. Since f is continuous, the level sets $L(\gamma) = \{\boldsymbol{\theta} : f(\boldsymbol{\theta}) \leq \gamma\}$ are closed. We have the following result.

PROPOSITION 4.2. *All level sets of f are bounded, and the SGSD model has an optimal solution.*

Proof. We have $\|\boldsymbol{\theta}\|^2 = 2I + \sum_{k=1}^K \|\mathbf{R}_k\|^2$. Hence, $\|\boldsymbol{\theta}_n\| \rightarrow \infty$ implies that $\|\mathbf{R}_k\| \rightarrow \infty$ for at least one k . Moreover,

$$f(\boldsymbol{\theta})^{1/2} = \sum_{k=1}^K \|\mathbf{Z}_k - \mathbf{Q}_a \mathbf{R}_k \mathbf{Q}_b^T\| \geq \sum_{k=1}^K \left| \|\mathbf{Z}_k\| - \|\mathbf{Q}_a \mathbf{R}_k \mathbf{Q}_b^T\| \right| = \sum_{k=1}^K \left| \|\mathbf{Z}_k\| - \|\mathbf{R}_k\| \right|,$$

which implies that $f(\boldsymbol{\theta}_n) \rightarrow \infty$ whenever $\|\boldsymbol{\theta}_n\| \rightarrow \infty$. From Lemma 4.1, it follows that all level sets of f are bounded. Since the level sets are also closed, f attains its infimum on any nonempty level set. This completes the proof. \square

Next, we present a relation between the CP model and the SGSD model, which was partly proven by De Lathauwer, De Moor, and Vandewalle [6]. We have the following result.

LEMMA 4.3. *Let $\mathbf{X} \in \mathbb{R}^{I \times I \times K}$. The following statements hold:*

- (i) *If \mathbf{X} has a full CP decomposition with $R = I$, then \mathbf{X} has a full SGSD.*
- (ii) *Suppose \mathbf{X}_1 is nonsingular. Then \mathbf{X} has a full CP decomposition with $R = I$ if and only if $\mathbf{X}_k \mathbf{X}_1^{-1}$, $k = 1, \dots, K$ have a simultaneous eigendecomposition with only real eigenvalues. Moreover, the full CP decomposition of \mathbf{X} is essentially unique if and only if $k_{\mathbf{C}} \geq 2$.*
- (iii) *Suppose \mathbf{X}_1 is nonsingular. If \mathbf{X} has an essentially unique full CP decomposition with $R = I$, then the indeterminacies in the full SGSD of \mathbf{X} are only due to the indeterminacies in the full CP decomposition of \mathbf{X} .*

Proof. First, we show (i). We have $\mathbf{X}_k = \mathbf{A} \mathbf{C}_k \mathbf{B}^T$, $k = 1, \dots, K$; see (1.3). Let $\mathbf{A} = \mathbf{Q}_a \mathbf{R}_a$ be a QR-decomposition of \mathbf{A} , with \mathbf{Q}_a orthonormal and \mathbf{R}_a upper triangular. Analogously, let $\mathbf{B} = \mathbf{Q}_b \mathbf{L}_b$ be a QL-decomposition of \mathbf{B} , with \mathbf{Q}_b orthonormal and \mathbf{L}_b lower triangular. Then $\mathbf{X}_k = \mathbf{Q}_a (\mathbf{R}_a \mathbf{C}_k \mathbf{L}_b^T) \mathbf{Q}_b^T$, $k = 1, \dots, K$ is a full SGSD for \mathbf{X} .

The first part of the proof of (ii) is due to De Lathauwer, De Moor, and Vandewalle [6]. Suppose \mathbf{X} has a full CP decomposition with $R = I$. Then we have $\mathbf{X}_k \mathbf{X}_1^{-1} = \mathbf{A} \mathbf{C}_k \mathbf{C}_1^{-1} \mathbf{A}^{-1}$, which is an eigendecomposition with real eigenvalues and shows that $\mathbf{X}_k \mathbf{X}_1^{-1}$, $k = 1, \dots, K$ have a simultaneous eigendecomposition. Next, suppose $\mathbf{X}_k \mathbf{X}_1^{-1} = \mathbf{A} \mathbf{C}_k \mathbf{A}^{-1}$ for diagonal matrices \mathbf{C}_k , $k = 2, \dots, K$. Then $\mathbf{X}_k = \mathbf{A} \mathbf{C}_k \mathbf{A}^{-1} \mathbf{X}_1$. Taking $\mathbf{C}_1 = \mathbf{I}_I$ and $\mathbf{B}^T = \mathbf{A}^{-1} \mathbf{X}_1$ now yields a full CP decomposition of \mathbf{X} with $R = I$.

In the CP decomposition of \mathbf{X} , we have $k_{\mathbf{A}} = k_{\mathbf{B}} = I$. Hence, Kruskal’s condition (1.4) for essential uniqueness is equivalent to $k_{\mathbf{C}} \geq 2$. See also Leurgans, Ross, and Abel [28]. Moreover, $k_{\mathbf{C}} \geq 2$ is also necessary for uniqueness as is shown in Stegeman and Sidiropoulos [42].

Next, we show (iii). From (ii), it follows that $\mathbf{X}_k \mathbf{X}_1^{-1} = \mathbf{A} \mathbf{C}_k \mathbf{A}^{-1}$, $k = 2, \dots, K$, and $k_{\mathbf{C}} \geq 2$. From the full SGSD of \mathbf{X} , we obtain that also $\mathbf{Q}_a^T \mathbf{X}_k \mathbf{X}_1^{-1} \mathbf{Q}_a = \mathbf{R}_k \mathbf{R}_1^{-1}$, $k = 2, \dots, K$ have a simultaneous eigendecomposition $\mathbf{R}_a \mathbf{C}_k \mathbf{R}_a^{-1}$, with \mathbf{R}_a upper triangular up to a column permutation. From Kruskal’s condition (1.4), it follows that $\mathbf{R}_k = \mathbf{R}_a \mathbf{C}_k \mathbf{R}_b$, with $\mathbf{R}_b = \mathbf{R}_a^{-1} \mathbf{R}_1$ and $\mathbf{C}_1 = \mathbf{I}_I$, is an essentially unique full CP decomposition. Thus we have $\mathbf{X}_k \mathbf{X}_1^{-1} = \mathbf{Q}_a \mathbf{R}_a \mathbf{C}_k \mathbf{R}_a^{-1} \mathbf{Q}_a^T = \mathbf{A} \mathbf{C}_k \mathbf{A}^{-1}$, $k = 2, \dots, K$, which implies $\mathbf{Q}_a \mathbf{R}_a = \mathbf{A}$ (since $k_{\mathbf{C}} \geq 2$). Looking at $\mathbf{X}_1^{-1} \mathbf{X}_k$, we get equivalently $\mathbf{Q}_b \mathbf{R}_b^T = \mathbf{B}$. Hence, there are no other indeterminacies in the full SGSD of \mathbf{X} than those implied by CP essential uniqueness. This completes the proof. \square

From the proof of Lemma 4.3, it follows that a CP decomposition of \mathbf{X} (if it exists) can be obtained from its full SGSD by computing the simultaneous eigendecomposi-

tion of $\mathbf{R}_k \mathbf{R}_1^{-1}$, $k = 2, \dots, K$. This method is analogous to the one proposed in De Lathauwer, De Moor, and Vandewalle [6]. For the case $I \leq K$ a different method is given in Van der Veen and Paulraj [47].

5. The GSD model for $I \times I \times 2$ arrays. Here, we consider the SGSD model for $I \times I \times 2$ arrays and discuss its relation with the CP model. Since a (complex-valued) SGSD for two slices ($K = 2$) is known as a GSD (see Golub and Van Loan [12]), we will use the abbreviation GSD. Next, we show which of the arrays in Lemma 2.1 have a full (real-valued) GSD.

LEMMA 5.1. For $\underline{\mathbf{X}} \in \mathcal{R}_I$, the following statements hold:

- (i) If $\mathbf{X}_2 \mathbf{X}_1^{-1}$ has I real eigenvalues and is diagonalizable, then $\underline{\mathbf{X}}$ has a full GSD.
- (ii) If $\mathbf{X}_2 \mathbf{X}_1^{-1}$ has at least one pair of complex eigenvalues, then $\underline{\mathbf{X}}$ does not have a full GSD.
- (iii) If $\mathbf{X}_2 \mathbf{X}_1^{-1}$ has I real eigenvalues but is not diagonalizable, then $\underline{\mathbf{X}}$ has a full GSD.

Proof. If (i) holds, then $\underline{\mathbf{X}}$ has a full CP decomposition with $R = I$ of the form (2.2). Hence, $\underline{\mathbf{X}}$ also has a full GSD. Next, suppose (ii) holds, and $\underline{\mathbf{X}}$ has a full GSD. Then $\mathbf{X}_2 \mathbf{X}_1^{-1} = \mathbf{Q}_a \mathbf{R}_2 \mathbf{R}_1^{-1} \mathbf{Q}_a^T$, and

$$\det(\mathbf{X}_2 \mathbf{X}_1^{-1} - \lambda \mathbf{I}_I) = \det(\mathbf{Q}_a^T \mathbf{X}_2 \mathbf{X}_1^{-1} \mathbf{Q}_a - \lambda \mathbf{I}_I) = \det(\mathbf{R}_2 \mathbf{R}_1^{-1} - \lambda \mathbf{I}_I).$$

Since $\mathbf{R}_2 \mathbf{R}_1^{-1}$ is upper triangular and has only real eigenvalues, it follows that also $\mathbf{X}_2 \mathbf{X}_1^{-1}$ has only real eigenvalues. But this contradicts (ii). Therefore, $\underline{\mathbf{X}}$ has no full GSD if (ii) holds.

Next, suppose (iii) holds. Then $\mathbf{X}_2 \mathbf{X}_1^{-1} = \mathbf{P} \mathbf{J} \mathbf{P}^{-1}$, where \mathbf{J} is the Jordan normal form. Let $\mathbf{P} = \mathbf{Q}_a \mathbf{R}_a$ be a QR-decomposition of \mathbf{P} , and let $\mathbf{X}_1^T \mathbf{Q}_a = \mathbf{Q}_b \mathbf{L}_b$ be a QL-decomposition of $\mathbf{X}_1^T \mathbf{Q}_a$. Then

$$(5.1) \quad \mathbf{X}_2 = \mathbf{Q}_a \mathbf{R}_a \mathbf{J} \mathbf{R}_a^{-1} \mathbf{Q}_a^T \mathbf{X}_1 = \mathbf{Q}_a (\mathbf{R}_a \mathbf{J} \mathbf{R}_a^{-1} \mathbf{L}_b^T) \mathbf{Q}_b^T \quad \text{and} \quad \mathbf{X}_1 = \mathbf{Q}_a \mathbf{L}_b^T \mathbf{Q}_b^T$$

is a full GSD of $\underline{\mathbf{X}}$. This completes the proof. \square

Note that a full GSD requires \mathbf{R}_1 and \mathbf{R}_2 to be upper triangular. This is not the same as the generalized real Schur decomposition (see Golub and Van Loan [12]), which always exists for two $I \times I$ matrices and which has \mathbf{R}_1 upper quasi-triangular.

As we see from Lemma 5.1, the arrays satisfying (iii) do not have a full CP decomposition with $R = I$ but do have a full GSD. Note that the CP decomposition of arrays satisfying (i) is essentially unique if and only if the eigenvalues of $\mathbf{X}_2 \mathbf{X}_1^{-1}$ are distinct; see (ii) of Lemma 4.3.

Since (iii) of Lemma 4.3 does not apply to the GSD in (5.1), one may wonder what the uniqueness properties of (5.1) are. The Jordan form $\mathbf{J} = \text{diag}(\lambda_1, \dots, \lambda_p, \mathbf{J}_{m_1}(\mu_1), \dots, \mathbf{J}_{m_r}(\mu_r))$ is unique up to the order of the Jordan blocks. If $\lambda_1, \dots, \lambda_p, \mu_1, \dots, \mu_r$ are distinct, then the columns of \mathbf{P} are unique up to the same ordering and up to scaling. Suppose there is a second GSD, i.e., $\mathbf{X}_k = \tilde{\mathbf{Q}}_a \tilde{\mathbf{R}}_k \tilde{\mathbf{Q}}_b^T$, $k = 1, 2$. Then there holds $\tilde{\mathbf{R}}_2 \tilde{\mathbf{R}}_1^{-1} = (\tilde{\mathbf{Q}}_a^T \mathbf{P}) \mathbf{J} (\tilde{\mathbf{Q}}_a^T \mathbf{P})^{-1}$. In fact, we have $\tilde{\mathbf{Q}}_a^T \mathbf{P} = \hat{\mathbf{R}} \mathbf{\Pi}$, with $\hat{\mathbf{R}}$ upper triangular and $\mathbf{\Pi}$ a permutation. Then $\tilde{\mathbf{R}}_2 \tilde{\mathbf{R}}_1^{-1} = \hat{\mathbf{R}} (\mathbf{\Pi} \mathbf{J} \mathbf{\Pi}^T) \hat{\mathbf{R}}$ is a Jordan form with a different ordering of the Jordan blocks. Hence, the GSD in (5.1) is unique up to the indeterminacies of the Jordan form of $\mathbf{X}_2 \mathbf{X}_1^{-1}$.

6. Using the GSD model to avoid diverging CP components. Here, we show how the relation between the GSD and CP models for $I \times I \times 2$ arrays can be used to avoid the problems of diverging CP components discussed in section 3.

First, we establish a relation between the set of $I \times I \times 2$ arrays that have a full CP decomposition with $R = I$, i.e., the set \mathcal{S}_I in (3.1), and the set of arrays that have a full GSD. Let

$$(6.1) \quad \mathcal{P}_I = \{\underline{\mathbf{Y}} \in \mathcal{R}_I : \underline{\mathbf{Y}} \text{ has a full GSD}\}.$$

Hence, the set \mathcal{P}_I consists of the arrays satisfying either (i) or (iii) in Lemma 5.1. From Lemmas 2.1 and 5.1, it follows that $\mathcal{S}_I \subset \mathcal{P}_I$. Moreover, Lemmas 3.1 and 5.1 show that \mathcal{P}_I is the closure of \mathcal{S}_I in \mathcal{R}_I and has the same interior points and boundary points as \mathcal{S}_I . For the boundary points $\underline{\mathbf{X}}$ of \mathcal{P}_I and \mathcal{S}_I , the matrix $\mathbf{X}_2\mathbf{X}_1^{-1}$ has I real eigenvalues which are not all distinct; see Lemma 3.1. As explained in Remark 3.2, the boundary points $\underline{\mathbf{X}}$ of type II, i.e., with $\mathbf{X}_2\mathbf{X}_1^{-1}$ not diagonalizable, lie dense on the boundary of \mathcal{P}_I .

Let $\underline{\mathbf{Z}}$ be a typical $I \times I \times 2$ array of rank $I + 1$, i.e., $\underline{\mathbf{Z}}$ satisfies (ii) of Lemma 5.1. Recall that the CP problem (3.2) for $\underline{\mathbf{Z}}$ usually does not have an optimal solution (see Remark 3.2). We define the analogue GSD problem as

$$(6.2) \quad \begin{aligned} &\text{Minimize } \|\underline{\mathbf{Z}} - \underline{\mathbf{Y}}\|^2 \\ &\text{subject to } \underline{\mathbf{Y}} \in \mathcal{P}_I. \end{aligned}$$

From the analysis in Stegeman [38], it follows that \mathcal{P}_I is a closed subset of \mathcal{R}_I . Hence, the GSD problem (6.2) has an optimal solution, and a GSD algorithm finds an optimal solution $\underline{\mathbf{X}}$ of problem (6.2) in terms of its full GSD. We will assume that the optimal solution $\underline{\mathbf{X}}$ obtained for the GSD problem (6.2) is a boundary point of \mathcal{P}_I of type II, i.e., $\mathbf{X}_2\mathbf{X}_1^{-1}$ has I real eigenvalues but is not diagonalizable. We conjecture (see Remark 3.2) that this is true almost everywhere for typical $\underline{\mathbf{Z}}$ of rank $I + 1$.

From the observations above and our discussion in section 3, it follows that the optimal solution $\underline{\mathbf{X}}$ of the GSD problem (6.2), if it is unique, is the limit point of the sequence of CP updates (featuring diverging components) which attempts to converge to the (nonexisting) optimal solution of the CP problem (3.2).

Next, we show how to extract the nondiverging CP components from the optimal GSD solution. The limit point of the diverging CP components can be obtained from the optimal GSD solution as a Tucker3 part from the Jordan form of $\mathbf{X}_2\mathbf{X}_1^{-1}$ or as a smaller GSD part. These CP+Jordan and CP+GSD representations will be discussed in sections 6.1 and 6.3, respectively. In section 6.2, we show how the GSD solution can be decomposed into rank-1 terms using the CP+Jordan representation. Here, the number of rank-1 terms equals the rank of the solution array.

6.1. Optimal GSD solution in CP+Jordan form. Let $\underline{\mathbf{X}}$ be the optimal solution of the GSD problem (6.2). As explained above, we assume that $\mathbf{X}_2\mathbf{X}_1^{-1}$ has only real eigenvalues but is not diagonalizable. Next, we show how to obtain the non-diverging CP components from $\underline{\mathbf{X}}$ and write the limit points of the groups of diverging CP components in Jordan form. We have $\mathbf{X}_k = \mathbf{Q}_a \mathbf{R}_k \mathbf{Q}_b^T$, $k = 1, 2$ from a GSD algorithm. Since $\underline{\mathbf{X}} \in \mathcal{R}_I$, the matrices \mathbf{R}_k , $k = 1, 2$ are nonsingular. Let the Jordan normal form $\mathbf{P} \mathbf{J} \mathbf{P}^{-1}$ of $\mathbf{R}_2\mathbf{R}_1^{-1}$ be given by $\mathbf{J} = \text{diag}(\lambda_1, \dots, \lambda_p, \mathbf{J}_{m_1}(\mu_1), \dots, \mathbf{J}_{m_r}(\mu_r))$, where $\mathbf{J}_{m_j}(\mu_j)$ denotes an $m_j \times m_j$ Jordan block with $m_j \geq 2$, and $r \geq 1$. Note that the Jordan form \mathbf{J} of $\mathbf{R}_2\mathbf{R}_1^{-1}$ is also the Jordan form of $\mathbf{X}_2\mathbf{X}_1^{-1}$. Hence, $\mathbf{R}_2\mathbf{R}_1^{-1}$ also has only real eigenvalues but is not diagonalizable.

Now the following decomposition of $\underline{\mathbf{X}}$ can be obtained. Let $\mathbf{C}_1 = \mathbf{I}_p$, $\mathbf{C}_2 = \text{diag}(\lambda_1, \dots, \lambda_p)$, and let \mathbf{A} contain the corresponding columns of $\mathbf{Q}_a\mathbf{P}$ and \mathbf{B}^T the corresponding rows of $\mathbf{P}^{-1}\mathbf{R}_1\mathbf{Q}_b^T$. For the r Jordan blocks \mathbf{J}_{m_j} , let \mathbf{K}_j contain the corresponding columns of $\mathbf{Q}_a\mathbf{P}$ and \mathbf{L}_j^T the corresponding rows of $\mathbf{P}^{-1}\mathbf{R}_1\mathbf{Q}_b^T$. Then

$$(6.3) \quad \mathbf{X}_2 = \mathbf{A} \mathbf{C}_2 \mathbf{B}^T + \sum_{j=1}^r \mathbf{K}_j \mathbf{J}_{m_j} \mathbf{L}_j^T,$$

$$(6.4) \quad \mathbf{X}_1 = \mathbf{A} \mathbf{C}_1 \mathbf{B}^T + \sum_{j=1}^r \mathbf{K}_j \mathbf{I}_{m_j} \mathbf{L}_j^T.$$

Hence, we have decomposed the optimal GSD solution $\underline{\mathbf{X}}$ into a nondiverging CP part and r parts with a Jordan block \mathbf{J}_{m_j} instead of a diagonal matrix. In this way, diverging CP components are avoided, i.e., the components $\mathbf{A}, \mathbf{K}_1, \dots, \mathbf{K}_r$ are linearly independent (since they are columns of $\mathbf{Q}_a \mathbf{P}$), the components $\mathbf{B}, \mathbf{L}_1, \dots, \mathbf{L}_r$ are linearly independent (since they are the rows of $\mathbf{P}^{-1} \mathbf{R}_1 \mathbf{Q}_b^T$), and none of the elements in the decomposition tends to infinity. Note that each part of the decomposition (6.3)–(6.4) can be written in GSD form by using QR- and QL-decompositions as in the proof of (i) of Lemma 4.3.

If the eigenvalues $\lambda_1, \dots, \lambda_p$ are distinct, then the CP-part of the representation (6.3)–(6.4) is essentially unique. Indeed, we have p components and k -ranks $k_{\mathbf{A}} = k_{\mathbf{B}} = p$ and $k_{\mathbf{C}} = 2$, and essential uniqueness follows from Kruskal’s condition (1.4). From the uniqueness properties of the Jordan form of $\mathbf{R}_2 \mathbf{R}_1^{-1}$ it follows that if μ_1, \dots, μ_r are distinct, then the representation of the non-CP part of (6.3)–(6.4) is unique up to the order of the Jordan blocks \mathbf{J}_{m_j} and the scaling of the principal vectors in \mathbf{P} .

Although the decomposition (6.3)–(6.4) features not only rank-1 terms, it is essentially unique and may be interpretable to the researcher. From a computational as well as a practical point of view, this is a considerable improvement with respect to facing diverging CP components.

In practice, the matrix $\mathbf{R}_2 \mathbf{R}_1^{-1}$ of the corresponding optimal GSD solution obtained from a GSD algorithm does not have exactly identical eigenvalues. To be able to “recognize” the identical eigenvalues of $\mathbf{R}_2 \mathbf{R}_1^{-1}$ and their geometric multiplicities, the GSD algorithm must have a sufficiently small stopping criterion. The identical eigenvalues can then be estimated as the average of the ones which are “close together.” The Jordan normal form of $\mathbf{R}_2 \mathbf{R}_1^{-1}$ can be estimated by using, e.g., the method proposed in Golub and Wilkinson [11]. Below, we present the algorithm to obtain representation (6.3)–(6.4). The algorithm is formulated for general R (instead of $R = I$) in order to make it applicable to the $I \times J \times 2$ case as well (see section 7).

ALGORITHM FOR CP+JORDAN REPRESENTATION OF OPTIMAL GSD SOLUTION.

Input: Optimal GSD solution $\mathbf{X}_k = \mathbf{Q}_a \mathbf{R}_k \mathbf{Q}_b^T$, $k = 1, 2$, where $\mathbf{R}_2 \mathbf{R}_1^{-1}$ has only real eigenvalues but is not diagonalizable.

Output: CP+Jordan representation (6.3)–(6.4).

1. Calculate the Jordan form $\mathbf{P} \mathbf{J} \mathbf{P}^{-1}$ of $\mathbf{R}_2 \mathbf{R}_1^{-1}$, where $\mathbf{J} = \text{diag}(\lambda_1, \dots, \lambda_p, \mathbf{J}_{m_1}(\mu_1), \dots, \mathbf{J}_{m_r}(\mu_r))$. Here, $\mathbf{J}_{m_j}(\mu_j)$ denotes an $m_j \times m_j$ Jordan block with $m_j \geq 2$, and $r \geq 1$.
2. Set $\mathbf{C}_1 = \mathbf{I}_p$, $\mathbf{C}_2 = \text{diag}(\lambda_1, \dots, \lambda_p)$. For eigenvalues $\lambda_1, \dots, \lambda_p$, let \mathbf{A} contain the corresponding columns of $\mathbf{Q}_a \mathbf{P}$ and \mathbf{B}^T the corresponding rows of $\mathbf{P}^{-1} \mathbf{R}_1 \mathbf{Q}_b^T$.
3. For Jordan block \mathbf{J}_{m_j} , let \mathbf{K}_j contain the corresponding columns of $\mathbf{Q}_a \mathbf{P}$ and \mathbf{L}_j^T the corresponding rows of $\mathbf{P}^{-1} \mathbf{R}_1 \mathbf{Q}_b^T$, $j = 1, \dots, r$.
4. The CP+Jordan representation (6.3)–(6.4) follows, with p nondiverging CP components in $\mathbf{A}, \mathbf{B}, \mathbf{C}_1, \mathbf{C}_2$ and r limit points of groups of diverging CP components (see section 3).

The following result states that (6.3)–(6.4) can be written as a Tucker3 model (1.2).

PROPOSITION 6.1. *Let the Jordan form of $\mathbf{R}_2\mathbf{R}_1^{-1}$ be given by $\text{diag}(\lambda_1, \dots, \lambda_p, \mathbf{J}_{m_1}(\mu_1), \dots, \mathbf{J}_{m_r}(\mu_r))$, where $\mathbf{J}_{m_j}(\mu_j)$ denotes an $m_j \times m_j$ Jordan block with $m_j \geq 2$. Set $M = p + r + 1$. The decomposition (6.3)–(6.4) can be written as a Tucker3 model with an $I \times I \times M$ core array and component matrices*

$$(6.5) \quad [\mathbf{A} \mid \mathbf{K}_1 \mid \dots \mid \mathbf{K}_r], \quad [\mathbf{B} \mid \mathbf{L}_1 \mid \dots \mid \mathbf{L}_r], \quad \left[\begin{array}{cccccc} 1 & \dots & 1 & 0 & 1 & \dots & 1 \\ \lambda_1 & \dots & \lambda_p & 1 & \mu_1 & \dots & \mu_r \end{array} \right].$$

The number of nonzeros in the core array equals $2I - (p + r)$.

Proof. The first p columns of the component matrices in (6.5) follow from the CP part in (6.3)–(6.4). Next, we consider a Jordan block $\mathbf{J}_m(\mu)$, with $m \geq 2$. The corresponding part in (6.3)–(6.4) can be written as

$$(6.6) \quad \sum_{i=1}^m \mathbf{k}_i \otimes \mathbf{l}_i \otimes \begin{pmatrix} 1 \\ \mu \end{pmatrix} + \sum_{i=1}^{m-1} \mathbf{k}_i \otimes \mathbf{l}_{i+1} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

where \mathbf{k}_i and \mathbf{l}_i are the columns of the corresponding matrices \mathbf{K} and \mathbf{L} , respectively. Hence, (6.6) uses the corresponding columns of the component matrices in (6.5) and adds $m + (m - 1)$ nonzeros to the Tucker3 core array.

Since the CP part adds p nonzeros to the Tucker3 core array, the total number of nonzeros equals

$$(6.7) \quad p + \sum_{j=1}^r (2m_j - 1) = p - r + 2 \sum_{j=1}^r m_j = p - r + 2(I - p) = 2I - (p + r).$$

This completes the proof. \square

Note that the restricted Tucker3 model in Proposition 6.1 is unique up to the indeterminacies in the CP+Jordan representation (6.3)–(6.4).

The result of Proposition 6.1 is in line with Harshman [15], who explains diverging CP components for $2 \times 2 \times 2$ arrays as ‘‘Parafac trying to model Tucker variation.’’ Paatero [33] also noticed that his constructed sequences of diverging CP components have a limit that can be written in Tucker3 form.

The decomposition (6.3)–(6.4) of \mathbf{X} into p rank-1 terms and r rank- $(m_j, m_j, 2)$ terms (i.e., the ranks of the vectors in the three modes are m_j, m_j , and 2) is an example of the *block-term decomposition* introduced in De Lathauwer [8].

Remark 6.2. Note that it is not our goal to find a CP+Tucker3 representation of \mathbf{Z} , for which $\mathbf{Z}_2\mathbf{Z}_1^{-1}$ has some complex eigenvalues. Such a representation exists if the eigenvalues of $\mathbf{Z}_2\mathbf{Z}_1^{-1}$ are distinct and can be obtained from the transformation

$$(6.8) \quad \mathbf{Z}_2\mathbf{Z}_1^{-1} = \mathbf{K} \mathbf{\Lambda} \mathbf{K}^{-1},$$

where $\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_s, \mathbf{\Gamma}_1, \dots, \mathbf{\Gamma}_t)$ and $\mathbf{\Gamma}_i$ is 2×2 and corresponds to a pair of complex eigenvalues of $\mathbf{Z}_2\mathbf{Z}_1^{-1}$; see, e.g., Horn and Johnson [19]. Instead, it is our goal to find the limit point \mathbf{X} of the sequence of CP updates featuring diverging components, and (6.3)–(6.4) is a representation of that point \mathbf{X} .

Next, we illustrate the CP+Jordan algorithm by revisiting the $4 \times 4 \times 2$ example in (1.7)–(1.10) that was also discussed at the end of section 3. Using the Jacobi algorithm of De Lathauwer, De Moor, and Vandewalle [6] with $R = 4$ and a convergence criterion

of $1e-9$, we obtain the following optimal GSD solution for \mathbf{Z} in (1.7):

$$(6.9) \quad \mathbf{Q}_a = \begin{bmatrix} 0.1279 & 0.8039 & -0.5519 & 0.1813 \\ -0.7946 & -0.1776 & -0.2749 & 0.5113 \\ -0.5895 & 0.3628 & 0.1606 & -0.7037 \\ 0.0690 & -0.4367 & -0.7708 & -0.4588 \end{bmatrix},$$

$$(6.10) \quad \mathbf{Q}_b = \begin{bmatrix} -0.6328 & 0.3387 & -0.0964 & -0.6896 \\ 0.6382 & 0.5502 & -0.4778 & -0.2486 \\ 0.1774 & 0.5110 & 0.8406 & -0.0294 \\ -0.4011 & 0.5670 & -0.2363 & 0.6795 \end{bmatrix},$$

$$(6.11) \quad \mathbf{R}_1 = \begin{bmatrix} -1.1875 & -1.3604 & 1.1724 & -1.5430 \\ 0 & -1.0758 & 0.4567 & -0.3733 \\ 0 & 0 & -0.9103 & -0.7889 \\ 0 & 0 & 0 & 1.5915 \end{bmatrix},$$

$$(6.12) \quad \mathbf{R}_2 = \begin{bmatrix} 1.8323 & 0.0832 & 0.0009 & -0.0168 \\ 0 & -0.5285 & -2.5802 & -0.9022 \\ 0 & 0 & -0.4472 & 1.4516 \\ 0 & 0 & 0 & 0.7818 \end{bmatrix}.$$

The GSD algorithm terminated after 24 sweeps with an error sum-of-squares of 0.051016. The latter is less than the value of 0.051204 obtained by the CP algorithm in section 1, indicating that the GSD solution is closer to \mathbf{Z} than the final CP update. The sum-of-squares distance between the GSD solution $\mathbf{X}_k = \mathbf{Q}_a \mathbf{R}_k \mathbf{Q}_b^T$, $k = 1, 2$ and the final CP update $\mathbf{Y}_k = \mathbf{A} \mathbf{C}_k \mathbf{B}^T$, $k = 1, 2$ is only $3.2144e-7$. For the GSD solution, the eigenvalues of $\mathbf{X}_2 \mathbf{X}_1^{-1}$ are

$$(6.13) \quad -1.5430, \quad 0.4912, \quad 0.4912, \quad 0.4912.$$

Hence, for the final CP update, the three eigenvalues of $\mathbf{Y}_2 \mathbf{Y}_1$ that were close together in (3.3) have become identical in the limit point \mathbf{X} .

Next, we apply the CP+Jordan algorithm to the obtained GSD solution above. For the CP-part, we obtain

$$(6.14) \quad \mathbf{A} = \begin{bmatrix} 0.1279 \\ -0.7946 \\ -0.5895 \\ 0.0690 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 0.8259 \\ 0.0385 \\ -0.4005 \\ -0.3950 \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} 2.8918 \\ -4.4621 \end{bmatrix},$$

where the columns of \mathbf{A} and \mathbf{B} are normalized to length 1. Comparing this to the final CP-update in (1.8)–(1.10), we see that (6.14) is the nondiverging CP component of the final CP update. For the non-CP part of the CP+Jordan representation, we obtain

$$(6.15) \quad \mathbf{K} = \begin{bmatrix} -0.6779 & -0.0194 & -0.0500 \\ 0.6690 & -0.0900 & -0.1191 \\ 0.1326 & -0.2662 & 0.1248 \\ 0.2744 & 0.3003 & 0.1064 \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} 0.8879 & -2.6832 & 5.3125 \\ 1.7433 & -2.6564 & 1.9149 \\ -0.7556 & 3.1066 & 0.2265 \\ 1.0387 & 1.3806 & -5.2348 \end{bmatrix},$$

$$(6.16) \quad \mathbf{J} = \begin{bmatrix} 0.4912 & 1 & 0 \\ 0 & 0.4912 & 1 \\ 0 & 0 & 0.4912 \end{bmatrix}.$$

Hence, the limit point of the three diverging CP components is represented as (6.15)–(6.16).

6.2. A rank-revealing decomposition of the optimal GSD solution. Here we discuss how one may obtain a decomposition into rank-1 terms of the optimal GSD solution, where the number of rank-1 terms equals the rank of the solution array $\underline{\mathbf{X}}$. We make use of the CP+Jordan representation (6.3)–(6.4). The Tucker3 representation of $\underline{\mathbf{X}}$ in Proposition 6.1 decomposes $\underline{\mathbf{X}}$ into $2I - (p + r)$ rank-1 terms. Lemma 2.2 states that $\underline{\mathbf{X}}$ has rank $I + r$. Hence, the number of rank-1 terms in the Tucker3 representation is equal to $\text{rank}_{\otimes}(\underline{\mathbf{X}}) = I + r$ if and only if $I = p + 2r$. That is, if all Jordan blocks $\mathbf{J}_{m_j}(\mu_j)$ have size $m_j = 2$. In this case, (6.3)–(6.4) itself is a rank-revealing decomposition of $\underline{\mathbf{X}}$. From (6.6), it follows that for $p = 0$, $r = 1$, and $m = 2$, the representation has the form (1.11) of De Silva and Lim [10] with $\mathbf{x}_1 = \mathbf{k}_1$, $\mathbf{x}_2 = \mathbf{l}_2$, $\mathbf{x}_3 = \begin{pmatrix} 1 \\ \mu \end{pmatrix}$, $\mathbf{y}_1 = \mathbf{k}_2$, $\mathbf{y}_2 = \mathbf{l}_1$, and $\mathbf{y}_3 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. For general p and r and $m_j = 2$ for $j = 1, \dots, r$, the representation (1.11) can be generalized to

$$(6.17) \quad \underline{\mathbf{X}} = \sum_{i=1}^p \mathbf{z}_1^{(i)} \otimes \mathbf{z}_2^{(i)} \otimes \mathbf{z}_3^{(i)} + \sum_{j=1}^r (\mathbf{x}_1^{(j)} \otimes \mathbf{x}_2^{(j)} \otimes \mathbf{y}_3 + \mathbf{x}_1^{(j)} \otimes \mathbf{y}_2^{(j)} \otimes \mathbf{x}_3^{(j)} + \mathbf{y}_1^{(j)} \otimes \mathbf{x}_2^{(j)} \otimes \mathbf{x}_3^{(j)}).$$

If there is a Jordan block $\mathbf{J}_{m_j}(\mu_j)$ with size $m_j \geq 3$, then the number of rank-1 terms in the decomposition (6.3)–(6.4) is larger than $\text{rank}_{\otimes}(\underline{\mathbf{X}}) = I + r$. However, a method to obtain a decomposition into $I + r$ rank-1 terms from (6.3)–(6.4) can be found in Ja’ Ja’ [21]. Consider the $m \times m \times 2$ array consisting of the slices \mathbf{I}_m and $\mathbf{J}_m(\mu)$, with $m \geq 2$. From Lemma 2.2, it follows that this array has rank $m + 1$. Let $\mathbf{w} = (w_0 \ w_1 \ \dots \ w_{m-1})^T$, and let \mathbf{e}_m denote the m th column of \mathbf{I}_m . Then $\mathbf{J}_m(\mu) - \mathbf{e}_m \mathbf{w}^T$ has characteristic polynomial $f(\lambda - \mu)$, with

$$(6.18) \quad f(x) = w_0 + w_1 x + \dots + w_{m-1} x^{m-1} - x^m.$$

It follows that we can pick \mathbf{w} such that $f(x)$ has m distinct real roots. By Lemma 2.1, the $m \times m \times 2$ array with slices \mathbf{I}_m and $\mathbf{J}_m(\mu) - \mathbf{e}_m \mathbf{w}^T$ has rank m , and a rank- m decomposition can be obtained from an eigendecomposition of its second slice. Since we have subtracted the rank-1 slice $\mathbf{e}_m \mathbf{w}^T$, this gives us a rank- $(m + 1)$ decomposition of the array with \mathbf{I}_m and $\mathbf{J}_m(\mu)$.

Applying this procedure to each Jordan block in (6.3)–(6.4) yields a decomposition of $\underline{\mathbf{X}}$ into $p + \sum_{j=1}^r (m_j + 1) = I + r$ rank-1 terms. Since we have freedom in choosing the vector \mathbf{w} , this decomposition is not essentially unique (also for $m_j = 2$).

6.3. Optimal GSD solution in CP+GSD form. Since the Jordan form has a discontinuous transition from diagonalizable to nondiagonalizable matrices, it is numerically unstable, and the obtained Jordan form is extremely sensitive to tolerances for “recognizing” identical eigenvalues; see the discussion in Golub and Van Loan [12]. It follows from (6.3)–(6.4) that the complete non-CP part may also be represented in a full GSD of size $I - p$. For this, one only has to determine the eigenvalues of $\mathbf{X}_2 \mathbf{X}_1^{-1}$ with algebraic multiplicity equal to 1, which is numerically more stable. Here, we show how the CP part and the GSD of the non-CP part can be computed without first computing the Jordan representation (6.3)–(6.4). Also, if one is only interested in obtaining the nondiverging CP components, computing the CP-part of the CP+GSD representation is an efficient way.

We assume that the optimal GSD solution $\underline{\mathbf{X}}$ has been obtained from a GSD algorithm and the GSD $\mathbf{X}_k = \mathbf{Q}_a \mathbf{R}_k \mathbf{Q}_b^T$, $k = 1, 2$ is known. Let the Jordan form of $\mathbf{R}_2 \mathbf{R}_1^{-1}$ be given by $\mathbf{J} = \text{diag}(\lambda_1, \dots, \lambda_p, \mathbf{J}_{m_1}(\mu_1), \dots, \mathbf{J}_{m_r}(\mu_r))$, where $\mathbf{J}_{m_j}(\mu_j)$ denotes an $m_j \times m_j$ Jordan block with $m_j \geq 2$, and $r \geq 1$. The eigenvalues and the Jordan form \mathbf{J} of $\mathbf{R}_2 \mathbf{R}_1^{-1}$ are the same as those of $\mathbf{X}_2 \mathbf{X}_1^{-1}$ and those of $\mathbf{R}_1^{-1} \mathbf{R}_2$. As mentioned above, we assume that $\mathbf{R}_2 \mathbf{R}_1^{-1}$ has only real eigenvalues but is not diagonalizable. In the following, we assume that the eigenvalues $\lambda_1, \dots, \lambda_p$ are known. For this, it is not necessary to compute the complete Jordan form \mathbf{J} .

First, we show how to obtain the CP-part of (6.3)–(6.4). For simplicity, we assume that none of the eigenvalues μ_j is equal to a λ_i . Let \mathbf{R}_a have as columns the eigenvectors of $\mathbf{R}_2 \mathbf{R}_1^{-1}$ corresponding to the eigenvalues $\lambda_1, \dots, \lambda_p$. From the discussion in section 6.1, it follows that $\mathbf{A} = \mathbf{Q}_a \mathbf{R}_a$. Next, we find \mathbf{B} . If $\mathbf{R}_2 \mathbf{R}_1^{-1} = \mathbf{P} \mathbf{J} \mathbf{P}^{-1}$, then $\mathbf{R}_1^{-1} \mathbf{R}_2 = (\mathbf{R}_1^{-1} \mathbf{P}) \mathbf{J} (\mathbf{R}_1^{-1} \mathbf{P})^{-1}$. Let \mathbf{R}_b have as rows the left eigenvectors of $\mathbf{R}_1^{-1} \mathbf{R}_2$ corresponding to the eigenvalues $\lambda_1, \dots, \lambda_p$, i.e., $\mathbf{R}_b \mathbf{R}_1^{-1} \mathbf{R}_2 = \text{diag}(\lambda_1, \dots, \lambda_p) \mathbf{R}_b$. Then we have $\mathbf{B} = \mathbf{Q}_b \mathbf{R}_b^T$ (see section 6.1). Since $\mathbf{R}_2 \mathbf{R}_1^{-1}$ and $\mathbf{R}_1^{-1} \mathbf{R}_2$ are upper triangular, the columns of \mathbf{R}_a and the rows of \mathbf{R}_b are the columns and rows, respectively, of an $I \times I$ upper triangular matrix. We normalize the rows of \mathbf{R}_b such that the first nonzero element becomes 1, and we normalize the columns of \mathbf{R}_a such that the last nonzero element becomes 1. Let \mathbf{C}_k be the $p \times p$ diagonal matrix containing the diagonal elements of \mathbf{R}_k corresponding to the locations of $\lambda_1, \dots, \lambda_p$ on the diagonal of $\mathbf{R}_2 \mathbf{R}_1^{-1}$. It now follows that the CP-part in (6.3)–(6.4) is equal (up to scaling/rescaling and a joint permutation of the p CP components) to $\mathbf{A} \mathbf{C}_k \mathbf{B}^T$, $k = 1, 2$.

Note that the eigenvalues $\lambda_1, \dots, \lambda_p$ may appear anywhere on the diagonal of $\mathbf{R}_2 \mathbf{R}_1^{-1}$. Hence, unlike the ordering in the Jordan form \mathbf{J} , the eigenvalues λ_j do not need to appear as the first p diagonal elements of $\mathbf{R}_2 \mathbf{R}_1^{-1}$. This is due to the permutation indeterminacy of the GSD solution. See also the discussion at the end of section 5.

Next, we show how to obtain the GSD of the non-CP part of (6.3)–(6.4). Define $\mathbf{T}_k = \mathbf{R}_k - \mathbf{R}_a \mathbf{C}_k \mathbf{R}_b$, $k = 1, 2$. Then $\mathbf{Y}_k = \mathbf{Q}_a \mathbf{T}_k \mathbf{Q}_b^T$, $k = 1, 2$ is the non-CP part of (6.3)–(6.4). From (6.3)–(6.4), it follows that $\mathbf{Y}_1 = \mathbf{K} \mathbf{I}_{I-p} \mathbf{L}^T$ and $\mathbf{Y}_2 = \mathbf{K} \tilde{\mathbf{J}} \mathbf{L}^T$ for $I \times (I-p)$ matrices \mathbf{K} and \mathbf{L} of full column rank and an $(I-p) \times (I-p)$ Jordan form $\tilde{\mathbf{J}}$. This implies that \mathbf{Y}_1 and \mathbf{Y}_2 have rank $I-p$ and identical column and row spaces. These properties of \mathbf{Y}_1 and \mathbf{Y}_2 also hold for \mathbf{T}_1 and \mathbf{T}_2 . Moreover, by definition, \mathbf{T}_k is upper triangular and has zeros on the diagonal corresponding to the locations of $\lambda_1, \dots, \lambda_p$ on the diagonal of $\mathbf{R}_2 \mathbf{R}_1^{-1}$. From the I locations on the diagonal of $\mathbf{R}_2 \mathbf{R}_1^{-1}$, let $1 \leq i_1 < i_2 < \dots < i_{I-p} \leq I$ be those not containing $\lambda_1, \dots, \lambda_p$. Let $\tilde{\mathbf{T}}_k$ contain the columns i_1, i_2, \dots, i_{I-p} of \mathbf{T}_k , in the same order as they appear in \mathbf{T}_k , $k = 1, 2$. Then each of these columns has a nonzero diagonal element in \mathbf{T}_k , and since \mathbf{T}_k is upper triangular, $\tilde{\mathbf{T}}_k$ has rank $I-p$. Since \mathbf{T}_k also has rank $I-p$, it follows that the column spaces of $\tilde{\mathbf{T}}_k$ and \mathbf{T}_k are identical. Also, the column spaces of $\tilde{\mathbf{T}}_1$ and $\tilde{\mathbf{T}}_2$ are identical. We write $\mathbf{T}_k = \tilde{\mathbf{T}}_k \mathbf{H}_k^T$, where $\mathbf{H}_k = \mathbf{T}_k^T \tilde{\mathbf{T}}_k (\tilde{\mathbf{T}}_k^T \tilde{\mathbf{T}}_k)^{-1}$, $k = 1, 2$. We need the following lemmas.

LEMMA 6.3. *There holds $\tilde{\mathbf{T}}_k = \tilde{\mathbf{Q}} \tilde{\mathbf{R}}_k$ for some $I \times (I-p)$ columnwise orthonormal $\tilde{\mathbf{Q}}$ and some $(I-p) \times (I-p)$ upper triangular $\tilde{\mathbf{R}}_k$, $k = 1, 2$.*

Proof. Let $\tilde{\mathbf{T}}_k$ contain columns i_1, \dots, i_{I-p} of \mathbf{T}_k , with $1 \leq i_1 < i_2 < \dots < i_{I-p} \leq I$. Let $\mathbf{t}_{i_n}^{(k)}$ denote column i_n of \mathbf{T}_k , which is column n of $\tilde{\mathbf{T}}_k$, $k = 1, 2$. Then $\mathbf{t}_{i_n}^{(k)}$ has the last $I - i_n$ elements equal to zero and element i_n nonzero. We obtain $\tilde{\mathbf{Q}}$ and $\tilde{\mathbf{R}}_1$ from a QR-decomposition of $\tilde{\mathbf{T}}_1$ by means of the Gram–Schmidt process.

Let

$$(6.19) \quad \mathbf{v}_1 = \mathbf{t}_{i_1}^{(1)} \quad \text{and} \quad \mathbf{v}_n = \mathbf{t}_{i_n}^{(1)} - \sum_{j=1}^{n-1} \text{proj}_{\mathbf{v}_j} \mathbf{t}_{i_n}^{(1)}, \quad n = 2, \dots, I - p,$$

where $\text{proj}_{\mathbf{v}} \mathbf{t} = (\mathbf{t}^T \mathbf{v}) / (\mathbf{v}^T \mathbf{v}) \mathbf{v}$ denotes the orthogonal projection of \mathbf{t} onto \mathbf{v} . The columns of $\tilde{\mathbf{Q}}$ are the unit length versions of $\mathbf{v}_1, \dots, \mathbf{v}_{I-p}$, and the elements of $\tilde{\mathbf{R}}_1$ follow from (6.19).

The columns of $\tilde{\mathbf{Q}}$ form an orthonormal basis for the column space of $\tilde{\mathbf{T}}_1$ and, hence, also for the column space of $\tilde{\mathbf{T}}_2$. This implies that for every column $\mathbf{t}_{i_n}^{(2)}$, there is a vector \mathbf{w} such that

$$(6.20) \quad \mathbf{t}_{i_n}^{(2)} = \tilde{\mathbf{Q}} \mathbf{w}.$$

From (6.19), it follows that column j of $\tilde{\mathbf{Q}}$ has the last $I - i_j$ elements equal to zero and element i_j nonzero, $j = 1, \dots, I - p$. Since $\mathbf{t}_{i_n}^{(2)}$ has the last $I - i_n$ elements equal to zero, (6.20) implies that $\mathbf{t}_{i_n}^{(2)}$ lies in the space spanned by the first n columns of $\tilde{\mathbf{Q}}$. Hence, \mathbf{w} in (6.20) has the last $I - p - n$ elements equal to zero. It follows that $\tilde{\mathbf{T}}_2 = \tilde{\mathbf{Q}} \tilde{\mathbf{R}}_2$ for some $(I - p) \times (I - p)$ upper triangular $\tilde{\mathbf{R}}_2$. Since $\tilde{\mathbf{Q}}$ has full column rank, the matrix $\tilde{\mathbf{R}}_2$ is uniquely determined. This completes the proof. \square

Recall that, since the column spaces of $\tilde{\mathbf{T}}_k$ and \mathbf{T}_k are identical, we may write $\mathbf{T}_k = \tilde{\mathbf{T}}_k \mathbf{H}_k^T$, $k = 1, 2$.

LEMMA 6.4. *Let \mathbf{H}_k satisfy $\mathbf{T}_k = \tilde{\mathbf{T}}_k \mathbf{H}_k^T$, $k = 1, 2$. Then $\mathbf{H}_1 = \mathbf{H}_2$.*

Proof. Since $\tilde{\mathbf{T}}_k$ contains columns i_1, \dots, i_{I-p} of \mathbf{T}_k , it follows that rows i_1, \dots, i_{I-p} of \mathbf{H}_k are equal to rows $1, \dots, I - p$ of \mathbf{I}_{I-p} , $k = 1, 2$. Let the row permutation $\mathbf{\Pi}$ be such that $\mathbf{\Pi} \mathbf{H}_k = \begin{bmatrix} \mathbf{I}_{I-p} \\ \tilde{\mathbf{H}}_k \end{bmatrix}$.

Since \mathbf{H}_k has full column rank, $\text{rank}(\mathbf{T}_k) = I - p$, and $\mathbf{T}_k^T = \mathbf{H}_k \tilde{\mathbf{T}}_k^T$, the column space of \mathbf{H}_k is identical to the column space of \mathbf{T}_k^T . Moreover, since the row spaces of \mathbf{T}_1 and \mathbf{T}_2 are identical, the column spaces of \mathbf{H}_1 and \mathbf{H}_2 are also identical. It follows that each column of $\mathbf{\Pi} \mathbf{H}_1$ must lie in the column space of $\mathbf{\Pi} \mathbf{H}_2$. Since both matrices have \mathbf{I}_{I-p} as their first $I - p$ rows, this yields that $\mathbf{\Pi} \mathbf{H}_1 = \mathbf{\Pi} \mathbf{H}_2$. Hence, $\mathbf{H}_1 = \mathbf{H}_2$, which completes the proof. \square

Using Lemmas 6.3 and 6.4, the GSD of the non-CP part of (6.3)–(6.4) can be computed as follows. From a QR-decomposition of $\tilde{\mathbf{T}}_1$, we obtain $\tilde{\mathbf{T}}_1 = \tilde{\mathbf{Q}} \tilde{\mathbf{R}}_1$. The matrix $\tilde{\mathbf{R}}_2$ in Lemma 6.3 follows from $\tilde{\mathbf{R}}_2 = \tilde{\mathbf{Q}}^T \tilde{\mathbf{T}}_2$. The matrix $\mathbf{H} = \mathbf{H}_1 = \mathbf{H}_2$ in Lemma 6.4 is obtained as $\mathbf{H} = \mathbf{T}_1^T \tilde{\mathbf{T}}_1 (\tilde{\mathbf{T}}_1^T \tilde{\mathbf{T}}_1)^{-1}$. Next, let $\mathbf{H} = \hat{\mathbf{Q}} \hat{\mathbf{R}}^T$ be a QL-decomposition of \mathbf{H} with an $I \times (I - p)$ columnwise orthonormal $\hat{\mathbf{Q}}$ and an $(I - p) \times (I - p)$ upper triangular $\hat{\mathbf{R}}$. It follows that

$$(6.21) \quad \mathbf{Y}_k = \mathbf{Q}_a \mathbf{T}_k \mathbf{Q}_b^T = \mathbf{Q}_a \tilde{\mathbf{T}}_k \mathbf{H}^T \mathbf{Q}_b^T = (\mathbf{Q}_a \tilde{\mathbf{Q}}) (\tilde{\mathbf{R}}_k \hat{\mathbf{R}}) (\mathbf{Q}_b \hat{\mathbf{Q}})^T, \quad k = 1, 2$$

is a full GSD of size $I - p$ of the non-CP part of (6.3)–(6.4). Below, we present the algorithm to obtain a CP+GSD representation of the optimal GSD solution $\underline{\mathbf{X}}$. The algorithm is formulated for general R (instead of $R = I$) in order to make it applicable to the $I \times J \times 2$ case as well (see section 7).

ALGORITHM FOR CP+GSD REPRESENTATION OF OPTIMAL GSD SOLUTION.

Input: Optimal GSD solution $\mathbf{X}_k = \mathbf{Q}_a \mathbf{R}_k \mathbf{Q}_b^T$, $k = 1, 2$, where $\mathbf{R}_2 \mathbf{R}_1^{-1}$ has only real eigenvalues but is not diagonalizable.

Output: CP+GSD representation $\mathbf{X}_k = \mathbf{A} \mathbf{C}_k \mathbf{B}^T + \mathbf{Q}_1 \mathbf{R}_k^{(0)} \mathbf{Q}_2^T$, $k = 1, 2$.

1. Calculate the eigenvalues $\lambda_1, \dots, \lambda_p$ of $\mathbf{R}_2 \mathbf{R}_1^{-1}$ with algebraic multiplicity 1. Set $\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_p)$.
2. Determine \mathbf{R}_a ($R \times p$) as $\mathbf{R}_2 \mathbf{R}_1^{-1} \mathbf{R}_a = \mathbf{R}_a \mathbf{\Lambda}$. Normalize the columns of \mathbf{R}_a such that the last nonzero element becomes 1. Determine \mathbf{R}_b ($p \times R$) as $\mathbf{R}_b \mathbf{R}_1^{-1} \mathbf{R}_2 = \mathbf{\Lambda} \mathbf{R}_b$. Normalize the rows of \mathbf{R}_b such that the first nonzero element becomes 1.
3. Set $\mathbf{A} = \mathbf{Q}_a \mathbf{R}_a$ and $\mathbf{B} = \mathbf{Q}_b \mathbf{R}_b^T$. Let \mathbf{C}_k be the diagonal matrix containing the diagonal elements of \mathbf{R}_k corresponding to the locations of $\lambda_1, \dots, \lambda_p$ on the diagonal of $\mathbf{R}_2 \mathbf{R}_1^{-1}$, $k = 1, 2$. The p nondiverging CP components are now obtained as $\mathbf{A} \mathbf{C}_k \mathbf{B}^T$, $k = 1, 2$.
4. Set $\mathbf{T}_k = \mathbf{R}_k - \mathbf{R}_a \mathbf{C}_k \mathbf{R}_b$, $k = 1, 2$. Let $\tilde{\mathbf{T}}_k$ contain the $R - p$ columns of \mathbf{T}_k with a nonzero diagonal element, in the same order as they appear in \mathbf{T}_k , $k = 1, 2$.
5. Compute the QR-decomposition $\tilde{\mathbf{T}}_1 = \tilde{\mathbf{Q}} \tilde{\mathbf{R}}_1$ and set $\tilde{\mathbf{R}}_2 = \tilde{\mathbf{Q}}^T \tilde{\mathbf{T}}_2$.
6. Set $\mathbf{H} = \mathbf{T}_1^T \tilde{\mathbf{T}}_1 (\tilde{\mathbf{T}}_1^T \tilde{\mathbf{T}}_1)^{-1}$ and compute the QL-decomposition $\mathbf{H} = \hat{\mathbf{Q}} \hat{\mathbf{R}}^T$.
7. Set $\mathbf{Q}_1 = \mathbf{Q}_a \hat{\mathbf{Q}}$, $\mathbf{Q}_2 = \mathbf{Q}_b \hat{\mathbf{Q}}$ and $\mathbf{R}_k^{(0)} = \tilde{\mathbf{R}}_k \hat{\mathbf{R}}$, $k = 1, 2$. The size- $(R - p)$ GSD representation of the limit point of the diverging CP components is now obtained as $\mathbf{Q}_1 \mathbf{R}_k^{(0)} \mathbf{Q}_2^T$, $k = 1, 2$.

To illustrate the CP+GSD algorithm, we return once again to the $4 \times 4 \times 2$ example in (1.7)–(1.10) that was also discussed at the end of sections 3 and 6.1. We apply the CP+GSD algorithm to the optimal GSD solution (6.9)–(6.12) for \mathbf{Z} in (1.7). For the CP-part, we obtain

$$(6.22) \quad \mathbf{R}_a = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{R}_b^T = \begin{bmatrix} 1.0000 \\ 0.3111 \\ 0.8314 \\ 2.0353 \end{bmatrix}, \quad \mathbf{C}_1 = -1.1875, \quad \mathbf{C}_2 = 1.8323.$$

Up to scaling/rescaling, the CP-part $\mathbf{A} = \mathbf{Q}_a \mathbf{R}_a$, $\mathbf{B} = \mathbf{Q}_b \mathbf{R}_b^T$, \mathbf{C}_1 , \mathbf{C}_2 in (6.22) is equal to the CP-part (6.14) of the CP+Jordan representation. For the GSD-part, we obtain

$$(6.23) \quad \mathbf{Q}_1 = \begin{bmatrix} -0.6779 & -0.0470 & 0.2357 \\ 0.6690 & -0.2187 & 0.5479 \\ 0.1326 & -0.6466 & -0.6812 \\ 0.2744 & 0.7293 & -0.4244 \end{bmatrix}, \quad \mathbf{Q}_2 = \begin{bmatrix} 0.3387 & -0.0964 & -0.6896 \\ 0.5502 & -0.4778 & -0.2486 \\ 0.5110 & 0.8406 & -0.0294 \\ 0.5670 & -0.2363 & 0.6795 \end{bmatrix},$$

$$(6.24) \quad \mathbf{R}_1^{(0)} = \begin{bmatrix} 1.4627 & -1.7991 & -0.3176 \\ 0 & 1.5699 & 1.1872 \\ 0 & 0 & 1.5963 \end{bmatrix}, \quad \mathbf{R}_2^{(0)} = \begin{bmatrix} 0.7185 & 2.9293 & 3.2016 \\ 0 & 0.7712 & -2.5885 \\ 0 & 0 & 0.7841 \end{bmatrix}.$$

Hence, the limit point of the three diverging CP components is represented as (6.23)–(6.24).

TABLE 7.1

Conjectures of Stegeman [40] on the occurrence of diverging CP components for a generic $I \times J \times 2$ array \mathbf{Z} . Here, $I \geq J \geq 2$ and $R \geq 2$.

Case	$\mathbf{Z} \in \mathbb{R}^{I \times J \times 2}$	$\text{Rank}_{\otimes}(\mathbf{Z})$	R	Diverging CP components
2	$I = J$	$I + 1$	$R = I$	almost everywhere
3	$I = J$	$I + 1$	$R < I$	positive volume
5	$I = J$	I	$R < I$	positive volume
8	$I > J$	$\min(I, 2J)$	$R = J$	positive volume
9	$I > J$	$\min(I, 2J)$	$R < J$	positive volume

7. Extension to $I \times J \times 2$ arrays and general R . Stegeman [40] has mathematically analyzed the cases of diverging CP components occurring for generic $I \times J \times 2$ arrays and all values of R . The cases in which diverging components occur are listed in Table 7.1, as well as the conjectures of Stegeman [40] on the frequency of their occurrence. A generic $I \times J \times 2$ array \mathbf{Z} has rank $\min(I, 2J)$ if $I > J$, and rank I or $I + 1$ (both on a set of positive volume) if $I = J$; see Ten Berge and Kiers [44].

It is shown in [40] that the cases of diverging CP components in Table 7.1 can be transformed to Case 2 (with $I = J = R$), which we have considered so far. Next, we extend our results in the previous sections by showing that in all cases in Table 7.1, the GSD approach may be used to avoid the problem of diverging CP components. Analogous to our previous results, the optimal GSD solution is the limit point of the sequence of CP updates (whether it features diverging components or not) and may be decomposed into a nondiverging CP-part and a Jordan part or into a nondiverging CP-part and a smaller GSD part.

The GSD model for an $I \times J \times 2$ array \mathbf{Z} is

$$(7.1) \quad \mathbf{Z}_k = \mathbf{Q}_a \mathbf{R}_k \mathbf{Q}_b^T + \mathbf{E}_k, \quad k = 1, 2,$$

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, $k = 1, 2$. Without loss of generality, we assume $I \geq J$. Also, we assume $R \leq J$ (and $R \leq I$) and $R < \text{rank}_{\otimes}(\mathbf{Z})$. From Table 7.1, it can be seen that this includes all cases. Finding \mathbf{Q}_a , \mathbf{Q}_b , \mathbf{R}_1 , and \mathbf{R}_2 , which minimize the sum-of-squares of the residuals in (7.1), can be achieved by a modification of the Jacobi algorithm of De Lathauwer, De Moor, and Vandewall [6]. This will be explained in section 7.1 below.

The proof of Proposition 4.2 can be used to show that the GSD model (7.1) for $I \times J \times 2$ arrays always has an optimal solution. Analogous to (6.1)–(6.2), we define

$$(7.2) \quad \mathcal{P}_{(I,J,R)} = \{\mathbf{Y} \in \mathbb{R}^{I \times J \times 2} : \mathbf{Y} \text{ has a full GSD (7.1) with } \mathbf{R}_1 \text{ and } \mathbf{R}_2 \text{ nonsingular}\}$$

and the GSD problem

$$(7.3) \quad \begin{aligned} &\text{Minimize } \|\mathbf{Z} - \mathbf{Y}\|^2 \\ &\text{subject to } \mathbf{Y} \in \mathcal{P}_{(I,J,R)}. \end{aligned}$$

From the analysis in Stegeman [40], it follows that the set $\mathcal{P}_{(I,J,R)}$ is closed, and hence, problem (7.3) always has an optimal solution. In Cases 3, 5, 8, and 9 of Table 7.1, the boundary of $\mathcal{P}_{(I,J,R)}$ is the set $\mathcal{P}_{(I,J,R)}$ itself, and the optimal solution \mathbf{X} of the GSD problem (7.3) has $\mathbf{R}_2 \mathbf{R}_1^{-1}$ with only real eigenvalues, some of which are identical. The problem of diverging CP components occurs if $\mathbf{R}_2 \mathbf{R}_1^{-1}$ is not diagonalizable; see [40]. In this case, the GSD of \mathbf{X} cannot be fully transformed to a CP representation, and

sequences of CP updates converging to $\underline{\mathbf{X}}$ feature diverging components. As in Case 2 of Table 7.1, two alternatives are a CP+Jordan or a CP+GSD representation. These can be obtained by using the algorithms in sections 6.1 and 6.3, respectively. As explained in section 6.2, a decomposition of $\underline{\mathbf{X}}$ into $\text{rank}_{\otimes}(\underline{\mathbf{X}})$ terms of rank 1 can be obtained from the CP+Jordan representation of $\underline{\mathbf{X}}$ using the method of Ja' Ja' [21].

If, in Cases 3, 5, 8, and 9 of Table 7.1, the optimal GSD solution $\underline{\mathbf{X}}$ has a GSD with $\mathbf{R}_2\mathbf{R}_1^{-1}$ diagonalizable, then the GSD can be transformed into a full CP representation of $\underline{\mathbf{X}}$, and the problems of diverging components do not occur. That is, $\underline{\mathbf{X}}$ is also an optimal solution of the CP problem. The CP representation of \mathbf{R}_1 and \mathbf{R}_2 can be obtained from the eigendecomposition of $\mathbf{R}_2\mathbf{R}_1^{-1}$ analogous to (2.2). Premultiplying by \mathbf{Q}_a and postmultiplying by \mathbf{Q}_b^T then yields the full CP representation for \mathbf{X}_1 and \mathbf{X}_2 .

7.1. The Jacobi algorithm for the GSD problem of $I \times J \times 2$ arrays.

Here, we show how the Jacobi algorithm of De Lathauwer, De Moor, and Vandewalle [6] for solving the GSD problem (6.2) can be modified to the case of $I \times J \times 2$ arrays and all values of R not larger than I and J . That is, the modified Jacobi algorithm can be used to solve the more general class of GSD problems (7.3).

Let $I = J = R$. The Jacobi algorithm of [6] sets out to find $(\mathbf{Q}_a, \mathbf{Q}_b, \mathbf{R}_1, \mathbf{R}_2)$ such that $\mathbf{Q}_a^T \mathbf{Z}_k \mathbf{Q}_b$, $k = 1, 2$ are as upper triangular as possible. Their upper triangular parts are then the estimates of \mathbf{R}_k , $k = 1, 2$. The estimates $(\mathbf{Q}_a, \mathbf{Q}_b, \mathbf{R}_1, \mathbf{R}_2)$ are updated by applying Givens rotations to the rows and columns of $\mathbf{Q}_a^T \mathbf{Z}_k \mathbf{Q}_b$, $k = 1, 2$, as follows. Let \mathbf{G}_{ij} be equal to \mathbf{I}_I except for the entries $(\mathbf{G}_{ij})_{ii} = (\mathbf{G}_{ij})_{jj} = \cos \alpha$ and $(\mathbf{G}_{ij})_{ji} = -(\mathbf{G}_{ij})_{ij} = \sin \alpha$, where α is the rotation angle. Let $\tilde{\mathbf{G}}_{ij}$ be defined as \mathbf{G}_{ij} for a rotation angle β . One sweep of the Jacobi algorithm determines for each (i, j) with $1 \leq i < j \leq I$, the optimal rotation angles α and β such that $\mathbf{G}_{ij} \mathbf{Q}_a^T \mathbf{Z}_k \mathbf{Q}_b \tilde{\mathbf{G}}_{ij}^T$, $k = 1, 2$ are as upper triangular as possible. The updated estimates of $(\mathbf{Q}_a, \mathbf{Q}_b, \mathbf{R}_1, \mathbf{R}_2)$ are given by $\mathbf{Q}_a \mathbf{G}_{ij}^T$, $\mathbf{Q}_b \tilde{\mathbf{G}}_{ij}^T$, and $\mathbf{G}_{ij} \mathbf{R}_k \tilde{\mathbf{G}}_{ij}^T$, $k = 1, 2$.

Next, consider the general case where possibly $I \neq J$ and $R \leq I$, $R \leq J$. In the modified Jacobi algorithm, we have the orthonormal variables $\tilde{\mathbf{Q}}_a$ ($I \times I$) and $\tilde{\mathbf{Q}}_b$ ($J \times J$). The modified Jacobi algorithm maximizes the sum-of-squares of the upper triangular parts of the first R rows and columns of $\tilde{\mathbf{R}}_k = \tilde{\mathbf{Q}}_a^T \mathbf{Z}_k \tilde{\mathbf{Q}}_b$, $k = 1, 2$. These $R \times R$ upper triangular parts are then the estimates of \mathbf{R}_k , $k = 1, 2$. The estimates of \mathbf{Q}_a and \mathbf{Q}_b are the first R columns of $\tilde{\mathbf{Q}}_a$ and $\tilde{\mathbf{Q}}_b$, respectively. Each sweep of the algorithm consists of two phases. In the first phase, the Givens rotations \mathbf{G}_{ij} ($I \times I$) and $\tilde{\mathbf{G}}_{ij}$ ($J \times J$) are determined as above for each (i, j) with $1 \leq i < j \leq R$. Within the first R rows and columns of $\tilde{\mathbf{R}}_k$, $k = 1, 2$, these rotations make the structure as upper triangular as possible.

In the second phase, rotations \mathbf{G}_i , $1 \leq i \leq R$ are determined such that they transfer as much energy as possible from rows $R + 1, \dots, I$ of $\tilde{\mathbf{R}}_k$ to row i of (the upper triangular part of) $\tilde{\mathbf{R}}_k$, $k = 1, 2$. Independently, rotations $\tilde{\mathbf{G}}_j$, $1 \leq j \leq R$ are determined such that they transfer as much energy as possible from columns $R + 1, \dots, J$ of $\tilde{\mathbf{R}}_k$ to column j of (the upper triangular part of) $\tilde{\mathbf{R}}_k$, $k = 1, 2$. We first show how to obtain \mathbf{G}_i . Let

$$\hat{\mathbf{R}}_i = \begin{bmatrix} (\tilde{\mathbf{R}}_1)_{ii} & \dots & (\tilde{\mathbf{R}}_1)_{iR} & (\tilde{\mathbf{R}}_2)_{ii} & \dots & (\tilde{\mathbf{R}}_2)_{iR} \\ (\tilde{\mathbf{R}}_1)_{R+1,i} & \dots & (\tilde{\mathbf{R}}_1)_{R+1,R} & (\tilde{\mathbf{R}}_2)_{R+1,i} & \dots & (\tilde{\mathbf{R}}_2)_{R+1,R} \\ \vdots & & \vdots & \vdots & & \vdots \\ (\tilde{\mathbf{R}}_1)_{I,i} & \dots & (\tilde{\mathbf{R}}_1)_{I,R} & (\tilde{\mathbf{R}}_2)_{I,i} & \dots & (\tilde{\mathbf{R}}_2)_{I,R} \end{bmatrix} = \mathbf{S} \mathbf{D} \mathbf{V}^T \tag{7.4}$$

be the singular value decomposition (SVD) of $\hat{\mathbf{R}}_i$. Then $\mathbf{S}^T \hat{\mathbf{R}}_i$ is an orthogonal rotation of the rows of $\hat{\mathbf{R}}_i$ such that its first row has maximum sum-of-squares. The square root of this is equal to the dominant singular value of $\hat{\mathbf{R}}_i$. From \mathbf{S}^T , the rotation \mathbf{G}_i can be obtained.

The computation of $\tilde{\mathbf{G}}_j$ is analogous. Let

$$(7.5) \quad \bar{\mathbf{R}}_j = \begin{bmatrix} (\tilde{\mathbf{R}}_1)_{1j} & (\tilde{\mathbf{R}}_1)_{1,R+1} & \cdots & (\tilde{\mathbf{R}}_1)_{1,J} \\ \vdots & \vdots & & \vdots \\ (\tilde{\mathbf{R}}_1)_{jj} & (\tilde{\mathbf{R}}_1)_{j,R+1} & \cdots & (\tilde{\mathbf{R}}_1)_{j,J} \\ (\tilde{\mathbf{R}}_2)_{1j} & (\tilde{\mathbf{R}}_2)_{1,R+1} & \cdots & (\tilde{\mathbf{R}}_2)_{1,J} \\ \vdots & \vdots & & \vdots \\ (\tilde{\mathbf{R}}_2)_{jj} & (\tilde{\mathbf{R}}_2)_{j,R+1} & \cdots & (\tilde{\mathbf{R}}_2)_{j,J} \end{bmatrix} = \mathbf{S} \mathbf{D} \mathbf{V}^T$$

be the SVD of $\bar{\mathbf{R}}_j$. Then $\bar{\mathbf{R}}_j \mathbf{V}$ is an orthogonal rotation of the columns of $\bar{\mathbf{R}}_j$ such that its first column has maximum sum-of-squares. The square root of this is equal to the dominant singular value of $\bar{\mathbf{R}}_j$. The rotation $\tilde{\mathbf{G}}_j$ can be obtained from \mathbf{V} .

Below, we present the steps of one sweep of the modified Jacobi algorithm.

ONE SWEEP OF THE MODIFIED JACOBI ALGORITHM FOR THE GSD PROBLEM.

Input: $I \times J \times 2$ array $\underline{\mathbf{Z}}$ with $I \times J$ slices \mathbf{Z}_k , $k = 1, 2$.

Previous GSD update: $\tilde{\mathbf{Q}}_a$ ($I \times I$) and $\tilde{\mathbf{Q}}_b$ ($J \times J$) orthonormal, and $\tilde{\mathbf{R}}_k$ ($I \times J$), $k = 1, 2$.

Output: New GSD update $\tilde{\mathbf{Q}}_a$, $\tilde{\mathbf{Q}}_b$, and $\tilde{\mathbf{R}}_k$, $k = 1, 2$.

1. (Do for $1 \leq i < j \leq R$.) Let \mathbf{G}_{ij} be equal to \mathbf{I}_I except for the entries $(\mathbf{G}_{ij})_{ii} = (\mathbf{G}_{ij})_{jj} = \cos \alpha$ and $(\mathbf{G}_{ij})_{ji} = -(\mathbf{G}_{ij})_{ij} = \sin \alpha$, where α is the rotation angle. Let $\tilde{\mathbf{G}}_{ij}$ be equal to \mathbf{I}_J and analogous to \mathbf{G}_{ij} for a rotation angle β . Using the Jacobi algorithm of [6], determine α and β such that the sum-of-squares of the upper triangular part of the first R rows and columns of $\mathbf{G}_{ij} \tilde{\mathbf{R}}_k \mathbf{G}_{ij}^T$, $k = 1, 2$ are maximal.

Update $\tilde{\mathbf{Q}}_a \rightarrow \tilde{\mathbf{Q}}_a \mathbf{G}_{ij}^T$, $\tilde{\mathbf{Q}}_b \rightarrow \tilde{\mathbf{Q}}_b \tilde{\mathbf{G}}_{ij}^T$, and $\tilde{\mathbf{R}}_k \rightarrow \mathbf{G}_{ij} \tilde{\mathbf{R}}_k \tilde{\mathbf{G}}_{ij}^T$, $k = 1, 2$.

2. (Do for $1 \leq i \leq R$.) Compute the SVD (7.4) and let s_{mn} denote the elements of \mathbf{S} . Let \mathbf{G}_i be equal to \mathbf{I}_I except $(\mathbf{G}_i)_{ii} = s_{11}$, $(\mathbf{G}_i)_{i,R+m} = s_{1,m+1}$ for $m = 1, \dots, I - R$, $(\mathbf{G}_i)_{R+m,i} = s_{m+1,1}$ for $m = 1, \dots, I - R$, and $(\mathbf{G}_i)_{mn} = s_{m-R+1,n-R+1}$ for $R + 1 \leq m, n \leq I$.

Update $\tilde{\mathbf{Q}}_a \rightarrow \tilde{\mathbf{Q}}_a \mathbf{G}_i^T$ and $\tilde{\mathbf{R}}_k \rightarrow \mathbf{G}_i \tilde{\mathbf{R}}_k$, $k = 1, 2$.

3. (Do for $1 \leq j \leq R$.) Compute the SVD (7.5) and let v_{mn} denote the elements of \mathbf{V}^T . Let \mathbf{G}_j be equal to \mathbf{I}_J except $(\mathbf{G}_j)_{jj} = v_{11}$, $(\mathbf{G}_j)_{j,R+m} = v_{1,m+1}$ for $m = 1, \dots, I - R$, $(\mathbf{G}_j)_{R+m,j} = v_{m+1,1}$ for $m = 1, \dots, I - R$, and $(\mathbf{G}_j)_{mn} = v_{m-R+1,n-R+1}$ for $R + 1 \leq m, n \leq I$.

Update $\tilde{\mathbf{Q}}_b \rightarrow \tilde{\mathbf{Q}}_b \mathbf{G}_j^T$ and $\tilde{\mathbf{R}}_k \rightarrow \tilde{\mathbf{R}}_k \tilde{\mathbf{G}}_j^T$, $k = 1, 2$.

8. Numerical experiments. Here, we illustrate the GSD method to avoid diverging CP components for generic $I \times J \times 2$ arrays. For each of the cases in Table 7.1, we randomly generate 50 arrays $\underline{\mathbf{Z}}$ of a chosen size. For each such $\underline{\mathbf{Z}}$, we use the (modified) Jacobi algorithm of De Lathauwer, De Moor, and Vandewall [6] to compute the optimal solution $\underline{\mathbf{X}}$ of the GSD problem (7.3), in terms of its full GSD representation $(\mathbf{Q}_a, \mathbf{Q}_b, \mathbf{R}_1, \mathbf{R}_2)$. The stopping criterion of the (modified) Jacobi algorithm is set to

TABLE 8.1

Types of optimal solutions encountered when solving the GSD problem (7.3) for randomly generated arrays $\underline{\mathbf{Z}}$ in the cases of Table 7.1. For each case, the value of (I, J, R) , the number of runs, and the average time to compute the GSD solution and the Jordan form of $\mathbf{R}_2\mathbf{R}_1^{-1}$ (on a Pentium 4 PC) are given. In all runs, the matrix $\mathbf{R}_2\mathbf{R}_1^{-1}$ has distinct eigenvalues $\lambda_1, \dots, \lambda_p, \mu_1, \dots, \mu_r$, where λ_j has algebraic multiplicity 1 and μ_i has algebraic multiplicity larger than 1 and geometric multiplicity 1. For each case, the number of solutions with the same (p, r) value are given.

Case, (I, J, R) , runs, time	(p, r)	Freq.	(p, r)	Freq.	(p, r)	Freq.	(p, r)	Freq.
Case 2 $(I, J, R) = (10, 10, 10)$ 48 runs, 58 sec.	(0,2)	4	(1,2)	7	(2,3)	2	(4,1)	3
	(0,3)	2	(1,3)	2	(3,1)	5	(4,2)	1
	(0,4)	2	(2,1)	2	(3,2)	4	(5,2)	1
	(1,1)	3	(2,2)	9	(3,3)	1		
Case 3 $(I, J, R) = (10, 10, 8)$ 49 runs, 12 sec.	(0,2)	5	(2,1)	1	(3,2)	5	(6,1)	1
	(1,1)	8	(2,2)	5	(4,1)	5		
	(1,2)	3	(2,3)	1	(4,2)	3		
	(1,3)	3	(3,1)	7	(5,1)	2		
Case 5 $(I, J, R) = (10, 10, 8)$ 50 runs, 32 sec.	(1,1)	2	(2,2)	2	(3,2)	6	(6,1)	15
	(1,3)	1	(2,3)	1	(4,2)	4	(8,0)	12
	(2,1)	1	(3,1)	2	(5,1)	4		
Case 8 $(I, J, R) = (10, 8, 8)$ 50 runs, 10 sec.	(0,2)	4	(1,2)	10	(3,1)	4	(4,2)	3
	(0,3)	2	(2,1)	1	(3,2)	2	(5,1)	2
	(1,1)	3	(2,2)	15	(4,1)	4		
Case 9 $(I, J, R) = (10, 8, 6)$ 49 runs, 3 sec.	(0,2)	4	(1,2)	7	(2,2)	4	(4,1)	9
	(1,1)	4	(2,1)	5	(3,1)	10	(6,0)	6

1e-9. Next, the Jordan normal form of $\mathbf{R}_2\mathbf{R}_1^{-1}$ is computed, which we denote as $\mathbf{J} = \text{diag}(\lambda_1, \dots, \lambda_p, \mathbf{J}_{m_1}(\mu_1), \dots, \mathbf{J}_{m_r}(\mu_r))$, where $\mathbf{J}_{m_j}(\mu_j)$ denotes an $m_j \times m_j$ Jordan block, with $m_j \geq 2$. Numerically, we treat two eigenvalues μ_1 and μ_2 as identical if $|\mu_1 - \mu_2| < 0.01$. The multiple eigenvalue μ is then estimated as the mean of all “identical” eigenvalues. The geometric multiplicity of an eigenvalue μ is determined as the number of singular values s_j of $(\mathbf{R}_2\mathbf{R}_1^{-1} - \mu \mathbf{I}_I)$ that satisfy $|s_j| < 0.0001$.

In the (modified) Jacobi algorithm, we use the following initial values for $(\mathbf{Q}_a, \mathbf{Q}_b, \mathbf{R}_1, \mathbf{R}_2)$. In Case 2 in Table 7.1, these are obtained from the “generalized real Schur decomposition” (GRSD) of \mathbf{Z}_1 and \mathbf{Z}_2 , which is computed by means of the QZ-method; see Golub and Van Loan [12]. In the other cases, the slices are first transformed to $\mathbf{U}_R^T \mathbf{Z}_k \mathbf{V}_R, k = 1, 2$, where \mathbf{U}_R contains the R dominant left singular vectors of $[\mathbf{Z}_1 | \mathbf{Z}_2]$ and \mathbf{V}_R contains the R dominant right singular vectors of $\begin{bmatrix} \mathbf{Z}_1 \\ \mathbf{Z}_2 \end{bmatrix}$. The initial values are then obtained from $\mathbf{U}_R, \mathbf{V}_R$ and the GRSD of $\mathbf{U}_R^T \mathbf{Z}_k \mathbf{V}_R, k = 1, 2$.

Table 8.1 summarizes the results of computing the optimal solutions $\underline{\mathbf{X}}$ of the GSD problem (7.3) and the Jordan forms of $\mathbf{R}_2\mathbf{R}_1^{-1}$. As can be seen, a wide variety of values (p, r) is encountered among the optimal solutions $\underline{\mathbf{X}}$. In a few of the 50 runs per case, some identical eigenvalues were not recognized. These runs do not appear in Table 8.1. In all runs in Table 8.1, the estimated eigenvalues $\lambda_1, \dots, \lambda_p, \mu_1, \dots, \mu_r$ are distinct. Hence, each μ_i has algebraic multiplicity larger than 1 and geometric multiplicity 1. As observed in Remark 3.2, this is probably due to the fact that the set of these arrays lies dense on the boundary of the set $\mathcal{P}_{(I, J, R)}$. For the solutions with $r \geq 1$, diverging CP components occur, and the GSD of the solution cannot be fully transformed into a CP solution. The solutions with $r = 0$ can be transformed into a nondiverging CP solution, i.e., diverging CP components do not occur.

As can be seen from Table 8.1, all runs in Cases 2, 3, and 8 have a solution with $r \geq 1$. For Case 2, this is in line with the conjecture of Stegeman [40] in Table 7.1. For Cases 3 and 8, this does not seem to support the conjectures of Stegeman [40] in Table 7.1, which state that diverging CP components occur on a set of positive volume (and not almost everywhere). However, trying different values of R in Case 3 yields 15 solutions with $r = 0$ (out of 50) for $R = 4$ and 3 solutions with $r = 0$ (out of 50) for $R = 6$. Hence, it seems that nondiverging CP solutions occur less frequently as R is increased. The same holds for Case 8, where we get 13 solutions with $r = 0$ (out of 50) for $R = J = 4$ and 5 solutions with $r = 0$ (out of 50) for $R = J = 6$. For Cases 5 and 9, there are both solutions with $r = 0$ as well as solutions with $r \geq 1$, which is in line with the conjectures of Stegeman [40] in Table 7.1.

Also listed in Table 8.1 are the average computational times (on a Pentium 4 PC) for the (modified) Jacobi algorithm to terminate and for the computation of the Jordan form of $\mathbf{R}_1 \mathbf{R}_1^{-1}$. For Case 2, this is 58 seconds. For comparison, we tried finding an approximate solution to the CP problem (3.2) for random \mathbf{Z} as in Case 2, by using the multilinear engine of Paatero [32]. For a convergence criterion of $1\text{e-}15$ over 1000 consecutive iterations, the algorithm terminated after 40 minutes. However, for the obtained approximate solution \mathbf{X} , the eigenvalues of $\mathbf{X}_2 \mathbf{X}_1^{-1}$ are all clearly distinct. On the other hand, running the Jacobi algorithm on the same \mathbf{Z} yields a solution with two groups of identical eigenvalues within 1 minute. Hence, to obtain an equally accurate estimate of the solution \mathbf{X} using a CP algorithm requires a very small stopping criterion and takes prohibitively long. This shows the spectacular improvement in efficiency when using the Jacobi GSD algorithm instead.

9. Discussion. We have proposed, analyzed, and demonstrated a method to avoid diverging components when trying to fit the CP model for generic $I \times J \times 2$ arrays and $R \leq I, J$ components. Instead of fitting the CP model, we fit the GSD model. The problems of diverging CP components are likely to occur because the CP model has no optimal solution in these cases. We showed that the GSD model always has an optimal solution. Moreover, the optimal GSD solution is the limit point of the sequence of CP updates, whether it features diverging components or not. Hereby we assume that the GSD model has a unique optimal solution (up to trivial indeterminacies) which is always satisfied in our numerical experiments. Also, we showed that the optimal GSD solution can be represented as the sum of the nondiverging CP components and a sparse Tucker3 part (CP+Jordan form) or as the sum of the nondiverging CP components and a smaller GSD part (CP+GSD form). The CP+Jordan form is essentially unique and sparse. Although it is not an outer-product decomposition, it may still be interpretable to the researcher. From the CP+Jordan representation, we can obtain a rank-revealing decomposition of the optimal GSD solution using the method of Ja' Ja' [21]. However, this decomposition is not essentially unique. The CP+GSD representation is numerically more stable and suitable if only the nondiverging CP components are of interest.

The GSD method not only yields an accurate solution, it is also much faster than trying to fit CP in the case of diverging components. Hence, to compute the CP solution for generic $I \times J \times 2$ arrays, it is advisable to compute the GSD solution instead and then transfer the nondiverging part of the solution into CP components. We may conclude that from a computational as well as a practical point of view, our method is a considerable improvement with respect to facing diverging CP components.

Our analysis is confined to arrays in the sets \mathcal{R}_I in (2.1) and $\mathcal{P}_{(I,J,R)}$ in (6.1). For a given array size, these sets are dense in the space of all arrays. The results

of our numerical experiments and those in Stegeman [38, 40], together with the fact that we consider generic arrays $\underline{\mathbf{Z}}$ to be approximated, lead us to conclude that this confinement is justified in practice. However, from a theoretical point of view, this leaves open the question whether the complement set of \mathcal{R}_I or $\mathcal{P}_{(I,J,R)}$ can contain all best rank- R approximations of a generic $I \times J \times 2$ array.

Stegeman [39] has mathematically analyzed diverging CP components occurring for several generic $I \times J \times 3$ arrays. Whether the SGSD method can also be used for arrays with three slices is currently under investigation.

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