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CP decomposition of semi-nonnegative semi-symmetric tensors based on QR matrix factorization

Lu Wang^{*†§}, Laurent Albera^{*†§¶}, Amar Kachenoura^{*†§}, Hua Zhong Shu^{‡§} and Lotfi Senhadji^{*†§}

^{*}INSERM, UMR 1099, Rennes, F-35000, France [†]Université de Rennes 1, LTSI, Rennes, F-35000, France

[§]Centre de Recherche en Information Biomédicale sino-français (CRIBs), Rennes, France

[‡]LIST, Southeast University, 2 Sipailou, 210096, Nanjing, China

[¶]INRIA, Centre Inria Rennes - Bretagne Atlantique, 35042 Rennes, France.

Email: wangLyu1986@hotmail.com

Abstract—The problem of Canonical Polyadic (CP) decomposition of semi-nonnegative semi-symmetric three-way arrays is often encountered in Independent Component Analysis (ICA), where the cumulant of a nonnegative mixing process is frequently involved, such as the Magnetic Resonance Spectroscopy (MRS). We propose a new method, called JD_{QR}^+ , to solve such a problem. The nonnegativity constraint is imposed by means of a square change of variable. Then the high-dimensional optimization problem is decomposed into several sequential rational subproblems using QR matrix factorization. A numerical experiment on simulated arrays emphasizes its good performance. A BSS application on MRS data confirms the validity and improvement of the proposed method.

I. INTRODUCTION AND PROBLEM FORMULATION

Canonical Polyadic (CP) decomposition of a multi-way array [1]–[3] plays an important role in Blind Source Separation (BSS), particularly in Independent Component Analysis (ICA) [4]. In this paper, we consider the following semi-nonnegative semi-symmetric CP decomposition problem:

Problem 1. *The semi-nonnegative semi-symmetric CP decomposition of a 3-way array $\mathcal{C} \in \mathbb{R}^{N \times N \times K}$, is the minimal linear combination of rank-1 3-way arrays that yields \mathcal{C} exactly:*

$$\mathcal{C} = \sum_{p=1}^P \mathbf{a}_p \circ \mathbf{a}_p \circ \mathbf{d}_p \quad (1)$$

subject to $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_P] \in \mathbb{R}^{N \times P}$ having nonnegative components, where \circ denotes the outer product. \mathbf{A} and $\mathbf{D} = [\mathbf{d}_1, \dots, \mathbf{d}_P] \in \mathbb{R}^{K \times P}$ are called the loading matrices of \mathcal{C} . P is then the rank of \mathcal{C} .

The decomposition is considered to be essentially unique when the uniqueness is guaranteed up to scaling and permutation indeterminacies. This problem is often encountered in ICA when a nonnegative mixing matrix is considered. For example, in Magnetic Resonance Spectroscopy (MRS), the mixing matrix contains the positive concentrations of the source metabolites. Then the 3-way array built by stacking the matrix slices of a cumulant is both nonnegative and symmetric in two modes. Equation (1) can also be described by using the frontal slices of \mathcal{C} : $\mathcal{C}^{(k)} = \mathcal{C}_{::,k} = \mathbf{A}\mathbf{D}^{(k)}\mathbf{A}^\top$, $\forall k \in \{1, 2, \dots, K\}$, where $\mathbf{D}^{(k)} \in \mathbb{R}^{P \times P}$ is a diagonal matrix whose diagonal contains the elements of the k -th row of \mathbf{D} , and $\mathcal{C}^{(k)} \in \mathbb{R}^{N \times N}$ is the k -th frontal slice \mathcal{C} . In this paper, we focus on computing the square matrix \mathbf{A} , where $N = P$. In order to compute

\mathbf{A} , we can resort to solve the following nonnegative Joint Diagonalization by Congruence (JDC) problem:

Problem 2. *Given a 3-way array $\mathcal{C} \in \mathbb{R}^{N \times N \times K}$ with K symmetric frontal slices $\mathcal{C}^{(k)} \in \mathbb{R}^{N \times N}$, find a matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$ and K diagonal matrices $\mathbf{D}^{(k)} \in \mathbb{R}^{N \times N}$ such that:*

$$\forall k \in \{1, 2, \dots, K\}, \mathcal{C}^{(k)} = \mathbf{A}\mathbf{D}^{(k)}\mathbf{A}^\top \quad (2)$$

subject to \mathbf{A} having nonnegative components.

Many existing CP algorithms handle the symmetry and the nonnegativity separately, such as in [5]–[7]. Several methods consider the combination of both constraints [8], [9], but they aim at solving different problems rather than problem 1. Only a few methods were proposed to solve the nonnegative JDC problem [10], [11]. In this paper, we propose a new algorithm, called JD_{QR}^+ , based on minimizing the following indirect least square criterion [6], [12]:

$$J_1(\mathbf{A}) = \sum_{k=1}^K \|\text{off}(\mathbf{A}^{-1}\mathcal{C}^{(k)}\mathbf{A}^{-\top})\|_F^2 \quad (3)$$

where $\text{off}(\cdot)$ vanishes the diagonal components of the input matrix, the superscript $^{-\top}$ denotes the inverse of the transposed matrix, and $\|\cdot\|_F$ computes the Frobenius norm. The nonnegativity constraint is imposed by means of a square change of variable. The QR matrix factorization of the Hadamard square root of \mathbf{A} decomposes the high-dimensional optimization problem into a sequential rational subproblems. In addition, the rotation matrix and the unit triangular matrix of the QR factorization have unit determinants, therefore the resulting matrix \mathbf{A} is nonsingular. A numerical experiment on simulated arrays emphasizes its good performance. A BSS application on MRS data confirms the validity and improvement of the proposed method.

II. THE JD_{QR}^+ METHOD

In order to avoid the inverse of \mathbf{A} in cost function (3), let us consider the following assumptions: *i)* $\mathbf{A} \in \mathbb{R}_+^{N \times N}$ is nonsingular; *ii)* $\mathbf{D} \in \mathbb{R}^{K \times N}$ is nonsingular and does not contain zero entries. Then each frontal slice of \mathcal{C} is nonsingular and its inverse can be expressed as follows:

$$(\mathcal{C}^{(k)})^{-1} = \mathbf{A}^{-\top}(\mathbf{D}^{(k)})^{-1}\mathbf{A}^{-1} \quad (4)$$

In practice, only the sufficiently well-conditioned matrix $\mathcal{C}^{(k)}$ is chosen when its condition number is below a predefined

threshold. We use $\mathbf{C}^{(k,-1)}$ to denote $(\mathbf{C}^{(k)})^{-1}$ for simplicity. Equation (4) shows that $\mathbf{C}^{(k,-1)}$ is jointly diagonalizable by \mathbf{A} . Then \mathbf{A} can be estimated by minimizing the following modified criterion of (3) directly:

$$J_2(\mathbf{A}) = \sum_{k=1}^K \|\text{off}(\mathbf{A}^\top \mathbf{C}^{(k,-1)} \mathbf{A})\|_F^2 \quad (5)$$

The nonnegativity constraint on \mathbf{A} can be imposed by a square change of variable: $\mathbf{A} = \mathbf{B} \square \mathbf{B} = \mathbf{B}^{\square 2}$, where $\mathbf{B} \in \mathbb{R}^{N \times N}$ and where \square denotes Hadamard product [13], [14]. Then we can find $\mathbf{A} \in \mathbb{R}_+^{N \times N}$ by estimating $\mathbf{B} \in \mathbb{R}^{N \times N}$, such that $\mathbf{A} = \mathbf{B}^{\square 2}$, and \mathbf{B} is the global minimum of the following cost function:

$$J_2(\mathbf{B}) = \sum_{k=1}^K \|\text{off}((\mathbf{B}^{\square 2})^\top \mathbf{C}^{(k,-1)} \mathbf{B}^{\square 2})\|_F^2 \quad (6)$$

Now let us recall the following definitions and lemmas:

Definition 1. A unit upper triangular matrix is an upper triangular matrix whose main diagonal entries are 1.

Definition 2. An elementary upper triangular matrix $\mathbf{R}^{(i,j)}(r_{i,j})$ is equal to an identity matrix except the (i, j) -th entry, which is equal to $r_{i,j}$.

Definition 3. A Givens rotation matrix $\mathbf{Q}^{(i,j)}(\theta_{i,j})$ is equal to an identity matrix except the (i, i) -th, (j, j) -th, (i, j) -th and (j, i) -th entries, which are equal to $\cos(\theta_{i,j})$, $\cos(\theta_{i,j})$, $-\sin(\theta_{i,j})$ and $\sin(\theta_{i,j})$, respectively.

Lemma 1. Any $(N \times N)$ unit upper triangular matrix can be factorized as a product of $N(N-1)/2$ elementary upper triangular matrices.

Lemma 2. Any $(N \times N)$ orthonormal matrix can be factorized as a product of, at most, $N(N-1)/2$ Givens rotation matrices.

For any nonsingular matrix $\mathbf{B} \in \mathbb{R}^{N \times N}$, the QR matrix factorization decomposes it as $\mathbf{B} = \mathbf{Q}\mathbf{R}\mathbf{A}$, where $\mathbf{Q} \in \mathbb{R}^{N \times N}$ is an orthonormal matrix, $\mathbf{R} \in \mathbb{R}^{N \times N}$ is a unit upper triangular matrix, and $\mathbf{A} \in \mathbb{R}^{N \times N}$ is a diagonal matrix. Due to the indeterminacies of the CP decomposition, the matrix \mathbf{B} solving (6) can be chosen as $\mathbf{B} = \mathbf{Q}\mathbf{R}$ without loss of generality. Moreover, lemma 1 and lemma 2 yield that \mathbf{B} can be written as a product of the following matrices:

$$\mathbf{B} = \prod_{i=1}^N \prod_{j=i+1}^N \mathbf{Q}^{(i,j)}(\theta_{i,j}) \prod_{i=1}^N \prod_{j=i+1}^N \mathbf{R}^{(i,j)}(r_{i,j}) \quad (7)$$

As a consequence, the minimization of (6) with respect to \mathbf{B} is converted to the estimation of $N(N-1)$ parameters: $\theta_{i,j}$ and $r_{i,j}$. We propose a Jacobi-like procedure, called JD_{QR}^+ , in order to compute these parameters sequentially.

A. Minimization with respect to $\mathbf{Q}^{(i,j)}(\theta_{i,j})$

Let $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{B}}$ denote the current estimate of \mathbf{A} and \mathbf{B} before estimating $\mathbf{Q}^{(i,j)}(\theta_{i,j})$, respectively. Let $\tilde{\mathbf{A}}^{(\text{new})}$ and $\tilde{\mathbf{B}}^{(\text{new})}$ stand for \mathbf{A} and \mathbf{B} updated by $\mathbf{Q}^{(i,j)}(\theta_{i,j})$, respectively. Furthermore, the update of $\tilde{\mathbf{B}}$ is defined as follows:

$$\tilde{\mathbf{B}}^{(\text{new})} = \tilde{\mathbf{B}} \mathbf{Q}^{(i,j)}(\theta_{i,j}) \quad (8)$$

In order to compute $\theta_{i,j}$, the natural way is to minimize criterion (6) with respect to $\theta_{i,j}$ by replacing matrix $\tilde{\mathbf{B}}$ by $\tilde{\mathbf{B}}^{(\text{new})}$. For the sake of convenience, we denote $J_2(\theta_{i,j})$

instead of $J_2(\tilde{\mathbf{B}}^{(\text{new})})$. $J_2(\theta_{i,j})$ can be expressed as follows:

$$J_2(\theta_{i,j}) = \sum_{k=1}^K \|\text{off}\{[(\tilde{\mathbf{B}}^{(\text{new})})^{\square 2}]^\top \mathbf{C}^{(k,-1)} [(\tilde{\mathbf{B}}^{(\text{new})})^{\square 2}]\}\|_F^2 \quad (9)$$

The Hadamard square of $\tilde{\mathbf{B}}^{(\text{new})}$ in (9) can be written as a function of $\theta_{i,j}$ as follows:

$$(\tilde{\mathbf{B}}^{(\text{new})})^{\square 2} = \tilde{\mathbf{B}}^{\square 2} (\mathbf{Q}^{(i,j)}(\theta_{i,j}))^{\square 2} + \sin(2\theta) (\tilde{\mathbf{b}}_i \square \tilde{\mathbf{b}}_j) (\mathbf{e}_i^\top - \mathbf{e}_j^\top) \quad (10)$$

where $\tilde{\mathbf{b}}_i$ denotes the i -th column of $\tilde{\mathbf{B}}$, and \mathbf{e}_i is the i -th column of the identity matrix $\mathbf{I} \in \mathbb{R}^{N \times N}$. Inserting (10) into the cost function (9), we obtain:

$$\begin{aligned} J_2(\theta_{i,j}) &= \sum_{k=1}^K \|\text{off}(\tilde{\mathbf{C}}^{(k,\text{new})})\|_F^2 \\ &= \sum_{k=1}^K \|\text{off}([(\mathbf{Q}^{(i,j)}(\theta_{i,j})]^{\square 2})^\top \tilde{\mathbf{C}}^{(k)} (\mathbf{Q}^{(i,j)}(\theta_{i,j})]^{\square 2} \\ &\quad + \sin(2\theta) [(\mathbf{Q}^{(i,j)}(\theta_{i,j})]^{\square 2})^\top \tilde{\mathbf{c}}^{(k,1)} (\mathbf{e}_i^\top - \mathbf{e}_j^\top) \\ &\quad + \sin(2\theta) (\mathbf{e}_i - \mathbf{e}_j) \tilde{\mathbf{c}}^{(k,2)} (\mathbf{Q}^{(i,j)}(\theta_{i,j})]^{\square 2} \\ &\quad + \sin^2(2\theta) \tilde{\mathbf{c}}^{(k,3)} (\mathbf{e}_i - \mathbf{e}_j) (\mathbf{e}_i^\top - \mathbf{e}_j^\top))\|_F^2 \end{aligned} \quad (11)$$

where $\tilde{\mathbf{C}}^{(k)} = \tilde{\mathbf{A}}^\top \mathbf{C}^{(k,-1)} \tilde{\mathbf{A}}$, $\tilde{\mathbf{c}}^{(k,1)} = \tilde{\mathbf{A}}^\top \mathbf{C}^{(k,-1)} (\tilde{\mathbf{b}}_i \square \tilde{\mathbf{b}}_j)$, $\tilde{\mathbf{c}}^{(k,2)} = (\tilde{\mathbf{c}}^{(k,1)})^\top$ and $\tilde{\mathbf{c}}^{(k,3)} = (\tilde{\mathbf{b}}_i \square \tilde{\mathbf{b}}_j)^\top \mathbf{C}^{(k,-1)} (\tilde{\mathbf{b}}_i \square \tilde{\mathbf{b}}_j)$ are a matrix, a column vector, a row vector and a scalar of constant values, respectively. (11) shows that just the i -th and j -th columns and rows of $\tilde{\mathbf{C}}^{(k,\text{new})}$ involve the parameter $\theta_{i,j}$. It is noteworthy that the (i, j) -th and (j, i) -th elements are twice affected by the transformation. Inspired by [12], we propose to minimize the sum of the squares of the (i, j) -th entries of the K symmetric matrices $\tilde{\mathbf{C}}^{(k,\text{new})}$, instead of minimizing all the off-diagonal entries. This simplified minimization criterion is denoted by $\tilde{J}_2(\theta_{i,j})$. The (i, j) -th element of $\tilde{\mathbf{C}}^{(k,\text{new})}$ can be expressed as a function of $\theta_{i,j}$ as follows:

$$\begin{aligned} \tilde{c}_{i,j}^{(k,\text{new})} &= -\sin^2(2\theta_{i,j}) \tilde{c}^{(k,3)} \\ &\quad + \sin^2(\theta_{i,j}) (\tilde{C}_{i,i}^{(k)} \cos^2(\theta_{i,j}) + \tilde{C}_{j,i}^{(k)} \sin^2(\theta_{i,j})) \\ &\quad + \cos^2(\theta_{i,j}) (\tilde{C}_{i,j}^{(k)} \cos^2(\theta_{i,j}) + \tilde{C}_{j,j}^{(k)} \sin^2(\theta_{i,j})) \\ &\quad + \sin(2\theta_{i,j}) (\tilde{c}_i^{(k,1)} \cos^2(\theta_{i,j}) + \tilde{c}_j^{(k,1)} \sin^2(\theta_{i,j})) \\ &\quad - \sin(2\theta_{i,j}) (\tilde{c}_j^{(k,2)} \cos^2(\theta_{i,j}) + \tilde{c}_i^{(k,2)} \sin^2(\theta_{i,j})) \end{aligned} \quad (12)$$

where $\tilde{C}_{i,j}^{(k)}$ is the (i, j) -th element of $\tilde{\mathbf{C}}^{(k)}$ and $\tilde{c}_i^{(k,q)}$ is the i -th element of vector $\tilde{\mathbf{c}}^{(k,q)}$ with $q \in \{1, 2\}$. By using the Weierstrass change of variable: $t_{i,j} = \tan(\theta_{i,j})$, the expression of (12) can be rewritten as follows:

$$\tilde{c}_{i,j}^{(k,\text{new})} = \frac{f_4^{(k)} t_{i,j}^4 + f_3^{(k)} t_{i,j}^3 + f_2^{(k)} t_{i,j}^2 + f_1^{(k)} t_{i,j} + f_0^{(k)}}{(1 + t_{i,j}^2)^2} \quad (13)$$

where $f_4^{(k)} = \tilde{C}_{j,i}^{(k)}$, $f_3^{(k)} = -2\tilde{c}_i^{(k,1)}$, $f_2^{(k)} = \tilde{C}_{i,i}^{(k)} + \tilde{C}_{j,j}^{(k)} + 2\tilde{c}_j^{(k,2)} - 4\tilde{c}^{(k,3)}$, $f_1^{(k)} = 2\tilde{c}_i^{(k,2)} - \tilde{c}_j^{(k,1)}$ and $f_0^{(k)} = \tilde{C}_{j,i}^{(k)}$. Equation (13) shows that the sum of the squares of $\tilde{c}_{i,j}^{(k,\text{new})}$, is a rational function in $t_{i,j}$, namely $\tilde{J}_2(t_{i,j})$, where the degrees of the numerator and the denominator are 8 and 8, respectively. The global minimum $t_{i,j}$ can be obtained by computing the roots of its derivative and selecting the one yielding the smallest value of $\tilde{J}_2(t_{i,j})$. Once $t_{i,j}$ is obtained, $\theta_{i,j}$ can be computed by $\theta_{i,j} = \arctan(t_{i,j})$. Then $\tilde{\mathbf{B}}$ is updated by (8) and $\tilde{\mathbf{A}}$ is updated by computing $(\tilde{\mathbf{B}}^{(\text{new})})^{\square 2}$.

B. Minimization with respect to $\mathbf{R}^{(i,j)}(r_{i,j})$

Let $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{B}}$ continue to denote the current estimate of \mathbf{A} and \mathbf{B} before estimating $\mathbf{R}^{(i,j)}(r_{i,j})$, respectively. The update of $\tilde{\mathbf{B}}$, denoted by $\tilde{\mathbf{B}}^{(\text{new})}$, is defined as follows:

$$\tilde{\mathbf{B}}^{(\text{new})} = \tilde{\mathbf{B}}\mathbf{R}^{(i,j)}(r_{i,j}) \quad (14)$$

By replacing matrix $\tilde{\mathbf{B}}$ by $\tilde{\mathbf{B}}^{(\text{new})}$ into criterion (6), the criterion $J_2(r_{i,j})$ can be expressed as follows:

$$J_2(r_{i,j}) = \sum_{k=1}^K \left\| \text{off} \left\{ [(\tilde{\mathbf{B}}^{(\text{new})})^{\square 2}]^T \mathbf{C}^{(k,-1)} [(\tilde{\mathbf{B}}^{(\text{new})})^{\square 2}] \right\} \right\|_F^2 \quad (15)$$

The Hadamard square of $\tilde{\mathbf{B}}^{(\text{new})}$ in (15) can be expressed as a function of $r_{i,j}$ as follows:

$$(\tilde{\mathbf{B}}^{(\text{new})})^{\square 2} = \tilde{\mathbf{B}}^{\square 2} \mathbf{R}^{(i,j)}(r_{i,j})^2 + 2r_{i,j}(\tilde{\mathbf{b}}_i \square \tilde{\mathbf{b}}_j) \mathbf{e}_j^T \quad (16)$$

where $\tilde{\mathbf{b}}_i$ denotes the i -th column of $\tilde{\mathbf{B}}$, and \mathbf{e}_j is the j -th column of the identity matrix $\mathbf{I} \in \mathbb{R}^{N \times N}$. Inserting (16) into the cost function (15), we have:

$$\begin{aligned} J_2(r_{i,j}) &= \sum_{k=1}^K \left\| \text{off} \left(\tilde{\mathbf{C}}^{(k,\text{new})} \right) \right\|_F^2 \\ &= \sum_{k=1}^K \left\| \text{off} \left(\mathbf{R}^{(i,j)}(r_{i,j})^2 \right)^T \tilde{\mathbf{C}}^{(k)} \mathbf{R}^{(i,j)}(r_{i,j}) + r_{i,j}^2 \tilde{\mathbf{c}}^{(k,3)} \mathbf{e}_j \mathbf{e}_j^T \right. \\ &\quad \left. + r_{i,j} \mathbf{R}^{(i,j)}(r_{i,j})^T \tilde{\mathbf{c}}^{(k,1)} \mathbf{e}_j^T + r_{i,j} \mathbf{e}_j \tilde{\mathbf{c}}^{(k,2)} \mathbf{R}^{(i,j)}(r_{i,j}) \right\|_F^2 \end{aligned} \quad (17)$$

where $\tilde{\mathbf{C}}^{(k)} = \tilde{\mathbf{A}}^T \mathbf{C}^{(k,-1)} \tilde{\mathbf{A}}$, $\tilde{\mathbf{c}}^{(k,1)} = 2\tilde{\mathbf{A}}^T \mathbf{C}^{(k,-1)} (\tilde{\mathbf{b}}_i \square \tilde{\mathbf{b}}_j)$, $\tilde{\mathbf{c}}^{(k,2)} = (\tilde{\mathbf{c}}^{(k,1)})^T$ and $\tilde{\mathbf{c}}^{(k,3)} = 4(\tilde{\mathbf{b}}_i \square \tilde{\mathbf{b}}_j)^T \mathbf{C}^{(k,-1)} (\tilde{\mathbf{b}}_i \square \tilde{\mathbf{b}}_j)$ are a matrix, a column vector, a row vector and a scalar of constant values, respectively. (17) shows that just the j -th column and row of $\tilde{\mathbf{C}}^{(k,\text{new})}$ involve the parameter $r_{i,j}$. Therefore, the minimization of the cost function (17) is equivalent to minimizing the sum of the squares of the j -th columns of all the symmetric matrices $\tilde{\mathbf{C}}^{(k,\text{new})}$ except their (j,j) -th elements. These elements can be expressed by a polynomial function of degree 2 in $r_{i,j}$ as follows, for every n value different of j :

$$\tilde{c}_{n,j}^{(k,\text{new})} = \tilde{c}_{n,i}^{(k)} r_{i,j}^2 + \tilde{c}_n^{(k,1)} r_{i,j} + \tilde{c}_{n,j}^{(k)} \quad (18)$$

where $\tilde{c}_{n,i}^{(k)}$ is the (n,i) -th component of $\tilde{\mathbf{C}}^{(k)}$, and $\tilde{c}_n^{(k,1)}$ is the n -th element of $\tilde{\mathbf{c}}^{(k,1)}$. Then the cost function (17), which is the total sum of squares of (18), is a polynomial function of degree 4 in $r_{i,j}$. The global minimum $r_{i,j}$ is one of the roots of its derivative, which yields the smallest value of (17). Once the optimal $r_{i,j}$ is computed, $\tilde{\mathbf{B}}$ is updated by (14) and $\tilde{\mathbf{A}}$ is updated by computing $(\tilde{\mathbf{B}}^{(\text{new})})^{\square 2}$.

The processing of all the $N(N-1)$ parameters $\theta_{i,j}$ and $r_{i,j}$, is called a QR sweep. The proposed JD_{QR}^+ algorithm is comprised of several QR sweeps in order to guarantee the convergence. In ICA, when a non-square matrix $\mathbf{A} \in \mathbb{R}_+^{N \times P}$ with $N > P$ is encountered, we can compress it by a matrix $\mathbf{W} \in \mathbb{R}_+^{N \times P}$ such that the resulting matrix $\tilde{\mathbf{A}} = \mathbf{W}^T \mathbf{A}$ is a nonnegative square matrix [15]. It is noteworthy that the proposed algorithm is different from the two published nonnegative JDC methods, which are based on the LU matrix factorization [10], [11]. We use QR factorization in this paper. The method in [10] estimates \mathbf{B} and $\mathbf{D}^{(k)}$ alternately, and its performance is sensitive to the initialization. The algorithm in [11] needs to compute the inverse of \mathbf{A} in all the $N(N-1)$ Jacobi-like iterations, leading to a high numerical complexity.

III. SIMULATION RESULTS

In this section, the proposed JD_{QR}^+ algorithm is compared with several existing JDC methods and BSS algorithms. The performance is measured in terms of the error between the true matrix \mathbf{A} and its estimate $\tilde{\mathbf{A}}$, as well as the source \mathbf{s} and its estimate $\tilde{\mathbf{s}}$ when a BSS context is considered. The following scale-invariant and permutation-blind distance is chosen as the preferred measure:

$$\alpha(\mathbf{A}, \tilde{\mathbf{A}}) = (1/N) \sum_{n=1}^N \min_{(n,n') \in I_n^2} d(\mathbf{a}_n, \tilde{\mathbf{a}}_{n'}) \quad (19)$$

where \mathbf{a}_n and $\tilde{\mathbf{a}}_{n'}$ are the n -th column of \mathbf{A} and the n' -th column of $\tilde{\mathbf{A}}$, respectively. I_n^2 is defined recursively by $I_1^2 = \{1, \dots, N\} \times \{1, \dots, N\}$, and $I_{n+1}^2 = I_n^2 - J_n^2$, where $J_n^2 = \text{argmin}_{(n,n') \in I_n^2} d(\mathbf{a}_n, \tilde{\mathbf{a}}_{n'})$. In addition, $d(\mathbf{a}_n, \tilde{\mathbf{a}}_{n'})$ is defined as the pseudo-distance between two vectors [4]:

$$d(\mathbf{a}_n, \tilde{\mathbf{a}}_{n'}) = 1 - \|\mathbf{a}_n^T \tilde{\mathbf{a}}_{n'}\|^2 / (\|\mathbf{a}_n\|^2 \|\tilde{\mathbf{a}}_{n'}\|^2) \quad (20)$$

The smaller the value of (19) is, the better estimation of \mathbf{A} is achieved.

A. Simulated semi-nonnegative semi-symmetric arrays

In this part, JD_{QR}^+ is compared with two classic JDC methods, namely ACDC [5] and FFdiag [6], and one nonnegative JDC method $\text{ACDC}_{\text{LU}}^+$ [10] with simulated semi-nonnegative semi-symmetric 3-way arrays \mathcal{C} . $\mathcal{C} \in \mathbb{R}^{3 \times 3 \times 5}$ is generated randomly according to equation (2). The loading matrices \mathbf{A} and \mathbf{D} are randomly drawn from a uniform distribution between 0 and 1. The pure array \mathcal{C} is perturbed by a semi-symmetric residual noise array \mathcal{V} . The loading matrices of \mathcal{V} obey the zero-mean unit-variance Gaussian distribution. The resulting noisy 3-way array can be written by $\mathcal{C}_N = \mathcal{C} / \|\mathcal{C}\|_F + \sigma_N \mathcal{V} / \|\mathcal{V}\|_F$, where σ_N is a scalar controlling the noise level. Then the Signal-to-Noise Ratio (SNR) is defined by $\text{SNR} = -20 \log_{10}(\sigma_N)$. All the algorithms stop either when the relative error of the corresponding criterion between two successive sweeps is less than 10^{-5} or when the number of sweeps exceeds 200. We repeat the experiment with SNR ranging from -10 dB to 30 dB with 500 Monte Carlo trials. Figure 1 shows the average curves of $\alpha(\mathbf{A}, \tilde{\mathbf{A}})$ of all the three algorithms as a function of SNR. It shows that ACDC performs better than FFdiag under higher SNR levels. The nonnegativity constraint obviously helps $\text{ACDC}_{\text{LU}}^+$ and JD_{QR}^+ to outperform the classic ones. The proposed JD_{QR}^+ algorithm maintains the best estimation accuracy, especially for the lower SNR levels.

B. BSS application on MRS data

In this section, the BSS performance of JD_{QR}^+ is compared with an effective ICA method CoM_2 [16] and a Nonnegative Matrix Factorization (NMF) method based on alternating Non-Negativity Least Squares (NNLS) [17], through an experiment carried out on simulated MRS data. Two metabolites, namely the Choline and Myo-inositol, serve as source signals $s_1(f)$ and $s_2(f)$. 32 observations are generated according to the noisy linear mixing model $\mathbf{x}(f) = \mathbf{A}\mathbf{s}(f) + \mathbf{v}(f)$, where $\mathbf{v}(f)$ is an additive white Gaussian noise. $\mathbf{A} \in \mathbb{R}_+^{32 \times 2}$ is similarly generated as in the previous section. For an ICA method based

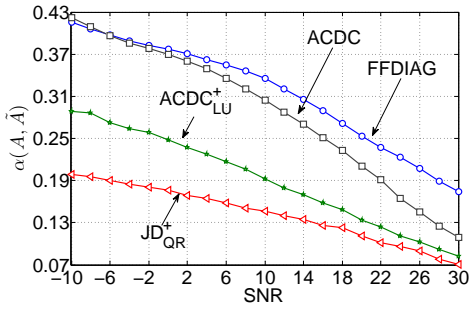


Fig. 1. Average error $\alpha(\mathbf{A}, \tilde{\mathbf{A}})$ evolution of ACDC, FFDIAG, $\text{ACDC}_{\text{LU}}^+$ and JD_{QR}^+ as a function of SNR on simulated arrays.

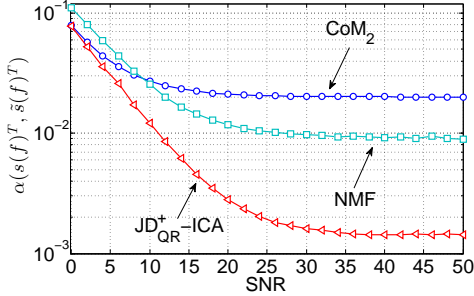


Fig. 2. Average error $\alpha(\{s(f)\}^T, \{\tilde{s}(f)\}^T)$ evolution of CoM_2 , NMF and JD_{QR}^+ -ICA as a function of SNR for BSS of 2 simulated MRS metabolites.

on JD_{QR}^+ , namely JD_{QR}^+ -ICA, $\{\mathbf{x}(f)\}$ is compressed by means of a matrix $\mathbf{W} \in \mathbb{R}_+^{32 \times 2}$ computed using the method proposed in [15], such that the number of observations is reduced to 2. The 3-way array \mathcal{C} is built by stacking four 4-th order cumulant matrix slices. We repeat the experiment with SNR ranging from 0 dB to 50 dB with 200 Monte Carlo trials. The average curves of the estimating error $\alpha(\{s(f)\}^T, \{\tilde{s}(f)\}^T)$ of all the three methods as a function of SNR are shown in figure 2. It shows that the proposed JD_{QR}^+ -ICA algorithm maintains competitive advantages when $\text{SNR} \geq 5$ dB. Figure 3 shows the separation results of all the methods with a SNR of 10 dB for one typical realization. Regarding CoM_2 and NMF, there are some obvious disturbances presented in the estimated metabolites. As far as JD_{QR}^+ -ICA is concerned, the estimated source metabolites are quasi-perfect.

IV. CONCLUSION

In this paper, we have addressed the problem of the CP decomposition of semi-nonnegative semi-symmetric 3-way arrays. We proposed a method, called JD_{QR}^+ , based on the QR factorization of the Hadamard square root of the nonnegative loading matrix. A numerical experiment on simulated arrays highlights its advantage. A BSS application on MRS signals also demonstrates the interest of the proposed method.

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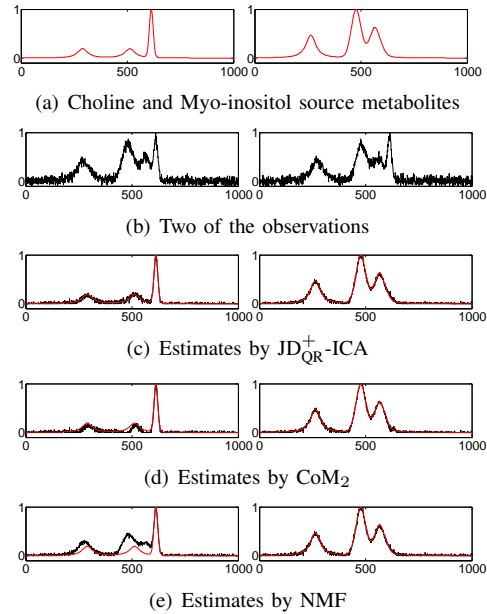


Fig. 3. MRS source metabolites, observations and estimated metabolites by JD_{QR}^+ -ICA, CoM_2 and NMF with SNR = 10 dB for one typical realization. The overlapping red lines in figures (c), (d) and (e) indicate the correct sources.

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