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CANONICAL POLYADIC DECOMPOSITION WITH ORTHOGONALITY CONSTRAINTS

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Abstract. Canonical Polyadic Decomposition (CPD) of a higher-order tensor is an important tool in mathematical engineering. In many applications at least one of the matrix factors is constrained to be column-wise orthonormal. We first derive a relaxed condition that guarantees uniqueness of the CPD under this constraint and generalize the result to the case where one of the factor matrices has full column rank. Second, we give a simple proof of the existence of the optimal low-rank approximation of a tensor in the case that a factor matrix is column-wise orthonormal. Third, we derive numerical algorithms for the computation of the constrained CPD. In particular, orthogonality-constrained versions of the CPD methods based on simultaneous matrix diagonalization and alternating least squares are presented. Numerical experiments are reported.

Key words. higher-order tensor, polyadic decomposition, canonical decomposition (CANDECOMP), parallel factor (PARAFAC), simultaneous matrix diagonalization, alternating least squares, orthogonality.

1. Introduction. A Nth-order rank-1 tensor $\mathcal{X} \in \mathbb{C}^{I_1 \times \cdots \times I_N}$ is defined as the tensor product of non-zero vectors $\mathbf{a}^{(n)} \in \mathbb{C}^{I_n}$, $1 \leq n \leq N$, such that $\mathcal{X}_{i_1 \dots i_N} = \prod_{n=1}^{N} a_{i_n}^{(n)}$. We write $\mathcal{X} = \mathbf{a}^{(1)} \circ \mathbf{a}^{(2)} \circ \cdots \circ \mathbf{a}^{(N)}$. The rank of a tensor $\mathcal{X}$ is equal to the minimal number of rank-1 tensors that yield $\mathcal{X}$ in a linear combination. Assume that the rank of $\mathcal{X}$ is R, then it can be written as

$$\mathcal{X} = \sum_{r=1}^{R} \mathbf{a}_r^{(1)} \circ \cdots \circ \mathbf{a}_r^{(N)}, \tag{1.1}$$

where $\mathbf{a}_r^{(n)} \in \mathbb{C}^{I_n}$. This decomposition is sometimes called the PARAllel FACtor (PARAFAC) [18] or the CANonical DECOMPosition (CANDECOMP) [5] of $\mathcal{X}$. In this paper we will use the term Canonical Polyadic Decomposition (CPD). Let us stack the vectors $\{\mathbf{a}_r^{(n)}\}$ into the matrices

$$\mathbf{A}^{(n)} = \left[\begin{array}{ccc} \mathbf{a}_1^{(n)}, & \cdots & , \mathbf{a}_R^{(n)} \end{array} \right] \in \mathbb{C}^{I_n \times R}, \quad 1 \leq n \leq N. \tag{1.2}$$

The matrices $\mathbf{A}^{(n)}$ in (1.2) will be denoted as factor matrices. In this paper we are interested in the case where one of the factor matrices is column-wise orthonormal. For convenience, we say that this matrix is semi-unitary (in the complex case) or semi-orthogonal (in the real case).

The CPD of a higher-order tensor is called unique if alternative representations involve the same rank-1 terms up to permutation. CPD is unique under mild conditions, see for instance [30, 12]. The first contribution of this paper is a relaxed

condition under which a semi-unitary constrained CPD is unique. Under this condition, the CPD may be computed by algebraic means. We extend the uniqueness result to the case where a factor matrix has full column rank (implying that it has at least as many rows as columns).

In applications, a CPD is rarely exact. Most often, a low-rank tensor is fitted to the given tensor in some approximate sense, e.g., in least-squares sense. However, the optimal solution does not necessarily exist, i.e., the cost function in the approximation problem may only have an infimum and not a minimum [15, 27]. One of the advantages of semi-unitary constrained CPD is that the approximation problem does always have an optimal solution, as was demonstrated in [27]. We give a very short proof of this basic fact.

For the computation of CPD with a semi-unitary factor matrix we derive new semi-unitary constrained versions of the Simultaneous matrix Diagonalization (SD-CP) [12] and Alternating Least Squares (ALS-CP) [18, 36] algorithms.

Besides being used for avoiding problems with the non-existence of the optimal low-rank approximation [19, 16], CPD with a semi-unitary factor matrix is used in signal processing in applications where the orthogonality constraints are due to zero-mean signals being uncorrelated. We mention applications in polarization sensitive array processing [32] and in multiple access wireless communication systems such as DS-CDMA [35]. The decomposition has further been used in the context of blind signal separation and Independent Component Analysis (ICA), e.g. for the blind identification of underdetermined mixtures [1, 13] and for structured ICA [2]. Further, CPD of fully or partially symmetric tensors with all or several factor matrices unitary has found application in ICA methods that involve a prewhitening [3, 7, 8, 11, 14]. The latter variants are commonly computed by means of Jacobi-type iterations. In image processing, unsymmetric CPD with unitary factor matrices has found use in data representation via a joint Singular Value Decomposition (SVD) [33]. Here the CPD is unsymmetric and two of the factor matrices are unitary. For the computation a Jacobi-type algorithm was proposed. Further, two iterative methods for the computation of an unsymmetric CPD involving only semi-orthogonal or semi-unitary factor matrices have been proposed in [31] and [6].

The paper is organized as follows. The rest of the introduction will present our notation. Next, in section 2 and 3 we discuss the uniqueness and low-rank approximation properties of a CPD with a semi-unitary matrix factor, respectively. Section 4 and 5 propose semi-unitary constrained versions of the SD-CP and ALS-CP methods, respectively. Parts of this work appeared in the conference papers [35, 8]. Section 6 briefly explains how the results can be extended to tensors of order higher than three. In section 7 numerical experiments are reported. We end the paper with a conclusion in section 8.

Notation Vectors, matrices and tensors are denoted by lower case boldface, upper case boldface and upper case calligraphic letters, respectively. The symbol $\otimes$ and $\odot$ denote the Kronecker and Khatri-Rao products, defined as

$$\mathbf{A} \otimes \mathbf{B} \triangleq \begin{bmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \dots \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \quad , \quad \mathbf{A} \odot \mathbf{B} \triangleq \begin{bmatrix} \mathbf{a}_1 \otimes \mathbf{b}_1 & \mathbf{a}_2 \otimes \mathbf{b}_2 & \dots \end{bmatrix},$$

in which $(\mathbf{A})_{mn} = a_{mn}$ and $\mathbf{a}_r$ and $\mathbf{b}_r$ denote the rth column vector of $\mathbf{A}$ and $\mathbf{B}$,

respectively. The Hadamard product is denoted by $*$ and is given by

$$\mathbf{A} * \mathbf{B} \triangleq \begin{bmatrix} a_{11}b_{11} & a_{12}b_{12} & \dots \\ a_{21}b_{21} & a_{22}b_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}.$$

The following three matrix representations of a CPD of a third-order tensor $\mathcal{X} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ will be used throughout the paper. Let $\mathbf{X}^{(i_1 \cdot \cdot)} \in \mathbb{C}^{I_2 \times I_3}$ denote the matrix such that $\mathbf{X}^{(i_1 \cdot \cdot)}_{i_2 i_3} = \mathcal{X}_{i_1 i_2 i_3}$, then

$$\mathbf{X}^{(i_1 \cdot \cdot)} = \mathbf{A}^{(2)} D_{i_1}\left(\mathbf{A}^{(1)}\right) \mathbf{A}^{(3)T}$$

and

$$\mathbb{C}^{I_1 I_2 \times I_3} \ni \mathbf{X}_{(1)} \triangleq \begin{bmatrix} \mathbf{X}^{(1 \cdot \cdot)} \\ \vdots \\ \mathbf{X}^{(I_1 \cdot \cdot)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{(2)} D_1\left(\mathbf{A}^{(1)}\right) \\ \vdots \\ \mathbf{A}^{(2)} D_{I_1}\left(\mathbf{A}^{(1)}\right) \end{bmatrix} \mathbf{A}^{(3)T} = \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right) \mathbf{A}^{(3)T}.$$

Similarly, let the matrices $\mathbf{X}^{(\cdot i_2 \cdot)} \in \mathbb{C}^{I_3 \times I_1}$ be constructed such that $\mathbf{X}^{(\cdot i_2 \cdot)}_{i_3 i_1} = \mathcal{X}_{i_1 i_2 i_3}$, then

$$\mathbf{X}^{(\cdot i_2 \cdot)} = \mathbf{A}^{(3)} D_{i_2}\left(\mathbf{A}^{(2)}\right) \mathbf{A}^{(1)T}$$

and

$$\mathbb{C}^{I_2 I_3 \times I_1} \ni \mathbf{X}_{(2)} \triangleq \begin{bmatrix} \mathbf{X}^{(\cdot 1 \cdot)} \\ \vdots \\ \mathbf{X}^{(\cdot I_2 \cdot)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{(3)} D_1\left(\mathbf{A}^{(2)}\right) \\ \vdots \\ \mathbf{A}^{(3)} D_{I_2}\left(\mathbf{A}^{(2)}\right) \end{bmatrix} \mathbf{A}^{(1)T} = \left(\mathbf{A}^{(2)} \odot \mathbf{A}^{(3)}\right) \mathbf{A}^{(1)T}.$$

Finally, let $\mathbf{X}^{(\cdot \cdot i_3)} \in \mathbb{C}^{I_1 \times I_2}$ satisfy $\mathbf{X}^{(\cdot \cdot i_3)}_{i_1 i_2} = \mathcal{X}_{i_1 i_2 i_3}$, then

$$\mathbf{X}^{(\cdot \cdot i_3)} = \mathbf{A}^{(1)} D_{i_3}\left(\mathbf{A}^{(3)}\right) \mathbf{A}^{(2)T}$$

and

$$\mathbb{C}^{I_1 I_3 \times I_2} \ni \mathbf{X}_{(3)} \triangleq \begin{bmatrix} \mathbf{X}^{(\cdot \cdot 1)} \\ \vdots \\ \mathbf{X}^{(\cdot \cdot I_3)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{(1)} D_1\left(\mathbf{A}^{(3)}\right) \\ \vdots \\ \mathbf{A}^{(1)} D_{I_3}\left(\mathbf{A}^{(3)}\right) \end{bmatrix} \mathbf{A}^{(2)T} = \left(\mathbf{A}^{(3)} \odot \mathbf{A}^{(1)}\right) \mathbf{A}^{(2)T}.$$

Further, $\mathrm{Tr}\,(\cdot)$, $(\cdot)^T$, $(\cdot)^*$, $(\cdot)^H$, $(\cdot)^\dagger$, $\|\cdot\|_F$, $\mathrm{Col}\,(\cdot)$, $\mathrm{Re}\,\{\cdot\}$ and $\mathrm{Im}\{\cdot\}$ denote the trace, transpose, conjugate, conjugate-transpose, Moore-Penrose pseudo-inverse, Frobenius norm, column space, real part and imaginary part of a matrix, respectively. The identity matrix and the all-ones vector are denoted by $\mathbf{I}_R \in \mathbb{C}^{R \times R}$ and $\mathbf{1}_R = [1, \dots, 1]^T \in \mathbb{C}^R$, respectively. Matlab index notation will be used to denote submatrices of a given matrix. For example, $\mathbf{A}(1:k,:)$ denotes the submatrix of $\mathbf{A}$ consisting of the rows from 1 to k. The notation $\mathrm{diag}\,(\cdot)$ is used to denote the operator that sets the off-diagonal elements of a matrix equal to zero. Let $\mathbf{A} \in \mathbb{C}^{I \times J}$, then $\mathrm{Vec}\,(\mathbf{A}) \in \mathbb{C}^{IJ}$ denotes the column vector defined by $(\mathrm{Vec}\,(\mathbf{A}))_{i+(j-1)I} = (\mathbf{A})_{ij}$. Let $\mathbf{a} \in \mathbb{C}^{IJ}$, then the reverse operation is $\mathrm{Unvec}\,(\mathbf{a}) = \mathbf{A} \in \mathbb{C}^{I \times J}$ such that $(\mathbf{a})_{i+(j-1)I} = (\mathbf{A})_{ij}$. Let $\mathbf{A} \in \mathbb{C}^{I \times I}$, then $\mathrm{Vecd}\,(\mathbf{A}) \in \mathbb{C}^I$ denotes the column vector defined by $(\mathrm{Vecd}\,(\mathbf{A}))_i = (\mathbf{A})_{ii}$. Let $\mathbf{A} \in \mathbb{C}^{I \times J}$, then $D_k\,(\mathbf{A}) \in \mathbb{C}^{J \times J}$ denotes the diagonal matrix holding row k of $\mathbf{A}$ on its diagonal.

The k-rank of a matrix $\mathbf{A}$ is denoted by $\mathrm{k}\,(\mathbf{A})$. It is equal to the largest integer $\mathrm{k}\,(\mathbf{A})$ such that every subset of $\mathrm{k}\,(\mathbf{A})$ columns of $\mathbf{A}$ is linearly independent.

2. Uniqueness of CPD with a Full Column Rank Matrix Factor. The CPD of a higher-order tensor is unique if all the N-tuplets $\left(\overline{\mathbf{A}}^{(1)}, \ldots, \overline{\mathbf{A}}^{(N)}\right)$ satisfying (1.1) are related via

$$\overline{\mathbf{A}}^{(n)} = \mathbf{A}^{(n)} \Pi \Delta_{\mathbf{A}^{(n)}}, \quad \forall n \in \{1, \ldots, N\},$$

where Π is a permutation matrix and $\{\Delta_{\mathbf{A}^{(n)}}\}$ are diagonal matrices satisfying $\prod_{n=1}^{N} \Delta_{\mathbf{A}^{(n)}} = \mathbf{I}_R$.

2.1. Deterministic Conditions. We first review two existing uniqueness conditions for CPD (Theorems 2.1 and 2.2). Next, we provide a new uniqueness condition for a complex CPD with a semi-unitary matrix factor (Theorem 2.3). This then leads to a new uniqueness condition for a complex CPD with a nonsingular matrix factor (Corollary 2.4). We consider the third-order case for simplicity. The results can however be extended to Nth-order tensors, as will be briefly discussed in section 6.

The following theorem presents the sufficient condition for essential CPD uniqueness that is known as Kruskal's condition.

THEOREM 2.1. *Consider the tensor* $X \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ *with rank R and matrix representation* $X_{(1)} = \left(A^{(1)} \odot A^{(2)}\right) A^{(3)T}$. *If*

$$k\left(A^{(1)}\right) + k\left(A^{(2)}\right) + k\left(A^{(3)}\right) \geq 2(R+1), \tag{2.1}$$

then the CPD of X is unique [30, 37].

Condition (2.1) is sufficient for essential uniqueness but not necessary [40]. The following uniqueness condition covers cases that are not covered by Kruskal's and vice-versa.

THEOREM 2.2. *Consider the tensor* $X \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ *with rank R and matrix representation* $X_{(1)} = \left(A^{(1)} \odot A^{(2)}\right) A^{(3)T}$. *Define* $C \in \mathbb{C}^{I_1^2 I_2^2 \times R(R-1)/2}$ *by*

$$c_{(i_1-1)(I_1 I_2^2)+(j_1-1)I_2^2+(i_2-1)I_2+j_2, \frac{(r_2-2)(r_2-1)}{2}+r_1} = \left(a_{i_1,r_1}^{(1)} a_{j_1,r_2}^{(1)} - a_{j_1,r_1}^{(1)} a_{i_1,r_2}^{(1)}\right)\left(a_{i_2,r_1}^{(2)} a_{j_2,r_2}^{(2)} - a_{j_2,r_1}^{(2)} a_{i_2,r_2}^{(2)}\right),$$

where $1 \leq i_1, j_1 \leq I_1$, $1 \leq i_2, j_2 \leq I_2$ and $1 \leq r_1 < r_2 \leq R$. If $A^{(3)}$ and C have full column rank, then the CPD of X is unique [12, 24].

When the matrix factor $\mathbf{A}^{(3)}$ is semi-unitary, it a forteriori has full column rank ($R \leq I_3$). Hence, the uniqueness condition stated in Theorem 2.2 also applies in the case of a CPD with a semi-unitary matrix factor.

We will now provide a new uniqueness condition for a complex CPD with a semi-unitary matrix factor.

THEOREM 2.3. *Consider the tensor* $X \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ *with rank R and matrix representation* $X_{(1)} = \left(A^{(1)} \odot A^{(2)}\right) A^{(3)T}$ *in which $A^{(3)}$ is semi-unitary. Let*

$$N_{\max} = \begin{cases} 2 & \text{if } I_2 \geq I_1 \\ 1 & \text{if } I_1 > I_2 \end{cases}, \quad N_{\min} = \begin{cases} 2 & \text{if } I_2 < I_1 \\ 1 & \text{if } I_1 \leq I_2 \end{cases} \tag{2.2}$$

$$I_{\max} = \max(I_1, I_2), \quad I_{\min} = \min(I_1, I_2). \tag{2.3}$$

Define $C \in \mathbb{C}^{I_{\max}^4 \times R(R-1)/2}$ *by*

$$c_{(i_1-1)I_{\max}^3+(j_1-1)I_{\max}^2+(i_2-1)I_{\max}+j_2, \frac{(r_2-2)(r_2-1)}{2}+r_1} = \left(a_{i_1,r_1}^{(N_{\max})*} a_{j_1,r_2}^{(N_{\max})*} - a_{j_1,r_1}^{(N_{\max})*} a_{i_1,r_2}^{(N_{\max})*}\right)\left(a_{i_2,r_1}^{(N_{\max})} a_{j_2,r_2}^{(N_{\max})} - a_{j_2,r_1}^{(N_{\max})} a_{i_2,r_2}^{(N_{\max})}\right)$$

$$\tag{2.4}$$

where $1 \leq i_1, j_1, i_2, j_2 \leq I_{\max}$ *and* $1 \leq r_1 < r_2 \leq R$. *If* $\mathbf{A}^{(N_{\min})*} \odot \mathbf{A}^{(N_{\min})} \in \mathbb{C}^{I_{\min}^2 \times R}$ *and* $\mathbf{C}$ *have full column rank, then the CPD of* $\mathcal{X}$ *is unique.*

Proof. Since $\mathbf{A}^{(3)}$ is semi-unitary we can construct the fourth order tensor $\mathcal{Y} \in \mathbb{C}^{I_2 \times I_2 \times I_1 \times I_1}$ with matrix slices

$$\mathbb{C}^{I_2 \times I_2} \ni \mathbf{Y}^{(\cdot \cdot i_3, i_4)} = \mathbf{X}^{(i_3 \cdot \cdot)} \mathbf{X}^{(i_4 \cdot \cdot)H}$$
$$= \mathbf{A}^{(2)} D_{i_3} \left(\mathbf{A}^{(1)} \right) D_{i_4} \left(\mathbf{A}^{(1)*} \right) \mathbf{A}^{(2)H}, \quad \forall i_3, i_4 \in \{1, \dots, I_1\},$$

and $\mathcal{Y}(:, :, i_3, i_4) = \mathbf{Y}^{(\cdot \cdot i_3, i_4)}, \forall i_3, i_4 \in \{1, \dots, I_1\}$. We have

$$\text{Vec}\left(\mathbf{Y}^{(\cdot \cdot i_3, i_4)} \right) = \left(\mathbf{A}^{(2)*} \odot \mathbf{A}^{(2)} \right) \text{Vecd} \left(D_{i_3} \left(\mathbf{A}^{(1)} \right) D_{i_4} \left(\mathbf{A}^{(1)*} \right) \right)$$

and

$$\mathbf{Y} = \left[\text{Vec}\left(\mathbf{Y}^{(\cdot \cdot 1, 1)} \right), \text{Vec}\left(\mathbf{Y}^{(\cdot \cdot 1, 2)} \right), \cdots, \text{Vec}\left(\mathbf{Y}^{(\cdot \cdot I_1, I_1)} \right) \right]$$
$$= \left(\mathbf{A}^{(2)*} \odot \mathbf{A}^{(2)} \right) \left(\mathbf{A}^{(1)*} \odot \mathbf{A}^{(1)} \right)^T. \tag{2.5}$$

Hence, if the fourth-order CPD with matrix representation $\mathbf{Y}$ in (2.5) is unique, then the semi-unitary constrained CPD of $\mathcal{X}$ is also unique. Due to Theorem 2.2 we know that the CPD (2.5) is unique If $\mathbf{A}^{(N_{\min})*} \odot \mathbf{A}^{(N_{\min})} \in \mathbb{C}^{I_{\min}^2 \times R}$ and $\mathbf{C} \in \mathbb{C}^{I_{\max}^4 \times R(R-1)/2}$ have full column rank, where the entries of $\mathbf{C}$ are determined by the relation (2.4). $\square$

In cases where Theorem 2.3 applies, the CPD of $\mathcal{X}$ may be computed as follows. First $\mathbf{A}^{(2)}$ may be obtained from the column space of $\mathbf{Y}$ in (2.5) by means of the unconstrained SD-CP method, which will be reviewed in section 4. Next, $\mathbf{A}^{(1)}$ may be obtained from (2.5) via a set of R decoupled best rank-1 matrix approximation problems, analogous to subsection 4.3. Finally, the semi-unitary matrix factor $\mathbf{A}^{(3)}$ may be computed by solving a unitary Procrustes-type problem, as will also be explained in subsection 4.3. In the rest of the paper we will find the matrix factors directly from $\mathcal{X}$, instead of working with $\mathcal{Y}$.

An important consequence of Theorem 2.3 is the following uniqueness result that extends it to the case where $\mathbf{A}^{(3)}$ only has full column rank.

COROLLARY 2.4. *Consider the tensor* $\mathcal{T} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ *with rank R and matrix representation* $\mathbf{T}_{(1)} = \left(A^{(1)} \odot A^{(2)} \right) A^{(3)T}$ *in which* $A^{(3)}$ *has full column rank. Let* $N_{\max}, N_{\min}, I_{\max}$ *and* $I_{\min}$ *be defined as (2.2) and (2.3) and let* $C \in \mathbb{C}^{I_{\max}^4 \times R(R-1)/2}$ *be constructed according to (2.4). If* $A^{(N_{\min})*} \odot A^{(N_{\min})} \in \mathbb{C}^{I_{\min}^2 \times R}$ *and* C *have full column rank, then the CPD of* $\mathcal{T}$ *is unique.*

Proof. Since $\mathbf{A}^{(3)}$ has full column rank we can compute

$$\mathbf{X}_{(1)} = \mathbf{T}_{(1)} \left(\mathbf{A}^{(3)T} \right)^{\dagger} = \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)} \right) \mathbf{I}_R. \tag{2.6}$$

As in the proof of Theorem 2.3 we obtain a matrix $\mathbf{Y}$ that can be decomposed as

$$\mathbf{Y} = \left(\mathbf{A}^{(2)*} \odot \mathbf{A}^{(2)} \right) \left(\mathbf{A}^{(1)*} \odot \mathbf{A}^{(1)} \right)^T. \tag{2.7}$$

Hence, if the fourth-order CPD with matrix representation $\mathbf{Y}$ in (2.7) is unique, then the CPD represented by the decomposition of $\mathbf{X}_{(1)}$ in (2.6) is also unique. Due to Theorem 2.3 we known that this is true if $\mathbf{A}^{(N_{\min})*} \odot \mathbf{A}^{(N_{\min})} \in \mathbb{C}^{I_{\min}^2 \times R}$ and $\mathbf{C} \in \mathbb{C}^{I_{\max}^4 \times R(R-1)/2}$ have full column rank. Finally, since $\mathbf{X}_{(1)} = \mathbf{T}_{(1)} \left(\mathbf{A}^{(3)T} \right)^{\dagger}$ with $\mathbf{A}^{(3)}$ full column rank, the CPD of $\mathcal{T}$ is unique. $\square$

By a similar reasoning we can also relax Theorem 2.1 in the case where one of the matrix factors has full column rank.

THEOREM 2.5. *Consider the tensor* $\mathcal{T} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ *with rank R and matrix representation* $T_{(1)} = \left(A^{(1)} \odot A^{(2)}\right) A^{(3)T}$ *in which* $A^{(3)}$*has full column rank. Let* $N_{\max}$ *and* $N_{\min}$ *be defined as in* (2.2). *If*

$$2k\left(A^{(N_{\max})}\right) + k\left(A^{(N_{\min})*} \odot A^{(N_{\min})}\right) \geq 2(R+1), \tag{2.8}$$

then the CPD of $\mathcal{T}$ *is unique.*

Proof. Since $\mathbf{A}^{(3)}$ has full column rank, then as in the proof of Corollary 2.4 we can construct the matrix

$$\mathbf{Y} = \left(\mathbf{A}^{(2)*} \odot \mathbf{A}^{(2)}\right)\left(\mathbf{A}^{(1)*} \odot \mathbf{A}^{(1)}\right)^T. \tag{2.9}$$

The matrix $\mathbf{Y}$ (2.9) can be seen as a representation of the third-order CPD with matrix factors $\mathbf{A}^{(N_{\max})}$, $\mathbf{A}^{(N_{\max})*}$ and $\mathbf{A}^{(N_{\min})*} \odot \mathbf{A}^{(N_{\min})}$. Hence, if the CPD with matrix representation $\mathbf{Y}$ in (2.9) is unique, then the CPD represented by the decomposition of $\mathbf{X}_{(1)}$ in (2.6) is also unique. Since $k\left(\mathbf{A}^{(N_{\max})}\right) = k\left(\mathbf{A}^{(N_{\max})*}\right)$, then due to Theorem 2.1 we known that this is true if condition (2.8) is satisfied. Finally, since $\mathbf{X}_{(1)} = \mathbf{T}_{(1)}\left(\mathbf{A}^{(3)T}\right)^{\dagger}$ with $\mathbf{A}^{(3)}$ full column rank, the CPD of $\mathcal{T}$ is unique. $\square$

2.2. Generic Conditions. A CPD property is called generic if it holds with probability one when the entries of the factor matrices are drawn from absolutely continuous probability density functions. Generically, Theorem 2.2 amounts to the following.

THEOREM 2.6. *Consider the tensor* $\mathcal{X} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ *with rank R. If*

$$2R(R-1) \leq I_1(I_1-1)I_2(I_2-1) \quad \text{and} \quad R \leq I_3, \tag{2.10}$$

then the CPD of $\mathcal{X}$ *is unique in the generic case* [12]. Condition (2.10) is also sufficient for generic uniqueness when $\mathbf{A}^{(1)} = \mathbf{A}^{(2)*}$, with $\mathbf{A}^{(1)} \in \mathbb{C}^{I_1 \times R}$. The condition $R \leq I_3$ is meant to make sure that $\mathbf{A}^{(3)}$ has full column rank.

Again, since the semi-unitary matrix factor $\mathbf{A}^{(3)}$ has full column rank, the generic uniqueness condition (2.10) also applies in the case of a CPD with a semi-unitary matrix factor.

We will now derive generic versions of Theorem 2.3 and Corollary 2.4. The derivations will make use of proposition 2.8, which in turn is based on the following lemma.

LEMMA 2.7. *Given an analytic function* $f : \mathbb{C}^n \to \mathbb{C}$. *If there exists an element* $x \in \mathbb{C}^n$ *such that* $f(x) \neq 0$, *then the set* $\{x \mid f(x) = 0\}$ *is of Lebesgue measure zero.*

Proof. For a proof, see for instance [23]. $\square$

PROPOSITION 2.8. *Let* $P \in \mathbb{C}^{L \times R}$, *then the matrix* $P \odot P^* \in \mathbb{C}^{L^2 \times R}$ *has generically rank* $\min(L^2, R)$.

Proof. Consider the transposed Vandermonde matrix

$$\begin{aligned}
\mathbf{P} &= \begin{bmatrix}
1 & d_1 & d_1^2 & \cdots & d_1^{R-1} \\
1 & d_2 & d_2^2 & \cdots & d_2^{R-1} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & d_L & d_L^2 & \cdots & d_L^{R-1}
\end{bmatrix} \\
&= \left[\mathbf{1}_L, \mathbf{D}\mathbf{1}_L, \mathbf{D}^2\mathbf{1}_L \ldots, \mathbf{D}^{R-1}\mathbf{1}_L\right] \in \mathbb{C}^{L \times R},
\end{aligned}$$

where $\mathbf{d} = [d_1, \ldots, d_L]^T \in \mathbb{C}^{1 \times L}$ and $D_1\left(\mathbf{d}^T\right)$, then we get

$$\mathbf{P} \odot \mathbf{P}^* = \begin{bmatrix} 1 & d_1 d_1^* & \cdots & (d_1 d_1^*)^{R-1} \\ 1 & d_1 d_2^* & \cdots & (d_1 d_2^*)^{R-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & d_L d_L^* & \cdots & (d_L d_L^*)^{R-1} \end{bmatrix}$$
$$= \left[\mathbf{1}_{L^2}, (\mathbf{d} \otimes \mathbf{d}^*), \ldots, (\mathbf{d} \otimes \mathbf{d}^*)^{R-1} \right]. \tag{2.11}$$

Matrix (2.11) is a transposed Vandermonde matrix. If its generators $\{d_m d_n^*\}$ are nonzero and distinct, then this matrix has full rank. Now that we have found one instance where $\mathbf{P} \odot \mathbf{P}^*$ has rank $\min(R, L^2)$, lemma 2.7 further implies that $\mathbf{P} \odot \mathbf{P}^*$ has rank $\min(R, L^2)$ generically. □

THEOREM 2.9. *Consider the third order tensor $\mathcal{X} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ with matrix representation*

$$\mathbb{C}^{I_2 \times I_3} \ni X^{(i_1 \cdot \cdot)} = A^{(2)} D_{i_1}\left(A^{(1)}\right) A^{(3)T}, \quad \forall i_1 \in \{1, \ldots, I_1\},$$

where $A^{(3)}$ is semi-unitary. Let $I_{\max}$ and $I_{\min}$ be defined as (2.3). If

$$R \leq I_{\min}^2 \quad and \quad 2R(R-1) \leq I_{\max}^2(I_{\max} - 1)^2, \tag{2.12}$$

then the semi-unitary constrained CPD of $\mathcal{X}$ is unique in the generic case.

Proof. Since $\mathbf{A}^{(3)}$ is semi-unitary we can construct the fourth order tensor $\mathcal{Y} \in \mathbb{C}^{I_2 \times I_2 \times I_1 \times I_1}$ with matrix representation

$$\mathbf{Y} = \left(\mathbf{A}^{(2)*} \odot \mathbf{A}^{(2)}\right)\left(\mathbf{A}^{(1)*} \odot \mathbf{A}^{(1)}\right)^T. \tag{2.13}$$

Due to proposition 2.11 we know that the matrix $\mathbf{A}^{(n)*} \odot \mathbf{A}^{(n)}$ has generically full column rank when $I_n^2 \geq R$. Let $\mathbf{Y} = \mathbf{U}\Sigma\mathbf{V}^H$ denote the compact SVD of $\mathbf{Y}$ and assume that $I_1^2, I_2^2 \geq R$, then there generically exists a nonsingular matrix $\mathbf{F} \in \mathbb{C}^{R \times R}$ such that

$$\left(\mathbf{A}^{(2)*} \odot \mathbf{A}^{(2)}\right)\mathbf{F}^T = \mathbf{U}. \tag{2.14}$$

The proof is completed by observing the comments following Theorem 2.6. □

Under the conditions in Theorem 2.9 the CPD may also be computed by means of the SD-CP method, as explained in subsection 2.1. From 2.1 it is clear that the constraint $\mathbf{A}^{(3)H}\mathbf{A}^{(3)} = \mathbf{I}_R$ (Theorems 2.6 or 2.9) allows us to algebraically compute the semi-unitary constrained CPD of $\mathcal{X}$ under mild conditions than the constraint $\mathbf{A}^{(3)\dagger}\mathbf{A}^{(3)} = \mathbf{I}_R$ (Theorem 2.6) does.

$(I_{\min}, I_{\max})$	(2,2)	(2,3)	(2,4)	(2,5)	(2,6)	(3,3)	(3,4)	(3,5)	(3,6)	(4,4)	(4,5)	(4,6)	(5,6)	(6,6)
$\mathbf{A}^{(3)\dagger}\mathbf{A}^{(3)} = \mathbf{I}_R$	2	3	4	5	6	4	6	8	10	9	11	13	17	21
$\mathbf{A}^{(3)H}\mathbf{A}^{(3)} = \mathbf{I}_R$	2	4	4	5	6	4	9	9	10	9	14	16	21	21

TABLE 2.1

Maximum value for R for which the SD-CP approach provides an algebraic solution of a generic complex CPD with a full column rank or semi-unitary matrix factor ($I_3 \geq R$). We denote $I_{\min} = \min(I_1, I_2)$ and $I_{\max} = \max(I_1, I_2)$.

We may relax the constraint on $\mathbf{A}^{(3)}$ in Theorem 2.9 to $\mathbf{A}^{(3)}$ having only full column rank.

COROLLARY 2.10. *Consider the third order tensor $\mathcal{X} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ with matrix representation*

$$\mathbb{C}^{I_2 \times I_3} \ni \mathbf{X}^{(i_1 \cdot \cdot)} = \mathbf{A}^{(2)} D_{i_1}\left(\mathbf{A}^{(1)}\right) \mathbf{A}^{(3)T}, \quad \forall i_1 \in \{1, \ldots, I_1\}.$$

Let $I_{\max}$ and $I_{\min}$ be defined as (2.3). If

$$R \leq I_{\min}^2 \quad , \quad 2R(R-1) \leq I_{\max}^2(I_{\max}-1)^2 \quad and \quad R \leq I_3, \tag{2.15}$$

then the CPD of $\mathcal{X}$ is unique in the generic case.

Proof. The result follows directly from Corollary 2.4 and Theorem 2.9. □

THEOREM 2.11. *Consider the tensor $\mathcal{T} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ with rank R and matrix representation $\mathbf{T}_{(1)} = \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right) \mathbf{A}^{(3)T}$ in which $\mathbf{A}^{(3)}$ has full column rank. Let $I_{\max}$ and $I_{\min}$ be defined as (2.3). If*

$$2 \min\left(I_{\max}, R\right) + \min\left(I_{\min}^2, R\right) \geq 2(R+1), \tag{2.16}$$

then the CPD of $\mathcal{T}$ is unique in the generic case.

Proof. Let $N_{\max}$ and $N_{\min}$ be defined as in (2.2). For a generic $\mathbf{A}^{(N_{\max})} \in \mathbb{C}^{I_{\max} \times R}$ it is well-known that generically $k\left(\mathbf{A}^{(N_{\max})}\right) = k\left(\mathbf{A}^{(N_{\max})*}\right) = \min\left(I_{\max}, R\right)$. Lemma 2.7 together with the generic example presented in the proof of Proposition 2.8 tell us that generically $k\left(\mathbf{A}^{(N_{\min})} \odot \mathbf{A}^{(N_{\min})*}\right) = \min\left(I_{\min}^2, R\right)$. The condition (2.16) now follows directly from Theorem 2.11. □

Conditions (2.15) and (2.16) may guarantee uniqueness for larger values of R than condition (2.10) in cases where $I_1 \neq I_2$. As an example, let $R = 7$, $I_1 = 3$ and $I_3 \geq R$, then condition (2.10) requires that $I_2 \geq 5$ while condition (2.12) only requires that $I_2 \geq 4$. In table 2.2 we give, for various values of I_1, the minimum value of I_2 for which uniqueness is established by Theorem 2.1, 2.6 and 2.11 and Corollary 2.10 assuming that $I_1^2 = R$ and $I_3 \geq R$. It is clear that in this case Corollary 2.10 provides

I_1	2	3	4	5	6	7	8	9	10
Theorem 2.1	4	8	14	22	32	44	58	74	92
Theorem 2.6	4	6	7	9	10	12	13	14	16
Corollary 2.10	3	4	6	7	8	9	10	12	13
Theorem 2.11	3	6	9	14	19	26	33	42	51

TABLE 2.2

Minimum value for I_2 as required for Theorem 2.1, 2.6 and 2.11 and Corollary 2.10 in order guarantee uniqueness of a complex CPD with $I_1^2 = R$ and a full column rank matrix factor ($I_3 \geq R$) in the generic case.

the most relaxed condition. Table 2.3 shows, for varying I_1 and I_2, the maximal value of R for which Theorem 2.1 and 2.6 and Corollary 2.10 and 2.11 guarantee uniqueness of a generic complex CPD with a full column rank matrix factor ($I_3 \geq R$). It is clear that the full column rank constraint allows us to establish uniqueness for higher rank values.

3. Low-rank Approximation of a Tensor by a CPD with a Semi-unitary Matrix Factor. In applications it is the optimal approximation of a given tensor $\mathcal{X} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ by a tensor that admits a CPD with semi-unitary factor that is of interest. The unknown matrices $\mathbf{A}^{(1)} \in \mathbb{C}^{I_1 \times R}$, $\mathbf{A}^{(2)} \in \mathbb{C}^{I_2 \times R}$ and semi-unitary $\mathbf{A}^{(3)} \in \mathbb{C}^{I_3 \times R}$ are typically found by minimizing the least-squares cost function

$$f\left(\mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \mathbf{A}^{(3)}\right) = \left\|\mathbf{X}_{(3)} - \left(\mathbf{A}^{(3)} \odot \mathbf{A}^{(1)}\right) \mathbf{A}^{(2)T}\right\|_F^2. \tag{3.1}$$

$(I_{\min}, I_{\max})$	(2,2)	(2,3)	(2,4)	(2,5)	(2,6)	(3,3)	(3,4)	(3,5)	(3,6)	(4,4)	(4,5)	(4,6)	(5,6)	(6,6)
Thm. 2.1	**2**	3	4	5	6	**4**	5	6	7	6	7	8	9	10
Thm. 2.6	**2**	3	4	5	6	**4**	6	8	**10**	9	11	13	17	**21**
Cor. 2.10	**2**	4	4	4	4	**4**	9	9	9	9	14	16	21	21
Thm. 2.11	**2**	4	5	6	7	**4**	6	8	9	6	8	10	10	10

TABLE 2.3

Maximum value for R for which Theorem 2.1, 2.6 and 2.11 and Corollary 2.10 guarantee uniqueness of a generic complex CPD with a full column rank matrix factor ($I_3 \geq R$). We denote $I_{\min} = \min(I_1, I_2)$ and $I_{\max} = \max(I_1, I_2)$.

In [27] it was shown using level sets that the optimal solution to (3.1) always exists, i.e., the cost function has a global minimum and not only an infimum. (In the unconstrained problem there is in general only an infimum [15, 27].) We give a very short proof of this fact.

PROPOSITION 3.1. *Consider a tensor $\mathcal{X} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ and let $\mathbf{A}^{(1)} \in \mathbb{C}^{I_1 \times R}$, $\mathbf{A}^{(2)} \in \mathbb{C}^{I_2 \times R}$ and $\mathbf{A}^{(3)} \in \mathbb{C}^{I_3 \times R}$ in which $\mathbf{A}^{(3)}$ is semi-unitary. Then (3.1) has a global minimum.*

Proof. Without loss of generality we can assume that the column vectors of $\mathbf{A}^{(1)}$ have unit norm. Since $\mathbf{A}^{(3)}$ is semi-unitary, $\mathbf{A}^{(3)} \odot \mathbf{A}^{(1)}$ is semi-unitary. Hence, given $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(3)}$, the optimal $\mathbf{A}^{(2)}$ is given by

$$\mathbf{A}^{(2)T} = \left(\mathbf{A}^{(3)} \odot \mathbf{A}^{(1)}\right)^H \mathbf{X}_{(3)}. \tag{3.2}$$

Substitution of (3.2) in (3.1) yields

$$g\left(\mathbf{A}^{(1)}, \mathbf{A}^{(3)}\right) = \left\|\mathbf{X}_{(3)} - \left(\mathbf{A}^{(3)} \odot \mathbf{A}^{(1)}\right)\left(\mathbf{A}^{(3)} \odot \mathbf{A}^{(1)}\right)^H \mathbf{X}_{(3)}\right\|_F^2. \tag{3.3}$$

Due to the continuity of g and the compactness of its domain, its global minimum exists. Consequently, (3.1) has a global minimum. □

4. SD-CPO: SD-CP with a semi-unitary matrix factor. In this section we explain how a semi-unitary constraint can be incorporated in the SD-CP method presented in [12]. The approach will be referred to as SD-CPO.

4.1. Problem formulation. The SD-CP method was developed to compute CPD under the condition in Theorem 2.2. We briefly explain how it works.

Let $\mathcal{X} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ be a rank-R tensor with matrix representation

$$\mathbb{C}^{I_1 I_2 \times I_3} \ni \mathbf{X}_{(1)} = \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)\mathbf{A}^{(3)T}. \tag{4.1}$$

The conditions in Theorem 2.2 imply that $\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}$ and $\mathbf{A}^{(3)}$ have full column rank. Let $\mathbf{X}_{(1)} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^H$ denote the compact SVD of $\mathbf{X}_{(1)}$, where $\mathbf{U} \in \mathbb{C}^{I_1 I_2 \times R}$, $\mathbf{V} \in \mathbb{C}^{I_3 \times R}$ are semi-unitary matrices and $\mathbf{\Sigma} \in \mathbb{C}^{R \times R}$ is a positive diagonal matrix. Since $\text{Col}(\mathbf{U}\mathbf{\Sigma}) = \text{Col}\left(\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)\mathbf{A}^{(3)T}\right) = \text{Col}\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)$, there exists a nonsingular matrix $\mathbf{F} \in \mathbb{C}^{R \times R}$ such that

$$\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)} = \mathbf{U}\mathbf{\Sigma}\mathbf{F}. \tag{4.2}$$

Together with the relation $\mathbf{X}_{(1)} = \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)\mathbf{A}^{(3)T} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^H$, this implies that

$$\mathbf{A}^{(3)T} = \mathbf{F}^{-1}\mathbf{V}^H. \tag{4.3}$$

It turns out that, under the conditions in Theorem 2.2, there exist R complex symmetric matrices $\mathbf{M}^{(r)} \in \mathbb{C}^{R \times R}$ and R diagonal matrices $\Lambda_r \in \mathbb{C}^{R \times R}$ satisfying

$$\mathbf{M}^{(1)} = \mathbf{F}\Lambda_1\mathbf{F}^T$$

$$\vdots \tag{4.4}$$

$$\mathbf{M}^{(R)} = \mathbf{F}\Lambda_R\mathbf{F}^T.$$

For the procedure to compute the matrices $\{\mathbf{M}^{(r)}\}$ we refer to [12]. The unknown matrix $\mathbf{F}$ may now be explicitly obtained from the generalized eigenvalue decomposition of a pencil consisting of two of the matrices $\{\mathbf{M}^{(r)}\}$ (or two linear combinations of these matrices). If $\mathcal{X}$ does not admit an exact CPD, i.e., if (4.1) holds only approximately, then it is recommended to use all matrices $\{\mathbf{M}^{(r)}\}$ in the estimation of an approximate matrix $\mathbf{F}$. Note that in this Simultaneous Matrix Diagonalization (SMD) problem (4.4) the unknowns $(\mathbf{F}, \{\Lambda_r\})$ have the same dimensions as the given matrices $(\{\mathbf{M}^{(r)}\})$, whereas in the original CPD (4.1) possibly $I_1, I_2 < R$.

When $\mathbf{A}^{(3)}$ is semi-unitary the reasoning above remains valid. However, we have $\mathbf{V}^H\mathbf{V} = \mathbf{F}\mathbf{A}^{(3)T}\mathbf{A}^{(3)*}\mathbf{F}^H = \mathbf{I}_R \Leftrightarrow \mathbf{F}\mathbf{F}^H = \mathbf{I}_R$ and hence $\mathbf{F}$ is a unitary matrix. This means that, in the case of semi-unitary $\mathbf{A}^{(3)}$, the estimation of the CPD of $\mathcal{X}$ has been converted into a *unitary* SMD problem. Subsection 4.2 will discuss how the unitary matrix $\mathbf{F}$ can be computed from the matrices $\{\mathbf{M}^{(r)}\}$. Subsection 4.3 will explain how subsequently the CPD factors $\mathbf{A}^{(1)}$, $\mathbf{A}^{(2)}$ and $\mathbf{A}^{(3)}$ may be found.

4.2. Computation of F. Equation (4.4) can be interpreted as a simultaneous Takagi factorization [20]. The algorithm that will be derived in this section has applications besides the computation of a CPD with semi-unitary factor. For instance, the simultaneous Takagi factorization problem also pops up in the blind separation of non-circular sources [8, 11].

Define the tensor $\mathcal{M} \in \mathbb{C}^{R \times R \times R}$ by $(\mathcal{M}_{r_1 r_2 r_3}) = (\mathbf{M}^{(r_3)})_{r_1 r_2}$, $r_1, r_2, r_3 \in \{1, 2, \ldots, R\}$, the vectors $\mathbf{d}_r \in \mathbb{C}^R$ by $(\mathbf{d}_r)_{r_1} = (\Lambda_{r_1})_{rr}$, $r, r_1 \in \{1, 2, \ldots, R\}$ and let $\mathbf{F} = [\mathbf{f}_1 \ \mathbf{f}_2 \ \ldots \ \mathbf{f}_R]$. Solving (4.4) in least-squares sense amounts to minimizing

$$g(\mathbf{F}, \{\Lambda_r\}) = \left\| \mathcal{M} - \sum_{r=1}^{R} \mathbf{f}_r \circ \mathbf{f}_r \circ \mathbf{d}_r \right\|_F^2.$$

This is a CPD problem with two unitary factors. According to proposition 3.1, g has a global minimum.

It is easy to show that the minimization of g is equivalent with the maximization of

$$f(\mathbf{F}) = \sum_{r=1}^{R} \left\| \text{diag}\left(\mathbf{F}^H \mathbf{M}^{(r)} \mathbf{F}^* \right) \right\|_F^2. \tag{4.5}$$

Objective function f may be maximized by means of a Jacobi-type algorithm. We work in analogy with the JADE algorithm for simultaneous diagonalization under a unitary congruence transformation [3, 4]. The idea behind the Jacobi approach is that any unitary matrix $\mathbf{F} \in \mathbb{C}^{R \times R}$ with determinant equal to one can be parameterized as

$$\mathbf{F} = \prod_{p=1}^{R-1} \prod_{q=p+1}^{R} \mathbf{F}[p, q],$$

where $\mathbf{F}[p, q]$ is a Givens rotation matrix, defined by

$$\mathbf{F}[p, q]_{kl} = \begin{cases} 1 & \text{if } k = l \text{ and } k \notin \{p, q\} \\ \cos(\theta) & \text{if } k = l = p \\ \cos(\theta) & \text{if } k = l = q \\ \sin(\theta)e^{i\phi} & \text{if } k = p \text{ and } l = q \\ -\sin(\theta)e^{-i\phi} & \text{if } k = q \text{ and } l = p \\ 0 & \text{otherwise} \end{cases}$$

with $\theta, \phi \in \mathbb{R}$. An outline of the sweeping procedure for the simultaneous Takagi factorization is presented as Algorithm 1.

Algorithm 1 Outline of sweeping procedure for simultaneous Takagi factorization.

Initialize: $\mathbf{F}$
Repeat until convergence
for $p = 1$ to $R - 1$ **do**
  for $q = p + 1$ to R **do**
    calculate optimal $\mathbf{F}[p, q]$ (subsection 4.2)
    $\mathbf{F} \leftarrow \mathbf{F}\,\mathbf{F}[p, q]$
    $\mathbf{M}^{(r)} \leftarrow \mathbf{F}[p, q]^H \mathbf{M}^{(r)} \mathbf{F}[p, q]^*$
  end for
end for

Let $\mathbf{F} = \mathbf{F}[p, q]$, then a technical derivation yields:

$$f(\mathbf{F}[p, q]) = \sum_{r=1}^{R} \left\| \text{diag}\left(\mathbf{F}[p, q]^H \mathbf{M}^{(r)} \mathbf{F}[p, q]^* \right) \right\|_F^2$$

$$= \mathbf{x}^T \begin{bmatrix} \alpha_1 & \beta_1/2 & \beta_2/2 \\ \beta_1/2 & \alpha_1/2 + \alpha_4/2 + \text{Re}\{\alpha_5\} & \text{Im}\{\alpha_5\} \\ \beta_2/2 & \text{Im}\{\alpha_5\} & \alpha_1/2 + \alpha_4/2 - \text{Re}\{\alpha_5\} \end{bmatrix} \mathbf{x}$$

$$= \mathbf{x}^T \mathbf{B} \mathbf{x},$$

where

$$\mathbf{x} = \left[\cos(2\theta), \sin(2\theta)\cos(\phi), \sin(2\theta)\sin(\phi) \right]^T$$

and

$$\alpha_1 = \sum_{r=1}^{R} \left| \mathbf{M}_{pp}^{(r)} \right|^2 + \left| \mathbf{M}_{qq}^{(r)} \right|^2 \qquad \alpha_2 = \sum_{r=1}^{R} \mathbf{M}_{qq}^{(r)*} \left(\mathbf{M}_{pq}^{(r)} + \mathbf{M}_{qp}^{(r)} \right)$$

$$\alpha_3 = \sum_{r=1}^{R} \mathbf{M}_{pp}^{(r)} \left(\mathbf{M}_{pq}^{(r)} + \mathbf{M}_{qp}^{(r)} \right)^* \qquad \alpha_4 = \sum_{r=1}^{R} \left| \mathbf{M}_{pq}^{(r)} + \mathbf{M}_{qp}^{(r)} \right|^2$$

$$\alpha_5 = \sum_{r=1}^{R} \mathbf{M}_{qq}^{(r)*} \mathbf{M}_{pp}^{(r)}$$

$$\beta_1 = \text{Re}\{\alpha_2\} + \text{Re}\{\alpha_3\} \qquad \beta_2 = \text{Im}\{\alpha_2\} - \text{Im}\{\alpha_3\}.$$

Note that the unknown $\mathbf{x}$ that characterizes the Givens rotation has unit norm. The function $f(\mathbf{F}[p, q])$ can be maximized by taking $\mathbf{x}$ equal to the dominant eigenvector of $\mathbf{B}$. Hence, the problem reduces to finding the eigenvector that corresponds to the largest eigenvalue of the above matrix $\mathbf{B}$.

4.3. Computation of $\mathbf{A}^{(1)}$, $\mathbf{A}^{(2)}$ and $\mathbf{A}^{(3)}$. Assume that the unitary matrix $\mathbf{F}$ has been found, then due to relation (4.2) the matrices $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(2)}$ can be found from a set of decoupled best rank-1 matrix approximation problems. Indeed, let $\mathbf{G} = \mathbf{U}\Sigma\mathbf{F}$, then

$$\left\| \mathrm{Unvec}\left(\mathbf{g}_r\right) - \mathrm{Unvec}\left(\mathbf{a}_r^{(1)} \otimes \mathbf{a}_r^{(2)}\right) \right\|_F^2 = \left\| \mathrm{Unvec}\left(\mathbf{g}_r\right) - \mathbf{a}_r^{(2)}\mathbf{a}_r^{(1)T} \right\|_F^2, \quad r \in \{1, \dots, R\},$$

where $\mathbf{g}_r$ and $\mathbf{a}_r^{(n)}$ denote the rth column of $\mathbf{G}$ and $\mathbf{A}^{(n)}$, respectively. Consequently, we can take $\mathbf{a}_r^{(1)} = \mathbf{t}_1^*$ and $\mathbf{a}_r^{(2)} = \sigma_1\mathbf{s}_1$, where σ_1 denotes the largest singular value of $\mathrm{Unvec}\left(\mathbf{g}_r\right)$ and $\mathbf{s}_1$ and $\mathbf{t}_1$ denote its dominant left and right singular vectors, respectively.

The matrix $\mathbf{A}^{(3)}$ can be found as the semi-unitary minimizer of the cost function

$$\begin{aligned}
f\left(\mathbf{A}^{(3)}\right) &= \left\| \mathbf{X}_{(1)} - \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)\mathbf{A}^{(3)T} \right\|_F^2 \\
&= \left\| \mathbf{X}_{(1)} \right\|_F^2 + \left\| \mathbf{A}^{(1)} \odot \mathbf{A}^{(2)} \right\|_F^2 - 2\mathrm{Re}\left\{ \mathrm{Tr}\left(\mathbf{A}^{(3)*}\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)} \right) \right\}.
\end{aligned} \quad (4.6)$$

The minimizer of (4.6) is equal to the minimizer of

$$\begin{aligned}
g\left(\mathbf{A}^{(3)}\right) &= \left\| \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)} - \mathbf{A}^{(3)T} \right\|_F^2 \\
&= \left\| \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)} \right\|_F^2 + \left\| \mathbf{A}^{(3)T} \right\|_F^2 - 2\mathrm{Re}\left\{ \mathrm{Tr}\left(\mathbf{A}^{(3)*}\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)} \right) \right\} \\
&= \left\| \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)} \right\|_F^2 + R - 2\mathrm{Re}\left\{ \mathrm{Tr}\left(\mathbf{A}^{(3)*}\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)} \right) \right\}.
\end{aligned} \quad (4.7)$$

Let $\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)} = \mathbf{P}\Lambda\mathbf{Q}^H$ denote the SVD of $\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)}$, then the optimal matrix is $\mathbf{A}^{(3)} = \mathbf{Q}(:, 1:R)^*\mathbf{P}(:, 1:R)^T$. This can be understood as a variant of the unitary Procrustes problem [20] for the semi-unitary case.

In the unconstrained CPD case it turned out that SD-CP finds the solution for rank values where optimization-based algorithms fail [12]. However, it also turned out that a few iterations of an optimization-based algorithm are sometimes useful to refine the estimate found by SD-CP. In the case with semi-unitary constraint one may use the constrained ALS algorithms discussed in section 5 for this purpose.

5. ALS-CPO: ALS-CP with semi-unitary matrix factor. This section explains how a semi-unitary constraint can be incorporated in the ALS method, which is the most popular algorithm for the computation of a CPD. Various unitary constrained ALS-type methods have been proposed in the literature. The first result seems to have been presented [28], where the unitary constraint was taken into account via the technique of Lagrange multipliers. In [39] an algorithm was given that makes use of a SVD. We will present variants of this algorithm. We first present an efficient implementation of the algorithm which we call ALS1-CPO. Next we recall the approach taken in [25], which we call ALS2-CPO.

5.1. ALS1-CPO. The ALS method attempts to minimize the cost function

$$f\left(\mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \mathbf{A}^{(3)}\right) = \left\| \mathbf{X}_{(1)} - \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)\mathbf{A}^{(3)T} \right\|_F^2 \quad (5.1)$$

by updating, in an alternating fashion, one of the matrices $\{\mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \mathbf{A}^{(3)}\}$ while keeping the other two fixed.

Assume that the matrix $\mathbf{A}^{(3)}$ is semi-unitary. Let us first consider an update of $\mathbf{A}^{(3)}$, i.e., the matrices $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(2)}$ are fixed. Let $\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^H$ denote the SVD of $\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)}$, then as explained in subsection 4.3 the optimal matrix is $\mathbf{A}^{(3)} = \mathbf{V}(:, 1:R)^* \mathbf{U}(:, 1:R)^T$.

Now let us consider the updates of $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(2)}$, for which we present an efficient implementation. Updating $\mathbf{A}^{(1)}$, given $\mathbf{A}^{(2)}$ and $\mathbf{A}^{(3)}$, is a classical linear Least Squares (LS) problem. The solution is:

$$\mathbf{A}^{(1)T} = \left(\mathbf{A}^{(2)} \odot \mathbf{A}^{(3)}\right)^{\dagger} \mathbf{X}_{(2)}.$$

The pseudo-inverse may be computed efficiently as [26]

$$\left(\mathbf{A}^{(2)} \odot \mathbf{A}^{(3)}\right)^{\dagger} = \left(\mathbf{A}^{(2)H}\mathbf{A}^{(2)} * \mathbf{A}^{(3)H}\mathbf{A}^{(3)}\right)^{-1}\left(\mathbf{A}^{(2)} \odot \mathbf{A}^{(3)}\right)^{H}. \tag{5.2}$$

By taking the semi-unitary constraint on $\mathbf{A}^{(3)}$ into account, we obtain

$$\left(\mathbf{A}^{(2)} \odot \mathbf{A}^{(3)}\right)^{\dagger} = \mathbf{D}^{(2)}\left(\mathbf{A}^{(2)} \odot \mathbf{A}^{(3)}\right)^{H}$$

in which

$$\mathbf{D}^{(2)} = \begin{bmatrix} \frac{1}{\|\mathbf{a}_1^{(2)}\|_F^2} & 0 & \cdots & 0 \\ 0 & \frac{1}{\|\mathbf{a}_2^{(2)}\|_F^2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \frac{1}{\|\mathbf{a}_R^{(2)}\|_F^2} \end{bmatrix} \in \mathbb{C}^{R \times R}, \tag{5.3}$$

where $\mathbf{a}_r^{(2)}$ denotes the rth column vector of $\mathbf{A}^{(2)}$. Hence, the update reduces to

$$\mathbf{A}^{(1)T} = \mathbf{D}^{(2)}\left(\mathbf{A}^{(2)} \odot \mathbf{A}^{(3)}\right)^{H} \mathbf{X}_{(2)}. \tag{5.4}$$

Note that (5.4) just involves row-wise scaling by $\mathbf{D}^{(2)}$, instead of computation of the inverse and matrix multiplication by $\left(\mathbf{A}^{(2)H}\mathbf{A}^{(2)} * \mathbf{A}^{(3)H}\mathbf{A}^{(3)}\right)^{-1}$ in (5.2).

Updating $\mathbf{A}^{(2)}$ is similar. As a matter of fact, because of the scaling ambiguity we may normalize the column vectors of $\mathbf{A}^{(1)}$,

$$\mathbf{a}_r^{(1)} \leftarrow \frac{\mathbf{a}_r^{(1)}}{\|\mathbf{a}_r^{(1)}\|_F}, \quad \forall r \in \{1, \ldots, R\},$$

so that the update of $\mathbf{A}^{(2)}$ reduces to

$$\mathbf{A}^{(2)T} = \left(\mathbf{A}^{(3)} \odot \mathbf{A}^{(1)}\right)^{H} \mathbf{X}_{(3)}.$$

This ALS1-CPO method is summarized as Algorithm 2.

Algorithm 2 Outline of ALS1-CPO method.

Initialize: $\mathbf{A}^{(1)}$, $\mathbf{A}^{(2)}$ and $\mathbf{A}^{(3)}$

Repeat until convergence

$\quad$ Compute SVD $\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)^H \mathbf{X}_{(1)} = \mathbf{U}\Sigma\mathbf{V}^H$

$\quad$ Update $\mathbf{A}^{(3)} = \mathbf{V}(:, 1:R)^* \mathbf{U}(:, 1:R)^T$

$\quad$ Compute $\mathbf{A}^{(1)T} = \mathbf{D}^{(2)}\left(\mathbf{A}^{(2)} \odot \mathbf{A}^{(3)}\right)^H \mathbf{X}_{(2)}$

$\quad$ Update $\mathbf{a}_r^{(1)} \leftarrow \frac{\mathbf{a}_r^{(1)}}{\|\mathbf{a}_r^{(1)}\|_F}, \quad \forall r \in \{1, \ldots, R\}$

$\quad$ Update $\mathbf{A}^{(2)T} = \left(\mathbf{A}^{(3)} \odot \mathbf{A}^{(1)}\right)^H \mathbf{X}_{(3)}$

Remark. For large tensors, the computation commonly starts with a dimensionality reduction. The original tensor is compressed by means of multilinear orthogonal projection to a tensor of which the dimension is equal to or slightly larger than the original tensor's multilinear rank. The CPD of the smaller tensor is computed and the results are expanded again. One may then perform a few refinement iterations in the original dimensions. For a discussion of dimensionality reduction and algorithms we refer to [41, 9, 10, 29, 34, 21, 22].

5.2. ALS2-CPO. Due to the semi-unitary constraint on $\mathbf{A}^{(3)}$ it is possible to simultaneously update $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(2)}$ in the ALS method. This can be understood as an extension of the method presented in [25] for the unitary case to the semi-unitary case.

The conditional update of $\mathbf{A}^{(3)}$ while $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(2)}$ are fixed is the same as in the ALS1-CPO method described in subsection 5.2.

Consider now the conditional update of $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(2)}$ while $\mathbf{A}^{(3)}$ is fixed. Let the column vectors of $\mathbf{A}^{(3)\perp} \in \mathbb{C}^{I_3 \times (I_3 - R)}$ constitute an orthogonal basis for the complementary subspace spanned by the column vectors of $\mathbf{A}^{(3)} \in \mathbb{C}^{I_3 \times R}$. Then

$$
\begin{aligned}
f\left(\mathbf{A}^{(1)}, \mathbf{A}^{(2)}\right) &= \left\|\mathbf{X}_{(1)} - \left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)\mathbf{A}^{(3)T}\right\|_F^2 \\
&= \left\|\mathbf{X}_{(1)} - \left[\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}, \mathbf{0}_{I_1 I_2, I_3 - R}\right]\left[\mathbf{A}^{(3)}, \mathbf{A}^{(3)\perp}\right]^T\right\|_F^2 \\
&= \left\|\mathbf{X}_{(1)}\left[\mathbf{A}^{(3)}, \mathbf{A}^{(3)\perp}\right]^* - \left[\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}, \mathbf{0}_{I_1 I_2, I_3 - R}\right]\right\|_F^2 . \qquad (5.5)
\end{aligned}
$$

Let $\mathbf{Y} = \mathbf{X}_{(1)}\mathbf{A}^{(3)*}$, then from (5.5) it is clear that $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(2)}$ follow from the best rank-1 approximation problems

$$
\text{Unvec}\left(\mathbf{y}_r\right) = \text{Unvec}\left(\mathbf{a}_r^{(1)} \otimes \mathbf{a}_r^{(2)}\right) = \mathbf{a}_r^{(2)}\mathbf{a}_r^{(1)T},
$$

where $\mathbf{y}_r$ and $\mathbf{a}_r^{(n)}$ denote the rth column vector of $\mathbf{Y}$ and $\mathbf{A}^{(n)}$, respectively. Hence, we can set $\mathbf{a}_r^{(1)} = \mathbf{v}_1^*$ and $\mathbf{a}_r^{(2)} = \sigma_1 \mathbf{u}_1$, where σ_1 denotes the largest singular value of $\text{Unvec}\left(\mathbf{y}_r\right)$ and $\mathbf{u}_1$ and $\mathbf{v}_1$ denote its dominant left and right singular vector, respectively. Again, an initial dimension reduction step may be used.

6. Extension to Nth-order tensors. The discussion so far has been limited to tensors of order three. The results can however be extended to tensors of arbitrary order, say N.

6.1. Existence and Uniqueness of Nth-Order CPD. Let $\mathcal{X} \in \mathbb{C}^{I_1 \times \cdots \times I_N}$ be a tensor of rank R constructed from the matrices $\mathbf{A}^{(n)} \in \mathbb{C}^{I_n \times R}$, $n \in \{1, \ldots, N\}$, such that

$$\mathcal{X} = \sum_{r=1}^{R} \mathbf{a}_r^{(1)} \circ \cdots \circ \mathbf{a}_r^{(N)}, \tag{6.1}$$

where $\mathbf{a}_r^{(n)}$ denotes the rth column vector of $\mathbf{A}^{(n)}$ and $\mathbf{A}^{(N)}$ is assumed to be a semi-unitary matrix. We generalize the construction of matrix $\mathbf{Y}$ in section 2. Let $\mathbf{X}^{(i_1, \ldots, i_{N-2})} \in \mathbb{C}^{I_{N-1} \times I_N}$ be constructed such that $\mathbf{X}_{i_{N-1}, i_N}^{(i_1, \ldots, i_{N-2})} = \mathcal{X}_{i_1, \ldots, i_N}$, then

$$\mathbf{X}^{(i_1, \ldots, i_{N-2})} = \sum_{r=1}^{R} \prod_{n=1}^{N-2} \mathbf{A}_{i_n r}^{(n)} \mathbf{a}_r^{(N-1)} \mathbf{a}_r^{(N)T} = \mathbf{A}^{(N-1)} \prod_{n=1}^{N-2} D_{i_n}\left(\mathbf{A}^{(n)}\right) \mathbf{A}^{(N)T},$$

Denoting $\mathbf{D}^{(i_1, \ldots, i_{N-2})} = \prod_{n=1}^{N-2} D_{i_n}\left(\mathbf{A}^{(n)}\right) \in \mathbb{C}^{R \times R}$, we have

$$\mathbf{X}^{(i_1, \ldots, i_{N-2})} = \mathbf{A}^{(N-1)} \mathbf{D}^{(i_1, \ldots, i_{N-2})} \mathbf{A}^{(N)T}. \tag{6.2}$$

and

$$\mathbf{X}_D = \left[\text{Vec}\left(\mathbf{X}^{(1, \ldots, 1)}\right), \text{Vec}\left(\mathbf{X}^{(1, \ldots, 2)}\right), \ldots, \text{Vec}\left(\mathbf{X}^{(I_1, \ldots, I_{N-2})}\right) \right]$$
$$= \left(\mathbf{D} \odot \mathbf{A}^{(N-1)}\right) \mathbf{A}^{(N)T} \tag{6.3}$$

with

$$\mathbb{C}^{\prod_{n=1}^{N-2} I_n \times R} \ni \mathbf{D} = \begin{bmatrix} \text{Vecd}\left(\mathbf{D}^{(1, \ldots, 1)}\right)^T \\ \text{Vecd}\left(\mathbf{D}^{(1, \ldots, 2)}\right)^T \\ \vdots \\ \text{Vecd}\left(\mathbf{D}^{(I_1, \ldots, I_{N-2})}\right)^T \end{bmatrix} = \mathbf{A}^{(1)} \odot \mathbf{A}^{(2)} \odot \cdots \odot \mathbf{A}^{(N-2)}.$$

Since $\mathbf{A}^{(N)}$ is semi-unitary, then as in section 2 one may construct the tensor of order $2(N-1)$ that has matrix representation

$$\mathbf{Y} = (\mathbf{D} \odot \mathbf{D}^*)\left(\mathbf{A}^{(N-1)} \odot \mathbf{A}^{(N-1)*}\right)^T$$
$$= \left(\mathbf{A}^{(1)} \odot \cdots \odot \mathbf{A}^{(N-2)} \odot \mathbf{A}^{(1)*} \odot \cdots \odot \mathbf{A}^{(N-2)*}\right)\left(\mathbf{A}^{(N-1)} \odot \mathbf{A}^{(N-1)*}\right)^T. \tag{6.4}$$

Assuming that $\mathbf{A}^{(N-1)} \odot \mathbf{A}^{(N-1)*}$ has full column rank, one may now deduce uniqueness from the results obtained in section 2 for a third-order CPD with a full column rank matrix factor or from the results presented in [12, 38] that take the higher-order CPD structure of $\mathbf{Y}$ in (6.4) into account. If $\mathbf{A}^{(N-1)} \odot \mathbf{A}^{(N-1)*}$ does not have full column rank, then it may still be possible to build a tensor of order less than $2(N-1)$ by combining different modes such that it has a full column rank matrix factor. Note that this result can also be used to obtain new uniqueness conditions for the CPD of an Nth-order tensor with a full column rank matrix factor that is not necessarily semi-unitary, as explained in section 2.

The discussion in section 3 may directly be generalized, i.e., under the semi-unitary constraint on $\mathbf{A}^{(N)}$ existence of the optimal solution is guaranteed for arbitrary N.

6.2. Computation of *N*th-Order CPD. The algorithms discussed in sections 4 and 5 may be generalized to *N*th-order tensors. We add that it is sometimes useful to reduce the computation of the CPD of a *N*th-order tensor to the computation of the CPD of a tensor of lower order. In applications, (6.1) is often a very highly overdetermined set of equations. Combining modes of the tensor, and ignoring the rank-1 structure in the combined mode, often still results in a highly overdetermined problem. In this way the computational load may be reduced with limited loss of accuracy.

SD-CPO for Nth-Order CPD. The procedure in section 4 remains valid with the exceptions that the matrices $\{\mathbf{M}^{(r)}\}$ are computed as in [12] and that subsection 4.2 involves the best rank-1 approximation of $(N-1)$th-order tensors instead of matrices, see further below.

In the SD-CP method the most expensive step is the computation of the symmetric matrices $\{\mathbf{M}^{(r)}\}$. We present a SD-CP variant that does not fully exploit the structure of the problem, but is must faster than the original SD-CP method. If we ignore the structure of $\mathbf{D}$ in (6.3), then we can interpret it as a third-order CPD with a semi-unitary matrix factor $\mathbf{A}^{(N)}$. Hence, we first compute $\mathbf{D}$, $\mathbf{A}^{(N-1)}$ and $\mathbf{A}^{(N)}$ via the procedures described in subsection 4.2 and 4.3. Next, we compute the remaining matrix factors from

$$\mathbf{D} = \mathbf{A}^{(1)} \odot \cdots \odot \mathbf{A}^{(N-2)}. \tag{6.5}$$

The Khatri-Rao product in the expression (6.5) indicates that every column of this matrix is the vector representation of a rank-1 term. Hence, the matrix factors follow from decoupled best rank-1 tensor approximation problems. In the case $N = 4$, the solution to (6.5) follows from R decoupled rank-1 matrix approximation problems.

ALS1-CPO for Nth-Order CPD. The extension of the ALS1-CPO method to *N*th-order tensors is straightforward. Simply notice that the conditional updates of the non-unitary matrix factors are given by

$$\mathbf{A}^{(n)T} = \left(\mathbf{A}^{(1)} \odot \cdots \odot \mathbf{A}^{(n-1)} \odot \mathbf{A}^{(n+1)} \odot \cdots \odot \mathbf{A}^{(N-1)} \odot \mathbf{A}^{(N)}\right)^{\dagger} \mathbf{X}_{[n]}$$

$$= \left(\prod_{\substack{m=1 \\ m \neq n}}^{N-1} \mathbf{D}^{(m)}\right) \left(\mathbf{A}^{(1)} \odot \cdots \odot \mathbf{A}^{(n-1)} \odot \mathbf{A}^{(n+1)} \odot \cdots \odot \mathbf{A}^{(N-1)} \odot \mathbf{A}^{(N)}\right)^{H} \mathbf{X}_{[n]},$$

where $\mathbf{X}_{[n]}$ is a matrix representation of (6.1) and $\mathbf{D}^{(m)} \in \mathbb{C}^{R \times R}$ are of the form (5.3).

ALS2-CPO for Nth-Order CPD. In ALS2-CPO the simultaneous update of $\mathbf{A}^{(1)}$, $\mathbf{A}^{(2)}$, ..., $\mathbf{A}^{(N-1)}$ involves the best rank-1 approximation of $(N-1)$th order tensors. To reduce the computational cost of ALS2-CPO the ORBIT method was proposed in [25]. It ignores the Khatri-Rao product structure of $\mathbf{D}$ in (6.3) and computes $\mathbf{A}^{(N-1)}$, $\mathbf{A}^{(N)}$ and $\mathbf{D}$ from (6.3) using the ALS2-CPO method as described in subsection 5.2. In ALS2-CPO the reduction to order three yields an update based on the best rank-1 approximation of a matrix, while the best rank-1 approximation of a higher-order tensor is a problem that sometimes has local minima.

7. Numerical Experiments. For the numerical tests we consider real-valued third order tensors. Let $\mathcal{T} \in \mathbb{R}^{I_1 \times I_2 \times I_3}$ with rank R denote the structured tensor of which we observe a noisy version $\mathcal{X} = \mathcal{T} + \beta \mathcal{N}$, where $\mathcal{N}$ is an unstructured perturbation tensor and $\beta \in \mathbb{R}$ controls the noise level. The entries of the matrix factors of $\mathcal{T}$ and

the perturbation tensor $\mathcal{N}$ are randomly drawn from a uniform distribution with support $[-\frac{1}{2}, \frac{1}{2}]$. The following Signal-to-Noise Ratio (SNR) measure will be used:

$$\text{SNR [dB]} = 10 \log \left(\frac{\left\| \mathbf{T}_{(1)} \right\|_F^2}{\left\| \beta \mathbf{N}_{(1)} \right\|_F^2} \right).$$

For $\mathbf{A}^{(n)} \in \mathbb{R}^{I_n \times R}$ with $I_n \geq R$, the estimation accuracy will be measured by

$$P\left(\mathbf{A}^{(n)} \right) = \min_{\Pi \Lambda} \frac{\left\| \mathbf{A}^{(n)} - \widehat{\mathbf{A}}^{(n)} \Pi \Lambda \right\|_F}{\left\| \mathbf{A}^{(n)} \right\|_F},$$

where $\widehat{\mathbf{A}}^{(n)}$ denotes the estimated matrix factor, Π denotes a permutation matrix and Λ denotes a diagonal matrix. For $\mathbf{A}^{(n)} \in \mathbb{R}^{I_n \times R}$ with $I_n < R \leq I_n^2$, the estimation accuracy will be measured by

$$Q\left(\mathbf{A}^{(n)} \right) = \min_{\Pi \Lambda} \frac{\left\| \mathbf{A}^{(n)} \odot \mathbf{A}^{(n)} - \left(\widehat{\mathbf{A}}^{(n)} \odot \widehat{\mathbf{A}}^{(n)} \right) \Pi \Lambda \right\|_F}{\left\| \mathbf{A}^{(n)} \odot \mathbf{A}^{(n)} \right\|_F}.$$

In order to find Π and Λ the greedy LS column matching algorithm between $\mathbf{A}^{(n)}$ and $\widehat{\mathbf{A}}^{(n)}$ proposed in [36] will be applied.

To measure the time in seconds needed to execute the algorithms in MATLAB, the built-in functions *tic*($\cdot$) and *toc*($\cdot$) are used.

The ALS methods are randomly initialized and we decide that they have converged when in an iteration step the cost function has changed less than $\epsilon_{\text{ALS}} = 10^{-8}$. We impose a maximum of 10000 iterations. We decide that the Jacobi iteration method has converged when in an iteration step the cost function has changed less than $\epsilon = 10^{-6}$. Here we impose a maximum of 1200 iterations.

If we let the SD-CP method be followed by at most 100 ALS refinement iterations, then it will be referred to as SD-ALS-CP. Similarly, if we let SD-CPO method be followed by at most 100 ALS1-CPO refinement iterations, then it will be referred to as SD-ALS-CPO.

In the following four experiments the matrix factor $\mathbf{A}^{(3)}$ is semi-orthogonal. In case 1 and 2 we consider a relatively simple problem ($I_1 = I_2 = I_3 \geq R$). In case 3 and 4 we consider a difficult problem ($I_3 \geq R$ and $I_1, I_2 < R$).

Case 1: CPD with $I_1 = I_2 = I_3 \geq R$. We first set $I_1 = I_2 = I_3 = R = 5$ and compare the performance of the semi-unitary constrained ALS1-CPO, ALS2-CPO, SD-CPO and SD-ALS-CPO methods with the unconstrained ALS-CP, SD-CP and SD-ALS-CP methods. This also corresponds to the case $I_1 = I_2 = I_3 \geq R$ after dimensionality reduction. The mean $P\left(\mathbf{A}^{(n)} \right)$ and time values over 100 trials as a function of SNR can be seen in figure 8.1.

In particular the plot for $P\left(\mathbf{A}^{(3)} \right)$ shows that the unconstrained methods do not obtain the same precision as their semi-unitary counterparts. We also notice that above 20 dB SNR the SD-CPO, ALS1-CPO and ALS2-CPO method perform about the same while below 20 dB SNR SD-CPO performs worse. The reason for this is that in the noise-free case SD-CPO yields the exact solution while at low SNR values the noise-free assumption is violated. In that case fine-tuning steps are necessary.

Indeed, we notice that the SD-ALS-CPO method performs about the same as the ALS1-CPO and ALS2-CPO methods.

We further notice that the ALS2-CPO method is more costly than the new semi-unitary constrained ALS1-CPO method. There is no substantial difference in computational complexity between SD-CPO and the unconstrained SD-CP. The refinement steps only mildly increase the computational cost in SD-ALS-CPO.

We conclude that imposing orthogonality when it applies is worthwhile, both in terms of accuracy and computational cost. In this simple case the ALS1-CPO seems to be best method.

Case 2: CPD with $I_1 = I_2 \geq R$ and $I_3 >> R$. As mentioned in the introduction, in signal separation applications, the orthogonality constraints often come from source signals being uncorrelated. In such applications $\mathbf{A}^{(3)}$ is often (very) tall. Therefore, we also compare the performance of the methods when $I_1 = I_2 = R = 5$ and $I_3 = 100$. The mean $\mathrm{P}\left(\mathbf{A}^{(n)}\right)$ and time values over 100 trials as a function of SNR can be seen in figure 8.2. In this case the SD-CP and SD-ALS-CPO method performs as as well as the ALS1-CPO and ALS2-CPO methods.

In this case, the CPD structure is stronger than in Case 1, regardless of the orthogonality constraint. We indeed observe that there is a less interest in imposing the orthogonality constraints than in Case 1, although there is still an improvement at low SNR. Due to the fact that $I_3 >> R$, a good estimate of $\mathrm{Col}\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)$ is obtained, such that the matrices $\{\mathbf{M}^{(r)}\}$ in the SD-CP and SD-CPO are reliable. This makes the SD-CP, SD-CPO, SD-ALS-CP and SD-ALS-CPO yield a good accuracy at low cost for sufficiently high SNR. It is noteworthy that the popular ALS-CP method does not obtain the same accuracy as the other methods for the same computational effort. The reasons are that ALS-CP does not start from a good initial value unlike SD-CP, SD-CPO, SD-ALS-CP and SD-ALS-CPO, and that it does not impose orthogonality.

Case 3: CPD with $I_3 = R$ and $I_1, I_2 < R$. We set $I_1 = 4$, $I_2 = 4$, $I_3 = 8$, $R = 8$ and compare the performance of the semi-unitary constrained ALS1-CPO, ALS2-CPO, SD-CPO and SD-ALS-CPO methods with the unconstrained ALS-CP, SD-CP and SD-ALS-CP methods. The mean $\mathrm{Q}\left(\mathbf{A}^{(1)}\right)$, $\mathrm{Q}\left(\mathbf{A}^{(2)}\right)$, $\mathrm{P}\left(\mathbf{A}^{(3)}\right)$ and time values over 100 trials as a function of SNR can be seen in figure 8.3.

We notice that the unconstrained methods perform significantly worse than their semi-orthogonal counterparts. There is a significant benefit in imposing the semi-unitary constraint in difficult cases. We also notice that at high SNR SD-CPO provides at low cost a very good estimate, which may then be refined. Starting from a random value, the ALS methods are more expensive at high SNR. At low SNR there is less interest in using SD-CPO.

Case 4: CPD with $I_3 >> R$ and $I_1, I_2 < R$. Again, we consider the variant with tall $\mathbf{A}^{(3)}$. We set $I_1 = 4$, $I_2 = 4$, $I_3 = 100$ and $R = 8$. The mean $\mathrm{Q}\left(\mathbf{A}^{(1)}\right)$, $\mathrm{Q}\left(\mathbf{A}^{(2)}\right)$, $\mathrm{P}\left(\mathbf{A}^{(3)}\right)$ and time values over 100 trials as a function of SNR can be seen in figure 8.4. Since a good estimate of $\mathrm{Col}\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)$ is obtained, we now observe that the SD-ALS-CPO method yields a higher accuracy than the ALS methods, even at a lower cost.

8. Conclusion. In many applications one of the factor matrices of the CPD is constrained to be semi-unitary. We first used a semi-unitary constraint to derive a new relaxed condition under which uniqueness of the decomposition is guaranteed. We then extended the result to the case where one of the matrix factors has full column rank. We also gave a simple explanation for the existence of the optimal low-rank

approximation of a tensor when a matrix factor is semi-unitary.

To numerically solve the semi-unitary constrained CPD problem we first presented a semi-unitary constrained version of the SD-CP method, which we called SD-CPO. This led to a simultaneous Takagi factorization problem which was solved by a Jacobi iteration scheme. Next, we discussed semi-unitary constrained ALS-CP methods. In particular, the efficient ALS1-CPO method was derived. We briefly explained how the results can be generalized to Nth-order tensors.

One generally expects that, when one of the factor matrices of the CPD is semi-unitary, taking this constraint into account will lead to more accurate results and a higher computational efficiency. This was confirmed by numerical experiments.

We considered a simple problem, in which the rank did not exceed the tensor dimensions, and a difficult problem, in which the rank was high. The gain obtained by imposing orthogonality was very high for the difficult problem. Overall we noticed that the new ALS1-CPO method is an efficient algorithm in its class. We saw that, when the given tensor can be well approximated by a low-rank tensor, the SD-CPO method is inexpensive and yields a higher accuracy than the ALS methods. When only a rough approximation can be obtained, the ALS methods yield better results than SD-CPO. The reason for this is that at high SNR the SD-CPO method starts close to the exact solution while at low SNR the working assumptions are violated. At low SNR, initializing ALS methods by SD-CPO may reduce the number of iterations.

We also considered variants of the experiments in which the semi-unitary matrix is tall, which is relevant for practice. Since one of the factor matrices is tall, the CPD structural constraint is already strong, such that a priori there is less of a need to impose orthogonality. However, orthogonality-constrained algorithms quickly yield a higher accuracy than unconstrained algorithms as soon as the problem is for some reason difficult. We saw this for a well-conditioned CPD at low SNR and for ill-conditioned CPD overall. Moreover, the orthogonality-constrained algorithms are less computationally expensive. The SD-CPO and SD-ALS-CPO methods performed remarkably well, due to the fact that in the case of tall $\mathbf{A}^{(3)}$ a good estimate of $\mathrm{Col}\left(\mathbf{A}^{(1)} \odot \mathbf{A}^{(2)}\right)$ was obtained. The popular unconstrained ALS-CP algorithm turned out not to be a good choice here.

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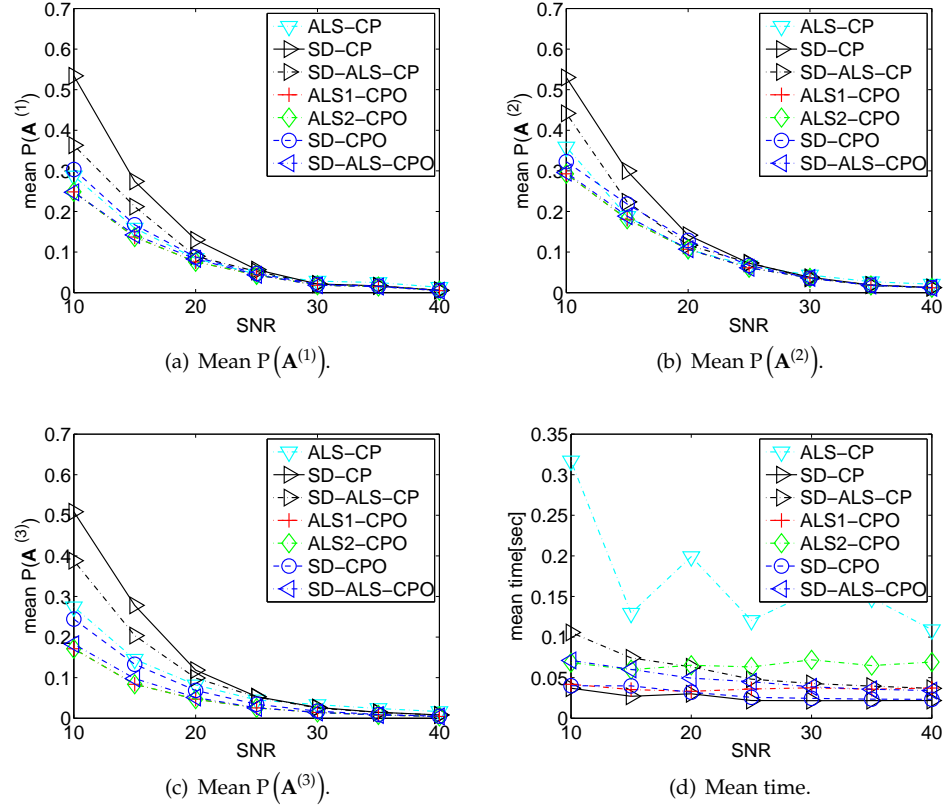[41] L. R. TUCKER, *Some Mathematical Notes on the Three-mode Factor Analysis*, Psychometrika, 31(1966), pp. 279-311.

(a) Mean $P\left(\mathbf{A}^{(1)}\right)$.

(b) Mean $P\left(\mathbf{A}^{(2)}\right)$.

(c) Mean $P\left(\mathbf{A}^{(3)}\right)$.

(d) Mean time.

FIG. 8.1. *Mean $P\left(\mathbf{A}^{(1)}\right)$, $P\left(\mathbf{A}^{(2)}\right)$, $P\left(\mathbf{A}^{(3)}\right)$ and time values over 100 trials while SNR is varying from 10 to 40 dB for the real third order tensor simulation, case 1.*

(a) Mean $P\left(\mathbf{A}^{(1)}\right)$.

(b) Mean $P\left(\mathbf{A}^{(2)}\right)$.

(c) Mean $P\left(\mathbf{A}^{(3)}\right)$.

(d) Mean time.

FIG. 8.2. *Mean* $P\left(A^{(1)}\right)$, $P\left(A^{(2)}\right)$, $P\left(A^{(3)}\right)$ *and time values over 100 trials while SNR is varying from* 10 *to* 40 *dB for the real third order tensor simulation, case 2.*
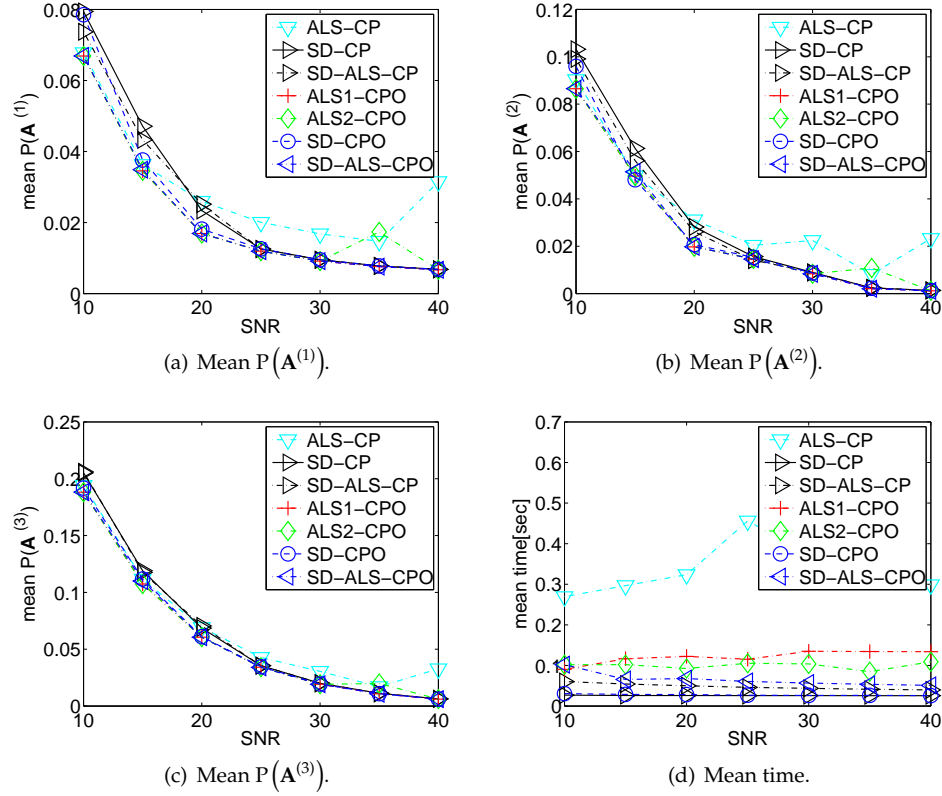
(a) Mean Q$\left(\mathbf{A}^{(1)}\right)$.

(b) Mean Q$\left(\mathbf{A}^{(2)}\right)$.

(c) Mean P$\left(\mathbf{A}^{(3)}\right)$.

(d) Mean time.

FIG. 8.3. *Mean and median* $Q\left(\mathbf{A}^{(1)}\right)$, $Q\left(\mathbf{A}^{(2)}\right)$, $P\left(\mathbf{A}^{(3)}\right)$ *and time values over 100 trials while SNR is varying from* 10 *to* 40 *dB for the real third order tensor simulation, case 3.*
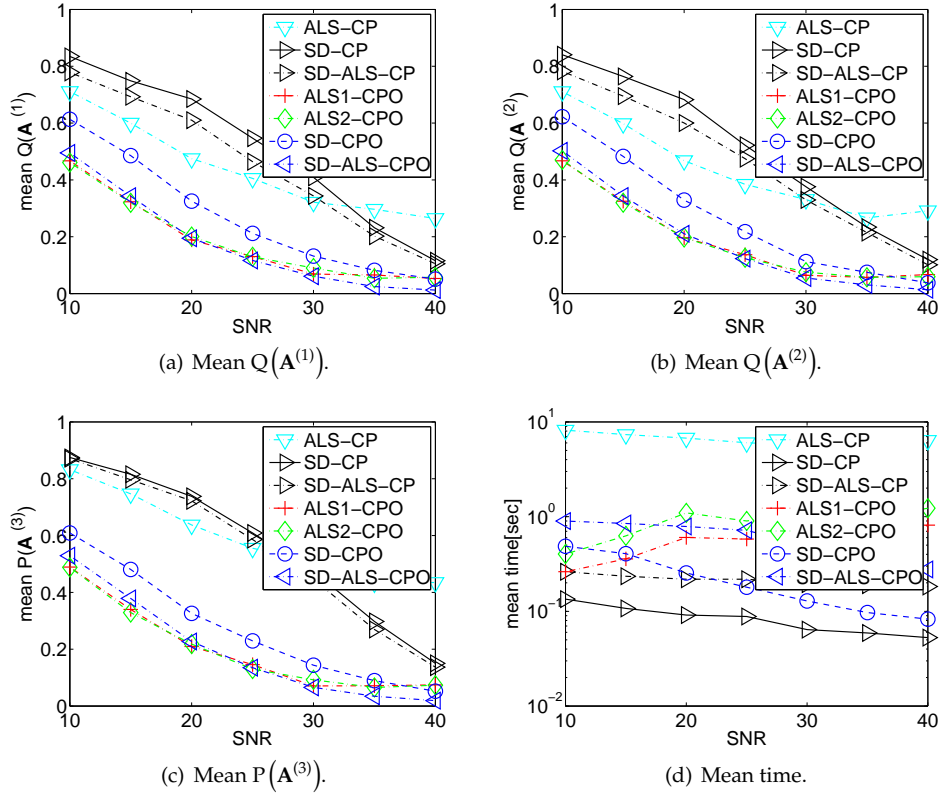
(a) Mean Q$\left(\mathbf{A}^{(1)}\right)$.

(b) Mean Q$\left(\mathbf{A}^{(2)}\right)$.

(c) Mean P$\left(\mathbf{A}^{(3)}\right)$.

(d) Mean time.

Fɪɢ. 8.4. *Mean and median* Q$\left(\boldsymbol{A}^{(1)}\right)$, Q$\left(\boldsymbol{A}^{(2)}\right)$, P$\left(\boldsymbol{A}^{(3)}\right)$ *and time values over 100 trials while SNR is varying from* 10 *to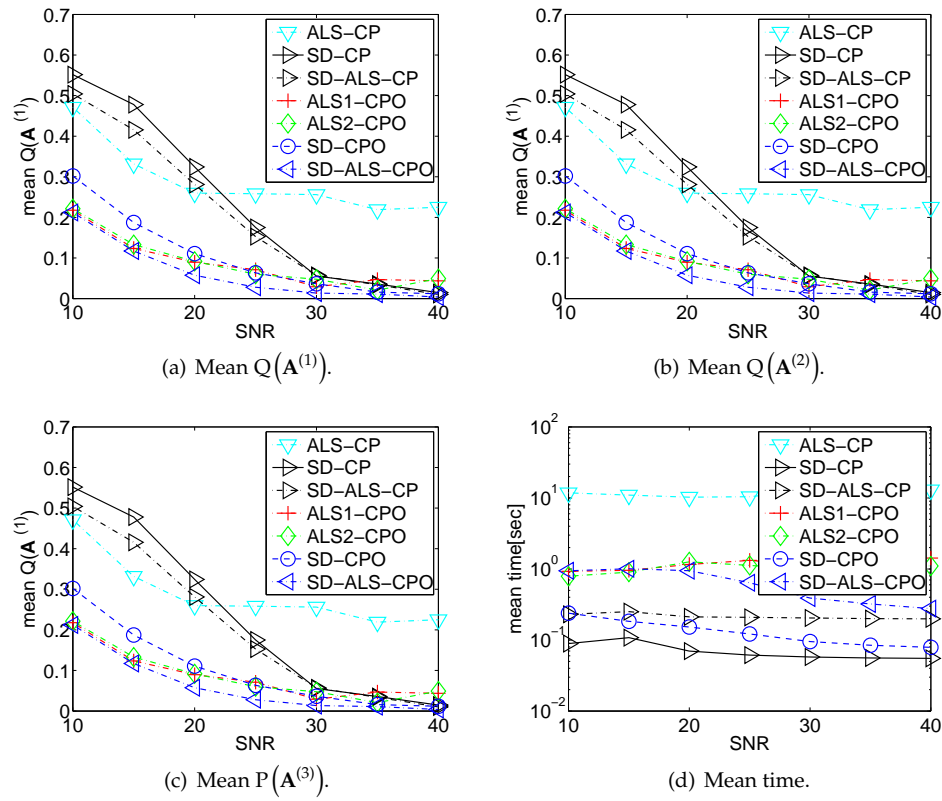* 40 *dB for the real third order tensor simulation, case 4.*