A link between the decomposition of a third-order tensor in rank-(L,L,1) terms and simultaneous matrix diagonalization

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May 20, 2009

Abstract

The decompositions of a higher-order tensor in block components are new multilinear algebra tools introduced in [10, 11, 19], that generalize the Parallel Factor (PARAFAC) decomposition. In this paper, we focus on one of these recently introduced decompositions, the Block-Component-Decomposition in rank-(L,L,1) terms, referred to as BCD-(L,L,1). An Alternating Least Squares (ALS) algorithm was proposed in [19] for the computation of the BCD-(L,L,1) and a sufficient bound for which uniqueness of this decomposition is guaranteed was given in [11]. In this paper, we show that the BCD-(L,L,1) can be equivalently reformulated as a problem of Simultaneous Diagonalization (SD) of a set of matrices. This reformulation has two major advantages. First, the resulting SD-based algorithm reveals to be more accurate and less sensitive to ill-conditioned data than the standard ALS algorithm. Second, the SD-based reformulation of the BCD-(L,L,1) involves itself a new sufficient uniqueness bound. The latter bound is more relaxed than the one derived in [11], in the sense that the number of rank-(L,L,1) terms that can be extracted from the tensor is significantly greater, under a few conditions on the dimensions. The major part of this paper consists of the derivation of the analytic expression for this new bound.

Key words. Multilinear Algebra, Third-Order Tensor, PARAFAC decomposition, Block Component Decomposition, Uniqueness Bound, Simultaneous Matrix Diagonalization.

AMS subject classifications. 15A18, 15A69

1 Introduction

In an increasing number of problems in signal processing, data analysis and scientific computing, the data have a multi-way structure, i.e., the samples are indexed by three or more independent indices, giving rise to a higher-order tensor or multi-way array, rather than a matrix (two-way array). Exploitation of this structure requires the use of signal processing tools based on multilinear algebra rather than standard linear algebra [5, 8, 16].

The Tucker decomposition and Higher-Order-Singular-Value-Decomposition (HOSVD) [17, 42, 43] are possible generalization of the matrix SVD to higher-order tensors, that have been used for applications such as face recognition [45], or image and signal denoising [28]. The Parallel

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Factor (PARAFAC) decomposition [1, 21, 39] and the Canonical Decomposition (CANDECOMP) [3] consist of writing a higher-order tensor as a sum of rank-one tensors. In this sense, they are also higher-order generalizations of the matrix SVD.

Recently, a new class of tensor decompositions that generalize PARAFAC has been introduced [10,11,19], the so-called *Block-Component-Decompositions* (BCD). These decompositions allow to handle the case where a given tensor results from a sum of components that are more structured than rank-1 tensors. In this context, the main idea of the BCD framework is to replace the vectors in each rank-1 term of PARAFAC by blocks (matrices or higher-order tensors). For instance, these new decompositions have found applications where the direct use of PARAFAC was not appropriate [15, 29, 30].

In this paper, we focus on the *Block-Component-Decomposition in rank-(L,L,1) terms* of a third-order tensor, which we denote by BCD-(L,L,1) [11]. Each term of this decomposition is built from two rank-L matrices and one vector, instead of three vectors for PARAFAC. In [11], a sufficient condition for uniqueness of this decomposition has been derived, and an ALS algorithm was proposed in [19] to compute the BCD-(L,L,1).

The two main contributions of this paper are the following:

i) First, we show that the BCD-(L,L,1) can be reformulated as a problem of Simultaneous Diagonalization (SD) of a set of matrices. As we will illustrate by numerical experiments, the resulting SD-based algorithm is more accurate than the standard ALS algorithm proposed in [19], especially in presence of ill-conditioned data,

ii) In a second contribution, we show that this SD-based reformulation involves a new uniqueness bound that is more relaxed than the sufficient bound of [11]. The analytic expression of this new uniqueness bound will first be derived for the particular case $L = 2$, and then generalized to the case $L \geq 2$.

The paper is organized as follows. In Section 2, we introduce multilinear algebra prerequisites. In Section 3, we discuss the PARAFAC decomposition. In Section 4, we re-introduce the BCD-(L,L,1). In Section 5, we derive the starting point for the reformulation of the BCD-(L,L,1) in terms of simultaneous diagonalization. In Section 6, we introduce an algebraic tool for rank-L detection. In Section 7, we consider the particular case $L = 2$ and we use this tool to derive a SD-based algorithm for the computation of the BCD-(2,2,1). In Section 8, we derive the analytic expression for the new uniqueness bound that results from the SD-based reformulation of the BCD-(2,2,1). In Section 9, we extend the results of Sections 7 and 8 to any value of L. Section 10 illustrates the performance of the proposed SD-based algorithm and Section 11 is the conclusion.

Notation. A calligraphic letter $\mathcal{Y}$ denotes a third-order tensor and a bold-face capital letter $\mathbf{Y}$ denotes a matrix. Vectors are written in bold-face lower-case $\mathbf{y}$ and $\mathbf{y}_k$ indicates the kth column of $\mathbf{Y}$. Scalars are lower-case y. The scalar y_i indicates the ith element of vector $\mathbf{y}$ and the scalar y_{ij} denotes the element on the ith row and jth column of $\mathbf{Y}$. Capitals are also used to denote index upper bounds ($i = 1, 2, \ldots, I$) and matrix dimensions $\mathbf{Y}^{(I \times J)}$. The transpose, complex conjugate and complex conjugate transpose are denoted by $\mathbf{Y}^T$, $\mathbf{Y}^*$ and $\mathbf{Y}^H$, respectively, and the pseudo-inverse by $\mathbf{Y}^\dagger$. The determinant of $\mathbf{Y}$ is denoted by $|\mathbf{Y}|$. Furthermore, the operator vec($\mathbf{Y}$) builds a vector from a matrix by stacking the columns of this matrix one above the other such that the element y_{ij} of the $(I \times J)$ matrix $\mathbf{Y}$ becomes the element at position $i + (j-1)I$ of the vector vec($\mathbf{Y}$). The reciprocal operator is denoted by unvec($\mathbf{Y}$). If $\mathbf{Y}$ is partitioned along only one dimension, i.e., $\mathbf{Y}$ is an $(I \times RJ)$ or $(RI \times J)$ matrix, then the rth $(I \times J)$ block is denoted by $\mathbf{Y}_r$. The Kronecker product of the $I \times 1$ vector $\mathbf{a}$ and the $J \times 1$ vector $\mathbf{b}$ is the $IJ \times 1$ vector denoted by $\mathbf{a} \otimes \mathbf{b}$. More generally, we will use $(\otimes_{i=1}^{I} \mathbf{a}_i)$ to denote $\mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \cdots \otimes \mathbf{a}_I$. The quantity C_n^k is defined by $C_n^k = \frac{n!}{k!(n-k)!}$. We will also use a Matlab-type notation for matrix sub-blocks, i.e., $[\mathbf{Y}]_{l:m,n:p}$ represents the matrix built after selection of $m - l + 1$ rows of $\mathbf{Y}$, from the lth to the mth, and $p - n + 1$ columns of $\mathbf{Y}$, from the nth to the pth. $[\mathbf{Y}]_{:,n:p}$ is used to denote selection of all rows and $[\mathbf{Y}]_{l:m,:}$ to denote selection of all columns.

2 Multilinear algebra prerequisites

Definition 2.1. (Outer product) *The outer product* $(\mathcal{A} \circ \mathcal{B})$ *of a Pth-order tensor* $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \cdots \times I_P}$ *and a Qth-order tensor* $\mathcal{B} \in \mathbb{C}^{J_1 \times J_2 \times \cdots \times J_Q}$ *is the* $(P+Q)$*th-order tensor defined by*

$$(\mathcal{A} \circ \mathcal{B})_{i_1 i_2 \ldots i_P j_1 j_2 \ldots j_Q} = a_{i_1 i_2 \ldots i_P} b_{j_1 j_2 \ldots j_Q},$$

for all values of the indices.

For instance, the outer product $(\mathbf{a} \circ \mathbf{b} \circ \mathbf{c})$ of three vectors $\mathbf{a} \in \mathbb{C}^{I \times 1}$, $\mathbf{b} \in \mathbb{C}^{J \times 1}$ and $\mathbf{c} \in \mathbb{C}^{K \times 1}$, is a third-order tensor $\mathcal{T} \in \mathbb{C}^{I \times J \times K}$ with elements defined by $t_{ijk} = a_i b_j c_k$, for all values of the indices.

Definition 2.2. (Rank-1 Tensor) *The third-order tensor* $\mathcal{T} \in \mathbb{C}^{I \times J \times K}$ *is rank-1 if its elements can be written as* $t_{ijk} = a_i b_j c_k$*, where* $\mathbf{a} \in \mathbb{C}^{I \times 1}$, $\mathbf{b} \in \mathbb{C}^{J \times 1}$ *and* $\mathbf{c} \in \mathbb{C}^{K \times 1}$*. Equivalently, the third-order tensor* $\mathcal{T} \in \mathbb{C}^{I \times J \times K}$ *is rank-1 if it can be written as the outer product of three vectors, i.e.* $\mathcal{T} = \mathbf{a} \circ \mathbf{b} \circ \mathbf{c}$*.*

This definition generalizes the definition of a rank-1 matrix: $\mathbf{T} \in \mathbb{C}^{I \times J}$ has rank 1 if $\mathbf{T} = \mathbf{a} \cdot \mathbf{b}^T$.

Definition 2.3. (Mode-n product) *The mode-1 product of a third-order tensor* $\mathcal{T} \in \mathbb{C}^{L \times M \times N}$ *by a matrix* $\mathbf{A} \in \mathbb{C}^{I \times L}$*, denoted by* $\mathcal{T} \bullet_1 \mathbf{A}$*, is an* $(I \times M \times N)$*-tensor with elements defined, for all index values, by*

$$(\mathcal{T} \bullet_1 \mathbf{A})_{imn} = \sum_{l=1}^{L} t_{lmn} a_{il}.$$

Similarly, the mode-2 product by a matrix $\mathbf{B} \in \mathbb{C}^{J \times M}$ *and the mode-3 product by* $\mathbf{C} \in \mathbb{C}^{K \times N}$ *are the* $(L \times J \times N)$ *and* $(L \times M \times K)$ *tensors respectively, with elements defined by*

$$(\mathcal{T} \bullet_2 \mathbf{B})_{ljn} = \sum_{m=1}^{M} t_{lmn} b_{jm},$$

$$(\mathcal{T} \bullet_3 \mathbf{C})_{lmk} = \sum_{n=1}^{N} t_{lmn} c_{kn}.$$

In this notation, the matrix product $\mathbf{T} = \mathbf{U} \cdot \mathbf{S} \cdot \mathbf{V}^T$ takes the form of $\mathbf{T} = \mathbf{S} \bullet_1 \mathbf{U} \bullet_2 \mathbf{V}$.

Definition 2.4. (Tensor Rank) *The rank of* $\mathcal{T}$ *is defined as the minimum number of rank-1 tensors that yield* $\mathcal{T}$ *in a linear combination.*

Definition 2.5. (Kruskal Rank of a matrix) *The Kruskal rank of a matrix* $\mathbf{A}$*, denoted by* $k_{\mathbf{A}}$*, is defined as the maximal number* k *such that* ***any*** *set of* k *columns of* $\mathbf{A}$ *is linearly independent* [27].

Definition 2.6. (Frobenius Norm) *The Frobenius Norm of the tensor* $\mathcal{T} \in \mathbb{C}^{I \times J \times K}$ *is defined by*

$$\|\mathcal{T}\|_F = \sqrt{\sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} |t_{ijk}|^2}.$$

Definition 2.7. (Khatri-Rao Product) *The Khatri-Rao Product (KRP) [33]* $\mathbf{A} \odot \mathbf{B}$ *of two matrices* $\mathbf{A} \in \mathbb{C}^{I \times RM}$ *and* $\mathbf{B} \in \mathbb{C}^{J \times RN}$*, that are partitioned in* R *submatrices* $\mathbf{A}_r \in \mathbb{C}^{I \times M}$ *and* $\mathbf{B}_r \in \mathbb{C}^{J \times N}$*, respectively, is and* $(IJ \times RMN)$ *matrix defined by*

$$\mathbf{A} \odot \mathbf{B} = [\mathbf{A}_1 \otimes \mathbf{B}_1, \ldots, \mathbf{A}_R \otimes \mathbf{B}_R],$$

where $\otimes$ *denotes the Kronecker product.*

The Khatri-Rao product is also referred to as block-wise Kronecker product. In the particular case $M = N = 1$, the KRP resumes to a column-wise Kronecker product, which we denote $\odot_c$, i.e., $\mathbf{A} \odot_c \mathbf{B} = [\mathbf{a}_1 \otimes \mathbf{b}_1, \ldots, \mathbf{a}_R \otimes \mathbf{b}_R]$, where $\mathbf{a}_r$ and $\mathbf{b}_r$ denote the rth column of $\mathbf{A}$ and $\mathbf{B}$, respectively.

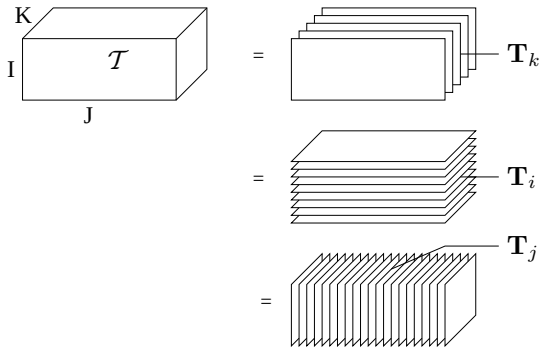


Figure 1: The three ways of matricizing a third-order tensor.

Definition 2.8. (Matrix representation of a third-order tensor) *The three standard matrix representations* $\mathbf{T}_{IK\times J}$, $\mathbf{T}_{JI\times K}$ *and* $\mathbf{T}_{KJ\times I}$ *of a third-order tensor* $\mathcal{T}\in\mathbb{C}^{I\times J\times K}$ *are the matrices of size* $(IK\times J)$, $(JI\times K)$ *and* $(KJ\times I)$, *respectively, defined by*

$$\left\{\begin{array}{lcl}(\mathbf{T}_{IK\times J})_{(i-1)K+k,j} & = & t_{ijk}\\ (\mathbf{T}_{JI\times K})_{(j-1)I+i,k} & = & t_{ijk}\\ (\mathbf{T}_{KJ\times I})_{(k-1)J+j,i} & = & t_{ijk}\end{array}\right. ,$$

for all values of the indices. Note that the matrices $\mathbf{T}_{IK\times J}$, $\mathbf{T}_{JI\times K}$ *and* $\mathbf{T}_{KJ\times I}$ *result from the row-wise concatenation of the* I *slices* $\mathbf{T}_i\in\mathbb{C}^{K\times J}$, *the* J *slices* $\mathbf{T}_j\in\mathbb{C}^{I\times K}$ *and the* K *slices* $\mathbf{T}_k\in\mathbb{C}^{J\times I}$, *respectively, as illustrated by Fig. 1.*

Definition 2.9. (Symmetric tensor) *An mth-order tensor* $\mathcal{T}$ *is symmetric if its elements satisfy* $(\mathcal{T})_{i_1,i_2,\ldots,i_m}=(\mathcal{T})_{i_{\Pi(1)},i_{\Pi(2)},\ldots,i_{\Pi(m)}}$ *for any permutation* Π *[7].*

Definition 2.10 (Completely anti-symmetric tensor) *An mth-order tensor is completely antisymmetric if it changes sign under the exchange of* ***any*** *pair of indices.*

Definition 2.11 (Anti-symmetric Kronecker product permutation matrix) *Let* $\mathbf{e}_i$ *be the* i*th column of the* $I\times I$ *identity matrix* $\mathbf{I}_I$. *The* L*th-order anti-symmetric Kronecker product permutation matrix* $\mathbf{\Delta}_I^{(L)}$, $L\leq I$, *is the* $I^L\times I^L$ *matrix defined by*

$$\mathbf{\Delta}_I^{(L)}=\frac{1}{L!}\sum_{i_1=1}^{I}\sum_{i_2=1}^{I}\cdots\sum_{i_L=1}^{I}\sum_{\sigma\in\Lambda_L}s(\sigma)\left(\otimes_{l=1}^{L}\mathbf{e}_{i_l}\cdot\mathbf{e}_{i_{\sigma(l)}}^T\right),$$

where Λ_L *is the set of* $L!$ *permutations of the elements* $\{1,2,\ldots,L\}$, σ *is a given permutation of this set,* $\sigma(l)$ *is the* l*th element of the corresponding permuted set, and* $s(\sigma)$ *is the signature of the permutation, i.e.,* $s(\sigma)=1$ *if* σ *is built from an even number of consecutive permutations of two elements in* $\{1,2,\ldots,L\}$, *and* $s(\sigma)=-1$ *otherwise.*

Definition 2.11 is similar to the one established in [35], where the symmetric case was considered, i.e., when $s(\sigma)$ is always equal to 1. As a particular case of Definition 2.11, we have

$$\begin{array}{rcl}\mathbf{\Delta}_I^{(3)} & = & \frac{1}{6}\sum_{i_1=1}^{I}\sum_{i_2=1}^{I}\sum_{i_3=1}^{I}\big(\mathbf{e}_{i_1}\cdot\mathbf{e}_{i_1}^T\otimes\mathbf{e}_{i_2}\cdot\mathbf{e}_{i_2}^T\otimes\mathbf{e}_{i_3}\cdot\mathbf{e}_{i_3}^T-\mathbf{e}_{i_1}\cdot\mathbf{e}_{i_1}^T\otimes\mathbf{e}_{i_2}\cdot\mathbf{e}_{i_3}^T\otimes\mathbf{e}_{i_3}\cdot\mathbf{e}_{i_2}^T\\ & & +\mathbf{e}_{i_1}\cdot\mathbf{e}_{i_2}^T\otimes\mathbf{e}_{i_2}\cdot\mathbf{e}_{i_3}^T\otimes\mathbf{e}_{i_3}\cdot\mathbf{e}_{i_1}^T-\mathbf{e}_{i_1}\cdot\mathbf{e}_{i_2}^T\otimes\mathbf{e}_{i_2}\cdot\mathbf{e}_{i_1}^T\otimes\mathbf{e}_{i_3}\cdot\mathbf{e}_{i_3}^T\\ & & +\mathbf{e}_{i_1}\cdot\mathbf{e}_{i_3}^T\otimes\mathbf{e}_{i_2}\cdot\mathbf{e}_{i_1}^T\otimes\mathbf{e}_{i_3}\cdot\mathbf{e}_{i_2}^T-\mathbf{e}_{i_1}\cdot\mathbf{e}_{i_3}^T\otimes\mathbf{e}_{i_2}\cdot\mathbf{e}_{i_2}^T\otimes\mathbf{e}_{i_3}\cdot\mathbf{e}_{i_1}^T\big).\end{array}$$

Property 2.12 *Let* $\mathbf{\Delta}_I^{(L)}$ *be the* $I^L\times I^L$ *anti-symmetric Kronecker product permutation matrix, and* $\{\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_L\}$ *be arbitrary* $I\times 1$ *vectors. Then, we have*

$$\mathbf{\Delta}_I^{(L)}\cdot(\otimes_{l=1}^{L}\mathbf{a}_l)=\frac{1}{L!}\sum_{\sigma\in\Lambda_L}s(\sigma)(\otimes_{l=1}^{L}\mathbf{a}_{\sigma(l)}).$$

Proof. The complete proof was established in [35] for the symmetric case. The proof for the anti-symmetric case follows directly from [35], since the only difference is the permutation signature term.

As a particular case of Property 2.12, we have

$$\begin{aligned}\boldsymbol{\Delta}_I^{(3)} \cdot (\mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3) &= \frac{1}{6}(\mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3 - \mathbf{a}_1 \otimes \mathbf{a}_3 \otimes \mathbf{a}_2 \\ &\quad +\mathbf{a}_2 \otimes \mathbf{a}_3 \otimes \mathbf{a}_1 - \mathbf{a}_2 \otimes \mathbf{a}_1 \otimes \mathbf{a}_3 \\ &\quad +\mathbf{a}_3 \otimes \mathbf{a}_1 \otimes \mathbf{a}_2 - \mathbf{a}_3 \otimes \mathbf{a}_2 \otimes \mathbf{a}_1).\end{aligned}$$

Property 2.12 will be useful in this paper to derive the analytic expression for a new sufficient uniqueness bound of the BCD-(L,L,1). More precisely, we will prove that $\text{rank}(\boldsymbol{\Delta}_I^{(L)}) = C_I^L$.

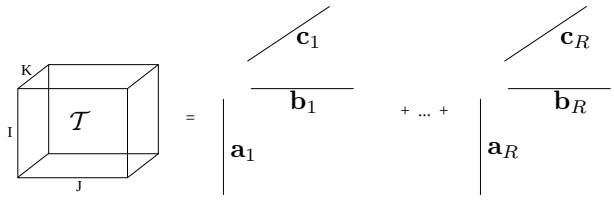


Figure 2: Schematic representation of the PARAFAC decomposition (third-order case).

3 PARAFAC decomposition

3.1 Principle

We now have enough material to introduce the PARAFAC decomposition.

Definition 3.1. (PARAFAC decomposition) *A Canonical or Parallel Factor Decomposition of a third-order tensor $\mathcal{T} \in \mathbb{C}^{I \times J \times K}$ is a decomposition of $\mathcal{T}$ as a linear combination of rank-1 terms:*

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

This decomposition is visualized in Fig. 2.

If the rank of $\mathcal{T}$ is R, its PARAFAC decomposition in R terms is *minimal*, i.e., $\mathcal{T}$ is decomposed as a linear combination of a minimal number of rank-1 terms. In this paper, we will only deal with minimal decompositions.

In terms of the standard matrix representations of $\mathcal{T}$, the PARAFAC decomposition can be written as:

$$\mathbf{T}_{IK \times J} = (\mathbf{A} \odot_c \mathbf{C}) \cdot \mathbf{B}^T, \tag{2}$$

$$\mathbf{T}_{JI \times K} = (\mathbf{B} \odot_c \mathbf{A}) \cdot \mathbf{C}^T, \tag{3}$$

$$\mathbf{T}_{KJ \times I} = (\mathbf{C} \odot_c \mathbf{B}) \cdot \mathbf{A}^T. \tag{4}$$

The decomposition of a tensor in a sum of rank-one tensors has a long history going back to Hitchcock in 1927 [22, 23]; but uniqueness was touched upon by Cattell in 1944 [4] and fleshed out by Harshman in 1970 [21]. Unlike the matrix-case, low-rank PARAFAC decomposition can be unique for rank higher than one, and this is a key strength of PARAFAC. Since 1970, PARAFAC has slowly found its way in various disciplines such as Chemometrics [39], exploratory data analysis [26], wireless communications and array processing [37, 38] and blind source separation [6, 13, 14].

3.2 Uniqueness

To a large extent, the practical importance of PARAFAC stems from its uniqueness properties. It is clear that one can arbitrarily permute the different rank-1 tensors of the sum. Also, the factors of a same rank-1 tensor may be arbitrarily scaled, as long as their outer-product remains the same. We call a PARAFAC decomposition *essentially unique* when it is only subject to these scaling and permutation ambiguities. In other words, the PARAFAC decomposition is *essentially unique* if any matrix triplet ($\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$) that also fits the model is linked to ($\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$) via

$$\mathbf{A} = \tilde{\mathbf{A}} \cdot \mathbf{\Pi} \cdot \mathbf{\Lambda}_1, \ \mathbf{B} = \tilde{\mathbf{B}} \cdot \mathbf{\Pi} \cdot \mathbf{\Lambda}_2, \ \mathbf{C} = \tilde{\mathbf{C}} \cdot \mathbf{\Pi} \cdot \mathbf{\Lambda}_3, \tag{5}$$

with $\mathbf{\Lambda}_1$, $\mathbf{\Lambda}_2$, $\mathbf{\Lambda}_3$ arbitrary diagonal matrices satisfying $\mathbf{\Lambda}_1 \cdot \mathbf{\Lambda}_2 \cdot \mathbf{\Lambda}_3 = \mathbf{I}_R$ and $\mathbf{\Pi}$ an arbitrary permutation matrix. The following theorem establishes a sufficient condition under which essential uniqueness is guaranteed.

Theorem 3.1: *The PARAFAC decomposition (1) is essentially unique if*

$$k_{\mathbf{A}} + k_{\mathbf{B}} + k_{\mathbf{C}} \geq 2R + 2. \tag{6}$$

This bound, known as Kruskal bound, was first proved for real third-order tensors in [27]. The result was generalized to tensors of arbitrary order in [36]. The overall proof was then reformulated in terms of accessible basic linear algebra in [40]. Note that (6) generically reduces to

$$\min(I, R) + \min(J, R) + \min(K, R) \geq 2R + 2. \tag{7}$$

(We call a property generic when it holds everywhere, except for a set of Lebesgue measure 0).

Recently, a new uniqueness bound for PARAFAC has been derived in [9,25]. This new sufficient bound, more relaxed than (7), is given by the following theorem.

Theorem 3.2: *The PARAFAC decomposition (1) is essentially unique, in the generic sense, if*

$$R \leq K \text{ and } \frac{1}{2}I(I-1)J(J-1) \geq R(R-1). \tag{8}$$

3.3 Algorithms

The R components of PARAFAC are usually estimated by minimization of the quadratic cost function

$$\phi(\mathbf{A}, \mathbf{B}, \mathbf{C}) = \|\mathcal{T} - \sum_{r=1}^{R} \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r\|^2. \tag{9}$$

This is most often achieved via the Alternating Least Squares (ALS) algorithm, in which $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are alternatingly updated in the least squares sense, from equations (2) to (4) [1, 38, 39]. Convergence of ALS is guaranteed, at least to a local minimum. In fact, the least squares conditional updates of a given matrix $\mathbf{A}$, $\mathbf{B}$ or $\mathbf{C}$, given previous updates of the two others, may either improve or maintain but cannot worsen the current fit to the model. However, convergence of ALS is sometimes slow and it is particularly sensitive to ill-conditioned data [24]. In addition, it is sometimes observed that the algorithm moves through a "swamp": the algorithm seems to converge, but then the convergence speed drastically decreases and remains small for several steps, after which it may suddenly increase again [34]. In order to escape from swamps quickly, a line search scheme can be inserted in the ALS loop [2, 21, 31, 32]. The optimization problem (9) can also be solved by a Newton type technique, such as the Levenberg-Marquardt algorithm [41].

In [18], an alternative to the aforementioned optimization techniques was proposed. It was shown that the PARAFAC decomposition can be calculated by means of simultaneous diagonalization of a set of matrices if *two* of the dimensions $\mathcal{T}$ are taller than its rank R. In [9], it was shown that SD can still be used if $\mathcal{T}$ is tall in one mode *only*, e.g. $R \leq \min(IJ, K)$. Apart from a new algorithm, the reformulation of PARAFAC in a SD problem proposed in [9] has led to the derivation of the new, and more relaxed, uniqueness bound given in Theorem 3.2.

The guideline of the work presented in this paper consists of the generalization of the results established for PARAFAC in [9] to the BCD-(L,L,1). In summary, we will first show that the BCD-(L,L,1) can be reformulated as a SD problem, after which we will demonstrate that this reformulation involves a new uniqueness bound, more relaxed than the sufficient bound derived in [11] for this decomposition. In the following section, we briefly reintroduce important results established in [10, 11, 19] for the BCD-(L,L,1).

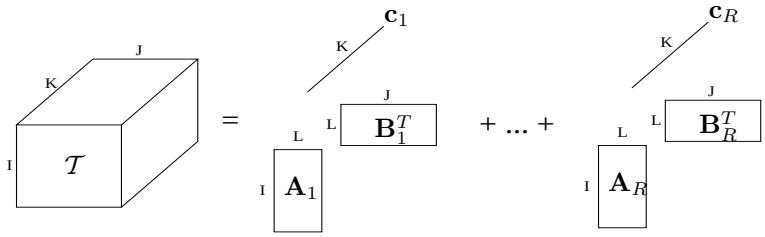


Figure 3: Visualization of the BCD-(L,L,1)

4 Decomposition in rank-(L,L,1) terms

4.1 Algebraic model

The PARAFAC decomposition of a third-order tensor $\mathcal{T}$ is a way to write this tensor as a sum of rank-1 tensors. The Block-Component-Decomposition in rank-(L,L,1) terms of $\mathcal{T}$ is more general than PARAFAC in the sense that the tensors that contribute to $\mathcal{T}$ do not consist of the outer product of three vectors, as stated by the following definition.

Definition 4.1. (Block Component Decomposition in rank-(L,L,1) terms) *The decomposition of a tensor $\mathcal{T} \in \mathbb{C}^{I \times J \times K}$ in a sum of rank-(L,L,1) terms is defined by*

$$\mathcal{T} = \sum_{r=1}^{R} (\mathbf{A}_r \cdot \mathbf{B}_r^T) \circ \mathbf{c}_r. \tag{10}$$

in which the $(I \times L)$ matrix $\mathbf{A}_r$ and the $(J \times L)$ matrix $\mathbf{B}_r$ are rank-L, $r = 1 \dots R$. This decomposition, introduced in [11], is visualized on Fig. 3.

Note that PARAFAC corresponds to the special case where $L = 1$ of the BCD-(L,L,1). If we define the rank-L matrices $\mathbf{X}_r \in \mathbb{C}^{I \times J}$, $r = 1, \dots, R$, by $\mathbf{X}_r = \mathbf{A}_r \cdot \mathbf{B}_r^T$, Eq. (10) is then equivalent to

$$\mathcal{T} = \sum_{r=1}^{R} \mathbf{X}_r \circ \mathbf{c}_r. \tag{11}$$

4.2 Matrix Representations of the model

Define the partitioned matrices $\mathbf{A} = [\mathbf{A}_1 \dots \mathbf{A}_R]$ of size $(I \times LR)$, $\mathbf{B} = [\mathbf{B}_1 \dots \mathbf{B}_R]$ of size $(J \times LR)$ and $\mathbf{C} = [\mathbf{c}_1 \dots \mathbf{c}_R]$ of size $(K \times R)$. In terms of the standard matrix representations of $\mathcal{T}$, (10) can be written as:

$$\mathbf{T}_{IK \times J} = (\mathbf{A} \odot \mathbf{C}) \cdot \mathbf{B}^T, \tag{12}$$

$$\mathbf{T}_{JI \times K} = [\mathrm{vec}(\mathbf{A}_1 \cdot \mathbf{B}_1^T), \dots, \mathrm{vec}(\mathbf{A}_R \cdot \mathbf{B}_R^T)] \cdot \mathbf{C}^T, \tag{13}$$

$$\mathbf{T}_{KJ \times I} = (\mathbf{C} \odot \mathbf{B}) \cdot \mathbf{A}^T. \tag{14}$$

4.3 Sufficient bounds for uniqueness

It is clear that in (10), one can arbitrarily permute the R different rank-(L,L,1) terms. Also, one can postmultiply $\mathbf{A}_r$ by any nonsingular $(L \times L)$ matrix $\mathbf{F}_r$, provided that $\mathbf{B}_r^T$ is premultiplied by $\mathbf{F}_r^{-1}$. Moreover, the factors of a same rank-(L,L,1) term may be arbitrarily scaled, as long as their product remains the same. We call the decomposition *essentially unique* when it is *only* subject to these indeterminacies.

In [11], it was established that essential uniqueness of the BCD-(L,L,1) is guaranteed, in the generic sense, if one of the following conditions is satisfied:

(i) $\min(I, J) \geq LR$ and $\mathbf{C}$ does not have proportional columns.

(ii) $K \geq R$ and $\min(\lfloor \frac{I}{L} \rfloor, R) + \min(\lfloor \frac{J}{L} \rfloor, R) \geq R + 2$.
(iii) $I \geq LR$ and $\min(\lfloor \frac{J}{L} \rfloor, R) + \min(K, R) \geq R + 2$
or $J \geq LR$ and $\min(\lfloor \frac{I}{L} \rfloor, R) + \min(K, R) \geq R + 2$.
(iv) $IJ \geq L^2 R$ and $\min(\lfloor \frac{I}{L} \rfloor, R) + \min(\lfloor \frac{J}{L} \rfloor, R) + \min(K, R) \geq 2R + 2$.

4.4 Algorithms

From the observation of the tensor $\mathcal{T}$ only, the calculation of its BCD-(L,L,1) consists of the estimation of the matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$, which is typically done by the minimization of the following quadratic cost function

$$\phi(\mathbf{A}, \mathbf{B}, \mathbf{C}) = \|\mathcal{T} - \sum_{r=1}^{R} (\mathbf{A}_r \cdot \mathbf{B}_r)^T \circ \mathbf{c}_r\|_F^2. \tag{15}$$

This can be achieved via the Alternating Least Squares (ALS) algorithm proposed in [19]. The principle of this algorithm is the same as for its PARAFAC counterpart, i.e., the least-squares update of $\mathbf{B}$, given previous estimates of $\mathbf{A}$ and $\mathbf{C}$, follows directly from Eq. (12), and so on.

In this paper, we propose another algorithmic strategy that starts from (11) and capitalizes on the rank-L property of $\mathbf{X}_r$, $r = 1, \ldots, R$. We will show that exploitation of this property leads to a simultaneous diagonalization problem. Apart from a new algorithm, we will also establish that this reformulation of the BCD-(L,L,1) allows the derivation of a new uniqueness bound.

5 Reformulation of the BCD-(L,L,1)

In this section, we show that, given several conditions on the dimensions, the BCD-(L,L,1) can be first rewritten under a matrix factorization problem. The latter is the starting point for the derivation of the SD-based technique, developed in Section 7 for $L = 2$ and generalized in Section 9 to $L \geq 2$.

5.1 Assumptions on the dimensions

Throughout the whole paper, we will assume that the two following conditions are satisfied.

- **Assumption 1(a):** the $K \times R$ matrix $\mathbf{C}$ is tall and full column-rank.

- **Assumption 1(b):** the $JI \times R$ matrix $\tilde{\mathbf{X}} \stackrel{def}{=} \left(\text{vec}(\mathbf{A}_1 \cdot \mathbf{B}_1^T), \ldots, \text{vec}(\mathbf{A}_R \cdot \mathbf{B}_R^T)\right)$ is tall and full column rank.

We first show that these conditions are both generically satisfied if

$$\min(IJ, K) \geq R. \tag{16}$$

Note that (16) implies that the "long" dimension of $\mathcal{Y}$, i.e. K, corresponds to the dimension of the rank-1 terms in the BCD-(L,L,1). The case where the long dimension is carried by one of the rank-L terms, i.e. $\min(IK, J) \geq R$ or $\min(JK, I) \geq R$, is outside the scope of this paper.

First, assuming (16) obviously guarantees that $\mathbf{C} \in \mathbb{C}^{K \times R}$ is generically rank-R. As stated by the following Lemma, (16) also guarantees that $\tilde{\mathbf{X}}$ is generically full column rank.

Lemma 5.1 *Consider $\mathbf{A} = [\mathbf{A}_1, \ldots, \mathbf{A}_R] \in \mathbb{C}^{I \times LR}$ and $\mathbf{B} = [\mathbf{B}_1, \ldots, \mathbf{B}_R] \in \mathbb{C}^{J \times LR}$, partitioned in $I \times L$ blocks $\mathbf{A}_r$ and $J \times L$ blocks $\mathbf{B}_r$, $r = 1 \ldots R$, respectively. Then, generically, we have*

$$\textit{rank}(\tilde{\mathbf{X}}) = \textit{min}(IJ, R),$$

where

$$\tilde{\mathbf{X}} \stackrel{def}{=} \left(\textit{vec}(\mathbf{A}_1 \cdot \mathbf{B}_1^T), \ldots, \textit{vec}(\mathbf{A}_R \cdot \mathbf{B}_R^T)\right).$$

Proof of Lemma 5.1 Denote $\tilde{R} = \text{rank}(\tilde{\mathbf{X}})$. Let us assume that $\tilde{R} < \min(IJ, R)$. The theorem follows from the observation that a generic perturbation of the vectors $\{\text{vec}(\mathbf{A}_r \cdot \mathbf{B}_r^T), r = 1 \ldots R\}$, makes the set linearly independent. Assume, without loss of generality, that the matrix $\mathbf{A}_1 \cdot \mathbf{B}_1^T$ lies in the vector space V generated by $\{\mathbf{A}_r \cdot \mathbf{B}_r^T, r = 2, 3, \ldots, R\}$. It suffices to prove that a generic perturbation of $\mathbf{A}_1 \cdot \mathbf{B}_1^T$ does not lie in V. We define the scalar product of two $I \times J$ matrices $\mathbf{A}$ and $\mathbf{B}$ as $\langle \mathbf{A}, \mathbf{B} \rangle = \sum_{i=1}^{I} \sum_{j=1}^{J} a_{ij} b_{ij}$. Let $\text{V}^\perp \in \mathbb{C}^{I \times J}$ be orthogonal to V, i.e., the scalar product of $\text{V}^\perp$ and any matrix in V is zero. We have $\left\langle \mathbf{A}_1 \cdot \mathbf{B}_1^T, \text{V}^\perp \right\rangle = 0$. Let the perturbed version of $\mathbf{A}_1 \cdot \mathbf{B}_1^T$ be denoted by $\tilde{\mathbf{A}}_1 \cdot \tilde{\mathbf{B}}_1^T$. Generically, $\left\langle \tilde{\mathbf{A}}_1 \cdot \tilde{\mathbf{B}}_1^T, \text{V}^\perp \right\rangle = \text{trace}\left(\tilde{\mathbf{A}}_1^T \cdot \text{V}^\perp \cdot \tilde{\mathbf{B}}_1\right)$ is different from 0, i.e., the perturbation has a component orthogonal to V. As a consequence $\text{vec}(\tilde{\mathbf{A}}_1 \cdot \tilde{\mathbf{B}}_1^T)$ has a component orthogonal to $\{\text{vec}(\mathbf{A}_r \cdot \mathbf{B}_r^T), r = 2, 3, \ldots, R\}$. ■

5.2 Reformulation of the BCD-(L,L,1) in terms of matrix factorizations

Let us now consider an $I \times J \times K$ tensor $\mathcal{T}$ and its decomposition in rank-$(L, L, 1)$ terms $\mathcal{T} = \sum_{r=1}^{R} \mathbf{X}_r \circ \mathbf{c}_r$, in which the $I \times J$ matrices $\mathbf{X}_r = \mathbf{A}_r \cdot \mathbf{B}_r^T$, $r = 1, \ldots, R$, are rank-L. From Eq. (13) the $JI \times K$ matrix reprensentation of $\mathcal{T}$ can be written as:

$$\left\{ \begin{array}{lcl} \mathbf{T}_{JI \times K} & = & \tilde{\mathbf{X}} \cdot \mathbf{C}^T, \\ \tilde{\mathbf{X}} & \stackrel{def}{=} & \left(\text{vec}(\mathbf{X}_1) \quad , \ldots, \quad \text{vec}(\mathbf{X}_R) \right), \\ \mathbf{X}_r & \stackrel{def}{=} & \mathbf{A}_r \cdot \mathbf{B}_r^T, \ r = 1, \ldots, R. \end{array} \right. \tag{17}$$

It is important to keep in mind that the $JI \times R$ matrix $\tilde{\mathbf{X}}$ has a particular structure, i.e., each column of $\tilde{\mathbf{X}}$ corresponds to the vectorized representation of a rank-L matrix $\mathbf{X}_r$. Exploitation of this structure is the core idea of the SD technique proposed in this paper.

From (16), and according to Lemma 5.1, the generic rank of $\tilde{\mathbf{X}} \in \mathbb{C}^{IJ \times R}$ and of $\mathbf{C} \in \mathbb{C}^{K \times R}$ is R. Thus, the generic rank of $\mathbf{T}_{JI \times K}$ in (17) is R. Consider then the economy size SVD of $\mathbf{T}_{JI \times K}$:

$$\mathbf{T}_{JI \times K} = \mathbf{U} \cdot \mathbf{\Sigma} \cdot \mathbf{V}^H, \tag{18}$$

in which $\mathbf{U} \in \mathbb{C}^{IJ \times R}$ and $\mathbf{V} \in \mathbb{C}^{K \times R}$ are column-wise orthonormal matrices and $\mathbf{\Sigma} \in \mathbb{C}^{R \times R}$ is positive diagonal. If we pose

$$\mathbf{E} \stackrel{def}{=} \mathbf{U} \cdot \mathbf{\Sigma}, \tag{19}$$

then we deduce from (17) and (18) that there exists an a priori unknown non-singular matrix $\mathbf{W} \in \mathbb{C}^{R \times R}$ that satisfies:

$$\left\{ \begin{array}{rcl} \tilde{\mathbf{X}} & = & \mathbf{E} \cdot \mathbf{W} \\ \mathbf{C}^T & = & \mathbf{W}^{-1} \cdot \mathbf{V}^H \end{array} \right. . \tag{20}$$

The estimation of the matrix $\mathbf{W}$ is sufficient to find $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$. Obviously, $\mathbf{C} = \mathbf{V}^* \cdot \mathbf{W}^{-T}$. Furthermore, the columns of $\mathbf{E} \cdot \mathbf{W}$ correspond to the vectorized representation of the rank-L matrices $\mathbf{X}_r = \mathbf{A}_r \cdot \mathbf{B}_r^T$. Thus, an estimate $\hat{\mathbf{A}}_r$ for $\mathbf{A}_r$ can be determined as the L dominant left singular vectors of $\mathbf{X}_r$ multiplied by the corresponding singular values, and an estimate $\hat{\mathbf{B}}_r$ for $\mathbf{B}_r$ corresponds to the conjugate L dominant right singular vectors. Of course, the true data matrices $\mathbf{A}_r$ and $\mathbf{B}_r$ to be estimated are not necessarily unitary. However, because of the intrinsic indeterminacies of the model (see Section 4.3), $\mathbf{X}_r$ can be written as

$$\mathbf{X}_r = \mathbf{A}_r \cdot \mathbf{B}_r^T = (\mathbf{A}_r \cdot \mathbf{F}_r) \cdot (\mathbf{F}_r^{-1} \cdot \mathbf{B}_r^T), \tag{21}$$

for any non-singular matrix $\mathbf{F}_r \in \mathbb{C}^{L \times L}$. Consequently, the matrices $\hat{\mathbf{A}}_r$ and $\hat{\mathbf{B}}_r$ given by the SVD technique correspond to an estimate for an orthogonal basis of the column-subspace of the true data matrices $\mathbf{A}_r$ and $\mathbf{B}_r$. This is an inherently unresolvable indeterminacy of the BCD-(L,L,1), i.e., the way the estimated basis vectors have to be linearly combined to yield $\mathbf{A}_r$ and $\mathbf{B}_r$ remains unknown in general. However, these degrees of freedom can possibly be reduced in practice if additional constraints specific to the application are available, e.g., when $\mathbf{A}$ and $\mathbf{B}$ have a particular structure (Toeplitz, Vandermonde, etc).

The task is now to find the matrix $\mathbf{W}$ in (20) that enforces the rank-L structure of all (unvectorized) columns of $\mathbf{E} \cdot \mathbf{W}$.

From the matrix $\mathbf{E} \in \mathbb{C}^{IJ \times R}$, we build the set of matrices $\mathbf{E}_1, \ldots, \mathbf{E}_R \in \mathbb{C}^{I \times J}$, defined by

$$\mathbf{E}_r = \text{unvec}([\mathbf{E}]_{:,r}), \ r = 1, \ldots, R. \tag{22}$$

We thus have

$$\begin{array}{rcl} \mathbf{E}_r & = & \text{unvec}([\tilde{\mathbf{X}} \cdot \mathbf{W}^{-1}]_{:,r}) \\ & = & \displaystyle\sum_{k=1}^{R} \mathbf{X}_k (\mathbf{W}^{-1})_{kr}. \end{array} \tag{23}$$

This means that the matrices $\mathbf{E}_r$ consist of linear combinations of the rank-L matrices $\mathbf{X}_k = \mathbf{A}_k \cdot \mathbf{B}_k^T$, $k = 1, \ldots, R$. Turned the other way around, we now have to find the linear combinations of the matrices $\mathbf{E}_r$ that yield rank-L matrices, because the coefficients of the linear combinations will yield the matrix $\mathbf{W}$ we are looking for.

In the following section, we introduce an algebraic tool for rank-L detection, that will be useful for the reformulation of the BCD-(L,L,1) in terms of simultaneous diagonalization.

6 Mapping for rank-L detection

6.1 Mapping for rank-1 detection

Theorem 6.1 Consider the mapping
$\Phi_1 : (\mathbf{X}, \mathbf{Y}) \in \mathbb{C}^{I\times J} \times \mathbb{C}^{I\times J} \mapsto \Phi_1(\mathbf{X}, \mathbf{Y}) \in \mathbb{C}^{I\times I\times J\times J}$ defined in [9]:

$$\begin{aligned}(\Phi_1(\mathbf{X},\mathbf{Y}))_{i_1i_2j_1j_2} &= x_{i_1j_1}y_{i_2j_2} + y_{i_1j_1}x_{i_2j_2} - x_{i_1j_2}y_{i_2j_1} - y_{i_1j_2}x_{i_2j_1} \\ &= \begin{vmatrix} x_{i_1j_1} & x_{i_1j_2} \\ y_{i_2j_1} & y_{i_2j_2} \end{vmatrix} + \begin{vmatrix} y_{i_1j_1} & y_{i_1j_2} \\ x_{i_2j_1} & x_{i_2j_2} \end{vmatrix}.\end{aligned}$$

Then, we have $\Phi_1(\mathbf{X}, \mathbf{X}) = \mathbf{0}$ if and only if $\mathbf{X}$ is at most rank-1.

Proof of Theorem 6.1. We refer to [9] for a complete proof. ∎

Properties of Φ_1. For any arbitrary $I \times J$ matrices $\mathbf{X}$ and $\mathbf{Y}$:
i) The entries of $\Phi_1(\mathbf{X}, \mathbf{Y})$ with indices $i_1 = i_2$ or $j_1 = j_2$ are all null,
ii) $(\Phi_1(\mathbf{X}, \mathbf{Y}))_{i_1i_2j_1j_2} = -(\Phi_1(\mathbf{X}, \mathbf{Y}))_{i_2i_1j_1j_2}$ and $(\Phi_1(\mathbf{X}, \mathbf{Y}))_{i_1i_2j_1j_2} = -(\Phi_1(\mathbf{X}, \mathbf{Y}))_{i_1i_2j_2j_1}$, since switching two rows or two columns changes the sign of the determinant,
iii) $\Phi_1(\mathbf{X}, \mathbf{Y}) = \Phi_1(\mathbf{Y}, \mathbf{X})$, i.e., Φ_1 is symmetric in its arguments,
iv) $\Phi_1(\alpha\mathbf{X} + \mathbf{Z}, \mathbf{Y}) = \alpha\Phi_1(\mathbf{X}, \mathbf{Y}) + \Phi_1(\mathbf{Z}, \mathbf{Y})$, for any arbitrary $I \times J$ matrix $\mathbf{Z}$ and arbitrary scalar α, i.e., Φ_1 is a multilinear form,
v) Furthermore, it is a matter of algebraic manipulations to show that, for arbitrary $I \times 1$ vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and arbitrary $J \times 1$ vectors $\mathbf{b}_1$, $\mathbf{b}_2$,

$$\begin{aligned}\mathcal{F}_1^{-1}(\Phi_1(\mathbf{a}_1 \cdot \mathbf{b}_1^T, \mathbf{a}_2 \cdot \mathbf{b}_2^T)) &= (\mathbf{a}_1 \otimes \mathbf{a}_2 - \mathbf{a}_2 \otimes \mathbf{a}_1) \otimes (\mathbf{b}_1 \otimes \mathbf{b}_2 - \mathbf{b}_2 \otimes \mathbf{b}_1) \\ &= \left(2\mathbf{\Delta}_I^{(2)} \cdot (\mathbf{a}_1 \otimes \mathbf{a}_2)\right) \otimes \left(2\mathbf{\Delta}_J^{(2)} \cdot (\mathbf{b}_1 \otimes \mathbf{b}_2)\right),\end{aligned}$$

where $\mathcal{F}_1$ is the bijective mapping of vectors in $\mathbb{C}^{I^2J^2}$ to tensors in $\mathbb{C}^{I\times I\times J\times J}$, defined by

$$(\mathcal{F}_1(\mathbf{x}))_{i_1i_2j_1j_2} = \mathbf{x}_{(i_1-1)IJ^2+(i_2-1)J^2+(j_1-1)J+j_2}.$$

From properties i) and ii), it is not necessary to check that the I^2J^2 entries of $\Phi_1(\mathbf{X}, \mathbf{X})$ are all null for $\mathbf{X}$ to be at most rank-1. It suffices that the $C_I^2C_J^2$ entries corresponding to indices $\{1 \le i_1 < i_2 \le I\} \cup \{1 \le j_1 < j_2 \le J\}$ all vanish. This is of practical interest, from the computational aspect, especially when dealing with long dimensions I and J.

The mapping for rank-1 detection given by Theorem 6.1 was used in [9] to reformulate the PARAFAC decomposition of a third-order tensor into a SD problem. In this paper we deal with the more general BCD-(L,L,1), thus we need a tool for rank-L detection. In the following, we first introduce a tool for rank-2 detection and then generalize to rank-L.

6.2 Mapping for rank-2 detection

Theorem 6.2 Consider the mapping
$\Phi_2 : (\mathbf{X}, \mathbf{Y}, \mathbf{Z}) \in \mathbb{C}^{I\times J} \times \mathbb{C}^{I\times J} \times \mathbb{C}^{I\times J} \to \Phi_2(\mathbf{X}, \mathbf{Y}, \mathbf{Z}) \in \mathbb{C}^{I\times I\times I\times J\times J\times J}$ defined by

$$\begin{aligned}(\Phi_2(\mathbf{X},\mathbf{Y},\mathbf{Z}))_{i_1i_2i_3j_1j_2j_3} &= \begin{vmatrix} x_{i_1j_1} & x_{i_1j_2} & x_{i_1j_3} \\ y_{i_2j_1} & y_{i_2j_2} & y_{i_2j_3} \\ z_{i_3j_1} & z_{i_3j_2} & z_{i_3j_3} \end{vmatrix} + \begin{vmatrix} x_{i_1j_1} & x_{i_1j_2} & x_{i_1j_3} \\ z_{i_2j_1} & z_{i_2j_2} & z_{i_2j_3} \\ y_{i_3j_1} & y_{i_3j_2} & y_{i_3j_3} \end{vmatrix} + \begin{vmatrix} y_{i_1j_1} & y_{i_1j_2} & y_{i_1j_3} \\ x_{i_2j_1} & x_{i_2j_2} & x_{i_2j_3} \\ z_{i_3j_1} & z_{i_3j_2} & z_{i_3j_3} \end{vmatrix} \\ &+ \begin{vmatrix} y_{i_1j_1} & y_{i_1j_2} & y_{i_1j_3} \\ z_{i_2j_1} & z_{i_2j_2} & z_{i_2j_3} \\ x_{i_3j_1} & x_{i_3j_2} & x_{i_3j_3} \end{vmatrix} + \begin{vmatrix} z_{i_1j_1} & z_{i_1j_2} & z_{i_1j_3} \\ x_{i_2j_1} & x_{i_2j_2} & x_{i_2j_3} \\ y_{i_3j_1} & y_{i_3j_2} & y_{i_3j_3} \end{vmatrix} + \begin{vmatrix} z_{i_1j_1} & z_{i_1j_2} & z_{i_1j_3} \\ y_{i_2j_1} & y_{i_2j_2} & y_{i_2j_3} \\ x_{i_3j_1} & x_{i_3j_2} & x_{i_3j_3} \end{vmatrix}.\end{aligned}$$

Then we have $\Phi_2(\mathbf{X},\mathbf{X},\mathbf{X}) = 0$ if and only if $\mathbf{X}$ is at most rank-2.

Proof of Theorem 6.2. The entries of $\Phi(\mathbf{X},\mathbf{X},\mathbf{X})/(3!)$ correspond to the determinants of the different (3×3) submatrices of $\mathbf{X}$. A necessary and sufficient condition for $\mathbf{X}$ to be at most rank-2, is that all these determinants vanish. ■

Properties of Φ_2. For any arbitrary $I \times J$ matrices $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$:

i) It is obvious that the entries of $\Phi_2(\mathbf{X},\mathbf{Y},\mathbf{Z})$ vanish as soon as two indices in the set $\{i_1,i_2,i_3\}$ are equal or two indices in the set $\{j_1,j_2,j_3\}$ are equal,

ii) Switching two indices in $\{i_1,i_2,i_3\}$ changes only the sign of $\Phi_2(\mathbf{X},\mathbf{Y},\mathbf{Z})$, and similarly for $\{j_1,j_2,j_3\}$, since switching two rows or columns changes the sign of the determinant,

iii) Φ_2 is symmetric in its arguments, i.e., Φ_2 is invariant under any permutation of its arguments $\{\mathbf{X},\mathbf{Y},\mathbf{Z}\}$,

iv) $\Phi_2(\alpha\mathbf{X}+\mathbf{Z},\mathbf{Y},\mathbf{W}) = \alpha\Phi_2(\mathbf{X},\mathbf{Y},\mathbf{W}) + \Phi_2(\mathbf{Z},\mathbf{Y},\mathbf{W})$, for any arbitrary $I \times J$ matrix $\mathbf{Z}$ and arbitrary scalar α, i.e., Φ_2 is a multilinear form,

v) Furthermore, it is a matter of algebraic manipulations to show that, for arbitrary $I \times 1$ vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ and arbitrary $J \times 1$ vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$,

$$\mathcal{F}_2^{-1}(\Phi_2(\mathbf{a}_1\cdot\mathbf{b}_1^T,\mathbf{a}_2\cdot\mathbf{b}_2^T,\mathbf{a}_3\cdot\mathbf{b}_3^T)) \;=\; \left(6\boldsymbol{\Delta}_I^{(3)}\cdot(\mathbf{a}_1\otimes\mathbf{a}_2\otimes\mathbf{a}_3)\right)\otimes\left(6\boldsymbol{\Delta}_J^{(3)}\cdot(\mathbf{b}_1\otimes\mathbf{b}_2\otimes\mathbf{b}_3)\right),$$

where $\mathcal{F}_2$ is the bijective mapping of vectors in $\mathbb{C}^{I^3J^3}$ to tensors in $\mathbb{C}^{I\times I\times I\times J\times J\times J}$:

$$(\mathcal{F}(\mathbf{x}))_{i_1i_2i_3j_1j_2j_3} = \mathbf{x}_{(i_1-1)I^2J^3+(i_2-1)IJ^3+(i_3-1)J^3+(j_1-1)J^2+(j_2-1)J+j_3}.$$

From properties i) and ii), it is not necessary to check that the I^3J^3 entries of $\Phi_2(\mathbf{X},\mathbf{X},\mathbf{X})$ are all null for $\mathbf{X}$ to be at most rank-2. It suffices that the $C_I^3C_J^3$ entries corresponding to indices $\{1 \le i_1 < i_2 < i_3 \le I\} \cup \{1 \le j_1 < j_2 < j_3 \le J\}$ all vanish. Similarly, for arbitrary matrices $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$, it suffices to compute the $C_I^3C_J^3$ entries of $\Phi_2(\mathbf{X},\mathbf{Y},\mathbf{Z})$ corresponding to these indices, since the remaining entries are then directly deduced.

6.3 Mapping for rank-L detection

Theorem 6.3 *Consider the mapping*

$$\begin{aligned}\Phi_L \;:\; (\mathbf{X}^{(1)},\mathbf{X}^{(2)},\ldots,\mathbf{X}^{(L+1)}) &\in (\mathbb{C}^{I\times J},\mathbb{C}^{I\times J},\ldots,\mathbb{C}^{I\times J})\\ \rightarrow\quad \Phi_L(\mathbf{X}^{(1)},\mathbf{X}^{(2)},\ldots,\mathbf{X}^{(L+1)}) &\in \mathbb{C}^{\overbrace{I\times I\times\cdots\times I}^{L+1\,times}\times\overbrace{J\times J\times\cdots\times J}^{L+1\,times}}\end{aligned}$$

defined by

$$(\Phi_L(\mathbf{X}^{(1)},\mathbf{X}^{(2)},\ldots,\mathbf{X}^{(L+1)}))_{i_1i_2\ldots i_{L+1}j_1j_2\cdots j_{L+1}} = \sum_{\sigma\in\Lambda_{L+1}}\begin{vmatrix} x_{i_1j_1}^{\sigma(1)} & x_{i_1j_2}^{\sigma(1)} & \cdots & x_{i_1j_{L+1}}^{\sigma(1)}\\ x_{i_2j_1}^{\sigma(2)} & x_{i_2j_2}^{\sigma(2)} & \cdots & x_{i_2j_{L+1}}^{\sigma(2)}\\ \vdots & \vdots & & \vdots\\ x_{i_{L+1}j_1}^{\sigma(L+1)} & x_{i_{L+1}j_2}^{\sigma(L+1)} & \cdots & x_{i_{L+1}j_{L+1}}^{\sigma(L+1)}\end{vmatrix},$$

where Λ_{L+1} is the set of $(L+1)!$ permutations of elements $\{1,2,\ldots,L+1\}$, σ is a given permutation of this set, and $x_{i_1j_1}^{\sigma(1)}$ is the element of $\mathbf{X}^{\sigma(1)}$ on i_1th row and j_1th column. Then we have $\Phi_L(\mathbf{X},\mathbf{X},\ldots,\mathbf{X}) = 0$ if and only if $\mathbf{X}$ is at most rank-L.

Proof of Theorem 6.3. The entries of $\Phi_L(\mathbf{X},\mathbf{X},\ldots,\mathbf{X})/(L+1)!$ correspond to the determinants of the different $(L+1)\times(L+1)$ submatrices of $\mathbf{X}$. A necessary and suffcient condition for

$\mathbf{X}$ to be at most rank-L, is that all these determinants vanish. ■

Properties of Φ_L. For any arbitrary $I \times J$ matrices $\mathbf{X}^{(1)}$, $\mathbf{X}^{(2)}$, ..., $\mathbf{X}^{(L+1)}$:

i) The entries of $\Phi_L(\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(L+1)})$ vanish as soon as two indices in the set $\{i_1, i_2, \ldots, i_{L+1}\}$ are equal or two indices in the set $\{j_1, j_2, \ldots, j_{L+1}\}$ are equal,

ii) Switching two indices in $\{i_1, i_2, \ldots, i_{L+1}\}$ changes only the sign of $\Phi_L(\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(L+1)})$, and similarly for $\{j_1, j_2, \ldots, j_{L+1}\}$, since switching two rows or columns changes the sign of the determinant,

iii) Φ_L is symmetric in its arguments, i.e., Φ_L is invariant under any permutation of its arguments $\{\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(L+1)}\}$,

iv) $\Phi_L(\alpha\mathbf{X}^{(1)} + \mathbf{Z}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(L+1)}) = \alpha\Phi_L(\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(L+1)}) + \Phi_L(\mathbf{Z}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(L+1)})$, for any arbitrary $I \times J$ matrix $\mathbf{Z}$ and arbitrary scalar α, i.e., Φ_L is a multilinear form,

v) Furthermore, it is a matter of algebraic manipulations to show that, for arbitrary $I \times 1$ vectors $\mathbf{a}_1$, $\mathbf{a}_2$, ..., $\mathbf{a}_{L+1}$ and arbitrary $J \times 1$ vectors $\mathbf{b}_1$, $\mathbf{b}_2$, ..., $\mathbf{b}_{L+1}$,

$$\mathcal{F}_L^{-1}(\Phi_L(\mathbf{a}_1 \cdot \mathbf{b}_1^T, \mathbf{a}_2 \cdot \mathbf{b}_2^T, \ldots, \mathbf{a}_{L+1} \cdot \mathbf{b}_{L+1}^T)) \quad = \quad \left((L+1)!\boldsymbol{\Delta}_I^{(L+1)} \cdot (\otimes_{l=1}^{L+1}\mathbf{a}_l)\right) \otimes \left((L+1)!\boldsymbol{\Delta}_J^{(L+1)} \cdot (\otimes_{l=1}^{L+1}\mathbf{b}_l)\right),$$

where $\mathcal{F}_L$ is the bijective mapping of vectors in $\mathbb{C}^{I^{L+1}J^{L+1}}$ to tensors in $\mathbb{C}^{I \times \cdots \times I \times J \times \cdots \times J}$:

$$(\mathcal{F}_L(\mathbf{x}))_{i_1 i_2 \ldots i_{L+1} j_1 j_2 \ldots j_{L+1}} = \mathbf{x}_{(i_1-1)I^L J^{L+1} + (i_2-1)I^{L-1}J^{L+1} + \cdots + (i_{L+1}-1)J^{L+1} + (j_1-1)J^L + \cdots + (j_L-1)J + j_{L+1}}.$$

From properties i) and ii), it follows that only the $C_I^{L+1}C_J^{L+1}$ entries of $\Phi_L(\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(L+1)})$ corresponding to indices $\{1 \leq i_1 < i_2 < \cdots < i_{L+1} \leq I\} \cup \{1 \leq j_1 < j_2 < \cdots < j_{L+1} \leq J\}$ have to be computed, since the remaining entries, if needed, can be deduced from these entries.

In the following, we use the tool for rank-L detection introduced in this section to show that the matrix $\mathbf{W}$ we are seeking for can be found by solving a problem of simultaneous diagonalization of a set of matrices. Since the derivation of this technique requires several algebraic manipulations, we first consider the particular case $L = 2$ in Section 7. The generalization to $L \geq 2$ will follow in the subsequent sections.

7 Simultaneous Diagonalization technique with $L = 2$

7.1 Derivation of the technique

In this section, we use the mapping Φ_2 for rank-2 detection to establish a link between the BCD-(2,2,1) and simultaneous diagonalization.

From the known matrices $\mathbf{E}_r = \sum_{k=1}^{R} \mathbf{X}_k (\mathbf{W}^{-1})_{kr}$ of Eq. (23), we first build the following set of R^3 tensors $\{\mathcal{P}_{rst}\}_{r,s,t\in[1,R]}$:

$$\mathcal{P}_{rst} = \Phi_2(\mathbf{E}_r, \mathbf{E}_s, \mathbf{E}_t). \tag{24}$$

Since Φ_2 is trilinear, we have :

$$\mathcal{P}_{rst} = \sum_{u,v,w=1}^{R} (\mathbf{W}^{-1})_{ur}(\mathbf{W}^{-1})_{vs}(\mathbf{W}^{-1})_{wt}\Phi_2\left(\mathbf{X}_u,\ \mathbf{X}_v,\ \mathbf{X}_w\right). \tag{25}$$

Assume at this point that there exists a symmetric third-order tensor $\mathcal{M} \in \mathbb{C}^{R\times R\times R}$ of which the entries m_{rst} satisfy the following set of homogeneous linear equations (we will justify this assumption below):

$$\sum_{r,s,t=1}^{R} m_{rst}\mathcal{P}_{rst} = 0. \tag{26}$$

Substitution of (25) in (26) yields:

$$\sum_{r,s,t=1}^{R}\sum_{u,v,w=1}^{R} (\mathbf{W}^{-1})_{ur}(\mathbf{W}^{-1})_{vs}(\mathbf{W}^{-1})_{wt}m_{rst}\Phi_2\left(\mathbf{X}_u,\ \mathbf{X}_v,\ \mathbf{X}_w\right) \quad = \quad 0. \tag{27}$$

According to Theorem 6.2, we have $\Phi_2\left(\mathbf{X}_u,\ \mathbf{X}_u,\ \mathbf{X}_u\right) = 0$, $1 \leqslant u \leqslant R$, which corresponds to the set of trivial solutions of (27). The non-trivial solutions satisfy

$$\sum_{r,s,t=1}^{R}\sum_{\substack{u,w,w=1\\ \neg(u=v=w)}}^{R} (\mathbf{W}^{-1})_{ur}(\mathbf{W}^{-1})_{vs}(\mathbf{W}^{-1})_{wt}m_{rst}\Phi_2\left(\mathbf{X}_u,\ \mathbf{X}_v,\ \mathbf{X}_w\right) \quad = \quad 0. \tag{28}$$

Furthermore, due to the symmetry of Φ_2 and $\mathcal{M}$, Eq. (28) can be written as:

$$\begin{array}{rl} & \sum_{r,s,t=1}^{R}\sum_{\substack{u,v=1\\ u<v}}^{R} 3\,(\mathbf{W}^{-1})_{ur}(\mathbf{W}^{-1})_{us}(\mathbf{W}^{-1})_{vt}m_{rst}\Phi_2\left(\mathbf{X}_u,\ \mathbf{X}_u,\ \mathbf{X}_v\right) \\ + & \sum_{r,s,t=1}^{R}\sum_{\substack{u,v=1\\ u<v}}^{R} 3\,(\mathbf{W}^{-1})_{ur}(\mathbf{W}^{-1})_{vs}(\mathbf{W}^{-1})_{vt}m_{rst}\Phi_2\left(\mathbf{X}_u,\ \mathbf{X}_v,\ \mathbf{X}_v\right) \\ + & \sum_{r,s,t=1}^{R}\sum_{\substack{u,v,w=1\\ u<v<w}}^{R} 6\,(\mathbf{W}^{-1})_{ur}(\mathbf{W}^{-1})_{vs}(\mathbf{W}^{-1})_{wt}m_{rst}\Phi_2\left(\mathbf{X}_u,\ \mathbf{X}_v,\ \mathbf{X}_w\right) \quad = \quad 0. \end{array} \tag{29}$$

Define the set Ω that holds the $C_{R+2}^3 - R$ tensors involved in (29):

$$\Omega = \{\Phi_2\left(\mathbf{X}_u,\ \mathbf{X}_v,\ \mathbf{X}_w\right) | \, 1 \leq u \leq v \leq w \leq R\} \backslash \{\Phi_2\left(\mathbf{X}_u,\ \mathbf{X}_u,\ \mathbf{X}_u\right) | 1 \leqslant u \leqslant R\}. \tag{30}$$

We make the crucial assumption that Ω is linearly independent.

As we will show in Section 8, this assumption implies a new bound on R that guarantees uniqueness of the BCD-(2,2,1). If the tensors of the set Ω are linearly independent, then (29) is satisfied if all the coefficients of the linear combinations of these tensors vanish. Finally, the trivial and non-trivial solutions of (26) can be written as:

$$\sum_{r,s,t=1}^{R} (\mathbf{W}^{-1})_{ur}(\mathbf{W}^{-1})_{vs}(\mathbf{W}^{-1})_{wt}m_{rst} \quad = \quad \lambda_{uvw}\delta_{uv}\delta_{vw} \qquad \forall u, v, w, \tag{31}$$

in which δ is the Kronecker delta ($\delta_{uv} = 1$ if $u = v$, $\delta_{uv} = 0$ if $u \neq v$) and λ_{uvw} is an arbitrary scalar.

Eq. (31) can be rewritten in tensor format as follows:

$$\mathcal{M} = \mathcal{D} \bullet_1 \mathbf{W} \bullet_2 \mathbf{W} \bullet_3 \mathbf{W}, \tag{32}$$

in which $\mathcal{D} \in \mathbb{C}^{R \times R \times R}$ is a diagonal tensor whose diagonal elements are arbitrary scalars λ_{uuu}, $u \in [1, R]$.

It can be verified that *any* symmetric tensor $\mathcal{M}$ of the form (32), with $\mathcal{D}$ an arbitrary diagonal tensor, satisfies (26). Note that linearly independent choices of $\mathcal{D}$ (of which diagonal entries are arbitrary) correspond to linearly independent solutions of (26). We conclude that if the set Ω is linearly independent, the kernel of (26) yields R linearly independent symmetric tensors $\mathcal{M}_r$, which can all be decomposed as in (32). We have:

$$\left\{ \begin{array}{rcl} \mathcal{M}_1 & = & \mathcal{D}_1 \bullet_1 \mathbf{W} \bullet_2 \mathbf{W} \bullet_3 \mathbf{W} \\ & \vdots & \\ \mathcal{M}_R & = & \mathcal{D}_R \bullet_1 \mathbf{W} \bullet_2 \mathbf{W} \bullet_3 \mathbf{W} \end{array} \right. , \tag{33}$$

in which $\mathcal{D}_1, \ldots, \mathcal{D}_R$ are diagonal. In terms of the matrix slices of $\mathcal{M}_1$, ..., $\mathcal{M}_R$, the set of R equations in (33) leads to the following set of R^2 equations:

$$\left\{ \begin{array}{rcll} (\mathcal{M}_1)_{:,:,r} & = & \mathbf{W} \cdot \mathbf{\Lambda}_{1,r} \cdot \mathbf{W}^T & \\ & \vdots & & \forall r \in [1, R] \, , \\ (\mathcal{M}_R)_{:,:,r} & = & \mathbf{W} \cdot \mathbf{\Lambda}_{R,r} \cdot \mathbf{W}^T & \end{array} \right. \tag{34}$$

in which $\mathbf{\Lambda}_{1,r}$, ..., $\mathbf{\Lambda}_{R,r}$, $1 \leqslant r \leqslant R$, are diagonal.

Finally $\mathbf{W}$ can be found by solving the simultaneous matrix diagonalization problem of the form (34). This can be done by means of the algorithms presented in, e.g., [12, 18, 44, 46]. The comparison between these algorithms is outside the scope of this paper. In Section 7.2.2, we will show that the set of R^2 matrices to be simultaneously diagonalized can be reduced to a set of R matrices only.

7.2 Computational aspect

7.2.1 Computation of symmetric tensors $\mathcal{M}_r$, $r = 1 \ldots R$

In this paragraph, we show how the R symmetric tensors $\mathcal{M}_r$ that are solutions of Eq. (26) can be computed in a numerically reliable way.

Let us stack the R^3 tensors $\mathcal{P}_{rst} \in \mathbb{C}^{I \times I \times I \times J \times J \times J}$, with $r, s, t \in [1, R]$, into a matrix $\mathbf{P} \in \mathbb{C}^{I^3 J^3 \times R^3}$, of which each column holds an $I^3 J^3$ vectorized representation of a given tensor $\mathcal{P}_{rst}$, i.e., $\mathcal{F}_2^{-1}(\Phi_2(\mathbf{E}_r, \mathbf{E}_s, \mathbf{E}_t))$. Then, (26) can be written as

$$\mathbf{P} \cdot \mathbf{m} = \mathbf{0}_{R^3}, \tag{35}$$

where $\mathbf{m}$ is an $R^3 \times 1$ vector that holds the entries m_{rst} of $\mathcal{M}$.

As explained in Section 6.2, it is indeed only necessary to build the $C_I^3 C_J^3$ rows of $\mathbf{P}$ corresponding to indices $\{1 \leq i_1 < i_2 < i_3 \leq I\} \cup \{1 \leq j_1 < j_2 < j_3 \leq J\}$ since the remaining rows are either redundant rows up to the sign (i.e., rows obtained by switching two indices in $\{i_1, i_2, i_3\}$ or in $\{j_1, j_2, j_3\}$) or null rows (if two indices in $\{i_1, i_2, i_3\}$ or in $\{j_1, j_2, j_3\}$ are equal).

Thus, the R tensors $\mathcal{M}_r$ can be built from the R right singular vectors of the $C_I^3 C_J^3 \times R^3$ reduced matrix $\bar{\mathbf{P}}$ associated to the R least significant singular values. However, if we choose R independent vectors in the kernel of $\bar{\mathbf{P}}$, there is no guarantee that the R^3 coefficients m_{rst} of each vector correspond to the entries of a symmetric tensor. For instance, it can be checked that any completely anti-symmetric tensor $\mathcal{M}$ is also solution of (26).

Let us show how symmetric solutions only can be found. Due to the symmetry of $\mathcal{M}$ and Φ_2, we can rewrite (26), after vectorization, as follows:

$$\mathcal{F}_2^{-1}(\sum_{r=1}^{R}\mathcal{P}_{rrr}m_{rrr}+3\sum_{\substack{r,s=1\\ r\neq s}}^{R}\mathcal{P}_{rrs}m_{rrs}+6\sum_{\substack{r,s,t=1\\ r<s<t}}^{R}\mathcal{P}_{rst}m_{rst})=\mathbf{0}_N, \tag{36}$$

where $N=C_R^1+2C_R^2+C_R^3=C_{R+2}^3$ is the number of tensors in the following set

$$\mathrm{G}=\{\mathcal{P}_{rrr}|\,1\leq r\leq R\}\cup\{3\,\mathcal{P}_{rrs}|\,1\leqslant r\neq s\leqslant R\}\cup\{6\,\mathcal{P}_{rst}|1\leqslant r<s<t\leqslant R\}. \tag{37}$$

Let us build the $C_I^3C_J^3\times C_{R+2}^3$ matrix $\tilde{\mathbf{P}}$ of which each column $\tilde{\mathbf{p}}_{rst}$ holds the $C_I^3C_J^3$ useful entries of $\alpha_{rst}\mathcal{F}_2^{-1}(\mathcal{P}_{rst})$, $\mathcal{P}_{rst}\in\mathrm{G}$, where α_{rst} takes values $\{1,3,6\}$, according to the values of indices r,s,t.

Eq. (35) can then be written in the equivalent compact form

$$\tilde{\mathbf{P}}\cdot\tilde{\mathbf{m}}=\mathbf{0}_N, \tag{38}$$

where $\tilde{\mathbf{m}}\in\mathbb{C}^{N\times 1}$ holds the N entries (out of R^3) that are necessary to build the symmetric tensor $\mathcal{M}$.

For instance, in the particular case $R=3$, (38) takes the form

$$(\tilde{\mathbf{p}}_{111},\tilde{\mathbf{p}}_{222},\tilde{\mathbf{p}}_{333},\tilde{\mathbf{p}}_{112},\tilde{\mathbf{p}}_{113},\tilde{\mathbf{p}}_{221},\tilde{\mathbf{p}}_{223},\tilde{\mathbf{p}}_{331},\tilde{\mathbf{p}}_{332},\tilde{\mathbf{p}}_{123})\cdot\begin{pmatrix}m_{111}\\ m_{222}\\ \vdots\\ m_{123}\end{pmatrix}=\begin{pmatrix}0\\ 0\\ \vdots\\ 0\end{pmatrix}.$$

Finally, the R symmetric tensors $\mathcal{M}_r$ are built from the R right singular vectors of $\tilde{\mathbf{P}}$ associated to the R lowest singular values. In summary, instead of computing the Kernel of an $I^3J^3\times R^3$ matrix $\mathbf{P}$, we only need to compute the Kernel of the $C_I^3C_J^3\times C_{R+2}^3$ reduced-size matrix $\tilde{\mathbf{P}}$ to build the set of R symmetric tensors $\mathcal{M}_r$.

7.2.2 Reduction of the number of matrices in (34)

In (34), $\mathbf{W}\in\mathbb{C}^{R\times R}$ can be found from simultaneous diagonalization of a set of R^2 matrices. However, each of these R^2 matrices is generated by the following set consisting of R rank-1 matrices $\{\mathbf{w}_r\cdot\mathbf{w}_r^T|1\leq r\leq R\}$. As a consequence, the R^2 matrices are linearly dependent and the simultaneous diagonalization algorithm can therefore be applied on a single set of R matrices instead of R^2. The task is then to select the R "most significant" matrices in (34). This is done by building the $R^2\times R^2$ matrix $[vec\,((\mathcal{M}_1)_{:,:,1})\ldots vec\,((\mathcal{M}_R)_{:,:,R})]$, from which the R left dominant singular vectors of size $R^2\times 1$ are selected. These vectors are then restacked into the new set $\{\check{\mathbf{M}}_1,\ldots,\check{\mathbf{M}}_R\}$ consisting of R symmetric matrices to be diagonalized.

The resulting SD-based technique for the computation of the BCD-(2,2,1) is given by Algorithm 1. In the very last step of this algorithm, we have inserted an ALS final refinement stage coupled with Enhanced Line Search (ELS) [31], initialized with the estimates of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ obtained from the SD stage. As we will illustrate through experimental results in Section 10, the number of ALS+ELS iterations needed in this final stage is small, which confirms that the SD stage provides a solution that is very close to the final least squares solution.

7.3 Conclusion of Section 7

In this section, we have shown that, in the particular case $L=2$, the BCD-(L,L,1) can be reformulated as a simultaneous diagonalization problem of a set of R matrices. The assumptions for this reformulation to be possible are:

Algorithm 1 SD-based algorithm for the decomposition in rank-(2,2,1) terms

• Stack the entries of $\mathcal{T}$ in an $(IJ \times K)$ matrix $\mathbf{T}_{JI\times K}$.
• Compute SVD $\mathbf{T}_{JI\times K} = \mathbf{U}\cdot\mathbf{\Sigma}\cdot\mathbf{V}^H = \mathbf{E}\cdot\mathbf{V}^H$.
• For $r = 1,\ldots,R$, stack the rth column of $\mathbf{E}$ in an $(I \times J)$ matrix $\mathbf{E}_r$.
• Build the $C_I^3 C_J^3 \times C_{R+2}^3$ matrix $\tilde{\mathbf{P}}$.
• Estimate the Kernel of $\tilde{\mathbf{P}}$ from the R right singular vectors associated with the R lowest singular values.
• The R symmetric tensors $\mathcal{M}_r$ are then built from the entries of these R vectors.
• Build the set of R^2 symmetric matrices of size $R \times R$ from the slices of the tensors $\mathcal{M}_r$, and select the R most significant $\check{\mathbf{M}}_r$.
• Estimate $\mathbf{W}$ by joint-diagonalization of the system

$$\left\{\begin{array}{rcl} \check{\mathbf{M}}_1 &=& \mathbf{W}\cdot\mathbf{\Lambda}_1\cdot\mathbf{W}^T \\ \check{\mathbf{M}}_2 &=& \mathbf{W}\cdot\mathbf{\Lambda}_2\cdot\mathbf{W}^T \\ &\vdots& \\ \check{\mathbf{M}}_R &=& \mathbf{W}\cdot\mathbf{\Lambda}_R\cdot\mathbf{W}^T \end{array}\right. \tag{39}$$

• Once $\mathbf{W}$ is known, the estimates of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are found as follows (see Section 5):
(a) Compute $\mathbf{C} = \mathbf{V}^*\cdot\mathbf{W}^{-T}$,
(b) Compute $\tilde{\mathbf{X}} = \mathbf{E}\cdot\mathbf{W}$. The rth column of $\tilde{\mathbf{X}}$ is an estimate of $\mathrm{vec}(\mathbf{A}_r\cdot\mathbf{B}_r^T)$. Apply unvec and compute the SVD of the so-obtained estimate of $\mathbf{X}_r = \mathbf{A}_r\cdot\mathbf{B}_r^T$. An estimate of $\mathbf{A}_r$ consists of the L dominant left singular vectors of $\mathbf{X}_r$ multiplied by the corresponding singular values. An estimate of $\mathbf{B}_r$ consists of the conjugate L dominant right singular vectors. Repeat this procedure for $r = 1,\ldots,R$.
• Final ALS+ELS refinement stage, initialized with the estimates of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ provided by the SD-based stage.

- **Assumptions 1(a) and 1(b) :** $\mathbf{C}$ and $\tilde{\mathbf{X}}$ are full-column rank, which is generically satisfied if $\min(IJ, K) \geq R$ (see Section 5),
- **Assumption 2 :** the set Ω defined in (30) is linearly independent.

In Section 8, we now examine the conditions for which linear independence of Ω is generically guaranteed. We will show that these conditions correspond to a new sufficient uniqueness bound for the BCD-(2,2,1).

In Section 8.1, we will emphasize the existence of this new bound through several numerical experiments. In Section 8.2, we will derive the analytic expression for this new bound. Generalization of this bound to any value of L will be addressed in Section 9.

8 A new uniqueness bound for the BCD-(2,2,1)

8.1 Numerical results

Under the assumption $\min(IJ, K) \geq R$, a sufficient generic condition that guarantees essential uniqueness of the BCD-(L,L,1) is given by (ii) in Section 4.3:

$$K \geq R \text{ and } \min(\left\lfloor \frac{I}{L} \right\rfloor, R) + \min(\left\lfloor \frac{J}{L} \right\rfloor, R) \geq R + 2. \tag{40}$$

The SD-based technique derived in the previous section for the particular case $L = 2$ relies on the crucial assumption that the set Ω defined in (30) is linearly independent. In this paragraph, we proceed to the following experiment: we set $L = 2$ and for given values of I, J and K that satisfy $\min(IJ, K) \geq R$, we look for the maximum value of R, such that the set $\mathbf{\Omega}$ is still numerically linearly independent. To test whether Ω is linearly independent, we build the $(I^3J^3 \times C^3_{R+2} - R)$ matrix $\bar{\mathbf{\Omega}}$ of which each column is an $I^3J^3 \times 1$ vectorized representation of a given tensor $\Phi_2(\mathbf{X}_u,\ \mathbf{X}_v,\ \mathbf{X}_w) \in \Omega$ and we compute the rank of $\bar{\mathbf{\Omega}}$. The maximum value of R thus obtained is then compared to the maximum value of R such that (40) is satisfied. The results are summarized in Table 1, which clearly indicates the existence of a new, more relaxed, uniqueness bound.

I	J	K	Bound 1	Bound 2
3	4	40	1	2
3	5	40	1	3
3	6	40	1	4
3	7	40	1	5
4	4	40	2	4
4	5	40	2	5
4	6	40	3	7
4	7	40	3	8
5	5	40	2	7
5	6	40	3	9
5	7	40	3	11
5	8	40	4	14

I	J	K	Bound 1	Bound 2
6	6	40	4	12
6	7	40	4	15
6	8	40	5	17
6	9	40	5	20
7	7	40	4	18
7	8	40	5	21
7	9	40	5	25
7	10	40	6	28
8	8	40	6	25
8	9	40	6	29
8	10	40	7	33
8	11	40	7	37

Table 1: Uniqueness bounds for the BCD-(2,2,1). Bound 1: maximum value of R that satisfies (40). Bound 2: maximum value of R such that Ω is linearly independent.

8.2 Analytic derivation of the new bound

In this section, we derive conditions that generically guarantee linear independence of the set Ω. We start with several preliminary Lemmas.

8.2.1 Preliminary Lemmas

Lemma 8.1 *Let $\mathbf{v}_1, \ldots, \mathbf{v}_M$ be linearly independent vectors in $\mathbb{C}^{N^3}$. Let $\mathbf{c}_1, \ldots, \mathbf{c}_R$ be vectors in $\mathbb{C}^N$, $N \geq 2$. If*

$$R \leq N - 1 \quad \textit{and} \quad (C^3_{R+2} - R) + M \leq N^3, \tag{41}$$

then the vectors $\mathbf{v}_m$, $1 \leq m \leq M$, and the $C^3_{R+2} - R$ vectors of the set

$$\Gamma_R \stackrel{def}{=} \{(\mathbf{c}_u \otimes \mathbf{c}_v \otimes \mathbf{c}_w) |\ 1 \leq u \leq v \leq w \leq R\ \} \backslash \{(\mathbf{c}_u \otimes \mathbf{c}_u \otimes \mathbf{c}_u) |\ 1 \leq u \leq R\ \}$$

are linearly independent for a generic choice of $\mathbf{c}_r$, $1 \leq r \leq R$.

Proof of Lemma 8.1 Define the sets

$V \stackrel{def}{=} \{\mathbf{v}_m | 1 \leq m \leq M\}$, and

$\Gamma_{R-1} = \{(\mathbf{c}_u \otimes \mathbf{c}_v \otimes \mathbf{c}_w) |\ 1 \leq u \leq v \leq w \leq R-1\ \} \backslash \{(\mathbf{c}_u \otimes \mathbf{c}_u \otimes \mathbf{c}_u) |\ 1 \leq u \leq R-1\ \}$.

The set Γ_R holds $C_{R+2}^3 - R$ vectors and the set Γ_{R-1} holds $C_{R+1}^3 - R + 1$ vectors. The proof is by induction. We first show that the lemma holds for $R = 2$. Then we show that, assuming that the lemma holds for $(M, R-1)$, it still holds for (M, R) if (41) is satisfied.

(i) Initialization ($R = 2$).

Let $V^\perp \in \mathbb{C}^{N^3}$ be orthogonal to the vectors in V. To initialize the induction, it suffices to show that $(\mathbf{c}_1 \otimes \mathbf{c}_1 \otimes \mathbf{c}_2)$ and $(\mathbf{c}_1 \otimes \mathbf{c}_2 \otimes \mathbf{c}_2)$ are linearly independent and both have components in the direction of $V^\perp$. The $N \times 2$ matrix $[\mathbf{c}_1, \mathbf{c}_2]$ is generically full column rank since we assumed $R \leq N - 1 < N$. By a property of the Kronecker product, $[\mathbf{c}_1, \mathbf{c}_2] \otimes [\mathbf{c}_1, \mathbf{c}_2] \otimes [\mathbf{c}_1, \mathbf{c}_2]$ is also generically full column rank. Thus, the vectors $(\mathbf{c}_1 \otimes \mathbf{c}_1 \otimes \mathbf{c}_2)$ and $(\mathbf{c}_1 \otimes \mathbf{c}_2 \otimes \mathbf{c}_2)$, which are two columns of the latter matrix, are linearly independent. Let us define a third-order tensor $\mathcal{V}^\perp \in \mathbb{C}^{N \times N \times N}$ by $(\mathcal{V}^\perp)_{n1,n2,n3} = (V^\perp)_{(n1-1)N^2+(n2-1)N+n3}$. Then we have $(\mathbf{c}_1 \otimes \mathbf{c}_1 \otimes \mathbf{c}_2)^T \cdot V^\perp = \mathcal{V}^\perp \bullet_1 \mathbf{c}_2 \bullet_2 \mathbf{c}_2 \bullet_3 \mathbf{c}_1$ and $(\mathbf{c}_1 \otimes \mathbf{c}_2 \otimes \mathbf{c}_2)^T \cdot V^\perp = \mathcal{V}^\perp \bullet_1 \mathbf{c}_1 \bullet_2 \mathbf{c}_1 \bullet_3 \mathbf{c}_2$, which are indeed generically different from zero.

(ii) Now we prove the induction step.

We suppose that the set $V \cup \Gamma_R$ is linearly dependent. We prove by contradiction that the set becomes linearly independent by a generic perturbation of the vector $\mathbf{c}_R$.

The matrix $[\mathbf{c}_1, \ldots, \mathbf{c}_R]$, of size $N \times R$, is generically full column rank since we assumed $R \leq N - 1 < N$ in (41). By a property of the Kronecker product, $[\mathbf{c}_1, \ldots, \mathbf{c}_R] \otimes [\mathbf{c}_1, \ldots, \mathbf{c}_R] \otimes [\mathbf{c}_1, \ldots, \mathbf{c}_R]$ is also generically full column rank. The set Γ_R, consisting of a selection of the columns of the latter matrix, is thus linearly independent. Let now $\mathbf{c}_R$ be replaced by a vector $\tilde{\mathbf{c}}_R$ that is not proportional to $\mathbf{c}_R$. The set Γ_R is consistently replaced by $\tilde{\Gamma}_R$. Suppose that $V \cup \tilde{\Gamma}_R$ is still linearly dependent. Generically, we may assume that $\mathbf{v}_1$ can be written as a linear combination of the vectors in $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_R$. We may also assume that $\mathbf{v}_1$ is a linear combination of the vectors in $(V \backslash \{\mathbf{v}_1\}) \cup \tilde{\Gamma}_R$. In other words, $\mathbf{v}_1$ is in the intersection of the subspaces W and $\tilde{W}$ generated by $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_R$ and $(V \backslash \{\mathbf{v}_1\}) \cup \tilde{\Gamma}_R$, respectively. W equals the sum of the subspace generated by $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_{R-1}$ and the subspace $\{\Gamma_R \backslash \Gamma_{R-1}\}$ generated by $\{(\mathbf{c}_u \otimes \mathbf{c}_R \otimes \mathbf{c}_R) |\ 1 \leq u \leq R-1\ \} \cup \{(\mathbf{c}_v \otimes \mathbf{c}_v \otimes \mathbf{c}_R) |\ 1 \leq v \leq R-1\ \} \cup \{(\mathbf{c}_u \otimes \mathbf{c}_v \otimes \mathbf{c}_R) | 1 \leq u < v \leq R-1\}$. $\tilde{W}$ equals the sum of the subspace generated by $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_{R-1}$ and the subspace $\{\tilde{\Gamma}_R \backslash \Gamma_{R-1}\}$ generated by $\{(\mathbf{c}_u \otimes \tilde{\mathbf{c}}_R \otimes \tilde{\mathbf{c}}_R) |\ 1 \leq u \leq R-1\ \} \cup \{(\mathbf{c}_v \otimes \mathbf{c}_v \otimes \tilde{\mathbf{c}}_R) |\ 1 \leq v \leq R-1\ \} \cup \{(\mathbf{c}_u \otimes \mathbf{c}_v \otimes \tilde{\mathbf{c}}_R) | 1 \leq u < v \leq R-1\}$. W can not be equal to $\mathbb{C}^{N^3}$ since $\dim(W) \leq M - 1 + C_{R+2}^3 - R < N^3$; neither can $\tilde{W}$ be equal to $\mathbb{C}^{N^3}$. The vectors of the set $\{\Gamma_R \backslash \Gamma_{R-1}\} \cup \{\tilde{\Gamma}_R \backslash \Gamma_{R-1}\}$ consist of a selection of the columns of the $N^3 \times 2(R+1)^2$ matrix $\mathbf{P} = [\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_R, \tilde{\mathbf{c}}_R] \otimes [\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_R, \tilde{\mathbf{c}}_R] \otimes [\mathbf{c}_R, \tilde{\mathbf{c}}_R]$. Both matrices $[\mathbf{c}_R, \tilde{\mathbf{c}}_R]$ and $[\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_R, \tilde{\mathbf{c}}_R]$ are generically full column rank since we assumed $R \leq N-1$, so by a property of the Kronecker product, the tall matrix $\mathbf{P}$ is generically full column-rank. It follows that the vectors of the set $\{\Gamma_R \backslash \Gamma_{R-1}\} \cup \{\tilde{\Gamma}_R \backslash \Gamma_{R-1}\}$ are linearly independent. We conclude that the intersection of W and $\tilde{W}$ is equal to the subspace generated by $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_{R-1}$. Since $\mathbf{v}_1$ is in the intersection of W and $\tilde{W}$, it is a linear combination of the vectors in $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_{R-1}$. This means that the set $V \cup \Gamma_{R-1}$ is linearly dependent.

As a conclusion, if $V \cup \Gamma_R$ is supposed to be linearly dependent, then $V \cup \Gamma_{R-1}$ is linearly dependent. By induction, if $V \cup \Gamma_{R-1}$ is linearly independent, then $V \cup \Gamma_R$ is linearly independent, which concludes the proof. ■

We now have the following Lemma.

Lemma 8.2 *Let $\mathbf{v}_1, \ldots, \mathbf{v}_M$ be linearly independent vectors in $\mathbb{C}^{I^3 J^3}$. Let $\mathbf{a}_1, \ldots, \mathbf{a}_R$ be vectors in $\mathbb{C}^I$ and let $\mathbf{b}_1, \ldots, \mathbf{b}_R$ be vectors in $\mathbb{C}^J$. If*

$$R \leq IJ - 1 \quad \textit{and} \quad (C_{R+2}^3 - R) + M \leq I^3 J^3, \tag{42}$$

then the vectors $\mathbf{v}_m$, $1 \leq m \leq M$, *and the* $C_{R+2}^3 - R$ *vectors of the set* $\{(\mathbf{a}_u \otimes \mathbf{b}_u \otimes \mathbf{a}_v \otimes \mathbf{b}_v \otimes \mathbf{a}_w \otimes \mathbf{b}_w) |\ 1 \leq u \leq v \leq w \leq R\ \} \backslash \{(\mathbf{a}_u \otimes \mathbf{b}_u \otimes \mathbf{a}_u \otimes \mathbf{b}_u \otimes \mathbf{a}_u \otimes \mathbf{b}_u) |\ 1 \leq u \leq R\ \}$ *are linearly independent for a generic choice of* $\mathbf{a}_r$ *and* $\mathbf{b}_r$, $1 \leq r \leq R$.

Proof of Lemma 8.2 The proof is analogous to the proof of Lemma 8.1. The role of $[\mathbf{c}_1, \ldots, \mathbf{c}_R]$ is now played by $[\mathbf{a}_1 \otimes \mathbf{b}_1, \ldots, \mathbf{a}_R \otimes \mathbf{b}_R]$. ■

Finally, we will also need the following preliminary Lemma.

Lemma 8.3 *Let* $\boldsymbol{\Delta}_I^{(3)}$ *be the* $I^3 \times I^3$ *anti-symmetric Kronecker product permutation matrix (see definition 2.11). Then, we have rank*$(\boldsymbol{\Delta}_I^{(3)}) = C_I^3$.

Proof of Lemma 8.3 Let $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ be $I \times 1$ arbitrary vectors. From property 2.12, we have:

$$\boldsymbol{\Delta}_I^{(3)} \cdot (\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}) = \frac{1}{6}[(\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}) - (\mathbf{a} \otimes \mathbf{c} \otimes \mathbf{b}) + (\mathbf{b} \otimes \mathbf{c} \otimes \mathbf{a}) - (\mathbf{b} \otimes \mathbf{a} \otimes \mathbf{c}) + (\mathbf{c} \otimes \mathbf{a} \otimes \mathbf{b}) - (\mathbf{c} \otimes \mathbf{b} \otimes \mathbf{a})]. \quad (43)$$

First, we notice that $(\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}) - (\mathbf{a} \otimes \mathbf{c} \otimes \mathbf{b}) + (\mathbf{b} \otimes \mathbf{c} \otimes \mathbf{a}) - (\mathbf{b} \otimes \mathbf{a} \otimes \mathbf{c}) + (\mathbf{c} \otimes \mathbf{a} \otimes \mathbf{b}) - (\mathbf{c} \otimes \mathbf{b} \otimes \mathbf{a})$ is a completely antisymmetric tensor (under vectorized form). Thus, $\boldsymbol{\Delta}_I^{(3)}$ maps a rank-1 tensor $(\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c})$ into a completely antisymmetric tensor. Since any linear combination of completely antisymmetric tensors is a completely antisymmetric tensor, $\boldsymbol{\Delta}_I^{(3)}$ maps any tensor into a completely antisymmetric tensor. The third-order completely antisymmetric $I \times I \times I$ tensors form an C_I^3-dimensional space, hence the rank of $\boldsymbol{\Delta}_I^{(3)}$ is *at most* C_I^3.

Let us now prove that the rank of $\boldsymbol{\Delta}_I^{(3)}$ is *at least* C_I^3. We denote by $\mathbf{e}_l$ the lth column of the $I \times I$ identity matrix. We define the set of C_I^3 vectors $E = \{(\mathbf{e}_l \otimes \mathbf{e}_m \otimes \mathbf{e}_n) | 1 \leq l < m < n \leq I\}$. A given $I^3 \times 1$ vector $(\mathbf{e}_l \otimes \mathbf{e}_m \otimes \mathbf{e}_n)$ holds only one non-zero entry, the element 1 at position $p = (l-1)I^2 + (m-1)I + n$. Thus, $\boldsymbol{\Delta}_I^{(3)} \cdot (\mathbf{e}_l \otimes \mathbf{e}_m \otimes \mathbf{e}_n)$ is the pth column of $\boldsymbol{\Delta}_I^{(3)}$. We now show that the subset of C_I^3 columns of $\boldsymbol{\Delta}_I^{(3)}$ defined by $\bar{E} = \{\boldsymbol{\Delta}_I^{(3)} \cdot (\mathbf{e}_l \otimes \mathbf{e}_m \otimes \mathbf{e}_n) | 1 \leq l < m < n \leq I\}$ is linearly independent. The vectors of $\bar{E}$ can be written as

$$\begin{array}{rcl} \bar{\mathbf{e}}_{l,m,n} & \stackrel{def}{=} & \boldsymbol{\Delta}_I^{(3)} \cdot (\mathbf{e}_l \otimes \mathbf{e}_m \otimes \mathbf{e}_n) \\ & = & \frac{1}{6}[(\mathbf{e}_l \otimes \mathbf{e}_m \otimes \mathbf{e}_n) - (\mathbf{e}_l \otimes \mathbf{e}_n \otimes \mathbf{e}_m) + (\mathbf{e}_m \otimes \mathbf{e}_n \otimes \mathbf{e}_l) \\ & & -(\mathbf{e}_m \otimes \mathbf{e}_l \otimes \mathbf{e}_n) + (\mathbf{e}_n \otimes \mathbf{e}_l \otimes \mathbf{e}_m) - (\mathbf{e}_n \otimes \mathbf{e}_m \otimes \mathbf{e}_l)]. \end{array} \quad (44)$$

For any given triplet (l_1, m_1, n_1), $\bar{\mathbf{e}}_{l_1,m_1,n_1}$ holds six non-zero elements, including a non-zero element at position $p_1 = (l_1 - 1)I^2 + (m_1 - 1)I + n_1$. Obviously, none of the $C_I^3 - 1$ vectors of the set $\bar{E} \backslash \{\bar{\mathbf{e}}_{l_1,m_1,n_1}\}$ can have a non-zero element at position p_1 since $\bar{\mathbf{e}}_{l_1,m_1,n_1}$ is the only vector of $\bar{E}$ built from $(\mathbf{e}_{l_1} \otimes \mathbf{e}_{m_1} \otimes \mathbf{e}_{n_1})$. It follows that $\bar{E}$ holds a set of C_I^3 linearly independent columns of $\boldsymbol{\Delta}_I^{(3)}$, the rank of which is at least C_I^3. As a conclusion, we have shown that the rank of $\boldsymbol{\Delta}_I^{(3)}$ is C_I^3. ■

8.2.2 New uniqueness bound for the BCD-(2,2,1)

With Lemmas 8.1, 8.2 and 8.3, we now have enough material to derive the analytic expression of the new uniqueness bound for the BCD-(2,2,1).

Theorem 8.4 *The decomposition of a third-order tensor* $\mathcal{Y} \in \mathbb{C}^{I \times J \times K}$ *in rank-(2,2,1) terms is generically unique if*

$$R \leq K \quad \textit{and} \quad C_I^3 . C_J^3 \geq C_{R+2}^3 - R. \quad (45)$$

Proof of Theorem 8.4 The second inequality implies that $R \leq IJ - 1 \leq IJ$, and combination with the first inequality gives $\min(IJ, K) \geq R$, which is a necessary requirement for $\tilde{\mathbf{X}}$ and $\mathbf{C}$ to

be generically full column rank (see Conditions 1(a) and 1(b)). We will now show that the second inequality generically guarantees linear independence of the set Ω defined in (30):

$$\begin{aligned}\Omega &= \{\Phi_2\left(\mathbf{A}_u \cdot \mathbf{B}_u^T, \mathbf{A}_v \cdot \mathbf{B}_v^T, \mathbf{A}_w \cdot \mathbf{B}_w^T\right) | \, 1 \leqslant u \leq v \leq w \leqslant R\} \\ &\quad \backslash \{\Phi_2\left(\mathbf{A}_u \cdot \mathbf{B}_u^T, \mathbf{A}_u \cdot \mathbf{B}_u^T, \mathbf{A}_u \cdot \mathbf{B}_u^T\right) | \, 1 \leqslant u \leqslant R\}.\end{aligned}$$

From Section 6.2, the image of the tensors $\Phi_2(\mathbf{X}_u, \mathbf{X}_v, \mathbf{X}_w) = \Phi_2(\mathbf{A}_u \cdot \mathbf{B}_u^T, \mathbf{A}_v \cdot \mathbf{B}_v^T, \mathbf{A}_w \cdot \mathbf{B}_w^T)$ under the inverse mapping $\mathcal{F}_2^{-1}$ are the vectors given by:

$$\begin{aligned}&\mathcal{F}_2^{-1}(\Phi_2(\mathbf{A}_u \cdot \mathbf{B}_u^T, \mathbf{A}_v \cdot \mathbf{B}_v^T, \mathbf{A}_w \cdot \mathbf{B}_w^T)) \\ =\ &\mathcal{F}_2^{-1}(\Phi_2(\textstyle\sum_{l_1=1}^{L=2}[\mathbf{A}_u]_{:,l_1} \cdot [\mathbf{B}_u]_{:,l_1}^T,\ \sum_{l_2=1}^{L=2}[\mathbf{A}_v]_{:,l_2} \cdot [\mathbf{B}_v]_{:,l_2}^T,\ \sum_{l_3=1}^{L=2}[\mathbf{A}_w]_{:,l_3} \cdot [\mathbf{B}_w]_{:,l_3}^T)) \\ =\ &\mathcal{F}_2^{-1}(\textstyle\sum_{l_1,l_2,l_3=1}^{2} \Phi_2([\mathbf{A}_u]_{:,l_1} \cdot [\mathbf{B}_u]_{:,l_1}^T, [\mathbf{A}_v]_{:,l_2} \cdot [\mathbf{B}_v]_{:,l_2}^T, [\mathbf{A}_w]_{:,l_3} \cdot [\mathbf{B}_w]_{:,l_3}^T)),\end{aligned} \tag{46}$$

where the trilinearity property of the mapping Φ_2 has been used. We denote by $\mathbf{a}_{u,l_1}$, $\mathbf{a}_{v,l_2}$ and $\mathbf{a}_{w,l_3}$ the $I \times 1$ vectors $[\mathbf{A}_u]_{:,l_1}$, $[\mathbf{A}_v]_{:,l_2}$ and $[\mathbf{A}_w]_{:,l_3}$, respectively. Similarly, we denote by $\mathbf{b}_{u,l_1}$, $\mathbf{b}_{v,l_2}$ and $\mathbf{b}_{w,l_3}$ the $J \times 1$ vectors $[\mathbf{B}_u]_{:,l_1}$, $[\mathbf{B}_v]_{:,l_2}$ and $[\mathbf{B}_w]_{:,l_3}$, respectively.

From Section 6.2, Eq. (46) can be written as:

$$\begin{aligned}&\mathcal{F}_2^{-1}(\Phi_2(\mathbf{A}_u \cdot \mathbf{B}_u^T, \mathbf{A}_v \cdot \mathbf{B}_v^T, \mathbf{A}_w \cdot \mathbf{B}_w^T)) \\ =\ &\textstyle\sum_{l_1,l_2,l_3=1}^{2} \left[\left(6\mathbf{\Delta}_I^{(3)} \cdot (\mathbf{a}_{u,l_1} \otimes \mathbf{a}_{v,l_2} \otimes \mathbf{a}_{w,l_3})\right) \otimes \left(6\mathbf{\Delta}_J^{(3)} \cdot (\mathbf{b}_{u,l_1} \otimes \mathbf{b}_{v,l_2} \otimes \mathbf{b}_{w,l_3})\right)\right] \\ =\ &36\mathbf{\Delta}_{IJ}^{(3)} \cdot \left(\textstyle\sum_{l_1,l_2,l_3=1}^{2} \mathbf{a}_{u,l_1} \otimes \mathbf{a}_{v,l_2} \otimes \mathbf{a}_{w,l_3} \otimes \mathbf{b}_{u,l_1} \otimes \mathbf{b}_{v,l_2} \otimes \mathbf{b}_{w,l_3}\right),\end{aligned} \tag{47}$$

where $\mathbf{\Delta}_{IJ}^{(3)} \stackrel{def}{=} \mathbf{\Delta}_I^{(3)} \otimes \mathbf{\Delta}_J^{(3)}$. Linear independence of tensors in Ω is equivalent to linear independence of the image vectors by the mapping $\mathcal{F}_2^{-1}$. The latter are linearly independent iff the intersection of the kernel of $\mathbf{\Delta}_{IJ}^{(3)}$ and the subspace generated by the $C_{R+2}^3 - R$ vectors of the set

$$\begin{aligned}\Gamma_{AB} &= \{\sum_{l_1,l_2,l_3=1}^{2} \mathbf{a}_{u,l_1} \otimes \mathbf{a}_{v,l_2} \otimes \mathbf{a}_{w,l_3} \otimes \mathbf{b}_{u,l_1} \otimes \mathbf{b}_{v,l_2} \otimes \mathbf{b}_{w,l_3} | \, 1 \leqslant u \leq v \leq w \leqslant R\} \\ &\quad \backslash \{\sum_{l_1,l_2,l_3=1}^{2} \mathbf{a}_{u,l_1} \otimes \mathbf{a}_{u,l_2} \otimes \mathbf{a}_{u,l_3} \otimes \mathbf{b}_{u,l_1} \otimes \mathbf{b}_{u,l_2} \otimes \mathbf{b}_{u,l_3} | \, 1 \leqslant u \leqslant R\}\end{aligned}$$

only contains the null vector. In other words, a basis of the kernel of $\mathbf{\Delta}_{IJ}^{(3)}$ and the latter vectors have to form a linearly independent set. The dimension of the kernel of $\mathbf{\Delta}_{IJ}^{(3)}$ is $I^3J^3 - \text{rank}(\mathbf{\Delta}_{IJ}^{(3)})$.

For any given triplet (l_1, l_2, l_3) with values in $(\{1,2\},\{1,2\},\{1,2\})$, according to Lemma 8.2, the set formed by a basis of the kernel of $\mathbf{\Delta}_{IJ}^{(3)}$ and the $(C_{R+2}^3 - R)$ vectors of the set

$$\begin{aligned}\Gamma_{AB}^{(l_1,l_2,l_3)} &= \{\mathbf{a}_{u,l_1} \otimes \mathbf{a}_{v,l_2} \otimes \mathbf{a}_{w,l_3} \otimes \mathbf{b}_{u,l_1} \otimes \mathbf{b}_{v,l_2} \otimes \mathbf{b}_{w,l_3} | \, 1 \leqslant u \leq v \leq w \leqslant R\} \\ &\quad \backslash \{\mathbf{a}_{u,l_1} \otimes \mathbf{a}_{u,l_2} \otimes \mathbf{a}_{u,l_3} \otimes \mathbf{b}_{u,l_1} \otimes \mathbf{b}_{u,l_2} \otimes \mathbf{b}_{u,l_3} | \, 1 \leqslant u \leqslant R\}\end{aligned}$$

is generically linearly independent if

$$I^3J^3 - \text{rank}(\mathbf{\Delta}_{IJ}^{(3)}) + (C_{R+2}^3 - R) \leq I^3J^3 \iff C_{R+2}^3 - R \leq \text{rank}(\mathbf{\Delta}_{IJ}^{(3)}). \tag{48}$$

Each vector of the set Γ_{AB} results from the sum of eight columns of the $I^3J^3 \times 2^6$ matrix $\mathbf{A}_u \otimes \mathbf{A}_v \otimes \mathbf{A}_w \otimes \mathbf{B}_u \otimes \mathbf{B}_v \otimes \mathbf{B}_w$, which is generically full column rank. Thus, each vector of Γ_{AB} results from the sum eight linearly independent vectors, none of which belongs to the kernel of $\mathbf{\Delta}_{IJ}^{(3)}$. It follows that the set formed by a basis of the kernel of $\mathbf{\Delta}_{IJ}^{(3)}$ and the $(C_{R+2}^3 - R)$ vectors of Γ_{AB} is generically linearly independent under the same condition (48). From Lemma 8.3, we have $\text{rank}(\mathbf{\Delta}_I^{(3)}) = C_I^3$ and $\text{rank}(\mathbf{\Delta}_J^{(3)}) = C_J^3$. Thus, by a property of the Kronecker product, we obtain

$$\text{rank}(\mathbf{\Delta}_{IJ}^{(3)}) = C_I^3 C_J^3. \tag{49}$$

Combining (48) with (49) yields that the set Ω is generically linearly independent iff

$$C_I^3 C_J^3 \geq C_{R+2}^3 - R,$$

which concludes the proof. ■

9 Generalization to any value of L

We now generalize the results of Sections 7 and 8 to any value of L. In Section 9.1, we show how the BCD-(L,L,1) can be reformulated in terms of simultaneous diagonalization via the tool for rank-L detection introduced in Section 6.3. In Section 9.2, we derive the expression of the new uniqueness bound for any value of L.

9.1 Link between the BCD-(L,L,1) and simultaneous diagonalization

From the known matrices $\mathbf{E}_r = \sum_{k=1}^{R} \mathbf{X}_k (\mathbf{W}^{-1})_{kr}$ of Eq. (23), we first build the following set of R^{L+1} tensors $\{\mathcal{P}_{r_1 r_2 \dots r_{L+1}}\}_{r_1,r_2,\dots,r_{L+1} \in [1,R]}$:

$$\mathcal{P}_{r_1 r_2 \dots r_{L+1}} = \Phi_L(\mathbf{E}_{r_1}, \mathbf{E}_{r_2}, \dots, \mathbf{E}_{r_{L+1}}). \tag{50}$$

Since Φ is multi-linear, we have:

$$\mathcal{P}_{r_1 r_2 \dots r_{L+1}} = \sum_{u_1,u_2,\dots,u_{L+1}=1}^{R} (\mathbf{W}^{-1})_{u_1 r_1} (\mathbf{W}^{-1})_{u_2 r_2} \dots (\mathbf{W}^{-1})_{u_{L+1} r_{L+1}} \Phi_L\left(\mathbf{X}_{u_1},\ \mathbf{X}_{u_2},\ \dots,\mathbf{X}_{u_{L+1}}\right). \tag{51}$$

Assume at this point that there exists an $(L+1)$th-order symmetric tensor $\mathcal{M} \in \mathbb{C}^{R \times R \times \dots \times R}$ of which the entries $m_{r_1 r_2 \dots r_{L+1}}$ satisfy the following set of homogeneous linear equations :

$$\sum_{r_1,r_2,\dots,r_{L+1}=1}^{R} m_{r_1 r_2 \dots r_{L+1}} \mathcal{P}_{r_1 r_2 \dots r_{L+1}} = 0. \tag{52}$$

Substitution of (51) in (52) yields:

$$\sum_{r_1,\dots,r_{L+1}=1}^{R} \sum_{u_1,\dots,u_{L+1}=1}^{R} (\mathbf{W}^{-1})_{u_1 r_1} \dots (\mathbf{W}^{-1})_{u_{L+1} r_{L+1}} m_{r_1 \dots r_{L+1}} \Phi_L\left(\mathbf{X}_{u_1},\dots,\mathbf{X}_{u_{L+1}}\right) = 0 \tag{53}$$

According to Theorem 6.3, we have $\Phi_L(\mathbf{X}_u,\ \dots,\ \mathbf{X}_u) = 0$, $1 \leqslant u \leqslant R$. Hence, (53) is equivalent to:

$$\sum_{r_1,\dots,r_{L+1}=1}^{R} \sum_{\substack{u_1,\dots,u_{L+1}=1 \\ \neg(u_1=\dots=u_{L+1})}}^{R} (\mathbf{W}^{-1})_{u_1 r_1} \dots (\mathbf{W}^{-1})_{u_{L+1} r_{L+1}} m_{r_1 \dots r_{L+1}} \Phi_L\left(\mathbf{X}_{u_1},\dots,\mathbf{X}_{u_{L+1}}\right) = 0 \tag{54}$$

Furthermore, due to the symmetry of Φ_L, Eq. (54) can be simplified by considering only the set of indices

$$\Theta_{L+1} = \{(u_1,u_2,\dots,u_{L+1}) | \mathrm{u}_1 \leq u_2 \leq \dots \leq u_{L+1}\} \backslash \{(u_1,u_2,\dots,u_{L+1}) | \mathrm{u}_1 = u_2 = \dots = u_{L+1}\},$$

and weighting each $(L+1)$-uplet of this set by its number of permutations. The number of all possible $(L+1)$-uplets containing n_1 times u_1, n_2 times u_2, ..., n_{L+1} times u_{L+1} is

$$\alpha_{L+1}(n_1,\dots,n_{L+1}) = \frac{(L+1)!}{n_1! n_2! \dots n_{L+1}!},$$

where $L+1 = \mathrm{n}_1 + n_2 + \dots + n_{L+1}$. For instance the term indexed by (u_1,u_1,u_1,u_2) is weighted by 4, the term indexed by (u_1,u_1,u_2,u_3) is weighted by 12, and so on.

It follows that Eq. (54) can be written as

$$\sum_{\substack{u_1,\dots,u_{L+1}=1,\dots,L \\ (u_1,\dots,u_{L+1}) \in \Theta_{L+1}}}^{R} \alpha_{L+1}(n_1,\dots,n_{L+1}) \Phi_L\left(\mathbf{X}_{u_1},\dots,\mathbf{X}_{u_{L+1}}\right) \sum_{r_1,\dots,r_{L+1}=1}^{R} (\mathbf{W}^{-1})_{u_1 r_1} \dots (\mathbf{W}^{-1})_{u_{L+1} r_{L+1}} m_{r_1 \dots r_{L+1}} = 0 \tag{55}$$

Define the set Ω_L that holds the $C_{R+L}^{L+1} - R$ tensors involved in (55):

$$\Omega_L = \{\Phi_L\left(\mathbf{X}_{u_1}, \ldots, \mathbf{X}_{u_{L+1}}\right) | \, 1 \leq u_1 \leq \cdots \leq u_{L+1} \leq R\} \backslash \{\Phi_L\left(\mathbf{X}_u, \ldots, \mathbf{X}_u\right) | 1 \leqslant u \leqslant R\}. \quad (56)$$

The quantity C_{R+L}^{L+1} is the number of ways to choose $L+1$ elements among R, with the possibility of choosing several times the same element. We substract R to this quantity, since it corresponds to the number of ways to choose $L+1$ times the same element.

We make the crucial assumption that Ω_L is linearly independent. As we will show in Section 9.2, this assumption implies a new bound on R that guarantees essential uniqueness of the BCD-(L,L,1) in the generic sense. The solution of (55) can then be written as:

$$\sum_{r_1,\ldots,r_{L+1}=1}^{R} (\mathbf{W}^{-1})_{u_1 r_1} \ldots (\mathbf{W}^{-1})_{u_{L+1} r_{L+1}} m_{r_1 \ldots r_{L+1}} = \lambda_{u_1 \ldots u_{L+1}} \delta_{u_1 u_2 u_3 \ldots u_{L+1}}, \quad (57)$$

in which $\delta_{u_1 u_2 u_3 \ldots u_{L+1}} = 1$ if $u_1 = u_2 = u_3 = \cdots = u_{L+1}$, and $\delta_{u_1 u_2 u_3 \ldots u_{L+1}} = 0$ otherwise. In fact, in the case $u_1 = u_2 = u_3 = \cdots = u_{L+1} = u$, the coefficients of the linear combinations of all tensors $\Phi_L\left(\mathbf{X}_u, \ldots, \mathbf{X}_u\right)$ in Eq. (55), $\forall u \in \{1, \ldots, R\}$, can be arbitrary scalars since $\Phi_L\left(\mathbf{X}_u, \ldots, \mathbf{X}_u\right) = 0$ by definition. If the indices u_l, $l = 1, \ldots, L+1$, are not all equal, then the coefficients of the linear combinations all have to be 0 since linear independence of Ω_L has been assumed.

Eq. (57) can be rewritten in tensor format as follows:

$$\mathcal{M} = \mathcal{D} \bullet_1 \mathbf{W} \bullet_2 \mathbf{W} \bullet_3 \cdots \bullet_{L+1} \mathbf{W}, \quad (58)$$

in which $\mathcal{D} \in \mathbb{C}^{R \times R \times \cdots \times R}$ is a diagonal tensor whose diagonal elements are arbitrary scalars $\lambda_{uu\ldots u}$, $u \in [1, R]$.

Note that linearly independent choices of $\mathcal{D}$ correspond to linearly independent solutions of (52). We conclude that if the set Ω_L is linearly independent, the kernel of (52) yields R linearly independent symmetric tensors $\mathcal{M}_r$, which can all be decomposed as in (58). We have:

$$\begin{cases} \mathcal{M}_1 = \mathcal{D}_1 \bullet_1 \mathbf{W} \bullet_2 \mathbf{W} \bullet_3 \cdots \bullet_{L+1} \mathbf{W} \\ \quad \vdots \\ \mathcal{M}_R = \mathcal{D}_R \bullet_1 \mathbf{W} \bullet_2 \mathbf{W} \bullet_3 \cdots \bullet_{L+1} \mathbf{W} \end{cases}, \quad (59)$$

in which $\mathcal{D}_1, \ldots, \mathcal{D}_R$ are diagonal. The set of R equations in (59) can be expressed in terms of the matrix slices of $\mathcal{M}_1, \ldots, \mathcal{M}_R$, after which $\mathbf{W}$ can be found by solving a simultaneous matrix diagonalization problem of a set of R^L matrices. As explained in Section 7.2.2 for the case $L = 2$, this set of R^L matrices can be reduced into a set of R matrices, with a SVD-based preliminary step that selects the R most significant ones. In order to build the R symmetric tensors $\mathcal{M}_r$, we proceed as explained in Section 7.2.1 for $L = 2$, i.e., we solve

$$\tilde{\mathbf{P}} \cdot \tilde{\mathbf{m}} = \mathbf{0}_N, \quad (60)$$

where $N = C_{R+L}^{L+1}$ is the number of entries that are necessary to build the symmetric tensors $\mathcal{M}_r$, and where each column of the $C_I^{L+1} C_J^{L+1} \times C_{R+L}^{L+1}$ matrix $\tilde{\mathbf{P}}$ holds the $C_I^{L+1} C_J^{L+1}$ useful entries (see Section 6.3) of $\alpha_{L+1}(n_1, \ldots, n_{L+1}) \mathcal{F}_L^{-1}(\mathcal{P}_{r_1 r_2 \ldots r_{L+1}})$.

We now derive the conditions that generically guarantee linear independence of Ω_L defined in (56).

9.2 Derivation of the new uniqueness bound

We start with the following Lemma:

Lemma 9.2 *Let $\mathbf{v}_1, \ldots, \mathbf{v}_M$ be linearly independent vectors in $\mathbb{C}^{N^{L+1}}$. Let $\mathbf{c}_1, \ldots, \mathbf{c}_R$ be vectors in $\mathbb{C}^N$. Let Γ_R be the set defined by*

$$\Gamma_R = \{(\mathbf{c}_{u_1} \otimes \mathbf{c}_{u_2} \otimes \cdots \otimes \mathbf{c}_{u_{L+1}}) | 1 \leq u_1 \leq \cdots \leq u_{L+1} \leq R\} \backslash \{(\mathbf{c}_u \otimes \mathbf{c}_u \otimes \cdots \otimes \mathbf{c}_u) | 1 \leq u \leq R\}.$$

If

$$R \leq N-1 \quad \textit{and} \quad (C_{R+L}^{L+1} - R) + M \leq N^{L+1}, \tag{61}$$

then the vectors $\mathbf{v}_m$, $1 \leq m \leq M$, and the $C_{R+L}^{L+1} - R$ vectors of the set Γ_R are linearly independent for a generic choice of $\mathbf{c}_r$, $1 \leq r \leq R$.

Proof of Lemma 9.2

Define $V = \{\mathbf{v}_m | 1 \leq m \leq M\}$, and

$$\begin{aligned} \Gamma_{R-1} = & \{(\mathbf{c}_{u_1} \otimes \mathbf{c}_{u_2} \otimes \cdots \otimes \mathbf{c}_{u_{L+1}}) | 1 \leq u_1 \leq \cdots \leq u_{L+1} \leq R-1\} \\ & \backslash \{(\mathbf{c}_u \otimes \mathbf{c}_u \otimes \cdots \otimes \mathbf{c}_u) | 1 \leq u \leq R-1\}. \end{aligned}$$

The set Γ_R holds $C_{R+L}^{L+1} - R$ vectors and the set Γ_{R-1} holds $C_{R+L-1}^{L+1} - R + 1$ vectors.

The proof is by induction. We first show that the lemma holds for $R = 2$. Then we show that, assuming that the lemma holds for $(M, R-1)$, it still holds for (M, R) if (61) is satisfied.

(i) Initialization.

Let $V^\perp \in \mathbb{C}^{N^{L+1}}$ be orthogonal to the vectors in V. To initialize the induction, it suffices to choose $R = 2$ and then show that the $L+1$ vectors of the set Γ_2 are linearly independent and all have components in the direction of $V^\perp$. The $N \times 2$ matrix $[\mathbf{c}_1, \mathbf{c}_2]$ is generically full column rank since we assumed $R \leq N-1 < N$. By a property of the Kronecker product, $\overbrace{[\mathbf{c}_1, \mathbf{c}_2] \otimes [\mathbf{c}_1, \mathbf{c}_2] \otimes \cdots \otimes [\mathbf{c}_1, \mathbf{c}_2]}^{L+1\, times}$ is also generically full column rank. Thus, the vectors of Γ_2, which is a subset of $L+1$ columns of the latter matrix, are linearly independent. Define the tensor $\mathcal{V}^\perp \in \mathbb{C}^{\overbrace{N \times N \times \cdots \times N}^{L+1\, times}}$ by $(\mathcal{V}^\perp)_{n_1, n_2, \ldots, n_{L+1}} = (V^\perp)_{(n_1-1)N^L + (n_2-1)N^{L-1} + \cdots + n_{L+1}}$. Then for each vector of Γ_2, we have $(\mathbf{c}_{u_1} \otimes \mathbf{c}_{u_2} \otimes \cdots \otimes \mathbf{c}_{u_{L+1}})^T \cdot V^\perp = \mathcal{V}^\perp \bullet_1 \mathbf{c}_{u_1} \bullet_2 \mathbf{c}_{u_2} \bullet_3 \cdots \bullet_{L+1} \mathbf{c}_{u_{L+1}}$ which is indeed generically different from zero.

(ii) Now we prove the induction step.

We suppose that the set $V \cup \Gamma_R$ is linearly dependent. We prove by contradiction that the set becomes linearly independent by a generic perturbation of the vector $\mathbf{c}_R$.

The $N \times R$ matrix $[\mathbf{c}_1, \ldots, \mathbf{c}_R]$ is generically full column since we assumed $R \leq N-1$. By a property of the Kronecker product, $\overbrace{[\mathbf{c}_1, \ldots, \mathbf{c}_R] \otimes [\mathbf{c}_1, \ldots, \mathbf{c}_R] \otimes \cdots \otimes [\mathbf{c}_1, \ldots, \mathbf{c}_R]}^{L+1\, times}$ is also generically full column rank. The set Γ_R, consisting of columns of the latter matrix, is thus linearly independent. Let now $\mathbf{c}_R$ be replaced by a vector $\tilde{\mathbf{c}}_R$ that is not proportional to $\mathbf{c}_R$. The set Γ_R is consistently replaced by $\tilde{\Gamma}_R$. Suppose that $V \cup \tilde{\Gamma}_R$ is still linearly dependent. Generically, we may assume that $\mathbf{v}_1$ can be written as a linear combination of the vectors in $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_R$. We may also assume that $\mathbf{v}_1$ is a linear combination of the vectors in $(V \backslash \{\mathbf{v}_1\}) \cup \tilde{\Gamma}_R$. In other words, $\mathbf{v}_1$ is in the intersection of the subspaces W and $\tilde{W}$ generated by $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_R$ and $(V \backslash \{\mathbf{v}_1\}) \cup \tilde{\Gamma}_R$, respectively. W equals the sum of the subspace generated by $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_{R-1}$ and the subspace $\{\Gamma_R \backslash \Gamma_{R-1}\}$ generated by $\{(\mathbf{c}_{u_1} \otimes \mathbf{c}_{u_2} \otimes \cdots \otimes \mathbf{c}_{u_L} \otimes \mathbf{c}_R) |\ 1 \leq u_1 \leq u_2 \leq \cdots \leq u_L \leq R\ \} \backslash \{(\mathbf{c}_R \otimes \mathbf{c}_R \otimes \cdots \otimes \mathbf{c}_R)\}$. $\tilde{W}$ equals the sum of the subspace generated by $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_{R-1}$ and the subspace $\{\tilde{\Gamma}_R \backslash \Gamma_{R-1}\}$ generated by $\{(\mathbf{c}_{u_1} \otimes \mathbf{c}_{u_2} \otimes \cdots \otimes \mathbf{c}_{u_L} \otimes \tilde{\mathbf{c}}_R) |\ 1 \leq u_1 \leq u_2 \leq \cdots \leq u_L \leq R\ \} \backslash \{(\tilde{\mathbf{c}}_R \otimes \tilde{\mathbf{c}}_R \otimes \cdots \otimes \tilde{\mathbf{c}}_R)\}$. W can not be equal to $\mathbb{C}^{N^{L+1}}$ since $\dim(W) \leq M - 1 + C_{R+L}^{L+1} - R < N^{L+1}$; neither can $\tilde{W}$ be equal to $\mathbb{C}^{N^{L+1}}$. The vectors of the set $\{\Gamma_R \backslash \Gamma_{R-1}\} \cup \{\tilde{\Gamma}_R \backslash \Gamma_{R-1}\}$ consist of a selection of the columns of the $N^{L+1} \times 2(R+1)^L$ matrix $\mathbf{P} = \overbrace{[\mathbf{c}_1, \ldots, \mathbf{c}_R, \tilde{\mathbf{c}}_R] \otimes \cdots \otimes [\mathbf{c}_1, \ldots, \mathbf{c}_R, \tilde{\mathbf{c}}_R]}^{L\, times} \otimes [\mathbf{c}_R, \tilde{\mathbf{c}}_R]$. Both matrices

$[\mathbf{c}_R, \tilde{\mathbf{c}}_R]$ and $[\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_R, \tilde{\mathbf{c}}_R]$ are generically full column rank since we assumed $R \leq N-1$, so by a property of the Kronecker product, the tall matrix $\mathbf{P}$ is generically full column-rank. It follows that the vectors of the set $\{\Gamma_R \backslash \Gamma_{R-1}\} \cup \{\tilde{\Gamma}_R \backslash \Gamma_{R-1}\}$ are linearly independent. We conclude that the intersection of W and $\tilde{W}$ is equal to the subspace generated by $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_{R-1}$. Since $\mathbf{v}_1$ is in the intersection of W and $\tilde{W}$, it is a linear combination of the vectors in $(V \backslash \{\mathbf{v}_1\}) \cup \Gamma_{R-1}$. This means that the set $V \cup \Gamma_{R-1}$ is linearly dependent.

As a conclusion, if $V \cup \Gamma_R$ is supposed to be linearly dependent, then $V \cup \Gamma_{R-1}$ is linearly dependent. By induction, if $V \cup \Gamma_{R-1}$ is linearly independent, then $V \cup \Gamma_R$ is linearly independent, which concludes the proof. ■

We now have the following Lemma.

Lemma 9.3 *Let $\mathbf{v}_1, \ldots, \mathbf{v}_M$ be linearly independent vectors in $\mathbb{C}^{(IJ)^{L+1}}$. Let $\mathbf{a}_1, \ldots, \mathbf{a}_R$ be arbitrary vectors in $\mathbb{C}^I$ and $\mathbf{b}_1, \ldots, \mathbf{b}_R$ arbitrary vectors in $\mathbb{C}^J$. If*

$$R \leq IJ - 1 \quad \textit{and} \quad (C_{R+L}^{L+1} - R) + M \leq (IJ)^{L+1}, \tag{62}$$

then the vectors $\mathbf{v}_m$, $1 \leq m \leq M$, and the $(C_{R+L}^{L+1} - R)$ vectors of the set

$$\begin{aligned} \Gamma_R \quad = \quad & \{(\mathbf{a}_{u_1} \otimes \mathbf{b}_{u_1} \otimes \mathbf{a}_{u_2} \otimes \mathbf{b}_{u_2} \otimes \cdots \otimes \mathbf{a}_{u_{L+1}} \otimes \mathbf{b}_{u_{L+1}}) | 1 \leq u_1 \leq \cdots \leq u_{L+1} \leq R\} \\ & \backslash \{(\mathbf{a}_u \otimes \mathbf{b}_u \otimes \mathbf{a}_u \otimes \mathbf{b}_u \otimes \cdots \otimes \mathbf{a}_u \otimes \mathbf{b}_u) | 1 \leq u \leq R\}. \end{aligned}$$

are linearly independent for a generic choice of $\mathbf{a}_r$ and $\mathbf{b}_r$, $1 \leq r \leq R$.

Proof of Lemma 9.3 The proof is analogous to the proof of Lemma 9.2. The role of $\mathbf{c}_r$ is now played by $\mathbf{a}_r \otimes \mathbf{b}_r$. ■

Finally, we will also need the following Lemma.

Lemma 9.4 *Let $\mathbf{\Delta}_I^{(L)}$ be the $I^L \times I^L$ anti-symmetric Kronecker product permutation matrix (see definition 2.11). Then, we have rank$(\mathbf{\Delta}_I^{(L)}) = C_I^L$.*

Proof of Lemma 9.4 First, we notice that $\mathbf{\Delta}_I^{(L)} \cdot (\otimes_{l=1}^L \mathbf{a}_l) = \frac{1}{L!} \sum_{\sigma \in \Lambda_L} s(\sigma)(\otimes_{l=1}^L \mathbf{a}_{\sigma(l)})$ (see Section 2) is the vectorized representation of an $(I \times I \times \cdots \times I)$ Lth-order completely antisymmetric rank-1 tensor. Thus, $\mathbf{\Delta}_I^{(L)}$ maps an Lth-order rank-1 tensor into an antisymmetric tensor. Since any linear combination of antisymmetric tensors is an antisymmetric tensor, $\mathbf{\Delta}_I^{(L)}$ maps any tensor into an antisymmetric tensor. The Lth-order$(I \times I \times \cdots \times I)$ antisymmetric tensors form an C_I^L-dimensional space, hence the rank of $\mathbf{\Delta}_I^{(L)}$ is at most C_I^L.

Let us now prove that the rank of $\mathbf{\Delta}_I^{(L)}$ is at least C_I^L. We denote by $\mathbf{e}_p$ the pth column of the $I \times I$ identity matrix. We define the set of C_I^L vectors $E = \{(\mathbf{e}_{p_1} \otimes \mathbf{e}_{p_2} \otimes \cdots \otimes \mathbf{e}_{p_L}) | 1 \leq p_1 < p_2 < \cdots < p_L \leq I\}$. A given $I^L \times 1$ vector $(\mathbf{e}_{p_1} \otimes \mathbf{e}_{p_2} \otimes \cdots \otimes \mathbf{e}_{p_L})$ holds only one non-zero entry, the element 1 at position $\bar{p} = (p_1 - 1)I^{L-1} + (p_2 - 1)I^{L-2} + \cdots + (p_{L-1} - 1)I + p_L$. Thus, $\mathbf{\Delta}_I^{(L)} \cdot (\mathbf{e}_{p_1} \otimes \mathbf{e}_{p_2} \otimes \cdots \otimes \mathbf{e}_{p_L})$ is the the $\bar{p}$th column of $\mathbf{\Delta}_I^{(L)}$. We now show that the subset of C_I^L columns of $\mathbf{\Delta}_I^{(L)}$ defined by $\bar{E} = \{\mathbf{\Delta}_I^{(L)} \cdot (\mathbf{e}_{p_1} \otimes \mathbf{e}_{p_2} \otimes \cdots \otimes \mathbf{e}_{p_L}) | 1 \leq p_1 < p_2 < \cdots < p_L \leq I\}$ is linearly independent. The vectors of $\bar{E}$ can be written as

$$\bar{\mathbf{e}}_{p_1, p_2, \ldots, p_L} \stackrel{def}{=} \mathbf{\Delta}_I^{(L)} \cdot (\otimes_{l=1}^L \mathbf{e}_{p_l}) = \frac{1}{L!} \sum_{\sigma \in \Lambda_L} s(\sigma)(\otimes_{l=1}^L \mathbf{e}_{\sigma(p_l)}). \tag{63}$$

For a given L-uplet $(p_1, p_2, \ldots, p_L)$, $\bar{\mathbf{e}}_{p_1, p_2, \ldots, p_L}$ is the only vector of $\bar{E}$ that holds a non-zero element at the position $\bar{p}$, since it is the only vector of $\bar{E}$ built from $(\mathbf{e}_{p_1} \otimes \mathbf{e}_{p_2} \otimes \cdots \otimes \mathbf{e}_{p_L})$. Consequently,

$\bar{\mathbf{e}}_{p_1,p_2,\ldots,p_L}$ and the $C_I^L - 1$ vectors of $\bar{E}\backslash\{\bar{\mathbf{e}}_{p_1,p_2,\ldots,p_L}\}$ are linearly independent. It follows that $\bar{E}$ holds a set of C_I^L linearly independent columns of $\boldsymbol{\Delta}_I^{(L)}$, the rank of which is at least C_I^L. As a conclusion, we have shown that the rank of $\boldsymbol{\Delta}_I^{(L)}$ is C_I^L. ■

We now have enough material to derive the analytic expression of a new sufficient uniqueness bound for the BCD-$(L,L,1)$.

Theorem 9.5 *The decomposition of a third-order tensor in rank-$(L,L,1)$ terms is generically unique if*

$$R \leq K \quad \textit{and} \quad C_I^{L+1}.C_J^{L+1} \geq C_{R+L}^{L+1} - R. \tag{64}$$

Proof of Theorem 9.5 We show that the second inequality generically guarantees linear independence of the set Ω_L defined in (56). We denote by $\mathbf{a}_{u_1 l_1}$, ...,$\mathbf{a}_{u_{L+1} l_{L+1}}$, the $I \times 1$ vectors $[\mathbf{A}_{u_1}]_{:,l_1}$, ..., $[\mathbf{A}_{u_{L+1}}]_{:,l_{L+1}}$, respectively. Similarly, we denote by $\mathbf{b}_{u_1 l_1}$, ...,$\mathbf{b}_{u_{L+1} l_{L+1}}$, the $J \times 1$ vectors $[\mathbf{B}_{u_1}]_{:,l_1}$, ..., $[\mathbf{B}_{u_{L+1}}]_{:,l_{L+1}}$, respectively. From Section 6.3, the image vectors of $\Phi_L(\mathbf{A}_{u_1} \cdot \mathbf{B}_{u_1}^T, \mathbf{A}_{u_2} \cdot \mathbf{B}_{u_2}^T, \ldots, \mathbf{A}_{u_{L+1}} \cdot \mathbf{B}_{u_{L+1}}^T)$ under the inverse mapping $\mathcal{F}_L^{-1}$ are given by:

$$\begin{array}{rl} & \mathcal{F}_L^{-1}(\Phi_L(\mathbf{A}_{u_1} \cdot \mathbf{B}_{u_1}^T, \mathbf{A}_{u_2} \cdot \mathbf{B}_{u_2}^T, \ldots, \mathbf{A}_{u_{L+1}} \cdot \mathbf{B}_{u_{L+1}}^T)) \\ = & \mathcal{F}_L^{-1}(\Phi_L(\sum_{l_1=1}^L \mathbf{a}_{u_1 l_1} \cdot \mathbf{b}_{u_1 l_1}^T,\ \sum_{l_2=1}^L \mathbf{a}_{u_2 l_2} \cdot \mathbf{b}_{u_2 l_2}^T\ , \ldots,\ \sum_{l_{L+1}=1}^L \mathbf{a}_{u_{L+1} l_{L+1}} \cdot \mathbf{b}_{u_{L+1} l_{L+1}}^T)) \\ = & \mathcal{F}_L^{-1}(\sum_{l_1,l_2,\ldots,l_{L+1}=1}^L \Phi_L(\mathbf{a}_{u_1 l_1} \cdot \mathbf{b}_{u_1 l_1}^T,\ \mathbf{a}_{u_2 l_2} \cdot \mathbf{b}_{u_2 l_2}^T, \ldots,\ \mathbf{a}_{u_{L+1} l_{L+1}} \cdot \mathbf{b}_{u_{L+1} l_{L+1}}^T)), \end{array} \tag{65}$$

where the multi-linearity property of the mapping Φ_L has been used. From Section 6.3, Eq. (65) can be written as:

$$\begin{array}{rl} & \mathcal{F}_L^{-1}(\Phi_L(\mathbf{A}_{u_1} \cdot \mathbf{B}_{u_1}^T, \ldots, \mathbf{A}_{u_{L+1}} \cdot \mathbf{B}_{u_{L+1}}^T)) \\ = & \sum_{l_1,\ldots,l_{L+1}=1}^L \left[(L+1)!\boldsymbol{\Delta}_I^{(L+1)} \cdot \left(\mathbf{a}_{u_1 l_1} \otimes \cdots \otimes \mathbf{a}_{u_{L+1} l_{L+1}}\right)\right] \otimes \left[(L+1)!\boldsymbol{\Delta}_J^{(L+1)} \cdot \left(\mathbf{b}_{u_1 l_1} \otimes \cdots \otimes \mathbf{b}_{u_{L+1} l_{L+1}}\right)\right] \\ = & 2(L+1)!\left(\boldsymbol{\Delta}_I^{(L+1)} \otimes \boldsymbol{\Delta}_J^{(L+1)}\right) \cdot \left(\sum_{l_1,\ldots,l_{L+1}=1}^L \mathbf{a}_{u_1 l_1} \otimes \cdots \otimes \mathbf{a}_{u_{L+1} l_{L+1}} \otimes \mathbf{b}_{u_1 l_1} \otimes \cdots \otimes \mathbf{b}_{u_{L+1} l_{L+1}}\right) \end{array} \tag{66}$$

Linear independence of the tensors in Ω_L is equivalent to linear independence of the image vectors by the mapping $\mathcal{F}_L^{-1}$. The latter are linearly independent iff the intersection of the kernel of $\boldsymbol{\Delta}_{IJ}^{(L+1)} \overset{def}{=} \left(\boldsymbol{\Delta}_I^{(L+1)} \otimes \boldsymbol{\Delta}_J^{(L+1)}\right)$ and the subspace generated by the $C_{R+L}^{L+1} - R$ vectors of the set

$$\begin{array}{rcl} \Gamma_{AB} & = & \{\displaystyle\sum_{l_1,\ldots,l_{L+1}=1}^{L} \mathbf{a}_{u_1 l_1} \otimes \cdots \otimes \mathbf{a}_{u_{L+1} l_{L+1}} \otimes \mathbf{b}_{u_1 l_1} \otimes \cdots \otimes \mathbf{b}_{u_{L+1} l_{L+1}} | \, 1 \leqslant u_1 \leq \cdots \leq u_{L+1} \leqslant R\} \\ & & \backslash\{\displaystyle\sum_{l_1,\ldots,l_{L+1}=1}^{L} \mathbf{a}_{u,l_1} \otimes \cdots \otimes \mathbf{a}_{u,l_{L+1}} \otimes \mathbf{b}_{u,l_1} \otimes \cdots \otimes \mathbf{b}_{u,l_{L+1}} | \, 1 \leqslant u \leqslant R\} \end{array}$$

only contains the null vector. In other words, a basis of the kernel of $\boldsymbol{\Delta}_{IJ}^{(L+1)}$ and the latter vectors have to form a linearly independent set. The dimension of the kernel of $\boldsymbol{\Delta}_{IJ}^{(L+1)}$ is $I^{L+1}J^{L+1} - \text{rank}(\boldsymbol{\Delta}_{IJ}^{(L+1)})$.

For any $(L+1)$-uplet $(l_1, \ldots, l_{L+1})$ with values in $(\{1,\ldots,L\}, \{1,\ldots,L\}, \ldots, \{1,\ldots,L\})$, according to Lemma 9.3, the set formed by a basis of the kernel of $\boldsymbol{\Delta}_{IJ}^{(L+1)}$ and the $(C_{R+L}^{L+1} - R)$ vectors of the set

$$\begin{array}{rcl} \Gamma_{AB}^{(l_1,l_2,\ldots,l_{L+1})} & = & \{\mathbf{a}_{u_1 l_1} \otimes \cdots \otimes \mathbf{a}_{u_{L+1} l_{L+1}} \otimes \mathbf{b}_{u_1 l_1} \otimes \cdots \otimes \mathbf{b}_{u_{L+1} l_{L+1}} | \, 1 \leqslant u_1 \leq \cdots \leq u_{L+1} \leqslant R\} \\ & & \backslash\{\mathbf{a}_{u,l_1} \otimes \cdots \otimes \mathbf{a}_{u,l_{L+1}} \otimes \mathbf{b}_{u,l_1} \otimes \cdots \otimes \mathbf{b}_{u,l_{L+1}} | \, 1 \leqslant u \leqslant R\} \end{array}$$

is generically linearly independent if

$$I^{L+1}J^{L+1} - \text{rank}(\boldsymbol{\Delta}_{IJ}^{(L+1)}) + (C_{R+L}^{L+1} - R) \leq I^{L+1}J^{L+1} \iff C_{R+L}^{L+1} - R \leq \text{rank}(\boldsymbol{\Delta}_{IJ}^{(L+1)}). \tag{67}$$

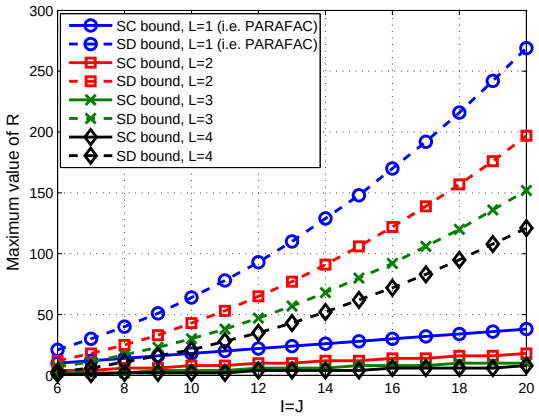


Figure 4: Maximum value of R such that the sufficient bound (denoted SC bound) of Eq. (40) and the new bound derived from the simultaneous diagonalization reformulation (denoted SD bound) of Eq. (64) are both satisfied.

Each vector of the set Γ_{AB} results from the sum of $L^{(L+1)}$ vectors of the $I^{L+1}J^{L+1} \times L^{2(L+1)}$ matrix $\mathbf{A}_{u_1} \otimes \mathbf{A}_{u_2} \otimes \cdots \otimes \mathbf{A}_{u_{L+1}} \otimes \mathbf{B}_{u_1} \otimes \mathbf{B}_{u_2} \otimes \cdots \otimes \mathbf{B}_{u_{L+1}}$, which is generically full column rank. Thus, each vector of Γ_{AB} results from the sum of $L^{(L+1)}$ linearly independent vectors, none of which belongs to the kernel of $\mathbf{\Delta}_{IJ}^{(L+1)}$. It follows that the set formed by a basis of the kernel of $\mathbf{\Delta}_{IJ}^{(L+1)}$ and the $(C_{R+L}^{L+1} - R)$ vectors of Γ_{AB} is generically linearly independent under the same condition 67. From Lemma 9.4, we have $\text{rank}(\mathbf{\Delta}_{I}^{(L+1)}) = C_I^{L+1}$ and $\text{rank}(\mathbf{\Delta}_{J}^{(L+1)}) = C_J^{L+1}$. Thus, by a property of the Kronecker product, we obtain

$$\text{rank}(\mathbf{\Delta}_{IJ}^{(L+1)}) = C_I^{L+1} C_J^{L+1}. \tag{68}$$

Combining (67) and (68) yields that the set Ω_L is generically linearly independent iff

$$C_I^{L+1} C_J^{L+1} \geq C_{R+L}^{L+1} - R,$$

which concludes the proof.

■

Fig. (4) is a comparison between the sufficient condition for uniqueness of the BCD-(L,L,1) derived in [11], given by Eq. (40), and the new bound given by Theorem 9.5. It is clear that the new bound derived in this paper is much more relaxed than the previous sufficient bound, in the sense that the number of rank-(L,L,1) terms that can de admitted in the decomposition is substantially greater.

10 Numerical experiments

10.1 Data generation

In this section, we illustrate the performance of the SD-based algorithm by means of numerical experiments. The data are generated as follows. The noisy tensor of observations $\mathcal{T} \in \mathbb{C}^{I \times J \times K}$ is generated in the following way:

$$\mathcal{T} = \frac{\tilde{T}}{\|\tilde{\mathcal{T}}\|_F} + \sigma_N \frac{\mathcal{N}}{\|\mathcal{N}\|_F}, \tag{69}$$

in which $\tilde{\mathcal{T}}$ can be exactly decomposed in rank-$(L,L,1)$ terms. The second term in (69) is a noise term. The entries of $\mathcal{N} \in \mathbb{C}^{I \times J \times K}$ are drawn from a zero-mean unit-variance Gaussian distribution and σ_N controls the noise level. To build the noise-free tensor $\tilde{\mathcal{T}}$, we first randomly generate the matrices $\{\mathbf{X}_r \in \mathbb{C}^{I \times J}, r = 1, \ldots, R\}$ from a zero-mean unit-variance Gaussian distribution, after which we compute the rank-L truncated SVD of these matrices, by keeping the first L singular vectors, i.e., $\mathbf{X}_r = \mathbf{U}_r \cdot \mathbf{\Sigma}_r \cdot \mathbf{V}_r^H$. For each of the R terms, we then change the L diagonal values of $\mathbf{\Sigma}_r$ to impose a given condition number $\kappa(\mathbf{X}_r)$ on $\mathbf{X}_r$, after which $\mathbf{A}_r \in \mathbb{C}^{I \times L}$ is set to $\mathbf{U}_r \cdot \mathbf{\Sigma}_r$ and $\mathbf{B}_r \in \mathbb{C}^{J \times L}$ is set to $\mathbf{V}_r^*$. For a given a value of $\kappa(\mathbf{X}_r)$, the first diagonal element of $\mathbf{\Sigma}_r$ is always set to 1, the last one is set to $\kappa(\mathbf{X}_r)$ and the $L-2$ others are linearly spaced values from 1 to $\kappa(\mathbf{X}_r)$. Throughout the experiments of this section, $\kappa(\mathbf{X}_1)$ is always set to 1 and we will compare the algorithms for chosen values of $\kappa(\mathbf{X}_R)$, the values of $\kappa(\mathbf{X}_r)$ for the $R-2$ other terms being linearly spaced from 1 to $\kappa(\mathbf{X}_R)$. For instance, with $R = 4$, $L = 3$ and $\kappa(\mathbf{X}_4) = 10$, the singular values associated to $\mathbf{X}_1$, $\mathbf{X}_2$, $\mathbf{X}_3$ and $\mathbf{X}_4$ are $\{1, 1, 1\}$, $\{1, 2.5, 4\}$, $\{1, 4, 7\}$ and $\{1, 5.5, 10\}$, respectively. Finally, the tall matrix $\mathbf{C} \in \mathbb{C}^{K \times R}$ is first randomly generated after which its SVD is computed and its R singular values are set to linearly spaced values between 1 and 3, in order to impose $\kappa(\mathbf{C}) = 3$.

10.2 Algorithms settings

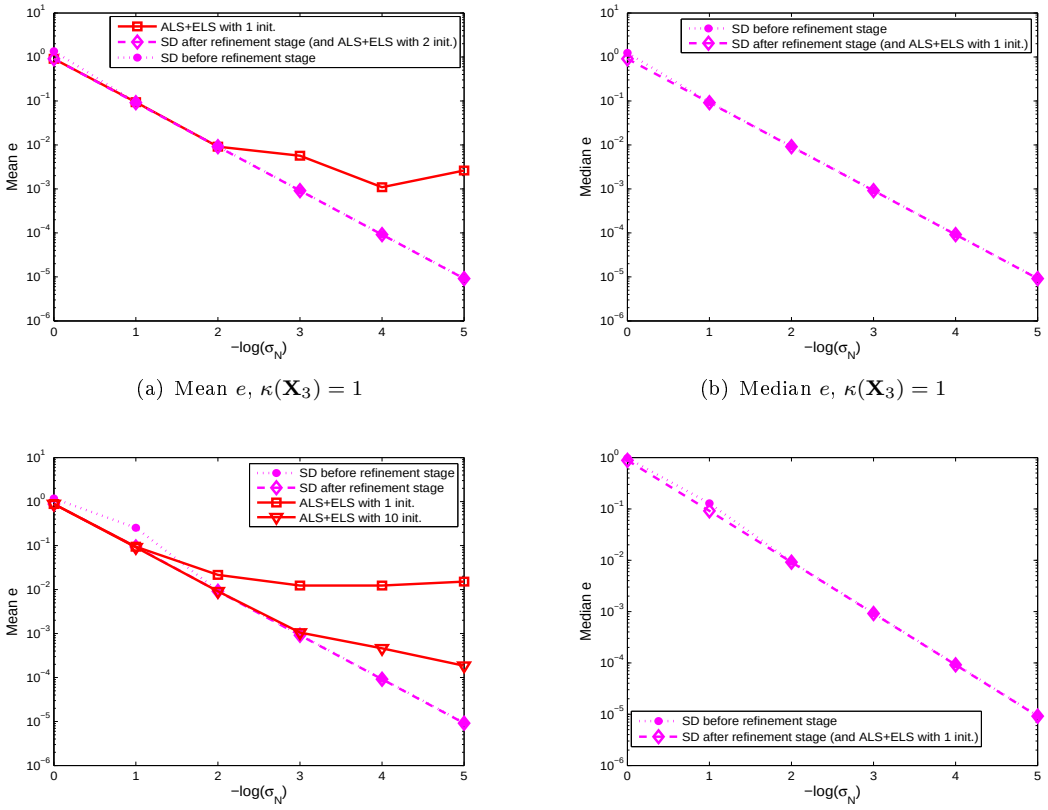
In the following experiments, the unknown components of the Decomposition in rank-$(L,L,1)$ terms are estimated in two different ways.

First, the ALS algorithm proposed in [19] is applied, coupled with an Enhanced Line Search (ELS) scheme to speed up convergence [31, 32]. The ALS+ELS algorithm is initialized with 10 different random starting points. In order to select the best initialization among the n first ($n \leq 10$), we choose the one that converges to the best fit to the model, where the Frobenius norm of the residual tensor $\|\mathcal{T} - \hat{\mathcal{T}}\|_F$ is minimal ($\hat{\mathcal{T}}$ being the estimated tensor, built from the estimates $\hat{\mathbf{A}}$, $\hat{\mathbf{B}}$ and $\hat{\mathbf{C}}$). Let k be the iteration index in the ALS+ELS algorithm and ϵ_k the quantity defined by $\epsilon_k = \|\mathcal{T} - \hat{\mathcal{T}}_{k-1}\|_F - \|\mathcal{T} - \hat{\mathcal{T}}_k\|_F$, which measures the decrease in fit to the model between two subsequent iterations. The algorithm is stopped when ϵ_k drops below a certain threshold (10^{-8} has been chosen in practice).

Second, the algorithm based on simultaneous diagonalization proposed in this paper is applied. The SD problem itself is solved by means of the efficient extended QZ-iteration proposed in [44]. This iteration is initialized by means of the generalized Schur decomposition [20] of $\check{\mathbf{M}}_1$ and $\check{\mathbf{M}}_2$ in (39). The iteration is stopped when a Q-step followed by a Z-step does no longer reduce the cost function of the extended QZ-iteration, defined in [44, Eq. (26)], by at least 10^{-3} percent. Finally the estimates provided by the QZ stage are used as starting points of an ALS+ELS final refinement stage, as explained in Section 7. The maximum number of ALS+ELS iterations in this stage is fixed to 500 and the stop criterion is the same as the one described previously for the full ALS+ELS algorithm. As we will illustrate further, only a few ALS+ELS refinement iterations are generally needed.

10.3 Performance

To assess performance of SD and ALS+ELS algorithms, we proceed as follows. First, the columns of the final estimate $\hat{\mathbf{C}} \in \mathbb{C}^{K \times R}$ are optimally reordered and rescaled to match the true data



(a) Mean e, $\kappa(\mathbf{X}_3) = 1$

(b) Median e, $\kappa(\mathbf{X}_3) = 1$

(c) Mean e, $\kappa(\mathbf{X}_3) = 10$

(d) Median e, $\kappa(\mathbf{X}_3) = 10$

Figure 5: Mean and median error for $\kappa(\mathbf{X}_3) = \{1, 10\}$. Dimensions: $I = 6$, $J = 6$, $K = 20$, $L = 2$, $R = 3$.

matrix $\mathbf{C}$. Once these permutation and scaling ambiguities have been fixed, the final error $e = \|\mathbf{C} - \hat{\mathbf{C}}\|_F / \|\mathbf{C}\|_F$ is computed.

10.4 Monte-Carlo simulations

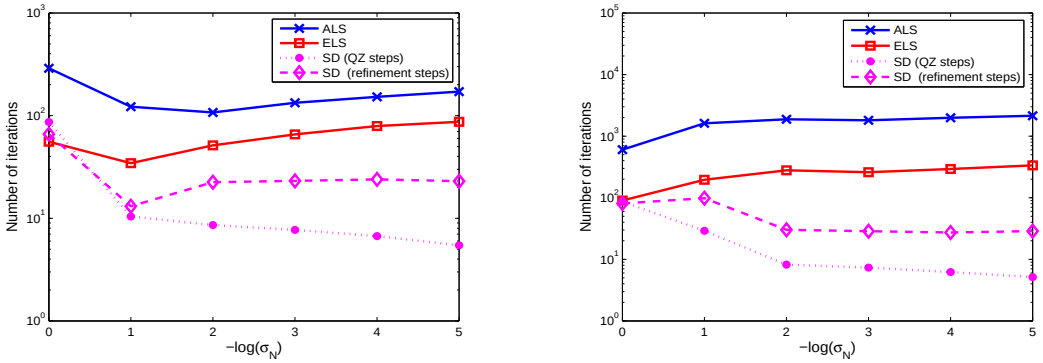
In this section, we compare the performance of the ALS+ELS and SD algorithms via Monte-Carlo simulations consisting of 200 independent runs for each value of $\sigma_N \in 10^{\{0,-1,-2,-3,-4,-5\}}$, all data being randomly regenerated for each run.

10.4.1 First experiment

In a first experiment (Figs. 5, 6 and 7), the dimensions are $I = 6$, $J = 6$, $K = 20$, $L = 2$, $R = 3$, i.e., uniqueness is covered by the sufficient bound (40), and a fortiori by the new bound (64) also. Performance is assessed in cases $\kappa(\mathbf{X}_3) = \{1, 10\}$. Fig. 5 represents the evolution of error (mean and median).

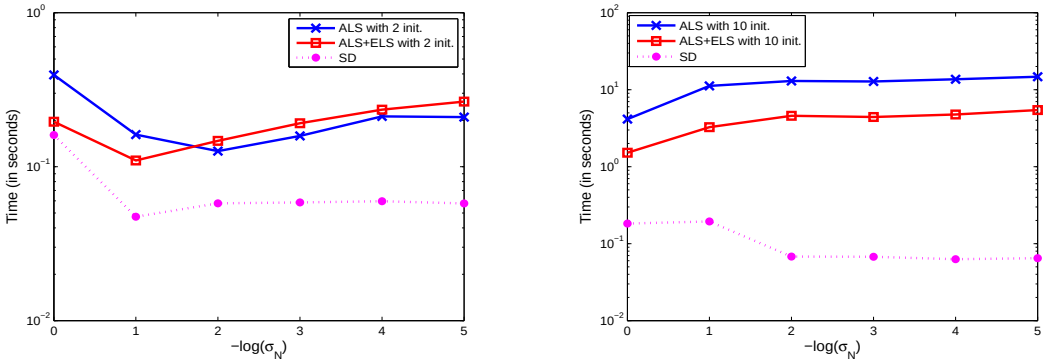
When $\kappa(\mathbf{X}_3) = 1$, ALS+ELS achieves the same mean error as SD after 2 random initializations, and the same median error after one initialization. The performance at the output of the SD stage, i.e., without the ALS+ELS refinement stage, is also plotted, and it is clear that in the case $\kappa(\mathbf{X}_3) = 1$, the refinement stage only slightly improves the error for high noise levels.

When $\kappa(\mathbf{X}_3) = 10$, the median error is also the same with one initialization, but there is a large performance gap in terms of the mean error between SD and ALS+ELS, even after 10 initializations of the latter algorithm. The relative bad performance of ALS+ELS algorithm in



(a) $\kappa(\mathbf{X}_3) = 1$ (b) $\kappa(\mathbf{X}_3) = 10$

Figure 6: Mean number of iterations (average over 10 initializations and 200 Monte-Carlo runs). Dimensions: $I = 6$, $J = 6$, $K = 20$, $L = 2$, $R = 3$.

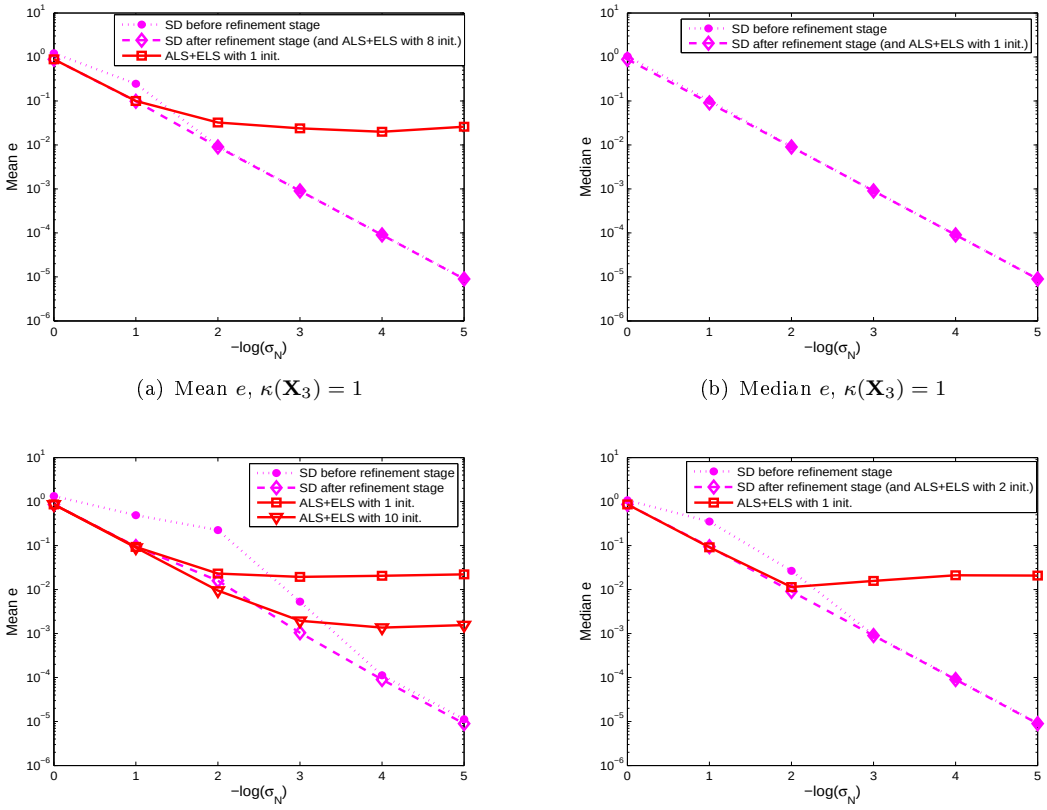


(a) $\kappa(\mathbf{X}_3) = 1$ (b) $\kappa(\mathbf{X}_3) = 10$

Figure 7: Total execution time (sum over the n needed initializations and average over the 200 Monte-Carlo runs). Dimensions: $I = 6$, $J = 6$, $K = 20$, $L = 2$, $R = 3$.

this case is caused by its sensibility to swamps, i.e., a region where the fit to the model $\|\mathcal{T} - \hat{\mathcal{T}}_k\|_F$ is almost constant for several consecutive iterations, after which it may suddenly decrease again. When a swamp is encountered, the stop criterion $\epsilon_k < 10^{-8}$ is likely to be satisfied before the algorithm reaches the global minimum (we call it a "bad run"). Of course, 10 random initializations may result in 10 bad runs, and this situation may occur several times among the 200 Monte-Carlo runs. Since swamps occur more often in presence of ill-conditioned data, this partly explains why more initializations are needed when $\kappa(\mathbf{X}_3)$ increases, since the global minimum becomes harder to reach. Note that these bad runs have less impact on the median error since it suffices that at least 50 percent of the Monte-Carlo runs converge to the global minimum for the bad runs to be excluded from the performance measure. Examination of the median error thus gives an idea on the number of bad runs. When $\kappa(\mathbf{X}_3) = 10$, one can also observe that the final refinement stage that follows the SD stage significantly lowers the final error for high noise levels, more than it does when $\kappa(\mathbf{X}_3) = 1$.

In Fig. 6, we represent the evolution of the number of iterations, averaged over the 200 Monte-Carlo runs. We compare SD to standard ALS (i.e., without line search) and to ALS+ELS. For ALS and ALS+ELS, the number of iterations is also averaged over the 10 random starting points. For SD, we distinguish between the number of QZ-iterations and the number of ALS+ELS iterations of the final refinement stage (initialized with the matrices obtained from the QZ-stage). We first observe that the ELS scheme allows a substantial reduction of the number of iterations, relatively



(a) Mean e, $\kappa(\mathbf{X}_3) = 1$

(b) Median e, $\kappa(\mathbf{X}_3) = 1$

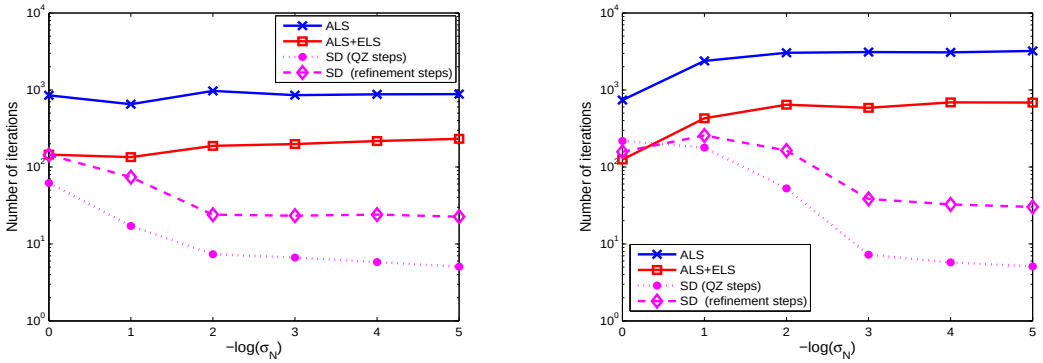
(c) Mean e, $\kappa(\mathbf{X}_3) = 10$

(d) Median e, $\kappa(\mathbf{X}_3) = 10$

Figure 8: Mean and median error for $\kappa(\mathbf{X}_3) = \{1, 10\}$. Dimensions: $I = 6$, $J = 6$, $K = 20$, $L = 3$, $R = 3$.

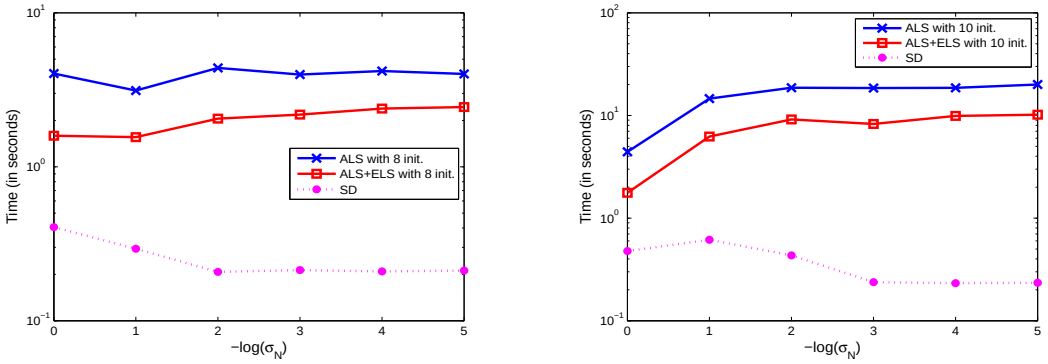
to standard ALS, which was expected since ELS has been derived to speed convergence of ALS (see [31, 32] for details). Note that the average number of iterations of both ALS and ALS+ELS increases by one decade when $\kappa(\mathbf{X}_3)$ increases from 1 to 10, which is caused by swamps. For both cases $\kappa(\mathbf{X}_3) = 1$ and $\kappa(\mathbf{X}_3) = 10$, the number of QZ-iterations is approximately the same (typically less than 10 below a certain noise level), and the number of ALS+ELS final refinement iterations is relatively small (typically less than 50), which confirms that the QZ-stage provides estimates that are already very close to the final least-squares solution.

In Fig. 7, we compare the execution times, averaged over the 200 Monte-Carlo runs. For ALS and ALS+ELS, we first find the number n of initializations needed for their respective mean error performance to match the performance of SD, i.e., from Fig. 5, 2 initializations when $\kappa(\mathbf{X}_3) = 1$ and more than 10 initializations when $\kappa(\mathbf{X}_3) = 10$. Then, the effective execution time is simply obtained from the sum of the n first execution times, and is compared to the total execution time of the SD-based algorithm (taking all QZ-steps and final ALS+ELS steps into account). It follows that the SD-based algorithm is substantially faster than ALS+ELS, at least for the dimensions considered in this section. This was expected from the observations on the number of iterations (Fig. 6), since on one side, we typically have less than 10 QZ-steps followed by less than 50 ALS+ELS steps for the SD algorithm, and around 100 ALS+ELS iterations multiplied by the number of initializations on the other side.



(a) $\kappa(\mathbf{X}_3) = 1$ (b) $\kappa(\mathbf{X}_3) = 10$

Figure 9: Mean number of iterations (average over 10 initializations and 200 Monte-Carlo runs). Dimensions: $I = 6$, $J = 6$, $K = 20$, $L = 3$, $R = 3$.

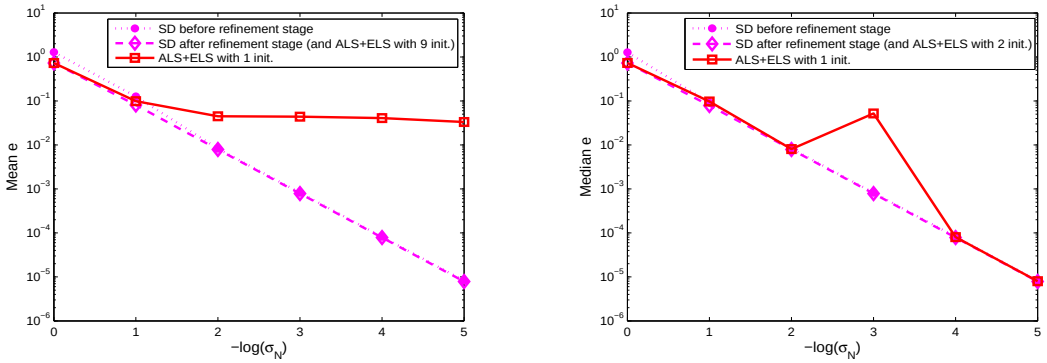


(a) $\kappa(\mathbf{X}_3) = 1$ (b) $\kappa(\mathbf{X}_3) = 10$

Figure 10: Total execution time (sum over the n needed initializations and average over the 200 Monte-Carlo runs). Dimensions: $I = 6$, $J = 6$, $K = 20$, $L = 3$, $R = 3$.

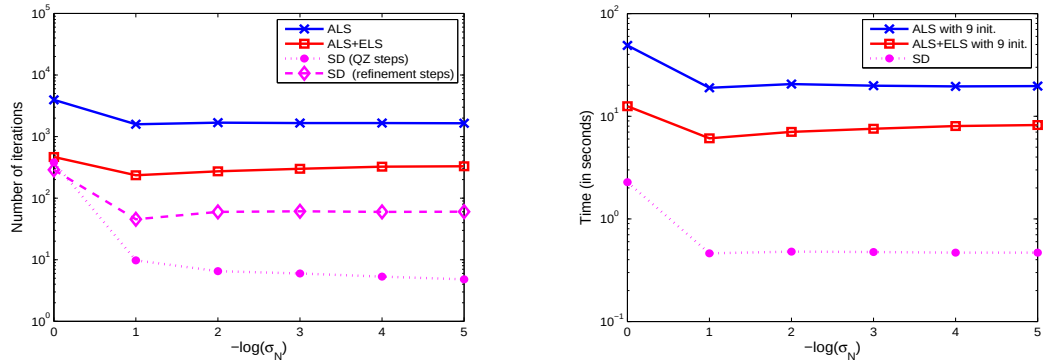
10.4.2 Second experiment

In this section, we proceed to the same experiments as in the previous section, except that now $L = 3$ instead of $L = 2$. Since the dimensions are $I = 6$, $J = 6$, $K = 20$, and $R = 3$, uniqueness is no longer covered by the sufficient bound (40), but it is nonetheless covered by the new bound (64). In Fig. 8, we represent the evolution of the mean and median error. When $\kappa(\mathbf{X}_3) = 1$, the mean error of ALS+ELS matches that of SD, after 8 initializations. In the same conditions but with $L = 2$, the performance of both algorithms matches after only 2 initializations (see Fig. 5). When $\kappa(\mathbf{X}_3) = 10$, a large mean error performance gap can be observed between SD and ALS+ELS. It is also interesting to note that, in the case $\kappa(\mathbf{X}_3) = 10$, the ALS+ELS median error curve with only one initialization does not match the SD curve at all. This means that among the 200 Monte-Carlo runs initialized once, at least 100 failed to converge to the global minimum. Compared to the results of Section 10.4.1, this clearly reveals that increasing L from 2 to 3 results in a considerably more difficult problem in average. It is also interesting to note that the final refinement stage now significantly improves the error. Nonetheless, the number of ALS+ELS iterations needed in this stage is still relatively small (see Fig. 9). This means that the solutions provided by the SD-stage may be considered as being not satisfactory in the least squares sense, but these solutions are still very good starting points for the ALS+ELS refinement stage, which may significantly reduce the error in a few iterations.



(a) Mean e

(b) Median e



(c) Number of iterations

(d) Execution time

Figure 11: Dimensions: $I = 6$, $J = 6$, $K = 20$, $L = 2$, $R = 7$. $\kappa(\mathbf{X}_7) = 1$.

In Fig. 10, we represent the evolution of the execution time. The observations are similar to the case $L = 2$ of Section 10.4.1, i.e., the number of QZ-iterations (followed by ALS+ELS iterations) being small compared to the number of ALS or ALS+ELS iterations, above from the fact that the two latter algorithms have to be initialized several times, it follows that the execution time for the SD-based algorithm is substantially smaller.

10.4.3 Third experiment

In this final experiment, the dimensions are set to $I = 6$, $J = 6$, $K = 20$, $L = 2$ and $R = 7$, such that uniqueness is guaranteed by the new bound only, and $\kappa(\mathbf{X}_7)$ is fixed to 1. In Fig. 11, we represent the evolution of the mean error, median error, number of iterations and execution time. Although the data are well conditioned, 9 initializations are needed for the mean error performance of ALS+ELS to match that of SD (2 initializations for the median error). The SD technique is clearly advantageous in terms of the number of iterations and execution time.

11 Conclusion

In this paper, we have considered the decomposition in rank-(L,L,1) terms of a third-order tensor. To a large extent, it is an important multilinear algebra tool that generalizes the standard rank-(1,1,1) (i.e., PARAFAC) decomposition. Under certain conditions on the dimensions of the tensor, we have shown that the BCD-(L,L,1) can be reformulated as a problem of Simultaneous Diagonalization (SD) of a set of matrices, via an algebraic tool for rank-L detection. The resulting SD-based algorithm followed by a few ALS+ELS refinement steps reveals to be faster and more accurate than the standard Alternating Least Squares algorithm proposed in [19], even when the latter is improved by an Enhanced Line Search scheme [31,32], especially when the problem is not well conditioned or when the number of rank-(L,L,1) terms is large.

Beyond the algorithmic aspect, another fundamental research axis which is still under intensive development concerns uniqueness of tensor decompositions. In [9], it was shown that the reformulation of PARAFAC into a simultaneous diagonalization problem results in a relaxed deterministic uniqueness bound. In this paper, we have generalized this result to the BCD-(L,L,1), i.e., we have shown that the reformulation of the BCD-(L,L,1) in terms of SD involves a new deterministic generic bound for its uniqueness. We have derived the analytic expression for this new bound, which is much more relaxed than the sufficient bound given in [11], in the sense that it allows extraction of a significantly greater number of rank-(L,L,1) terms. A possible extension of the work proposed in this paper would consist in the derivation of a new uniqueness bound when the long dimension of the tensor is carried by one of the rank-L matrix, i.e., $R \leq \min(IK, J)$ or $R \leq \min(JK, I)$, instead of the condition $R \leq \min(IJ, K)$ considered in this paper.

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