CANONICAL POLYADIC DECOMPOSITION OF COMPLEX-VALUED MULTI-WAY ARRAYS BASED ON SIMULTANEOUS SCHUR DECOMPOSITION

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ABSTRACT

In this paper, we propose a new semi-algebraic algorithm to compute the Canonical Polyadic (CP) decomposition of complex-valued multi-way arrays. The proposed algorithm is based on the Simultaneous Schur Decomposition (SSD) of particular matrices derived from the array to process. This CP algorithm solves some convergence problems of classical iterative techniques and its identifiability assumptions are less restrictive than those of other semi-algebraic methods. We also propose a new Jacobi-like algorithm to calculate the SSD of several complex-valued matrices. Finally the usefulness of the proposed method is illustrated in the context of fluorescence spectroscopy and epileptic source localization.

Index Terms— Canonical Polyadic Decomposition, CANDECOMP/PARAFAC model, Simultaneous Schur Decomposition, Jacobi-like optimization, epileptic source localization.

1. INTRODUCTION

The Canonical Polyadic or CANDECOMP/PARAFAC (CP) decomposition consists in decomposing a Higher Order (HO) array as a linear combination of a minimal number of rank-1 terms. The CP decomposition can then be seen as a generalization of the Singular Value Decomposition (SVD) of two-way data to multi-way data. But the main difference is that, under weak assumptions [1], [2], no orthogonality constraint is needed to ensure uniqueness of the CP decomposition. This advantage makes the CP decomposition very useful in various applications [3], [4], [5], [6], [7], [8].

Several different methods were proposed to solve the CP problem. Generally, they can be divided into two categories: fully iterative and semi-algebraic methods. The fully iterative methods, such as the Alternative Least Squares (ALS) [9], Levenberg-Marquardt (LM) [10], [11] and nonlinear conjugate gradient approaches [12], try to estimate factors by starting from an initial point and iteratively decreasing the corresponding cost function. As the general iterative algorithms, these algorithms suffer from converging to local minima. To cope with this problem, different initial points must be used, which results to a time-consuming procedure. Unlike the iterative algorithms, the semi-algebraic algorithms do not require any initialization. These algorithms try to rewrite the CP problem into a more classical matrix problem such as joint eigenvalue decomposition [13], [14], simultaneous diagonalization by congruence [15] or Simultaneous Generalized Schur Decomposition (SGSD) [16], [17] of several matrices. These reformulated problems are usually solved by means of a Jacobi-like procedure.

In this paper, we propose a new semi-algebraic algorithm for CP decomposition of complex-valued HO arrays which is based on Simultaneous Schur Decomposition (SSD) of several matrices. Previously, a CP algorithm based on SGSD originally introduced in [18]

was proposed in [16]. This CP algorithm aims at decomposing real-valued three-way arrays. In fact, as other algorithms proposed in [17], it consists in reformulating the CP problem into an unsymmetric simultaneous triangularization problem. To deal with the latter, two QR decompositions are assumed and the problem is solved by using a QZ iteration method followed by an algorithm to compute the triangular matrices (three different methods are introduced in [17]). Note that some constraints on the rank of the loading matrices must be assumed for identifiability of these algorithms [16], [17]. Compared with these CP algorithms, our formulation differs in such a way that results in a symmetric simultaneous triangularization problem. In addition, the proposed CP algorithm imposes no limitation on the order of the complex-valued arrays to decompose and the identification constraints are also less restrictive. Also a new SSD algorithm for decomposition of several complex-valued matrices is proposed. Finally the usefulness of the proposed method is illustrated in the context of fluorescence spectroscopy and epileptic source localization.

2. METHODOLOGY

In the following sections, bold uppercase letters (e.g. $\mathbf{A}$), bold lowercase letters (e.g. $\boldsymbol{a}$) and calligraphic letters (e.g. $\mathcal{A}$) are used to denote matrices, vectors and HO arrays, respectively. The superscripts $*, \sharp, ^{\mathsf{T}}, ^{\mathsf{H}}$ stand for the complex conjugate, the Moore-Penrose pseudoinverse, the transpose and the complex conjugated transpose, respectively.

2.1. Complex Simultaneous Schur Decomposition

In this section, we introduce a new Jacobi-like algorithm in order to calculate the SSD of several complex-valued matrices. It is a non trivial extension of a method proposed in the nineties for real-valued matrices only [19].

The SSD problem can be expressed as the following simultaneous triangularization problem. Given R matrices $\boldsymbol{Y}^{(r)} \in \mathbb{C}^{d \times d}$ that have the following structure:

$$\boldsymbol{Y}^{(r)} = \boldsymbol{\Theta}^{(o)} \boldsymbol{X}^{(r)} \boldsymbol{\Theta}^{(o)\mathsf{H}} \tag{1}$$

where $\boldsymbol{\Theta}^{(o)} \in \mathbb{C}^{d \times d}$ is a unitary matrix and where the R matrices $\boldsymbol{X}^{(r)} \in \mathbb{C}^{d \times d}$ are upper triangular matrices, our objective is the simultaneous triangularization of the R matrices $\boldsymbol{Y}^{(r)}$ by finding the appropriate unitary matrix $\boldsymbol{\Theta}^{(o)}$. In the presence of noise, the matrices $\boldsymbol{Y}^{(r)}$ do not exactly fit (1), so $\boldsymbol{\Theta}^{(o)}$ should be computed as an approximate solution to the problem of simultaneous upper triangularization. Indeed, we should find matrix $\boldsymbol{\Theta}^{(o)}$ which minimizes the following cost function:

$$\psi(\boldsymbol{\Theta}^{(o)}) = \sum_{r=1}^{R} \|\mathcal{L}(\boldsymbol{\Theta}^{(o)\mathsf{H}} \boldsymbol{Y}^{(r)} \boldsymbol{\Theta}^{(o)})\|_F^2 \tag{2}$$

where $\mathcal{L}(\boldsymbol{Y}^{(r)})$ extracts the strictly lower triangular part of its matrix-valued argument by replacing the upper triangular part with zeros and where $\|.\|_F$ denotes the Frobenius norm.

Minimizing the function ψ in several variables is a hard optimization problem, except for small dimensions. The idea is to reformulate this multivariate optimization problem in a finite sequence of monovariate optimization problems using a Jacobi-like optimization scheme. Since any unitary matrix can be written as a product of elementary Givens rotation matrices, we can parameterize the orthogonal matrix $\boldsymbol{\Theta}^{(o)}$ as follows:

$$\boldsymbol{\Theta}^{(o)} = \prod_{sw=1}^{\#ofsweeps} \prod_{q=1}^{d} \prod_{p=1}^{q-1} \boldsymbol{\Theta}^{(o,p,q)} \qquad (3)$$

where each elementary Givens rotation matrix $\boldsymbol{\Theta}^{(o,p,q)}$ is obtained from an identity matrix in which we have $\Theta_{p,p}^{(p,q)} = c$, $\Theta_{p,q}^{(p,q)} = s$, $\Theta_{q,p}^{(p,q)} = -s^*$ and $\Theta_{q,q}^{(p,q)} = c$, where $(c,s) \in \mathbb{R} \times \mathbb{C}$ such that $c^2 + |s|^2 = 1$. An appropriate parameterization of c and s in the complex domain used in the proposed algorithm is:

$$s = \frac{t}{\sqrt{1+|t|^2}}, \quad c = \frac{1}{\sqrt{1+|t|^2}}, \quad t \in \mathbb{C} \qquad (4)$$

In each iteration, a new elementary Givens rotation matrix $\boldsymbol{\Theta}^{(o,p,q)}$ which defines $\boldsymbol{\Theta}^{(o)}$ (3) is computed in order to minimize the cost function (2). So, for each p and q, the R complex-valued matrices $\boldsymbol{Y}^{(r)}$ are transformed as:

$$\boldsymbol{Y}^{(r)\prime} = \boldsymbol{\Theta}^{(o,p,q)^{\mathsf{H}}} \boldsymbol{Y}^{(r)} \boldsymbol{\Theta}^{(o,p,q)} \qquad (5)$$

Since this orthogonal similarity transformation changes only the elements of $\boldsymbol{Y}^{(r)}$ which appear in rows and columns p and q, the change in the cost function can be expressed as:

$$\begin{aligned} \Delta\psi(\boldsymbol{\Theta}_{q,p}) =& (1+|t|^2)^{-2} \left(v_8 + 2Re\{t(v_3^* - v_9^*)\} - 2Re\{t^2(v_4^*)\} \right. \\ &+ |t|^4 v_6 + |t|^2 (v_1 + v_{10} - 2Re\{v_7\}) + 2Re\{t|t|^2(v_5^* - v_2^*)\} \big) \\ &+ (1+|t|^2)^{-1} \left(u_1 - 2Re\{tu_2\} + |t|^2 u_3 + w_1 + 2Re\{tw_2\} \right. \\ &+ |t|^2 w_3 \big) - \sum_{r=1}^{R} \left(|Y_{q,p}^{(r)}|^2 + \sum_{k=p+1}^{q-1} \left(|Y_{k,p}^{(r)}|^2 + |Y_{q,k}^{(r)}|^2 \right) \right) \quad (6) \end{aligned}$$

where the coefficients v_1-v_{10}, u_1-u_3 and w_1-w_3 are defined in appendix. To calculate an appropriate complex value for t in each iteration, we use the parameterization $t = \rho e^{i\phi}$ and then we differentiate (6) with respect to ρ and ϕ separately. Note that the roots of the following equation system are the stationary points of $\Delta\psi(\boldsymbol{\Theta}_{q,p})$.

$$\frac{\partial \Delta\psi(\rho,\phi)}{\partial \rho} = 0 \quad \text{and} \quad \frac{\partial \Delta\psi(\rho,\phi)}{\partial \phi} = 0 \qquad (7)$$

It can be shown that by merging both equations of (7) and simplifying the resulting equation, the wanted ϕ value can be obtained by rooting a single 14-th degree polynomial in variable $x = e^{i2\phi}$ whose coefficients A_ℓ are given in appendix. By rooting this polynomial numerically, fourteen complex values $\overline{x}_k$ are extracted. Now, we should choose the optimum solution $\overline{x}^{(o)}$ among all possible $\overline{x}_k$s that minimizes the cost function (6). Since the equation (6) is a function of t, we should first calculate the corresponding value t_k for each $\overline{x}_k$ in order to choose the best solution. To this end, we do the following computations.

By using the values $\overline{x}_k$, the corresponding values $\hat{\phi}_k$ can be computed as follows:

$$\hat{\phi}_k = \frac{\text{angle}\{\overline{x}_k\}}{2}, 1 \le k \le 14 \qquad (8)$$

Afterwards for each $\hat{\phi}_k$, two corresponding values $\hat{\rho}_k^{(+)}$ and $\hat{\rho}_k^{(-)}$ are calculated by rooting the second degree polynomial $\frac{\partial \Delta\psi(\rho,\hat{\phi}_k)}{\partial \hat{\phi}_k}$ in variable ρ:

$$\hat{\rho}_k^{(+/-)} = \frac{-Re\{b_1 e^{i2\hat{\phi}_k}\} \pm \sqrt{\left(Re\{b_1 e^{i2\hat{\phi}_k}\}\right)^2 - 4Re\{b_0 e^{i\hat{\phi}_k}\}Re\{b_2 e^{i\hat{\phi}_k}\}}}{2Re\{b_0 e^{i\hat{\phi}_k}\}} \qquad (9)$$

where b_0, b_1 and b_2 are given in appendix.

So, for each $\overline{x}_k$, two couples $(\hat{\phi}_k, \hat{\rho}_k^{(+)})$ and $(\hat{\phi}_k, \hat{\rho}_k^{(-)})$ are obtained. Then, for each couple $(\hat{\phi}_k, \hat{\rho}_k^{(+/-)})$, $\hat{t}_k^{(+/-)}$ is calculated as follows:

$$\hat{t}_k^{(+/-)} = \hat{\rho}_k^{(+/-)} e^{i\hat{\phi}_k} \qquad (10)$$

To select the optimum solution $t^{(o)}$, the cost function (6) is computed for the twenty-eight values $\hat{t}_k^{(+/-)}$ and the argument of the minimum of (6) that makes it negative (to ensure that the cost function (2) is reduced in each step) is chosen as follows:

$$t^{(o)} = \arg\min_{\hat{t}_k^{(+/-)}} \Delta\psi(\boldsymbol{\Theta}_{q,p}) \qquad (11)$$

By using the selected $t^{(o)}$, $\boldsymbol{\Theta}^{(o,p,q)}$ is computed and the matrices $\boldsymbol{Y}^{(r)}$ are updated using (5).

2.2. Canonical polyadic decomposition

Let $\circ$ be the outer product operator [20], the CP decomposition of a q-th order complex-valued array $\boldsymbol{\mathcal{T}}$ of size $(N_1 \times N_2 \times \ldots \times N_q)$ is defined by the following minimal linear combination:

$$\boldsymbol{\mathcal{T}} = \sum_{p=1}^{P} \boldsymbol{u}_p^{(1)} \circ \boldsymbol{u}_p^{(2)} \circ \cdots \circ \boldsymbol{u}_p^{(q)} \qquad (12)$$

where for each integer $i \in \{1, ..., q\}$ the P complex-valued vectors $\boldsymbol{u}_p^{(i)}$ are the column vectors of a $(N_i \times P)$ matrix $\boldsymbol{U}^{(i)}$ called loading matrix. The aim of the CP problem is to determine the q loading matrices $\boldsymbol{U}^{(i)}$ of $\boldsymbol{\mathcal{T}}$ up to a diagonal scaling matrix and a permutation which are the classical indeterminacies of the CP decomposition.

Generally, people prefer handle unfolding matrices of multi-way arrays. All possible matricizations of a q-way array $\boldsymbol{\mathcal{T}}$ can be defined by using two parameters, a permutation function π and an integer $L \in \{1, \ldots, q\}$:

$$T(\pi, L)_{k,\ell} = \mathcal{T}_{n_1, n_2, \ldots, n_q} \qquad (13)$$

$$k = n_{\pi(1)} + \sum_{j=2}^{L} (n_{\pi(j)} - 1) N^{(\pi(1), \pi(2), \ldots, \pi(j-1))}$$

$$\ell = n_{\pi(L+1)} + \sum_{j=L+2}^{q} (n_{\pi(j)} - 1) N^{(\pi(L+1), \pi(L+2), \ldots, \pi(j-1))}$$

with $N^{(a_1, \ldots, a_K)} = N_{a_1} N_{a_2} \ldots N_{a_K}$. In the proposed algorithm, we use two different unfolding matrices, namely $\boldsymbol{T}^{(1)} = \boldsymbol{T}(\pi, L_1)$ and $\boldsymbol{T}^{(2)} = \boldsymbol{T}(\pi, L_2)$, where the permutation matrix π, the constants L_1 and L_2 ($L_1 < L_2$) are defined in such a way that the smallest value of the three values $N^{(\pi(1), \pi(2), \ldots, \pi(L_1))}$, $N^{(\pi(L_1+1), \pi(L_1+2), \ldots, \pi(L_2))}$ and $N^{(\pi(L_2+1), \pi(L_2+2), \ldots, \pi(q))}$, which is an upper bound of P, is the largest among all possible triples (π, L_1, L_2). Indeed, our purpose is to propose an algorithm able to compute a CP decomposition with the maximal rank P. For the sake of simplicity, we assume in the following that π is the identity permutation.
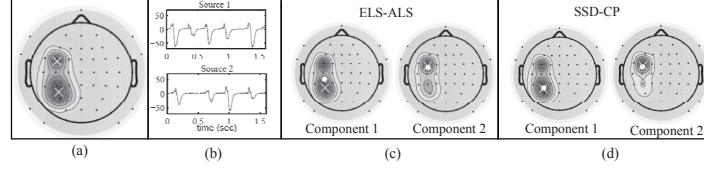
Fig. 1. An example of the localization process: (a) the location of two epileptic sources and the average potential distribution on the scalp, (b) the epileptic activity in the dipole sources of part (a), (c) the extracted components by using the ELS-ALS algorithm, (d) the extracted components by using the proposed algorithm. White crosses and white points represent the original and the estimated dipole locations respectively.

Then, it can be easily shown that $\boldsymbol{T}^{(1)} = \widetilde{\boldsymbol{U}}^{(L_1:1)} \widetilde{\boldsymbol{U}}^{(q:L_1+1)^\mathsf{T}}$ with $\widetilde{\boldsymbol{U}}^{(k:l)} = \boldsymbol{U}^{(k)} \odot \boldsymbol{U}^{(k-1)} \odot \ldots \odot \boldsymbol{U}^{(l)}$ where $\odot$ denotes the Khatri-Rao product operator. Note that the $\widetilde{\boldsymbol{U}}^{(q:L_1+1)}$ matrix can also be written as follows:

$$\widetilde{\boldsymbol{U}}^{(q:L_1+1)^\mathsf{T}} = \left(\widetilde{\boldsymbol{U}}^{(q:L_2+1)} \odot \widetilde{\boldsymbol{U}}^{(L_2:L_1+1)}\right)^\mathsf{T}$$
$$= \left[\Phi^{(1)}\widetilde{\boldsymbol{U}}^{(L_2:L_1+1)^\mathsf{T}}, \ldots, \Phi^{(N^*)}\widetilde{\boldsymbol{U}}^{(L_2:L_1+1)^\mathsf{T}}\right] \quad (14)$$

with $N^* = N^{(L_2+1,\ldots,q)}$ and where $\Phi^{(i)}$ is a $(P \times P)$ diagonal matrix for which diagonal is equal to the elements of the i-th row of $\widetilde{\boldsymbol{U}}^{(q:L_2+1)}$. By comparing the SVD $\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^\mathsf{H}$ of $\boldsymbol{T}^{(1)}$ truncated at order P with the previous factorized expression of $\boldsymbol{T}^{(1)}$, we conclude that it exists a $(P \times P)$ non-singular matrix $\boldsymbol{W}$ such that:

$$\boldsymbol{V}^\mathsf{H} = \boldsymbol{W}\widehat{\boldsymbol{U}}^{(q:L_1+1)^\mathsf{T}} \quad (15)$$

Now by inserting (14) into (15), we can rewrite $\boldsymbol{V}^\mathsf{H}$ as follows:

$$\boldsymbol{V}^\mathsf{H} = \left[\boldsymbol{W}\Phi^{(1)}\widetilde{\boldsymbol{U}}^{(L_2:L_1+1)^\mathsf{T}}, \ldots, \boldsymbol{W}\Phi^{(N^*)}\widetilde{\boldsymbol{U}}^{(L_2:L_1+1)^\mathsf{T}}\right] \quad (16)$$

Now let's define the N^* matrices $\boldsymbol{\Gamma}^{(i)}$ of size $(P \times N^{(L_1+1,\ldots,L_2)})$ by $\boldsymbol{\Gamma}^{(i)} = \boldsymbol{W}\Phi^{(i)}\widetilde{\boldsymbol{U}}^{(L_2:L_1+1)^\mathsf{T}}$. By assuming that each matrix $\boldsymbol{\Gamma}^{(i)}$ is full row rank, all matrices $\boldsymbol{\Gamma}^{(i)}$ admit a Moore-Penrose matrix inverse $\boldsymbol{\Gamma}^{(i)\sharp}$. So, we define $N^{*2} - N^*$ matrices $\boldsymbol{Y}^{(i,j)}$ by $\boldsymbol{Y}^{(i,j)} = \boldsymbol{\Gamma}^{(i)}\boldsymbol{\Gamma}^{(j)\sharp}$. It can be shown that $\boldsymbol{Y}^{(i,j)} = \boldsymbol{W}\boldsymbol{D}^{(i,j)}\boldsymbol{W}^{-1}$ where, for each couple (i, j), $\boldsymbol{D}^{(i,j)} = \Phi^{(i)}\Phi^{(j)\sharp}$ is a diagonal matrix. Thus, let us write $\boldsymbol{W} = \boldsymbol{Q}\boldsymbol{R}$, namely the QR decomposition of matrix $\boldsymbol{W}$ where $\boldsymbol{Q}\boldsymbol{Q}^\mathsf{H} = \boldsymbol{I}$ and $\boldsymbol{R}$ is an upper triangular matrix. Then we can rewrite $\boldsymbol{Y}^{(i,j)}$ as follows:

$$\boldsymbol{Y}^{(i,j)} = \boldsymbol{Q}\boldsymbol{R}\boldsymbol{D}^{(i,j)}\boldsymbol{R}^{-1}\boldsymbol{Q}^{-1} = \boldsymbol{Q}\boldsymbol{X}^{(i,j)}\boldsymbol{Q}^\mathsf{H} \quad (17)$$

where the matrices $\boldsymbol{X}^{(i,j)} = \boldsymbol{R}\boldsymbol{D}^{(i,j)}\boldsymbol{R}^{-1}$ are upper triangular matrices. Since the elements on the diagonal of $\boldsymbol{X}^{(i,j)}$ are equal to the diagonal components of $\boldsymbol{D}^{(i,j)}$, by applying the proposed SSD algorithm to matrices $\boldsymbol{Y}^{(i,j)}$, the upper triangularized matrices $\boldsymbol{X}^{(i,j)}$ and consequently the diagonal matrices $\boldsymbol{D}^{(i,j)}$ are extracted. Now let's see how the components of $\widetilde{\boldsymbol{U}}^{(q:L_2+1)}$ can be identified from those of the matrices $\boldsymbol{D}^{(i,j)}$. Since $\boldsymbol{D}^{(i,j)} = \Phi^{(i)}\Phi^{(j)\sharp}$, for each column of $\widetilde{\boldsymbol{U}}^{(q:L_2+1)}$, we have $R = N^{*2} - N^*$ equations. If we define $\boldsymbol{U}^* = \widetilde{\boldsymbol{U}}^{(q:L_2+1)}$, for column p, we have:

$$\forall i, j, \; i \neq j, \quad \frac{U^*_{i,p}}{U^*_{j,p}} = D^{(i,j)}_{p,p} \Rightarrow U^*_{i,p} - D^{(i,j)}_{p,p}U^*_{j,p} = 0 \quad (18)$$

These equations can be written in a matrix form:

$$\boldsymbol{M}^{(p)}\boldsymbol{u}^*_p = \boldsymbol{0}_{R \times 1} \quad (19)$$

where $\boldsymbol{u}^*_p$ is the p-th column of matrix $\boldsymbol{U}^*$ and the matrix $\boldsymbol{M}^{(p)}$ of size $((N^{*2} - N^*) \times N^*)$ is defined as follows. For each ordered pair $\{(i, j), i \neq j, 1 \leq i, j \leq N^*\}$, we consider one row in matrix $\boldsymbol{M}^{(p)}$ such that the element in the i-th column is equal to 1, the element in the j-th column is equal to $-D^{(i,j)}_{p,p}$ and the other elements are 0. Note that the order of the rows are unimportant in the solution. It is also noteworthy that the system (19) has an infinite number of solutions due to the scaling indeterminacies of the CP decomposition. So we set the elements of the first row of $\boldsymbol{U}^* = \widetilde{\boldsymbol{U}}^{(q:L_2+1)}$ equal to one and then we extract the elements of the other rows from (19). Now, since we have $\boldsymbol{T}^{(2)} = \widetilde{\boldsymbol{U}}^{(L_2:1)} \widetilde{\boldsymbol{U}}^{(q:L_2+1)^\mathsf{T}}$, by assuming the full column rank of $\widetilde{\boldsymbol{U}}^{(q:L_2+1)}$, $\widetilde{\boldsymbol{U}}^{(L_2:1)}$ can be calculated as follows:

$$\widetilde{\boldsymbol{U}}^{(L_2:1)} = \boldsymbol{U}^{(L_2)} \odot \ldots \odot \boldsymbol{U}^{(1)} = \boldsymbol{T}^{(2)}(\pi, L_2)\left(\widetilde{\boldsymbol{U}}^{(q:L_2+1)^\mathsf{T}}\right)^\sharp \quad (20)$$

Next, the $(N_{L_2} \times \ldots \times N_1)$ rank-1 array $\widetilde{\boldsymbol{\mathcal{U}}}^{(L_2:1)}_p$ associated to the p-th column $\boldsymbol{u}^{(p)}$ of $\widetilde{\boldsymbol{U}}^{(L_2:1)}$ is generated as follows:

$$\widetilde{\mathcal{U}}^{(L_2:1)}_{p,i_{L_2},\ldots,i_2,i_1} = u^{(p)}_{i_{L_2}+\sum_{i=i_{L_2}-1}^{i_1}\left((i-1)N^{(L_2,\ldots,i+1)}\right)} \quad (21)$$

Then by computing a simple rank-1 HOSVD [21] of $\widetilde{\boldsymbol{\mathcal{U}}}^{(L_2:1)}_p$, the p-th columns of matrices $\boldsymbol{U}^{(1)}, \ldots, \boldsymbol{U}^{(L_2)}$ are extracted. The same procedure can be applied to the matrix $\widetilde{\boldsymbol{U}}^{(q:L_2+1)}$ to extract the other loading matrices $\boldsymbol{U}^{(j)}$ for $j \in \{L_2 + 1, \ldots, q\}$.

3. SIMULATIONS

3.1. Multiway analysis of amino acids fluorescence data

In this section, we examine the effect of overfactoring, say an overestimation of the array rank, on the performance of different CP methods. To this end, we use the Amino acids fluorescence data downloaded from [22] and described in [22], [23]. This data set comprises five simple laboratory-made samples. Each sample is composed of different amounts of tyrosine, tryptophan and phenylalanine dissolved in phosphate buffered water. The samples were measured by fluorescence on a PE LS50B spectrofluorometer with excitation slit-width of 2.5 nm, an emission slit-width of 10 nm and a scan-speed of 1500 nm/s [22]. Since each individual amino acid gives a rank-1 contribution to the data, ideally we can describe these data with three CP components [22]. We applied three classical CP methods, namely ALS [9], ELS-ALS [10], LM [10] and the SSD-CP method proposed in this paper, to canonically decompose the amino acids fluorescence data. Then we compared the emission-mode factors estimated by the four methods by varying the rank P of the CP decomposition from 3 to 5 as shown in Fig.2. Note that, regarding the three fully iterative methods, they are run several times with different random initial guess in order to use the best initialization.
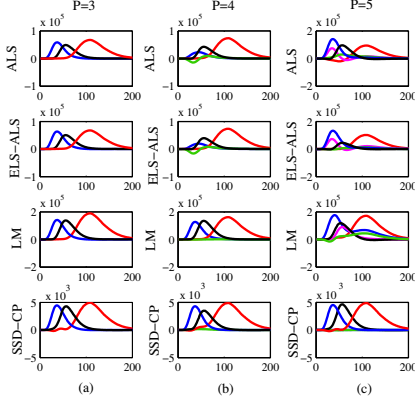
Fig. 2. The emission mode factors with the estimated number of components equal to (a) $P = 3$, (b) $P = 4$ and (c) $P = 5$

As displayed in Fig.2(a), for $P = 3$, all CP algorithms generate almost the same emission factors corresponding to three amino acids. As shown in Fig.2(b-c), in the case of $P = 4$ and $P = 5$, the factors obtained from the three iterative algorithms change, however the SSD-CP proposed technique generates three factors that match with the true factors while the forth and the fifth estimated factors are very small. These results show that SSD-CP is robust with respect to overfactoring.

3.2. Localization of Epileptic Sources

In this section, the efficiency of the proposed algorithm in extracting loading matrices of complex-valued arrays is studied in the context of the localization of epileptic electroencephalographic sources. A 3-shell spherical head model, two superficial, radically oriented dipole sources (with random positions) and the Jansen model [24] are considered to construct 64 channels of epileptic data [7]. Then, the STFT of these data is used to construct the HO array $\mathcal{T} \in \mathbb{C}^{N_1 \times N_2 \times N_3}$ where the three dimensions represent time, frequency and channel respectively. By using the CP algorithms, the location of the dipoles is estimated by extracting the corresponding factors. The efficiency of the proposed algorithm and the ELS-ALS algorithm to estimate the location of the sources is compared in 100 monte-carlo trials. In each trial, we calculate the Root Mean square Error (RMSE) [7] between the estimated and the original locations of the sources. Fig.1 (a) shows the location of two epileptic sources and the average potential distribution on the scalp while Fig.1 (b) displays the epileptic activity of these dipole sources. Fig.1 (c) and (d) show the original and the estimated locations of the sources by using the ELS-ALS algorithm [20] and the proposed algorithm, respectively. In this figure, white crosses and white points represent the original and the estimated dipole locations, respectively. The average localization errors of the proposed algorithm and the ELS-ALS algorithm are 2.53 and 2.78 cm, respectively.

4. CONCLUSION

In this paper, a new semi-algebraic SSD-based algorithm to compute the CP decomposition of multi-way complex-valued arrays was proposed. We also proposed a new Jacobi-like algorithm to calculate SSD of several complex-valued matrices. We compared the efficiency of the proposed algorithm with the ELS-ALS algorithm in the context of source localization. We show that the localization error of the proposed algorithm is lower than that of the ELS-ALS algorithm and conclude that our algorithm can be used in the source localization context. We also show that the proposed method is robust with respect to the overestimation of the number of factors.

5. APPENDIX

To calculate the values of coefficients A_ℓ, first we define the values v_1 to v_{10}, u_1 to u_3 and w_1 to w_3 as functions of elements of matrices $\boldsymbol{Y}^{(r)}$, $1 \leq r \leq R$ as follows:

$$v_1 = \sum_{r=1}^{R} |Y_{p,p}^{(r)}|^2, \quad v_2 = \sum_{r=1}^{R} Y_{p,p}^{(r)} Y_{p,q}^{(r)*}, \quad v_3 = \sum_{r=1}^{R} Y_{p,p}^{(r)} Y_{q,p}^{(r)*}$$

$$v_4 = \sum_{r=1}^{R} Y_{p,p}^{(r)} Y_{q,q}^{(r)*}, \quad v_5 = \sum_{r=1}^{R} Y_{p,q}^{(r)} Y_{q,q}^{(r)*}, \quad v_6 = \sum_{r=1}^{R} |Y_{p,q}^{(r)}|^2$$

$$v_7 = \sum_{r=1}^{R} Y_{p,q}^{(r)} Y_{q,p}^{(r)*}, \quad v_8 = \sum_{r=1}^{R} |Y_{q,p}^{(r)}|^2, \quad v_9 = \sum_{r=1}^{R} Y_{q,p}^{(r)} Y_{q,q}^{(r)*}$$

$$v_{10} = \sum_{r=1}^{R} |Y_{q,q}^{(r)}|^2, \quad u_1 = \sum_{r=1}^{R} \sum_{k=p+1}^{q-1} |Y_{kp}^{(r)}|^2, \quad w_1 = \sum_{r=1}^{R} \sum_{k=p+1}^{q-1} |Y_{qk}^{(r)}|^2$$

$$u_2 = \sum_{r=1}^{R} \sum_{k=p+1}^{q-1} Y_{kp}^{(r)} Y_{kq}^{(r)*}, \quad w_2 = \sum_{r=1}^{R} \sum_{k=p+1}^{q-1} Y_{qk}^{(r)} Y_{pk}^{(r)*}$$

$$u_3 = \sum_{r=1}^{R} \sum_{k=p+1}^{q-1} |Y_{kq}^{(r)}|^2, \quad w_3 = \sum_{r=1}^{R} \sum_{k=p+1}^{q-1} |Y_{pk}^{(r)}|^2 \tag{22}$$

Then we define $b_0 - b_4$, $c_0 - c_4$, $t_0 - t_7$ and $s_0 - s_5$ as follows:

$$b_0 = j(v_5^* - v_2 - u_2 + w_2), \quad b_1 = -j2v_7^*, \quad b_2 = j(v_3^* - v_9 - v_2 + w_2)$$
$$b_3 = -2v_1 + 4v_6 + 4\mathrm{Re}\{v_4\} - 2v_{10} + 2u_3 - 2u_1 + 2w_3 - 2w_1$$
$$b_4 = 2v_1 - 4\mathrm{Re}\{v_4\} - 4v_8 + 2v_{10} + 2u_3 - 2u_1 + 2w_3 - 2w_1 \tag{23}$$
$$c_0 = c_4^* = b_1^2, \quad c_1 = c_3^* = -4b_2 b_0^*, \quad c_2 = 2|b_1|^2 - 8\mathrm{Re}\{b_2 b_0^*\} \tag{24}$$

$$t_0 = t_7^* = 2jb_2^* b_1^{*2} b_0^{*2} - 2jb_0 b_1^{*4} - 2jb_1^{*2} b_0^{*3} + b_3 b_1^{*3} b_0^* \tag{25}$$
$$t_1 = t_6^* = -4jb_2^* b_0^{*3} + 4jb_2^* b_0^{*4} - 4jb_2 b_1^{*2} b_0^{*2} + b_0 b_3 b_1^{*3}$$
$$\quad + 2jb_1 b_1^{*3} b_0^* + b_4 b_1^* b_0^{*3} + 12jb_0 b_2^* b_1^{*2} b_0^* - 3b_3 b_2^* b_1^* b_0^{*2}$$
$$t_2 = t_5^* = 10jb_0^2 b_2^* b_1^{*2} - 16jb_0 b_2^{*2} b_0^{*2} + 6jb_0^2 b_1^{*2} b_0^* - 6jb_1 b_0 b_1^{*3}$$
$$\quad + 8jb_2 b_0^{*4} + 4jb_2 b_2^* b_0^{*3} + 4jb_0 b_2^* b_0^{*3} - 6jb_1 b_1^* b_0^{*3} + 3b_1 b_3 b_1^{*2} b_0^*$$
$$\quad - 2jb_1 b_2^* b_1^* b_0^{*2} - 3b_2 b_3 b_1^* b_0^{*2} + 3b_0 b_4 b_1^* b_0^{*2} - 6b_0 b_3 b_2^* b_1^* b_0^*$$
$$t_3 = t_4^* = 8jb_2^* b_0^{*3} + 4jb_0^3 b_1^{*2} - 12jb_0^2 b_2^* b_0^{*2} - 20jb_0^2 b_2^* b_0^*$$
$$\quad + 6jb_1^2 b_1^{*2} b_0^* + 20jb_2 b_0 b_0^{*3} + b_1 b_4 b_0^{*3} + 4jb_2 b_0 b_1^{*2} - 3b_0^2 b_3 b_2^* b_1^*$$
$$\quad + 3b_1 b_0 b_3 b_1^{*2} + 4jb_2 b_0 b_2^* b_0^{*2} - 14jb_2 b_1 b_1^* b_0^{*2} - 6b_2 b_0 b_3 b_1^* b_0^*$$
$$\quad - 6jb_1 b_0 b_1^* b_0^{*2} - 3b_1 b_3 b_2^* b_0^{*2} + 3b_0^2 b_4 b_1^* b_0^* + 12jb_1 b_0 b_2^* b_1^* b_0^*$$

$$s_0 = s_5^* = -2jb_0 b_1^{*3} - 2jb_1^* b_0^{*3} + b_3 b_1^{*2} b_0^* + 2jb_2^* b_1^* b_0^{*2} \tag{26}$$
$$s_1 = s_4^* = b_4 b_0^{*3} + b_0 b_3 b_1^{*2} - 4jb_2 b_1^* b_0^{*2} + 2jb_1 b_1^{*2} b_0^*$$
$$\quad - b_3 b_2^* b_0^{*2} + 8jb_0 b_2^* b_1^* b_0^*$$
$$s_2 = s_3^* = -4jb_1 b_0^{*3} - 4jb_1 b_0 b_1^{*2} - b_2 b_3 b_0^{*2} + 3b_0 b_4 b_0^{*2} - 2b_0 b_3 b_2^* b_0^*$$
$$\quad + 6jb_0^2 b_2^* b_1^* + 6jb_0^2 b_0^* b_1^* b_0^* - 4jb_2 b_0 b_1^* b_0^* + 2b_1 b_3 b_1^* b_0^*$$

Finally, we can calculate the fifteen coefficients A_ℓ according to the predefined parameters:

$$A_\ell = \sum_{k=\max(0,\ell-7)}^{\min(7,\ell)} t_k t_{\ell-k} - \sum_{i=\max(0,\ell-9)}^{\min(5,\ell)} \sum_{j=\max(0,\ell-9,\ell-i-4)}^{\min(5,\ell-i)} s_i s_j c_{\ell-i-j}$$

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