CP decomposition of semi-nonnegative semisymmetric tensors based on QR matrix factorization
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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\textsuperscript{QR}, to solve such a problem. The nonnegativity constraint is imposed by means of a square 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 \( C \in \mathbb{R}^{N \times N \times K} \), is the minimal linear combination of rank-1 3-way arrays that yields \( C \) exactly:

\[
C = \sum_{p=1}^{P} a_p \circ a_p \circ d_p
\]

subject to \( A = [a_1, \cdots, a_P] \in \mathbb{R}^{N \times P} \) having nonnegative components, where \( \circ \) denotes the outer product. \( A \) and \( D = [d_1, \cdots, d_P] \in \mathbb{R}^{K \times P} \) are called the loading matrices of \( C \). \( P \) is then the rank of \( C \).

The decomposition is considered to be essentially unique when the uniqueness is guaranteed up to scaling and permuting 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 \( C \): \( C^{(k)} = C_{:, :, k} = AD^{(k)}A^T, \forall k \in \{1, 2, \cdots, K\} \), where \( D^{(k)} \in \mathbb{R}^{P \times P} \) is a diagonal matrix whose diagonal contains the elements of the \( k \)-th row of \( D \), and \( C^{(k)} \in \mathbb{R}^{N \times N} \) is the \( k \)-th frontal slice \( C \). In this paper, we focus on computing the square matrix \( A \), where \( N = P \). In order to compute \( A \), we can resort to solve the following nonnegative Joint Diagonalization by Congruence (JDC) problem:

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

\[
\forall k \in \{1, 2, \cdots, K\}, \ C^{(k)} = AD^{(k)}A^T
\]

subject to \( A \) 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 constrains [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\textsuperscript{QR}, based on minimizing the following indirect least square criterion [6], [12]:

\[
J_1(A) = \sum_{k=1}^{K} \left\| \text{off}(A^{-1}C^{(k)}A^{-T}) \right\|_F^2
\]

where \( \text{off}(.) \) vanishes the diagonal components of the input matrix, the superscript \(-T\) denotes the inverse of the transposed matrix, and \( \| \cdot \|_F \) computes the Frobenius norm. The nonnegativity constraint is imposed by means of a square of variable. The QR matrix factorization of the Hadamard square root of \( A \) 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 \( A \) 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\textsuperscript{QR} METHOD

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

\[
(C^{(k)})^{-1} = A^{-T}(D^{(k)})^{-1}A^{-1}
\]

In practice, only the sufficiently well-conditioned matrix \( C^{(k)} \) is chosen when its condition number is below a predefined
threshold. We use $C^{(k-1)}$ to denote $(C^k)^{-1}$ for simplicity. Equation (4) shows that $C^{(k-1)}$ is jointly diagonalizable by $A$. Then $A$ can be estimated by minimizing the following modified criterion of (3) directly:

$$J_2(A) = \sum_{k=1}^{K} \| \text{off} \left( A^T C^{(k-1)} A \right) \|_F^2.$$  (5)

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

$$J_2(B) = \sum_{k=1}^{K} \| \text{off} \left( (B^{oxprod 2})^T C^{(k-1)} B^{oxprod 2} \right) \|_F^2.$$  (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 $R^{(i-j)}(r_{i,j})$ 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 $Q^{(i,j)}(\theta_{i,j})$ 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 $\cos(\theta_{i,j})$, $\cos(\theta_{j,i})$, $-\sin(\theta_{i,j})$ and $\sin(\theta_{j,i})$, 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 $B \in \mathbb{R}^{N \times N}$, the QR matrix factorization decomposes it as $B = QR \Lambda$, where $Q \in \mathbb{R}^{N \times N}$ is an orthonormal matrix, $R \in \mathbb{R}^{N \times N}$ is a unit upper triangular matrix, and $\Lambda \in \mathbb{R}^{N \times N}$ is a diagonal matrix. Due to the indeterminacies of the CP decomposition, the matrix $B$ solving (6) can be chosen as $B = QR$ without loss of generality. Moreover, lemma 1 and lemma 2 yield that $B$ can be written as a product of the following matrices:

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

As a consequence, the minimization of (6) with respect to $B$ 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 $Q^{(i,j)}(\theta_{i,j})$**

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

$$\tilde{B}^{(\text{new})} = B Q^{(i,j)}(\theta_{i,j}).$$  (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 $\tilde{B}$ by $\tilde{B}^{(\text{new})}$. For the sake of convenience, we denote $J_2^*(\theta_{i,j})$ instead of $J_2(\tilde{B}^{(\text{new})})$. $J_2(\theta_{i,j})$ can be expressed as follows:

$$J_2(\theta_{i,j}) = \sum_{k=1}^{K} \| \text{off} \left\{ (\tilde{B}^{(\text{new})})^T C^{(k-1)} (\tilde{B}^{(\text{new})}) \right\} \|_F^2.$$  (9)

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

$$\| (\tilde{B}^{(\text{new})})^T C^{(k-1)} (\tilde{B}^{(\text{new})}) \|_F^2 = \sum_{k=1}^{K} \| \text{off} \left\{ (\tilde{B}^{(\text{new})})^T C^{(k-1)} (\tilde{B}^{(\text{new})}) \right\} \|_F^2$$  (10)

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

$$J_2(\theta_{i,j}) = \sum_{k=1}^{K} \| \text{off} \left\{ \left( \tilde{b}_i^T C^{(k-1)} \tilde{b}_i \right) e_i - e_i^T \right\} \|_F^2$$  (11)

where $\tilde{C}^{(k)}(\tilde{b}_i^T) = \tilde{A}^T C^{(k)}(\tilde{b}_i^T)$. Equation (11) shows that the sum of the squares of $\theta_{i,j}$ can be written as a function of $\theta_{i,j}$ as follows:

$$\| \tilde{b}_i^T C^{(k-1)} \tilde{b}_i \|_2^2 = \sum_{i,j} \| \text{off} \left\{ (\tilde{b}_i^T C^{(k-1)} \tilde{b}_i) e_i - e_i^T \right\} \|_F^2$$  (12)

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

$$\| \tilde{b}_i^T C^{(k-1)} \tilde{b}_i \|_2^2 = \frac{f_i^4 + f_j^4 + f_i^2 f_j^4 + 4 f_i^4 f_j^4 + f_i^2 + f_j^4 + f_i^2 f_j^4}{(1 + t_{i,j}^2)^2}$$  (13)

where $f_i^4 = \tilde{c}^{(k)}_{i,j} - \tilde{c}^{(k)}_{j,i}$, $f_j^4 = -\tilde{c}^{(k)}_{i,j} + \tilde{c}^{(k)}_{j,i}$, $f_i^2 = \tilde{c}^{(k)}_{i,j} + \tilde{c}^{(k)}_{j,i}$, $f_j^2 = 2 \tilde{c}^{(k)}_{i,j} - \tilde{c}^{(k)}_{j,i}$ and $f_i^0 = \tilde{c}^{(k)}_{i,j}$.

Equation (13) shows that the sum of the squares of $\tilde{c}^{(k)}_{i,j}$ 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 $B$ is updated by (8) and $A$ is updated by computing $(\tilde{B}^{(\text{new})})^2$. 

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

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

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

(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:

$$
J_2(r_{i,j}) = \sum_{k=1}^{K} \|\tilde{\mathbf{B}}^{(\text{new})} \tilde{\mathbf{C}}_{(k,-1)}(r_{i,k})\|^2_F
$$

(15)

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

$$
\tilde{\mathbf{B}}^{(\text{new})} = \tilde{\mathbf{B}}\mathbf{R}^{(i,j)}(r_{i,j}) + 2r_{i,j}(\hat{b}_i \boxdot \hat{b}_j)e_j^T
$$

(16)

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

$$
J_2(r_{i,j}) = \sum_{k=1}^{K} \|\tilde{\mathbf{C}}^{(k)}_{(\text{new})}\|^2_F
$$

where $\tilde{\mathbf{C}}^{(k)} = \tilde{\mathbf{A}}^T\tilde{\mathbf{C}}^{(k,-1)}\tilde{\mathbf{A}}$, and $\tilde{\mathbf{C}}^{(k)}_2 = \mathbf{R}^{(i,j)}(r_{i,j})e_j^T + r_{i,j}e_j^T + \mathbf{R}^{(i,j)}(r_{i,j})e_j^T + r_{i,j}e_j^T$

(17)

where $\tilde{\mathbf{C}}^{(k)}_{(\text{new})}$ is the $(n,i,j)$-th component of $\tilde{\mathbf{C}}^{(k)}$, and $\tilde{\mathbf{C}}^{(k)}_n$ is the $n$-th element of $\tilde{\mathbf{C}}^{(k)}$. 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 $\tilde{\mathbf{B}}^{(\text{new})} \boxdot \tilde{\mathbf{B}}^{(\text{new})}$.

The processing of all the $N(N-1)$ parameters $\theta_{i,j}$ and $r_{i,j}$, is called a QR sweep. The proposed $\text{JD}_{QR}$ 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 $\mathbf{A} = \mathbf{W}^\top \mathbf{A}$ 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 $\text{JD}_{QR}$ 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 $\hat{\mathbf{A}}$, as well as the source $\mathbf{s}$ and its estimate $\hat{\mathbf{s}}$ when a BSS context is considered. The following scale-invariant and permutation-blind distance is chosen as the preferred measure:

$$
\alpha(A, \hat{A}) = \left(\frac{1}{N}\right) \sum_{n=1}^{N} \min_{(n,n') \in \mathcal{P}_2} d(a_n, \hat{a}_{n'})
$$

(19)

where $a_n$ and $\hat{a}_{n'}$ are the $n$-th column of $\mathbf{A}$ and the $n'$-th column of $\hat{\mathbf{A}}$, respectively. $I_n^2$ is defined recursively by $I_n^2 = \{1, \cdots, N\} \times \{1, \cdots, N\}$, and $I_{n+1}^2 = I_n^2 - J_n^2$, where $J_n = \min_{(n,n') \in \mathcal{P}_2} d(a_n, \hat{a}_{n'})$. In addition, $d(a_n, \hat{a}_{n'})$ is defined as the pseudo-distance between two vectors $[4]$:

$$
d(a_n, \hat{a}_{n'}) = 1 - \frac{\|a_n\|^2}{\|a_n\|^2 + \|\hat{a}_{n'}\|^2}
$$

(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, $\text{JD}_{QR}$ is compared with two classic JDC methods, namely ACDC [5] and FFDIAG [6], and one nonnegative JDC method ACDC*$_{LU}$ [10] with simulated semi-nonnegative semi-symmetric 3-way arrays $\mathbf{C}$. $\mathbf{C} \in \mathbb{R}^{3 \times 3 \times 5}$ 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 $\mathbf{C}$ is perturbed by a semi-symmetric residual noise array $\mathbf{V}$. The loading matrices of $\mathbf{V}$ obey the zero-mean unit-variance Gaussian distribution. The resulting noisy 3-way array can be written by $\mathbf{C} = \mathbf{C}/\|\mathbf{C}\|_F + \sigma_N \mathbf{V}/\|\mathbf{V}\|_F$, where $\sigma_N$ 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 $\alpha(A, \hat{A})$ 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 ACDC*$_{LU}$ and $\text{JD}_{QR}$ to outperform the classic ones. The proposed $\text{JD}_{QR}$ 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 $\text{JD}_{QR}$ is compared with an effective ICA method CoMz [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 $x(f) = A s(f) + v(f)$, where $v(f)$ is an additive white Gaussian noise. $\mathbf{A} \in \mathbb{R}_+^{N \times 2}$ is similarly generated as in the previous section. For an ICA method based
on $\text{JD}_{QR}$, namely $\text{JD}_{QR}^{+}$-ICA, $\{s(f)\}$ is compressed by means of a matrix $W \in \mathbb{R}^{32 \times 2}$ computed using the method proposed in [15], such that the number of observations is reduced to 2. The 3-way array $C$ 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 $\alpha(\{u(f)\}^T, \{\hat{s}(f)\}^T)$ of all the three methods as a function of SNR are shown in figure 2. It shows that the proposed $\text{JD}_{QR}^{+}$-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 $\text{JD}_{QR}^{+}$-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 $\text{JD}_{QR}^{+}$, 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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