Blind Identification of Underdetermined Mixtures by Simultaneous Matrix Diagonalization

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***Abstract*—In this paper, we study simultaneous matrix diagonalization-based techniques for the estimation of the mixing matrix in underdetermined independent component analysis (ICA). This includes a generalization to underdetermined mixtures of the well-known SOBI algorithm. The problem is reformulated in terms of the parallel factor decomposition (PARAFAC) of a higher-order tensor. We present conditions under which the mixing matrix is unique and discuss several algorithms for its computation.**

***Index Terms*—Canonical decomposition, higher order tensor, independent component analysis (ICA), parallel factor (PARAFAC) analysis, simultaneous diagonalization, underdetermined mixture.**

I. Introduction

CONSIDER the following basic linear mixture model:

$$\mathbf{x}_t = \mathbf{A}\mathbf{s}_t + \mathbf{n}_t. \tag{1}$$

The stochastic vector $\mathbf{x}_t \in \mathbb{C}^J(\mathbb{R}^J)$ represents multichannel observations, the components of the stochastic vector $\mathbf{s}_t \in \mathbb{C}^R(\mathbb{R}^R)$ correspond to unobserved source signals, and $\mathbf{n}_t \in \mathbb{C}^J(\mathbb{R}^J)$ denotes additive noise. The *a priori* unknown mixing matrix $\mathbf{A} \in \mathbb{C}^{J\times R}(\mathbb{R}^{J\times R})$ characterizes the way the sources are combined in the observations. The goal of independent component analysis (ICA) [12], [37], or blind source separation (BSS), consists of the estimation of the source signals and/or the mixing matrix from observations of $\mathbf{x}_t$, assuming that the sources are statistically independent. The literature on ICA addresses for the most part the so-called *overdetermined* case, where $J \geqslant R$. Here, we consider the *underdetermined* or *overcomplete* case, where $J < R$.

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A large class of algorithms for underdetermined ICA starts from the assumption that the sources are (quite) sparse [5], [27], [32], [42], [63]. In this case, the scatter plot typically shows high signal values in the directions of the mixing vectors. These extrema may be localized by maximization of some clustering measure [5], [27], [63]. Some of the clustering-based techniques perform an exhaustive search in the mixing vector space, and are therefore very expensive when there are more than two observation channels. In a preprocessing step, a linear transform may be applied such that the new representation of the data is sparser (e.g., short-time Fourier transform in the case of audio signals) [5]. The method in [1] only requires that for each source one area in the time-frequency plane can be found where only that particular source is active; the signals may overlap anywhere else. In [24], the difference between long-time stationary sources and sources that are only short-time stationary is exploited to separate the latter.

There are two aspects to ICA: estimation of the mixing matrix and separation of the sources. In the overdetermined case, sources are usually separated by multiplying the observations with the pseudoinverse of the mixing matrix estimate. This is no longer possible in the case of underdetermined mixtures: for each sample $\mathbf{x}_t$, the corresponding source sample $\mathbf{s}_t$ that satisfies $\mathbf{x}_t = \mathbf{A}\mathbf{s}_t$ is only known to belong to an affine variety of dimension $R - J$—hence the term "underdetermined." However, the mixing matrix and the source densities are still unique under mildly restrictive conditions [28]. Uniqueness of the source distributions allows for the joint estimation of sources and mixing matrix in a probabilistic framework [43]. However, even in the case of underdetermined mixtures, the estimation of the mixing matrix is an overdetermined problem, such that it makes sense to estimate the mixing matrix first, and then estimate the sources. The source values $\mathbf{s}_t$ may subsequently be estimated by maximizing the log posterior likelihood [43]. In the case of sparse sources, characterized by Laplacian densities, this can be formulated in terms of a linear programming problem [5], [9], [42]. If at most $J - 1$ sources can be active at the same time, then for each sample, the active mixing vectors may be determined and the corresponding mixture inverted [32]. In the case of finite alphabet signals in telecommunication, one may perform an exhaustive search over all possible combinations. In this paper we focus on the estimation of the mixing matrix. The estimate of the mixing matrix may subsequently be used to separate the sources by means of the techniques mentioned earlier.

This paper presents new contributions to the class of algebraic algorithms for underdetermined ICA. In [14], [16], and [17], algorithms are derived for the specific case of two mixtures and three sources. An arbitrary number of mixing vectors

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can be estimated from two observation channels by sampling derivatives of sufficiently high order of the second characteristic function [62]. A more stable version of [62] is presented in [15]. Algebraic underdetermined ICA is based on the decomposition of a higher order tensor in a sum of rank-1 terms. Some links with the literature on homogeneous polynomials are discussed in [13]. A simultaneous matrix diagonalization technique that may still be used when the number of sources exceeds the number of sensors, is presented in [69]. In [21], the algebraic structure of the fourth-order cumulant tensor is exploited. On the other hand, the algebraic structure of the sixth-order cumulant tensor is partially exploited in [2]. A similar idea can be applied to a set of fourth-order cumulant tensors, corresponding to different time lags, when the individual source signals are dependent over some time interval [31].

In this paper, we assume that the sources are individually correlated in time. The spatial covariance matrices of the observations then satisfy [3]

$$\begin{aligned} \mathbf{C}_1 &\stackrel{\text{def}}{=} E\left\{\mathbf{x}_t \mathbf{x}_{t+\tau_1}^H\right\} = \mathbf{A}\cdot\mathbf{D}_1\cdot\mathbf{A}^H \\ &\vdots \\ \mathbf{C}_K &\stackrel{\text{def}}{=} E\left\{\mathbf{x}_t \mathbf{x}_{t+\tau_K}^H\right\} = \mathbf{A}\cdot\mathbf{D}_K\cdot\mathbf{A}^H \end{aligned} \tag{2}$$

in which $\mathbf{D}_k \stackrel{\text{def}}{=} E\{\mathbf{s}_t \mathbf{s}_{t+\tau_k}^H\}$ is diagonal, $k = 1, \ldots, K$. One of the delays τ_k can be equal to zero. For simplicity, we have dropped the noise terms; they can be considered as a perturbation of (2). The problem we want to solve is the estimation of $\mathbf{A}$ from the set $\{\mathbf{C}_k\}$, in the case $J < R$. This is the underdetermined version of the SOBI problem [3]. The solution will obtained by interpreting (2) as a tensor decomposition.

Stack the matrices $\mathbf{C}_1, \ldots, \mathbf{C}_K$ in a tensor $\mathcal{C} \in \mathbb{C}^{J\times J\times K}$ as follows: $(\mathcal{C})_{ijk} \stackrel{\text{def}}{=} (\mathbf{C}_k)_{ij}$, $i = 1, \ldots, J, j = 1, \ldots, J, k = 1, \ldots, K$. Define a matrix $\mathbf{D} \in \mathbb{C}^{K\times R}$ by $(\mathbf{D})_{kr} \stackrel{\text{def}}{=} (\mathbf{D}_k)_{rr}$, $k = 1, \ldots, K$, $r = 1, \ldots, R$. Then, we have

$$c_{ijk} = \sum_{r=1}^{R} a_{ir} a_{jr}^* d_{kr} \tag{3}$$

which we write as

$$\mathcal{C} = \sum_{r=1}^{R} \mathbf{a}_r \circ \mathbf{a}_r^* \circ \mathbf{d}_r \tag{4}$$

in which $\circ$ denotes the tensor outer product and in which $\{\mathbf{a}_r\}$ and $\{\mathbf{d}_r\}$ are the columns of $\mathbf{A}$ and $\mathbf{D}$, respectively.

Stack the entries of tensor $\mathcal{C}$ in matrices $\mathbf{C} \in \mathbb{C}^{J^2\times K}$, $\bar{\mathbf{C}} \in \mathbb{C}^{KJ\times J}$, $\bar{\bar{\mathbf{C}}} \in \mathbb{C}^{JK\times J}$ as follows:

$$(\mathbf{C})_{(i-1)J+j,k} = (\bar{\mathbf{C}})_{(k-1)K+i,j} = (\bar{\bar{\mathbf{C}}})_{(j-1)J+k,i} = c_{ijk}, \quad i = 1, \ldots, J, j = 1, \ldots, J, k = 1, \ldots K.$$

Then, (4) can be written in a matrix format as

$$\mathbf{C} = (\mathbf{A}\odot\mathbf{A}^*)\cdot\mathbf{D}^T \tag{5}$$

$$\bar{\mathbf{C}} = (\mathbf{D}\odot\mathbf{A})\cdot\mathbf{A}^H \tag{6}$$

$$\bar{\bar{\mathbf{C}}} = (\mathbf{A}^*\odot\mathbf{D})\cdot\mathbf{A}^T \tag{7}$$

in which $\odot$ denotes the Khatri–Rao product (for a definition, see the end of this section).

Equation (4) is a decomposition of tensor $\mathcal{C}$ in a sum of R rank-1 terms. It is a constrained version of a so-called "canonical decomposition" (CANDECOMP) [8] or "parallel factors model" (PARAFAC) [34]. The minimal number of rank-1 tensors in which a higher order tensor can be decomposed, is called its rank. Note that each rank-1 term in (4) consists of the contribution of one distinct source to $\mathcal{C}$. Hence, in terms of this tensor, "mixture identification" amounts to the computation of decomposition (4), provided it is unique. In contrast to the matrix case, PARAFAC can be unique (up to some trivial indeterminacies) even when i) the rank-1 terms are not mutually orthogonal and ii) the rank is greater than the smallest tensor dimension. This allows for the determination of the mixing matrix (up to a scaling and permutation of its columns) in the overcomplete case.

Although our formulation is in terms of spatial covariance matrices for different time lags, our results apply to any ICA technique that is based on a simultaneous matrix diagonalization like (2). An example is the algorithm proposed in [47] for the separation of non-stationary sources subject to a constant mixing, where the matrices $\{\mathbf{C}_k\}$ correspond to spatial covariance matrices measured at different time instances. In [4] the matrices $\{\mathbf{C}_k\}$ are observed spatial time-frequency distributions. In [68], one works with Hessian matrices of the second characteristic function of the observations, sampled at different working points.

The paper is organized as follows. PARAFAC and its uniqueness properties are discussed in Section II. Sections III and IV present algorithms for the computation of decomposition (4). Section III deals with algorithms that can be applied when $R > K$. More powerful results are obtained for the case where $R \leqslant K$ in Section IV. Section V shows the results of some simulations. Section VI is the conclusion. The presentation is in terms of complex signals. Whenever the results cannot be directly applied to real data, this will be explicitly mentioned.

A short version of this manuscript appeared as the conference paper [22]. The foundations of Section IV were laid in [7]. Some mathematical aspects are developed in more detail in [20].

Notation: Scalars are denoted by lower-case italic letters $(a, b, \ldots)$, vectors by lower-case boldface letters $(\mathbf{a}, \mathbf{b}, \ldots)$, matrices by boldface capitals $(\mathbf{A}, \mathbf{B}, \ldots)$ and tensors by calligraphic letters $(\mathcal{A}, \mathcal{B}, \ldots)$. Italic capitals are used to denote index upper bounds $(i = 1, 2, \ldots, I)$. The entry with row index i and column index j in a matrix $\mathbf{A}$, i.e., $(\mathbf{A})_{ij}$, is symbolized by a_{ij}. Likewise, we have $(\mathcal{A})_{ijk} = a_{ijk}$. The columns of $\mathbf{A}$ are denoted by $\mathbf{a}_1, \mathbf{a}_2, \ldots$. Conversely, the matrix with columns $\mathbf{a}_1, \mathbf{a}_2, \ldots$ is denoted by $\mathbf{A}$. The superscripts $\cdot^T$, $\cdot^*$ and $\cdot^H$ denote the transpose, the complex conjugate, and the complex conjugated transpose, respectively. We will often stack $(I \times J)$ matrices in IJ-dimensional vectors

$$\mathbf{m} = \text{vec}(\mathbf{M}) \Leftrightarrow (\mathbf{m})_{(i-1)J+j} = (\mathbf{M})_{ij}.$$

The inverse of this operation is denoted by $\mathbf{M} = \text{unvec}(\mathbf{m})$. Vectorization of an $(I \times J \times K \times L)$ tensor is done as follows:

$$\mathbf{m} = \text{vec}(\mathcal{M}) \Leftrightarrow (\mathbf{m})_{(i-1)JKL+(j-1)KL+(k-1)L+l} = (\mathcal{M})_{ijkl}.$$

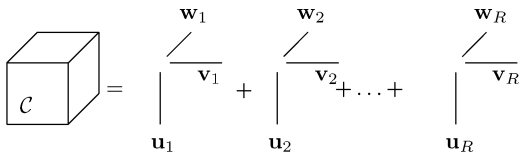

Fig. 1. Visualization of third-order PARAFAC.

The symbol δ_{ij} stands for the Kronecker delta, i.e., $\delta_{ij} = 1$ if $i = j$ and 0 otherwise. The identity matrix is denoted by $\mathbf{I}$. Finally, we recall the definition of the Kronecker product $\otimes$ and the Khatri–Rao product $\odot$ [50]

$$\mathbf{A} \otimes \mathbf{H} \stackrel{\text{def}}{=} \begin{pmatrix} a_{11}\mathbf{H} & a_{12}\mathbf{H} & \cdots \\ a_{21}\mathbf{H} & a_{22}\mathbf{H} & \cdots \\ \vdots & \vdots & \end{pmatrix}$$

$$\mathbf{A} \odot \mathbf{H} \stackrel{\text{def}}{=} (\mathbf{a}_1 \otimes \mathbf{h}_1 \quad \mathbf{a}_2 \otimes \mathbf{h}_2 \quad \cdots).$$

II. Parallel Factor Analysis

We have the following definitions.

Definition 1: The *outer product* of three vectors $\mathbf{u} \in \mathbb{C}^I$, $\mathbf{v} \in \mathbb{C}^J$, $\mathbf{w} \in \mathbb{C}^K$, is the tensor $\mathcal{C} \in \mathbb{C}^{I \times J \times K}$ defined by

$$c_{ijk} = u_i v_j w_k \quad i = 1, \ldots, I, j = 1, \ldots, J, k = 1, \ldots, K.$$

The outer product of $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$ is denoted by $\mathbf{u} \circ \mathbf{v} \circ \mathbf{w}$.

Definition 2: A tensor $\mathcal{C} \in \mathbb{C}^{I \times J \times K}$ has *rank 1* if it equals the outer product of three vectors $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$.

Definition 3: The *rank* of a tensor $\mathcal{C}$ is the minimal number of rank-1 tensors that yield $\mathcal{C}$ in a linear combination.

Definition 4: A *Canonical* or *Parallel Factor Decomposition* of a tensor $\mathcal{C} \in \mathbb{C}^{I \times J \times K}$ is a decomposition of $\mathcal{C}$ as a linear combination of a minimal number of rank-1 terms:

$$\mathcal{C} = \sum_{r=1}^{R} \mathbf{u}_r \circ \mathbf{v}_r \circ \mathbf{w}_r. \tag{8}$$

The decomposition is visualized for third-order tensors in Fig. 1.

The fully symmetric variant in which $\mathbf{u}_r = \mathbf{v}_r = \mathbf{w}_r$, $r = 1, \ldots, R$, was already studied in the Nineteenth Century in the context of invariant theory [13]. The unsymmetric decomposition was introduced by Hitchcock in 1927 [35], [36]. Around 1970, it was independently reintroduced in psychometrics [8] and phonetics [34]. Later on, the decomposition was also applied in chemometrics and food industry [57]. In these various disciplines PARAFAC is used for the purpose of multiway factor analysis. The term "canonical decomposition" is standard in psychometrics, while in chemometrics the decomposition is called a "parallel factors model." Recently, PARAFAC has found important applications in signal processing. In wireless communications, it provides powerful means for the exploitation of different types of diversity [53], [54], [56]. It also describes the basic tensor structure on which all algebraic ICA methods are (implicitly) based [12], [18], [37]. Moreover, PARAFAC is intimately linked with the harmonic analysis problem [38], [55].

To a large extent, the practical importance of PARAFAC stems from its uniqueness properties. It is clear that PARAFAC can only be unique up to permutation of the rank-1 terms and scaling and counterscaling of the factors of the rank-1 terms. We call the unsymmetric decomposition in (8) essentially unique if any other matrix triplet $(\mathbf{U}', \mathbf{V}', \mathbf{W}')$ that satisfies (8) is related to $(\mathbf{U}, \mathbf{V}, \mathbf{W})$ via

$$\mathbf{U} = \mathbf{U}' \cdot \mathbf{P} \cdot \mathbf{\Omega}_1, \quad \mathbf{V} = \mathbf{V}' \cdot \mathbf{P} \cdot \mathbf{\Omega}_2, \quad \mathbf{W} = \mathbf{W}' \cdot \mathbf{P} \cdot \mathbf{\Omega}_3 \tag{9}$$

with $\mathbf{\Omega}_1, \mathbf{\Omega}_2, \mathbf{\Omega}_3 \in \mathbb{C}^{R \times R}$ diagonal matrices, satisfying $\mathbf{\Omega}_1 \cdot \mathbf{\Omega}_2 \cdot \mathbf{\Omega}_3 = \mathbf{I}$, and $\mathbf{P} \in \mathbb{R}^{R \times R}$ a permutation matrix. Likewise, we call the constrained decomposition (4) essentially unique if any other matrix pair $\mathbf{A}'$ and $\mathbf{D}'$ that satisfies (4) is related to $\mathbf{A}$ and $\mathbf{D}$ via

$$\mathbf{A} = \mathbf{A}' \cdot \mathbf{P} \cdot \mathbf{\Omega}_1, \quad \mathbf{D} = \mathbf{D}' \cdot \mathbf{P} \cdot \mathbf{\Omega}_2 \tag{10}$$

with $\mathbf{\Omega}_1, \mathbf{\Omega}_2 \in \mathbb{C}^{R \times R}$ diagonal matrices, satisfying $\mathbf{\Omega}_1 \cdot \mathbf{\Omega}_1^* \cdot \mathbf{\Omega}_2 = \mathbf{I}$, and $\mathbf{P} \in \mathbb{R}^{R \times R}$ a permutation matrix.

A first uniqueness result requires the notion of Kruskal-rank of a matrix [40].

Definition 5: The *Kruskal rank* or *k-rank* of a matrix $\mathbf{A}$, denoted by $k_{\mathbf{A}}$, is the maximal number r such that any set of r columns of $\mathbf{A}$ is linearly independent.

Example 1: Consider the matrix

$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 4 \\ 2 & 1 & 2 \end{pmatrix}$$

which has rank 2. The k-rank of $\mathbf{A}$ is 1, because its last two columns are proportional.

The following theorem establishes a condition under which essential uniqueness is guaranteed [39], [40], [53], [59].

Theorem 1: The PARAFAC decomposition (8) is essentially unique if

$$k_{\mathbf{U}} + k_{\mathbf{V}} + k_{\mathbf{W}} \geqslant 2R + 2. \tag{11}$$

From (11), we have immediately that decomposition (4) is essentially unique when

$$2k_{\mathbf{A}} + k_{\mathbf{D}} \geqslant 2(R + 1). \tag{12}$$

We call a property generic when it holds with probability one when the parameters it involves are drawn from continuous probability densities. Generically, a matrix is full rank and full k-rank. Hence, in practice, $k_{\mathbf{A}} = \min(J, R) = J$ and $k_{\mathbf{D}} = \min(K, R)$. Equation (12) then guarantees identifiability when the number of sources is bounded as follows:

$$R \leqslant J - 1 + K/2 \qquad \text{if} \quad R \geqslant K \tag{13}$$

$$R \leqslant 2J - 2 \qquad \text{if} \quad R \leqslant K. \tag{14}$$

These conditions are sufficient for essential uniqueness but not always necessary. They hold both in the real and the complex case.

Remark 1: It is well-known that in the SOBI algorithm for overdetermined mixtures the sources all need to have a different spectrum [3]. This constraint is also implicit in the bounds above. Assume that sources r and s, $1 \leqslant r \neq s \leqslant R$, have proportional vectors $\mathbf{d}_r$ and $\mathbf{d}_s$. Then $k_{\mathbf{D}} = 1$, such that (12) can impossibly be satisfied.

For a second uniqueness condition we assume that $R \leqslant K$. It has been proven that the unsymmetric decomposition (8) is generically essentially unique when $2R(R-1) \leqslant IJ(I-1)(J-1)$ [20]. Likewise, in the complex case the constrained decomposition (4) is generically essentially unique when

$$2R(R-1) \leqslant J^2(J-1)^2. \tag{15}$$

Numerically, this means that generic essential uniqueness is guaranteed for $R \leqslant R_{\max,c}$, given by

J	2	3	4	5	6	7	8
$R_{\max,c}$	2	4	9	14	21	30	40

In the real case a different condition applies. Here, we have generic essential uniqueness for $R \leqslant R_{\max,r}$, given by [58]

J	2	3	4	5	6	7	8
$R_{\max,r}$	2	4	6	10	15	20	26

In [58], an algorithm is derived that allows one to compute $R_{\max,r}$ for any value of J. It is conjectured that the theoretical expression of the bound in the real case is given by

$$\frac{R(R-1)}{2} \leqslant \frac{J(J-1)}{4}\left(\frac{J(J-1)}{2}+1\right) - \frac{J!}{(J-4)!4!}1_{\{J\geqslant 4\}} \tag{16}$$

where

$$1_{\{J\geqslant 4\}} = \begin{cases} 0, & \text{if } J<4 \\ 1, & \text{if } J \geqslant 4. \end{cases}$$

Conditions (15) and (16) are also sufficient but not always necessary for essential uniqueness. Note that these conditions are more relaxed than (14). A (nongeneric) deterministic version will be given in Remark 6.

Remark 2: In [10], [11], and [25] it is explained that in antenna array applications, the characteristics of the antennas and the geometry of the array may induce a structure in the entries of the mixing matrix that limits the number of sources that can effectively be dealt with. Such a structure is neglected in condition (15). As a result, the number of sources that can be allowed is bounded by the minimum of i) the number of sources in condition (15) and ii) the maximal number of virtual sensors (VSs), N_e, derived in [10], [11], and [25]. For instance, for a uniform circular array (UCA) consisting of J identical antennas, the maximum number of VSs is given by

J	2	3	4	5	6	7	8
$N_{e,UCA}$	3	7	9	21	19	43	33

From this table and the table for $R_{\max,c}$ above, we have, e.g., that in the case of a UCA formed by six antennas, the number of sources is bounded by $\min(19,21) = 19$.

III. Computation: General Case

In this section we review some methods for the computation of PARAFAC. The standard way to compute the decomposition, is by means of an "alternating least squares" (ALS) algorithm [34], [53], [57]. The aim is to minimize the (squared) Frobenius norm of the difference between $\mathcal{C}$ and its estimated decomposition in rank-1 terms by means of an iteration in which each step consists of fixing a subset of unknown parameters to their current estimates, and optimizing with regard to the remaining unknowns, followed by fixing an other subset of parameters, and optimizing with regard to the complimentary set, etc. More specifically, one optimizes the cost function

$$f(\mathbf{U},\mathbf{V},\mathbf{W}) = \left\| \mathcal{C} - \sum_{r=1}^{R} \mathbf{u}_r \circ \mathbf{v}_r \circ \mathbf{w}_r \right\|^2 \tag{17}$$

$$\stackrel{\text{def}}{=} \sum_{ijk} \left| c_{ijk} - \sum_{r=1}^{R} u_{ir}v_{jr}w_{kr} \right|^2. \tag{18}$$

Due to the multilinearity of the model, estimation of one of the arguments, given the other two, is a classical linear least squares problem. One alternates between updates of $\mathbf{U}$, $\mathbf{V}$, and $\mathbf{W}$. After updating $\mathbf{U}$ and $\mathbf{V}$, their columns are rescaled to unit length, to avoid under- and overflow. Although, in the case of the constrained decomposition (4), during the iteration the symmetry of the problem is broken, one supposes that eventually $\mathbf{U}$ and $\mathbf{V}^*$ will both converge to an estimate of $\mathbf{A}$. If some difference remains, then the mixing vector $\mathbf{a}_r$ can be estimated as the dominant left singular vector of the matrix $[\mathbf{u}_r\ \mathbf{v}_r^*]$, $r = 1,\ldots,R$. The rank of $\mathcal{C}$ is estimated by trial-and-error. In [48] and [49], an exact line search (ELS) is proposed to enhance the convergence of the ALS algorithm. This means that one looks for the new estimates on the line between the ALS estimates and the current values. The discussion in [48] and [49] is limited to the real case. The complex case is addressed in [44] and [45].

TABLE I
SOBIUM—General Case

1) Estimate the covariance matrices $\mathbf{C}_1,\ldots,\mathbf{C}_K$ and stack them in a tensor $\mathcal{C}$.
2) Compute the PARAFAC decomposition $\mathcal{C} = \sum_{r=1}^{R} \mathbf{a}_r \circ \mathbf{a}_r^* \circ \mathbf{d}_r$, for instance by means of the ALS+ELS algorithm in [44], [47], [48].

In [46], a Gauss–Newton method is described, in which all the factors are updated simultaneously; in addition, the inherent indeterminacy of the decomposition has been fixed by adding a quadratic regularization constraint on the component entries. Instead of the least-squares error (18), one can also minimize the least absolute error. To this end, an alternating linear programming algorithm as well as a weighted median filtering iteration are derived in [67].

It has been proven that in some cases cost function (18) (or any other measure of the difference between $\mathcal{C}$ and its approximation) only has an infimum, and not a minimum [23], [41], [51], [60], [61]. However, this did not seem to pose major problems in our simulations.

The general scheme for *second-order blind identification of underdetermined mixtures* (SOBIUM) is outlined in Table I. We refer to this algorithm as Alg. I.

Remark 3: The choice of $\tau_1,\ldots,\tau_K$ in (2) may affect the condition of the problem. Condition aspects of PARAFAC have

been little studied in the literature. Since we are looking for the factor matrices $\mathbf{A}$, $\mathbf{A}^*$, and $\mathbf{D}$, it is clear from (5)–(7) that it is advantageous to choose $\tau_1, \ldots, \tau_K$ such that $\mathbf{D} \odot \mathbf{A}$, $\mathbf{A}^* \odot \mathbf{D}$, and the $(K \times K)$ submatrices of $\mathbf{D}$ are well conditioned.

IV. Computation: Case $R \leqslant K$

In this case, one can still work as in the previous section. However, more powerful results can be derived. We assume that the second uniqueness condition in Section II is satisfied. This implies in particular that $R < J^2$. We develop a reasoning similar to the one in [7] and [21].

We start from the matrix equation (5). We assume at this point that $\mathbf{A} \odot \mathbf{A}^*$ and $\mathbf{D}$ are full column rank. In the complex case, this is generically true if $R \leqslant \min(J^2, K)$. In the real case, the condition is $R \leqslant \min(J(J+1)/2, K)$ [20]. (Also recall Remark 2.) The full column rank property of $\mathbf{A} \odot \mathbf{A}^*$ and $\mathbf{D}$ implies that the number of sources R is simply equal to the rank of $\mathbf{C}$. Instead of determining it by trial-and-error, as in the previous section, it can be estimated as the number of significant singular values of $\mathbf{C}$. Let the "economy size" singular value decomposition (SVD) of $\mathbf{C}$ be given by

$$\mathbf{C} = \mathbf{U} \cdot \mathbf{\Sigma} \cdot \mathbf{V}^H \tag{19}$$

in which $\mathbf{U} \in \mathbb{C}^{J^2 \times R}$ and $\mathbf{V} \in \mathbb{C}^{K \times R}$ are columnwise orthonormal matrices and in which $\mathbf{\Sigma} \in \mathbb{R}^{R \times R}$ is positive diagonal. We deduce from (5) and (19) that there exists an *a priori* unknown matrix $\mathbf{F} \in \mathbb{C}^{R \times R}$ that satisfies

$$\mathbf{A} \odot \mathbf{A}^* = \mathbf{U} \cdot \mathbf{\Sigma} \cdot \mathbf{F}. \tag{20}$$

Since both $\mathbf{A} \odot \mathbf{A}^*$ and $\mathbf{U} \cdot \mathbf{\Sigma}$ are full column rank, $\mathbf{F}$ is nonsingular. If we knew $\mathbf{F}$, then the mixing matrix $\mathbf{A}$ would immediately follow. Define $\tilde{\mathbf{A}} = \mathbf{A} \odot \mathbf{A}^* \in \mathbb{C}^{J^2 \times R}$ and $\tilde{\mathbf{A}}_r = \mathrm{unvec}(\tilde{\mathbf{a}}_r) \in \mathbb{C}^{J \times J}$, $r = 1, \ldots, R$. Then $\tilde{\mathbf{A}}_r$ is theoretically a rank-one matrix: $\tilde{\mathbf{A}}_r = \mathbf{a}_r \mathbf{a}_r^H$. This means that $\mathbf{a}_r$ can, up to an irrelevant scaling factor, be determined as the left singular vector associated with the largest singular value of $\tilde{\mathbf{A}}_r$, $r = 1, \ldots, R$.

We will now explain how the matrix $\mathbf{F}$ in (20) can be found. Define $\mathbf{H} = \mathbf{U}\mathbf{\Sigma} \in \mathbb{C}^{J^2 \times R}$ and $\mathbf{H}_r = \mathrm{unvec}(\mathbf{h}_r) \in \mathbb{C}^{J \times J}$, $r = 1, \ldots, R$. We have

$$\mathbf{H}_r = \sum_{k=1}^{R} \left(\mathbf{a}_k \mathbf{a}_k^H\right) (\mathbf{F}^{-1})_{kr}. \tag{21}$$

This means that the matrices $\mathbf{H}_r$ consist of linear combinations of the rank-one matrices $\mathbf{a}_k \mathbf{a}_k^H$ and that the linear combinations are the entries of the nonsingular matrix $\mathbf{F}^{-1}$. It would be helpful to have a tool that allows us to determine whether a matrix is rank-one or not. Such a tool is offered by the following theorem.

Theorem 2: Consider the mapping $\Phi : (\mathbf{X}, \mathbf{Y}) \in \mathbb{C}^{J \times J} \times \mathbb{C}^{J \times J} \longmapsto \Phi(\mathbf{X}, \mathbf{Y}) = \mathcal{P} \in \mathbb{C}^{J \times J \times J \times J}$ defined by

$$p_{ijkl} = x_{ij} y_{kl} + y_{ij} x_{kl} - x_{il} y_{kj} - y_{il} x_{kj}$$

for all index values. Given $\mathbf{X} \in \mathbb{C}^{J \times J}$, $\Phi(\mathbf{X}, \mathbf{X}) = 0$ if and only if the rank of $\mathbf{X}$ is at most one.

Proof: A proof for unsymmetric $\mathbf{X}$ was given in [20]. The reasoning remains valid when $\mathbf{X}$ is real symmetric or complex Hermitean. ∎

From the set of matrices $\{\mathbf{H}_r\}$ we construct the set of R^2 tensors $\{\mathcal{P}_{st} \stackrel{\text{def}}{=} \Phi(\mathbf{H}_s, \mathbf{H}_t)\}_{1 \leqslant s,t \leqslant R}$. Now, let $\mathbf{\Lambda}$ be any diagonal matrix and let $\mathbf{M} = \mathbf{F} \cdot \mathbf{\Lambda} \cdot \mathbf{F}^T$. Then, using the bilinearity of Φ, its rank-one detecting feature, and (20), it is readily found that $\sum_{s,t=1}^{R} (\mathbf{M})_{st} \mathcal{P}_{st} = 0$. This suggests to determine matrices $\mathbf{M}$ from the latter equation, and find $\mathbf{F}$ as the matrix that jointly diagonalizes the set by congruence. More specifically, we have the following theorem.

Theorem 3: Assume that the tensors $\Phi(\mathbf{a}_u \mathbf{a}_u^H, \mathbf{a}_v \mathbf{a}_v^H)$, $1 \leqslant u < v \leqslant R$, are linearly independent. Then there exist precisely R linearly independent complex symmetric[1] matrices $\mathbf{M}_r \in \mathbb{C}^{R \times R}$ that satisfy

$$\sum_{s,t=1}^{R} (\mathbf{M}_r)_{st} \mathcal{P}_{st} = 0. \tag{22}$$

The matrix $\mathbf{F}$ diagonalizes each of these matrices by congruence, i.e.,

$$\begin{aligned} \mathbf{M}_1 &= \mathbf{F} \cdot \mathbf{\Lambda}_1 \cdot \mathbf{F}^T \\ &\vdots \\ \mathbf{M}_R &= \mathbf{F} \cdot \mathbf{\Lambda}_R \cdot \mathbf{F}^T \end{aligned} \tag{23}$$

in which $\mathbf{\Lambda}_1, \ldots, \mathbf{\Lambda}_R \in \mathbb{R}^{R \times R}$ are diagonal.

Proof: A proof for the unsymmetric PARAFAC decomposition (8) was given in [20]. The reasoning remains valid when $\mathbf{U} = \mathbf{V}^* = \mathbf{A}$. ∎

Equations (22) and (23) provide the means to find $\mathbf{F}$. Equation (22) is just an homogeneous set of linear equations, from which the matrices $\mathbf{M}_r$ may be computed. Then, the matrix $\mathbf{F}$ follows from the simultaneous diagonalization (23). We now consider these two steps in more detail.

In practice, we work with noisy covariance estimates, such that (22) will only approximately be satisfied. The matrices $\mathbf{M}_r$ are then determined as follows. Due to the symmetry of $\mathbf{M}_r$, and the fact that $\mathcal{P}_{st} = \mathcal{P}_{ts}$, $s, t = 1, \ldots, R$, (22) can be written as

$$\sum_{s=1}^{R} (\mathbf{M}_r)_{ss} \mathcal{P}_{ss} + 2 \sum_{\substack{s,t=1 \\ s<t}}^{R} (\mathbf{M}_r)_{st} \mathcal{P}_{st} = 0. \tag{24}$$

In the usual form of a set of homogeneous linear equations, we have

$$\begin{aligned} \mathbf{P} \cdot \big((\mathbf{M}_r)_{1,1}, \ldots, (\mathbf{M}_r)_{R,R}, \\ 2(\mathbf{M}_r)_{1,2}, 2(\mathbf{M}_r)_{1,3}, \ldots, 2(\mathbf{M}_r)_{R-1,R}\big)^T = 0 \end{aligned} \tag{25}$$

in which the coefficient matrix $\mathbf{P} \in \mathbb{C}^{J^4 \times R(R+1)/2}$ is given by

$$\begin{aligned} \mathbf{P} = \big(\mathrm{vec}(\mathcal{P}_{11}), \ldots, \mathrm{vec}(\mathcal{P}_{RR}), \mathrm{vec}(\mathcal{P}_{12}), \mathrm{vec}(\mathcal{P}_{13}), \ldots, \\ \mathrm{vec}(\mathcal{P}_{R-1,R})\big). \end{aligned} \tag{26}$$

[1]The matrices satisfy $\mathbf{M}_r = \mathbf{M}_r^T$, also in the complex case.

TABLE II
SOBIUM, CASE $R \leqslant K$

1) Estimate the covariance matrices $\mathbf{C}_1, \ldots, \mathbf{C}_K$. Define $\mathbf{C} = [\mathrm{vec}(\mathbf{C}_1) \ \cdots \ \mathrm{vec}(\mathbf{C}_K)]$.
2) Compute the SVD $\mathbf{C} = \mathbf{U} \cdot \mathbf{\Sigma} \cdot \mathbf{V}^H$. $\mathbf{H} = \mathbf{U} \cdot \mathbf{\Sigma}$. The number of sources R equals rank($\mathbf{C}$).
3) Compute $\mathcal{P}_{st} = \Phi(\mathbf{H}_s, \mathbf{H}_t)$, $1 \leqslant s \leqslant t \leqslant R$. Stack the results in $\mathbf{P}$.
4) Compute the R right singular vectors $\mathbf{w}_r$ of $\mathbf{P}$ that correspond to the smallest singular values. Stack these vectors in upper triangular matrices $\mathbf{W}_r$. Compute $\mathbf{M}_r = \frac{1}{2}(\mathbf{W}_r + \mathbf{W}_r^T)$, $r = 1, \ldots, R$.
5) Compute nonsingular $\mathbf{F}$ that best simultaneously diagonalizes the matrices $\mathbf{M}_r$.
6) Compute $\tilde{\mathbf{A}} = \mathbf{U} \cdot \mathbf{\Sigma} \cdot \mathbf{F}$.
7) Estimate mixing vector $\mathbf{a}_r$ as the dominant left singular vector of $\tilde{\mathbf{A}}_r = \mathrm{unvec}(\tilde{\mathbf{a}}_r)$, $r = 1, \ldots, R$.

The least-squares solution of (25) consists of the R right singular vectors $\mathbf{w}_r$ of $\mathbf{P}$ that correspond to the smallest singular values. After stacking these vectors in upper triangular matrices $\mathbf{W}_r \in \mathbb{C}^{R \times R}$, in the manner suggested by (25), the matrices $\mathbf{M}_r$ are obtained as $\mathbf{M}_r = (1/2)(\mathbf{W}_r + \mathbf{W}_r^T)$.

After computation of the matrices $\mathbf{M}_r$, $\mathbf{F}$ is obtained from (23). Note that we have turned the underdetermined problem (2) into a (square) overdetermined problem. In the absence of noise, $\mathbf{F}$ already follows from the eigenvalue decomposition (EVD)

$$\mathbf{M}_1 \cdot \mathbf{M}_2^{-1} = \mathbf{F} \cdot (\mathbf{\Lambda}_1 \cdot \mathbf{\Lambda}_2^{-1}) \cdot \mathbf{F}^{-1} \tag{27}$$

in which we assumed that $\mathbf{\Lambda}_2$, and hence $\mathbf{M}_2$, is nonsingular. Stated otherwise, $\mathbf{F}^{-T}$ is a generalized eigenmatrix of the pencil $(\mathbf{M}_1, \mathbf{M}_2)$; see [6], [26], [33], and [52], and references therein. In practice, it is more reliable to take all matrices in (23) into account. The set can be simultaneously diagonalized by means of the algorithms presented in [19], [34], [48], [49], [64]–[66], [69], and [70]. Comparing these algorithms is outside the scope of this paper. The generalized eigenmatrix of the pencil $(\mathbf{M}_1, \mathbf{M}_2)$ can be used as initial value.

The overall SOBIUM algorithm for the case $R \leqslant K$ is outlined in Table II. We refer to this algorithm as Alg. II.

Remark 4: In the derivation above, we assumed that the matrices $\mathbf{A} \odot \mathbf{A}^*$ and $\mathbf{D}$ are both full column rank and that the tensors $\Phi(\mathbf{a}_u \mathbf{a}_u^H, \mathbf{a}_v \mathbf{a}_v^H)$, $1 \leqslant u < v \leqslant R$, are linearly independent. The derivation shows that these deterministic conditions are sufficient for essential uniqueness of the PARAFAC decomposition (4). This result has independently, in an entirely different way, been obtained in [39]. For generic mixtures, the conditions reduce to the dimensionality constraints (15) and (16) [20], [58].

Remark 5: Recall that in the SOBI algorithm for overdetermined mixtures, the sources all need to have a different spectrum [3]. The conditions above are stronger. It is not only needed that $\mathbf{D}$ does not have proportional columns; this matrix should be full column rank.

Remark 6: As already stated in Remark 3, the choice of $\tau_1, \ldots, \tau_K$ in (2) may affect the condition of the problem. From (5) and (19), we recall that the matrix $\mathbf{D}$ is used to determine the dominant R-dimensional subspace of the column space of $\mathbf{C}$. The more accurately this subspace can be estimated, the better for the overall accuracy of the method. It is thus advantageous to choose $\tau_1, \ldots, \tau_K$ such that $\mathbf{D}$ is well conditioned.

V. SIMULATIONS

We consider R narrowband sources, received by a UCA of $J = 4$ identical sensors of radius R_a. We assume free space propagation. This means that the entries of the mixing matrix before normalization are given by

$$\tilde{a}_{jr} = \exp\left(2\pi \jmath \left(x_j \cos(\theta_r)\cos(\phi_r) + y_j \cos(\theta_r)\sin(\phi_r)\right)\right)$$

where $x_j = (R_a/\lambda)\cos(2\pi(j-1)/J)$, $y_j = (R_a/\lambda)\sin(2\pi(j-1)/J)$, and $\jmath = \sqrt{-1}$. We have $R_a/\lambda = 0.55$. The mixing matrix $\mathbf{A}$ is obtained by dividing the columns of $\tilde{\mathbf{A}}$ by their Frobenius norm. The sources are unit-variance quadrature phase-shift keying (QPSK) (taking their values equally likely in the set $\{\pm 1/\sqrt{2} \pm \jmath/\sqrt{2}\}$), shaped by a raise cosine pulse shape filter with roll-off $\mu = 0.3$. All sources have the same symbol duration $T = 8T_e$, where T_e is the sample period. The number of snapshots $L = 8N$, in which N is the number of transmitted symbols. The directions-of-arrival (DOAs) of the different sources are given by $\theta_1 = 3\pi/10$, $\theta_2 = 3\pi/10$, $\theta_3 = 2\pi/5$, $\theta_4 = 0$, $\theta_5 = \pi/10$, $\theta_6 = 3\pi/5$ and $\phi_1 = 7\pi/10$, $\phi_2 = 9\pi/10$, $\phi_3 = 3\pi/5$, $\phi_4 = 4\pi/5$, $\phi_5 = 3\pi/5$, $\phi_6 = \pi/5$. We consider two cases: $R = 5$ and $R = 6$. In the case $R = 5$, we only consider the first five sources. There is a residual carrier, characterized by $\Delta f_1 \times T_e = 0$, $\Delta f_2 \times T_e = 1/2$, $\Delta f_3 \times T_e = 1/3$, $\Delta f_4 \times T_e = 1/5$, $\Delta f_5 \times T_e = 0.74$, $\Delta f_6 \times T_e = 0.58$. Additive zero-mean complex Gaussian noise is added to the data. Although the signals are cyclostationary, their statistics are estimated by means of an empirical estimator. It is explained in [29], [30] that the empirical estimator of the second-order statistics of the data is unbiased for zero-mean sources whatever the circularity properties of the latter. The time delays in (2) are defined by $\tau_k = k - 1$. The mixing matrix is estimated by means of i) the SOBIUM algorithm (the scheme of Alg. I when $K < R$ and the scheme of Alg. II when $K \geqslant R$, unless stated otherwise) and ii) the FOBIUM algorithm [31], which uses the fourth-order cumulant of the observations. In FOBIUM, we used the cumulants $\mathrm{Cum}(\mathbf{x}_t, \mathbf{x}_{t+\tau_k}^*, \mathbf{x}_t^*, \mathbf{x}_t)$, $k = 1, \ldots, K$, like in [31]. In Step 2 of Alg. I, we use the ALS+ELS algorithm of [48], [49]. Since the data are complex, the step size is computed as in [44] and [45]. The precision is measured in terms of the mean relative error

$$\text{error} = E\left\{\frac{\|\mathbf{A} - \hat{\mathbf{A}}\|}{\|\mathbf{A}\|}\right\} \tag{28}$$

in which the norm is the Frobenius norm and in which $\hat{\boldsymbol{A}}$ represents the optimally ordered and scaled estimate of $\mathbf{A}$. We conduct Monte Carlo experiments consisting of 100 runs.

Figs. 2–6 compare Alg. I and FOBIUM for the case $K = 4$ and $R = 5$. Fig. 2 shows the accuracy as a function of the signal-to-noise ratio (SNR) when $N = 1000$ symbols are transmitted. Figs. 3 and 4 show the accuracy and the computational cost, respectively, as a function of the number of data symbols, when the SNR is 10 dB. (The computation time varies little as a function of the SNR.) We see that the length of the data set determines which of the two methods is more accurate. SOBIUM

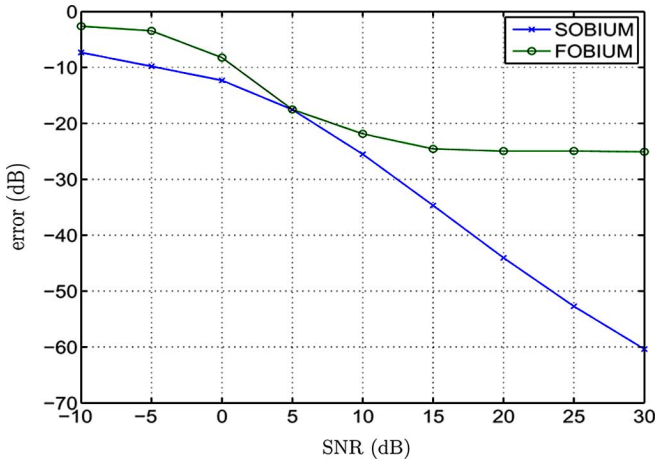

Fig. 2. Accuracy as a function of SNR in the first experiment ($K = 4$; $R = 5$; $N = 1000$).

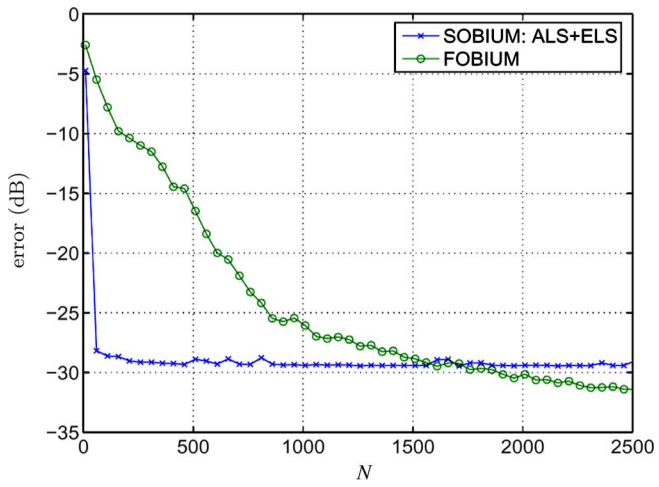

Fig. 3. Accuracy as a function of data length in the first experiment ($K = 4$; $R = 5$; 10 dB).

is more accurate than FOBIUM when data blocks are short. FOBIUM is more reliable when data sets are long. (Recall that the signal is oversampled by a factor 8.) This is as expected. On one hand, for the estimation of the fourth-order cumulants in FOBIUM more samples are needed than for the estimation of the covariance matrices in SOBIUM. On the other hand, fourth-order cumulants are blind to additive Gaussian noise. Fig. 4 shows us that Alg. I is computationally cheaper than FOBIUM, except for short data sets.

Fig. 5 shows the accuracy as a function of the condition of the problem. In this figure, ϕ_1 is varied from $7\pi/10$ to $0.95\pi/10$, thereby passing the value of ϕ_2). The SNR was taken equal to 10 dB and 1000 symbols were transmitted. Fig. 6 shows the same results using the following error measure:

$$\text{error}_2 = \max_m \left(1 - \max_i \left(\frac{\left| \mathbf{a}_m^H \hat{\mathbf{a}}_i \right|}{\sqrt{\left(\mathbf{a}_m^H \mathbf{a}_m \right) \left(\hat{\mathbf{a}}_i^H \hat{\mathbf{a}}_i \right)}} \right) \right). \quad (29)$$

This error takes a value between 0 and 1. It is zero when $\mathbf{A}$ and $\hat{\mathbf{A}}$ are equal up to permutation and scaling of the columns. The

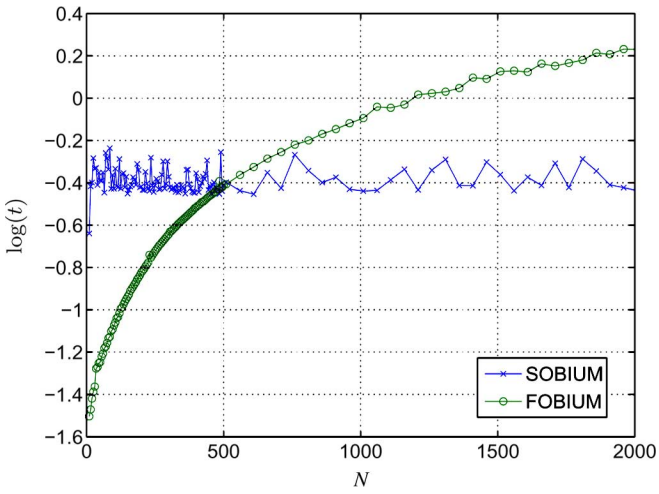

Fig. 4. Computation time as a function of data length in the first experiment ($K = 4$; $R = 5$; 10 dB).

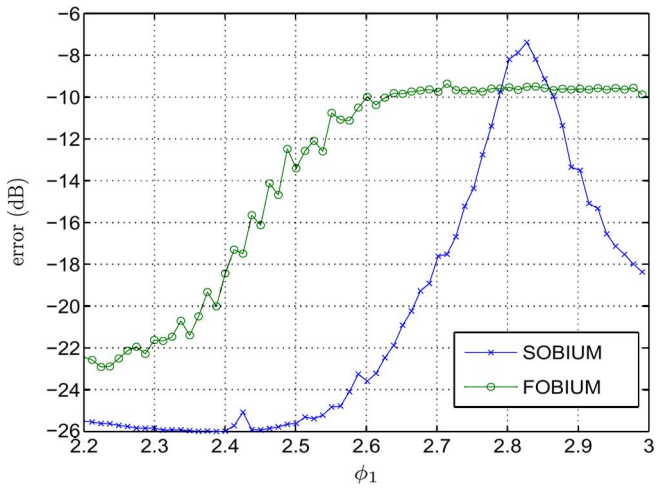

Fig. 5. Accuracy as a function of angle of first mixing vector in the first experiment ($K = 4$; $R = 5$; 10 dB; $N = 1000$).

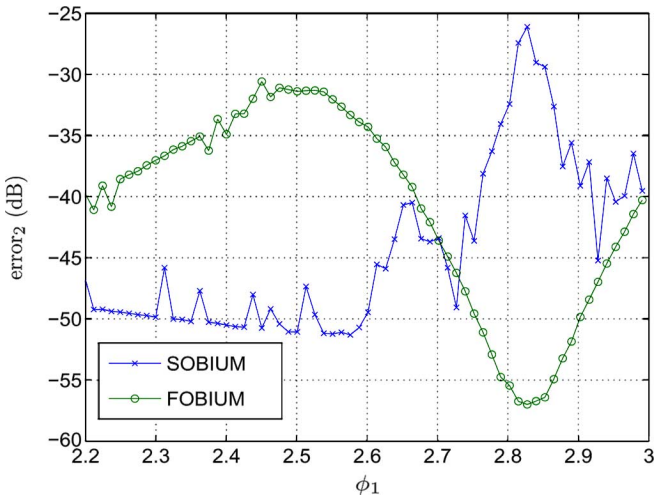

Fig. 6. Accuracy as a function of angle of first mixing vector in the first experiment ($K = 4$; $R = 5$; 10 dB; $N = 1000$).

criterion (29) gives the error associated to the mixing vector that has been estimated the least well. Figs. 5 and 6 do not contradict. When ϕ_1 approaches ϕ_2, it is possible that an algorithm finds one vector, say $\hat{\mathbf{a}}_1$, that is a good approximation of both $\mathbf{a}_1$ and $\mathbf{a}_2$, while an other estimated vector, say $\hat{\mathbf{a}}_2$, does not particularly

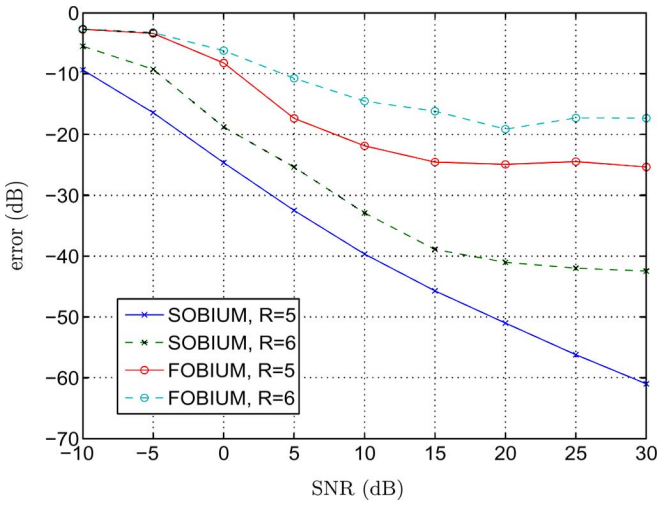

Fig. 7. Accuracy as a function of SNR in the second experiment ($K = 12$; $R = 5, 6$; $N = 1000$).

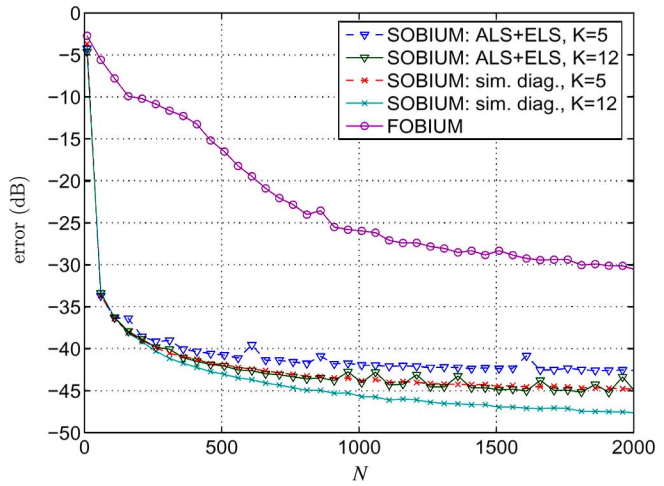

Fig. 8. Accuracy as a function of data length in the second experiment ($R = 5$; 10 dB).

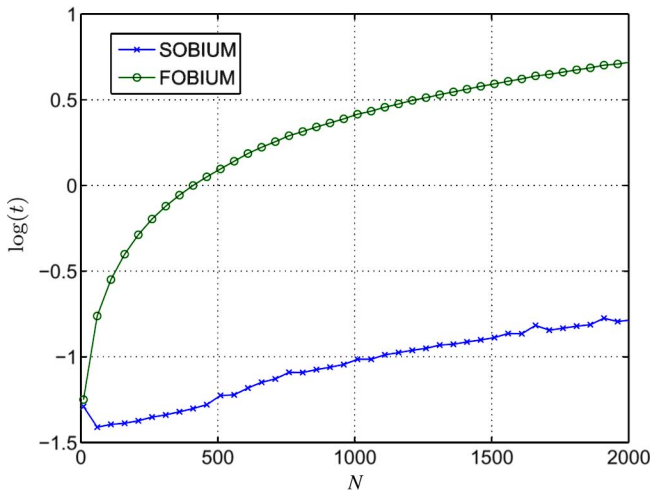

Fig. 9. Computation time as a function of data length in the second experiment ($K = 12$; $R = 5$; 10 dB).

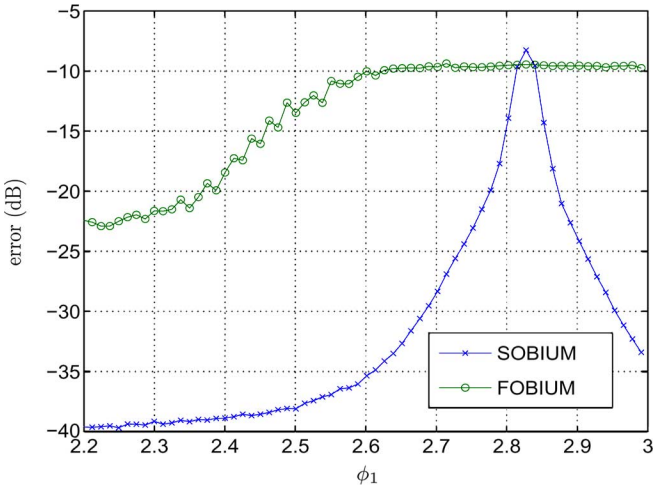

Fig. 10. Accuracy as a function of angle of first mixing vector in the second experiment ($K = 12$; $R = 5$; 10 dB; $N = 1000$).

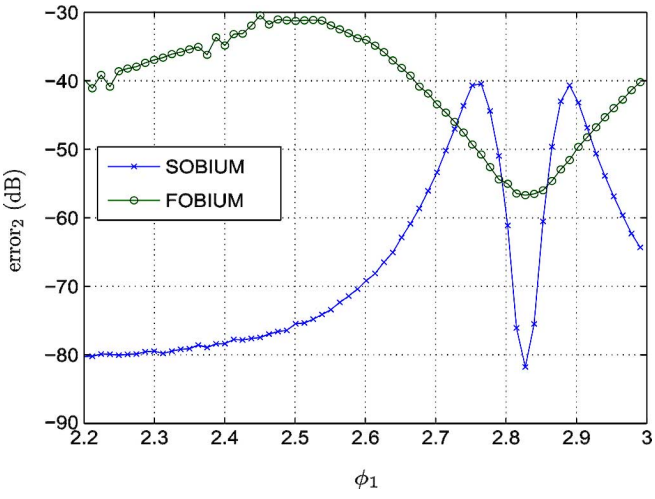

Fig. 11. Accuracy as a function of angle of first mixing vector in the second experiment ($K = 12$; $R = 5$; 10 dB; $N = 1000$).

well estimate any of the mixing vectors. This is detected by error (28) but not by error (29): in (28) $\hat{\mathbf{a}}_2$ has to be assigned to one of the columns of $\mathbf{A}$, while $\hat{\mathbf{a}}_1$ can be assigned to both $\mathbf{a}_1$ and $\mathbf{a}_2$ in (29). This causes the FOBIUM curve to stabilize around -10 dB in Fig. 5, while it decreases in Fig. 6. We also mention that the vectors $\mathbf{a}_1 \otimes \mathbf{a}_1^*$ and $\mathbf{a}_2 \otimes \mathbf{a}_2^*$ are less close than the vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ (cf. [11]), such that higher order methods have a conceptual advantage when mixing vectors are close.

Figs. 7–11 are the counterparts of Figs. 2–6, respectively, when $K = 12$ and when Alg. II is used instead of Alg. I. In Fig. 8, we have also checked what happens when fewer matrices are taken into account $(K = 5)$. The result was as expected: by adding more rows to $\mathbf{D}$, the condition number of $\mathbf{D}$ generally decreased, which in turn improved the accuracy. We have also compared to Alg. I in Fig. 8. In this simulation Alg. II turned out to be somewhat more accurate than Alg. I. This is not necessarily generally true: in [19] and [20], we have observed that an algorithm that directly optimizes the cost function (17), initialized with an algebraic solution, sometimes yields a modest gain in precision. Finally, we mention that Alg. II can be initialized with the noise-free solution (27), while Alg. I has to work

its way to the solution without guidance, which makes it much less efficient.

VI. Conclusion

In this paper, we exploited differences in autocovariance to estimate the mixing matrix in underdetermined ICA. The joint decomposition of a set of spatial covariance matrices was interpreted as a PARAFAC decomposition of the third-order tensor in which these matrices are stacked. We distinguished between two cases, depending on whether the number of covariance matrices K exceeds the number of sources R or not. For both cases, we presented theoretical bounds on the number of sources that can be allowed and discussed algebraic algorithms. We explained that, in the case $K \geqslant R$, the noise-free solution can be obtained by means of an EVD. The performance of the main algorithms was illustrated by means of simulations. Our results can be used to generalize any ICA technique, based on a simultaneous matrix diagonalization like (4), to the underdetermined case.

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