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CP decomposition of semi-nonnegative semi-symmetric 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_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 $C \in \mathbb{R}^{N \times N \times K}$, 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 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 $C$: $C^{(k)} = C_{:, :, k} = AD^{(k)}A^T$, $\forall k \in \{1, 2, \cdots, K\}$, 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:

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

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_QR, based on minimizing the following indirect least square criterion [6], [12]:

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

where $\text{off}(\cdot)$ 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 change 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_QR METHOD

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

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

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:

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

(5)

The nonnegativity constraint on $A$ can be imposed by a square change of variable: $A = B \Box B = B^{(2)}$, where $B \in \mathbb{R}^{N \times N}$ and where $\Box$ 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 $A = B^{(2)}$, and $B$ is the global minimum of the following cost function:

$$J_2(B) = \sum_{k=1}^{K} \| \text{off}((B^{(2)})^T C^{(k,-1)} B^{(2)}) \|_F^2.$$  

(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 $B = Q R A$, 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 $A \in \mathbb{R}^{N \times N}$ is a diagonal matrix. Due to the in-determinacies 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 JDQG, in order to compute these parameters sequentially.

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

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

$$\hat{B}^{(\text{new})} = B Q^{(i,j)}(\theta_{i,j}).$$  

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

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

(9)

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

$$\hat{B}^{(\text{new})^2} = \hat{B}^{(\text{new})} \cdot \hat{B}^{(\text{new})^2} = \sin(2\theta)(\hat{b}_i \odot \hat{b}_j)(e_i^T - e_j^T) + \sin^2(\theta)(\hat{c}_i(1)+\hat{c}_j(1)),$$

(10)

where $\hat{b}_i$ denotes the $i$-th column of $\hat{B}$, 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:

$$J_2(\theta_{i,j}) = \sum_{k=1}^{K} \| \text{off}(\hat{C}^{(k,\text{new})}) \|_F^2,$$

(11)

where $\hat{C}^{(k,\text{new})} = \hat{A}^T C^{(k,-1)} \hat{A}$, $\hat{c}^{(k,1)} = \hat{A}^T C^{(k,-1)}(\hat{b}_i \odot \hat{b}_j)$, $\hat{c}^{(k,2)} = (\hat{e}_i^T - \hat{e}_j^T)$, $\hat{c}^{(k,3)} = \hat{b}_i \odot \hat{b}_j C^{(k,-1)}(\hat{b}_i \odot \hat{b}_j)$ 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 $C^{(k,\text{new})}$ involve the parameter $\theta_{i,j}$. It is noteworthy that the $(i,i)$-th and $(j,j)$-th elements are twice affected by the transformation. Inspired by [12], we propose to minimize the sum of the squares of the $(i,i)$-th entries of the $K$ symmetric matrices $C^{(k,\text{new})}$, instead of minimizing all the off-diagonal entries. This simplified minimization criterion is denoted by $J_2(\theta_{i,j})$. The $(i,i)$-th element of $C^{(k,\text{new})}$ can be expressed as a function of $\theta_{i,j}$ as follows:

$$\hat{c}^{(i,k,\text{new})}(\theta_{i,j}) = -\sin^2(2\theta_{i,j})\hat{c}^{(i,k,3)} + \sin^2(\theta_{i,j})(\hat{c}^{(i,k,3)} cos(\theta_{i,j}) + \hat{c}^{(i,k,1)} sin(\theta_{i,j}))$$

$$+ \cos^2(\theta_{i,j})(\hat{c}^{(i,k,3)} cos(\theta_{i,j}) + \hat{c}^{(i,k,2)} sin(\theta_{i,j}))$$

(12)

$$\sin(2\theta_{i,j})(\hat{c}^{(i,k,1)} cos(\theta_{i,j}) + \hat{c}^{(i,k,2)} sin(\theta_{i,j}))$$

$$+ \sin^2(\theta_{i,j})(\hat{c}^{(i,k,1)} cos(\theta_{i,j}) + \hat{c}^{(i,k,2)} sin(\theta_{i,j}))$$

(12)

where $\hat{c}^{(i,k,1)}$ is the $(i,j)$-th element of $\hat{C}^{(k,\text{new})}$ and $\hat{c}^{(i,k,q)}$ is the $i$-th element of vector $\hat{c}^{(k,q)}$ 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:

$$\hat{c}^{(i,k,\text{new})}(t_{i,j}) = \frac{f_{d,k}(t_{i,j})^4 + f_{d,k}(t_{i,j})^2 + f_{d,k}^2(t_{i,j})^2 + f_{d,k}^4(t_{i,j})}{(1 + t_{i,j}^2)^2},$$

(13)

where $f_{d,k}(t_{i,j}) = \hat{c}^{(i,k)} + \hat{c}^{(j,k)} - 2\hat{c}^{(i,j)}$, $f_{d,k}^2(t_{i,j}) = \hat{c}^{(i,k)} + \hat{c}^{(j,k)} + 2\hat{c}^{(i,j)} - 4\hat{c}^{(k,3)}$, $f_{d,k}(t_{i,j}) = \hat{c}^{(i,k)} - \hat{c}^{(j,k)}$, and $f_{d,k}^2(t_{i,j}) = \hat{c}^{(i,k)} - \hat{c}^{(j,k)}$.

Equation (13) shows that the sum of the squares of $\hat{c}^{(i,k,\text{new})}$, is a rational function in $t_{i,j}$, namely $J_2(t_{i,j})$, 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 $J_2(t_{i,j})$. Once $t_{i,j}$ is obtained, $\theta_{i,j}$ can be computed by $\theta_{i,j} = \arctan(t_{i,j})$. Then $\hat{B}$ is updated by (8) and $\hat{A}$ is updated by computing $(\hat{B}^{(\text{new})})^2$. 


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

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

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

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

$$J_2(r_{i,j}) = \sum_{k=1}^{K} \| \text{off} \left( \left[ (\tilde{B}^{\text{new}})_{\square 2} \right] C(k_{\cdot j}) \| (\tilde{B}^{\text{new}})_{\square 2} \right) \|^2_F$$

(15)

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

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

(16)

where $\hat{b}_i$ denotes the $i$-th column of $\hat{B}$, 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:

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

= \sum_{k=1}^{K} \| \text{off} \left( (R^{(i,j)}(r_{i,j})^T C^{(k)}(r_{i,j}) + r_{i,j}c^{(k,3)} e_j^T + r_{i,j}c^{(k,2)} R^{(i,j)}(r_{i,j}) e_j^T \right) \|^2_F$$

(17)

where $\tilde{C}^{(k)} = \tilde{A}^T C^{(k),-1} \tilde{A}$, $c^{(k,1)} = 2 \tilde{A}^T C^{(k),-1}(\hat{b}_i \boxdot \hat{b}_j)$, $c^{(k,2)} = (c^{(k,1)})^T$ and $c^{(k,3)} = 4 (\hat{b}_i \boxdot \hat{b}_j)^T C^{(k),-1} (\hat{b}_i \boxdot \hat{b}_j)$ 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 $\tilde{C}^{(k),\text{new}}$ 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 $\tilde{C}^{(k),\text{new}}$ except their $(i,j)$-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:

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

(18)

where $c^{(k,1)}_{n,i}$ is the $(n,i)$-th component of $\tilde{C}^{(k)}$, and $c^{(k,1)}_{n,j}$ is the n-th component of $c^{(k,1)}$. 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, $\tilde{B}$ is updated by (14) and $\tilde{A}$ is updated by computing $(\tilde{B}^{\text{new}})_{\square 2}$.

The processing of all the $N(N-1)$ parameters $\theta_{i,j}$ and $r_{i,j}$, is called 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 $A \in \mathbb{R}_{N \times P}$ with $N > P$ is encountered, we can compress it by a matrix $W \in \mathbb{R}_{N \times P}$ such that the resulting matrix $\tilde{A} = W^T A$ 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 $B$ and $D^{(k)}$ alternately, and its performance is sensitive to the initialization. The algorithm in [11] needs to compute the inverse of $A$ 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 $A$ and its estimate $\hat{A}$, as well as the source vector $s$ and its estimate $\hat{s}$ when a BSS context is considered. The following scale-invariant and permutation-blind distance is chosen as the preferred measure:

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

(19)

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

$$d(a_n, \hat{a}_{n'}) = 1 - \frac{\|a_n^T \hat{a}_{n'}\|^2}{\|a_n\|^2 \|\hat{a}_{n'}\|^2}$$

(20)

The smaller the value of (19) is, the better estimation of $A$ 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 ACDC$^+_{LU}$ [10] with simulated semi-nonnegative semi-symmetric 3-way arrays $C$, $C \in \mathbb{R}_{3 \times 3 \times 5}$ is generated randomly according to $\text{equation (2)}$. The loading matrices $A$ and $D$ are randomly drawn from a uniform distribution between 0 and 1. The pure array $C$ is perturbed by a semi-nonsymmetric 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 $C_N = C + \sigma\mathbb{N}(\mathbf{V})$, 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 $-10 \text{ dB}$ to $30 \text{ dB}$ 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 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 $x(f) = As(f) + v(f)$, where $v(f)$ is an additive white Gaussian noise. $A \in \mathbb{R}_{32 \times 2}$ is similarly generated as in the previous section. For an ICA method based
on JDQR, namely JDQR-ICA, \{\alpha(f)\} is compressed by means of a matrix \(W \in \mathbb{R}^{D \times 2}\) 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 \(\alpha(\{\hat{s}(f)\}^T, \{\tilde{s}(f)\}^T)\) of all the three methods as a function of SNR are shown in figure 2. It shows that the proposed JDQR-ICA algorithm maintains competitive advantages when 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 CoM2 and NMF, there are some obvious disturbances presented in the estimated metabolites. As far as JDQR-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 JDQR, 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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