

Second-Order Blind Identification of Underdetermined Mixtures*

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Abstract. In this paper we show that the underdetermined ICA problem can be solved using a set of spatial covariance matrices, in case the sources have sufficiently different temporal autocovariance functions. The result is based on a link with the decomposition of higher-order tensors in rank-one terms. We discuss two algorithms and present theoretical bounds on the number of sources that can be allowed.

1 Introduction

Let us use the following notation for the basic Independent Component Analysis (ICA) model:

$$\mathbf{x}_t = \mathbf{A}\mathbf{s}_t + \mathbf{n}_t, \quad (1)$$

in which the observation vector $\mathbf{x}_t \in \mathbb{C}^J$, the noise vector $\mathbf{n}_t \in \mathbb{C}^J$ and the source vector $\mathbf{s}_t \in \mathbb{C}^R$ are zero-mean. The mixing matrix $\mathbf{A} \in \mathbb{C}^{J \times R}$. The goal is to exploit the assumed mutual statistical independence of the source components to estimate the mixing matrix and/or the source signals from the observations. The literature on ICA addresses for the most part the so-called *overdetermined* case, where $J \geq R$. Here, we consider the *underdetermined* or *overcomplete* case, where $J < R$.

A large class of algorithms for underdetermined ICA starts from the assumption that the sources are (quite) sparse [2, 12, 15, 22]. 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 [2, 12]. Some of these techniques are based on 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) [2].

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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 pseudo-inverse 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 $J - R$ — hence the term “underdetermined”. One could estimate the sources and the mixing matrix simultaneously by exploiting prior knowledge on the sources [15, 22]. An other approach is to estimate the mixing matrix first, and then estimate the sources. In this paper we will show that the estimation of the mixing matrix is actually an overdetermined subproblem, even in the case of underdetermined mixtures. If the source densities are known, then \mathbf{s}_t may subsequently be estimated by maximizing the log posterior likelihood [15]. In the case of Laplacian probability densities, modelling sparse sources, this can be formulated in terms of a linear programming problem [2, 15]. In the case of finite alphabet signals in telecommunication, one may perform an exhaustive search over all possible combinations. In this paper we will focus on the estimation of the mixing matrix.

This paper presents new contributions to the class of algebraic algorithms for underdetermined ICA. In [6, 7, 8] algorithms are derived for the case of two mixtures and three sources. An arbitrary number of mixing vectors can be estimated from two observation channels by sampling derivatives of sufficiently high order of the second characteristic function [19]. 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 [5].

In this paper we assume that the sources are individually correlated in time. The spatial covariance matrices of the observations then satisfy [1]:

$$\begin{aligned} \mathbf{C}_1 &\equiv E\{\mathbf{x}_t\mathbf{x}_{t+\tau_1}^H\} = \mathbf{A} \cdot \mathbf{D}_1 \cdot \mathbf{A}^H \\ &\vdots \\ \mathbf{C}_K &\equiv E\{\mathbf{x}_t\mathbf{x}_{t+\tau_K}^H\} = \mathbf{A} \cdot \mathbf{D}_K \cdot \mathbf{A}^H \end{aligned} \quad (2)$$

in which $\mathbf{D}_k \equiv E\{\mathbf{s}_t\mathbf{s}_{t+\tau_k}^H\}$ is diagonal, $k = 1, \dots, K$. For simplicity, we have dropped the noise terms; they can be considered as a perturbation of (2).

Let us stack the matrices $\mathbf{C}_1, \dots, \mathbf{C}_K$ in Eq. (2) in a tensor $\mathcal{C} \in \mathbb{C}^{J \times J \times K}$. Define a matrix $\mathbf{D} \in \mathbb{C}^{K \times R}$ by $(\mathbf{D})_{kr} \equiv (\mathbf{D}_k)_{rr}$, $k = 1, \dots, K$, $r = 1, \dots, R$. Then we have

$$c_{ijk} = \sum_{r=1}^R a_{ir} a_{jr}^* d_{kr}, \quad (3)$$

which we write as

$$\mathcal{C} = \sum_{r=1}^R \mathbf{a}_r \circ \mathbf{a}_r^* \circ \mathbf{d}_r, \quad (4)$$

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. Eq. (4) is a decomposition of tensor \mathcal{C} in

a sum of R rank-1 terms. In the literature, this is called a ‘‘Canonical Decomposition’’ (CANDECOMP) [4] or a ‘‘Parallel Factors Model’’ (PARAFAC) [13]. 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, ‘‘source separation’’ 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.

Uniqueness issues are discussed in Section 2. Section 3 and 4 present algorithms for the computation of decomposition (4). Section 3 deals with the case where $R > K$. More powerful results are obtained for the case where $R \leq K$ in Section 4. Section 5 shows the results of some simulations. The presentation is in terms of complex signals. Whenever the results cannot be directly applied to real data, this will be explicitly mentioned.

This paper is a short version of [11]. The foundations of Section 4 were laid in [3]. Some mathematical aspects are developed in more detail in [10].

2 PARAFAC Uniqueness

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 decomposition in (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

$$\mathbf{A} = \mathbf{A}' \cdot \mathbf{P} \cdot \mathbf{\Omega}_1 \quad \mathbf{D} = \mathbf{D}' \cdot \mathbf{P} \cdot \mathbf{\Omega}_2, \quad (5)$$

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

A first uniqueness result requires the notion of Kruskal-rank or k -rank $k(\mathbf{A})$ of a matrix \mathbf{A} [14]. It is defined as the maximal number k such that any set of k columns of \mathbf{A} is linearly independent. From [14, 18] we have then immediately that decomposition (4) is essentially unique when

$$2k(\mathbf{A}) + k(\mathbf{D}) \geq 2(R + 1). \quad (6)$$

For a second uniqueness condition we assume that the number of sources R does not exceed the number of covariance matrices K . We call decomposition (4) generic when the (noiseless) entries of \mathbf{A} and \mathbf{D} can be considered drawn from continuous probability densities. It turns out that in the complex case the generic decomposition is essentially unique when $2R(R-1) \leq J^2(J-1)^2$ [10, 11]. For real-valued tensors, we have uniqueness if $R \leq R_{max}$, given by [18]:

$$\begin{array}{c|cccccccc} J & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \hline R_{max} & 2 & 4 & 6 & 10 & 15 & 20 & 26 \end{array}$$

3 Case 1: $R > K$

Generically, a matrix is full rank and full k -rank. Hence, in practice, $k(\mathbf{A}) = \min(J, R) = J$ and $k(\mathbf{D}) = \min(K, R) = K$ if $R > K$. Eq. (6) then guarantees identifiability if $2J + K \geq 2R + 2$, i.e., when the number of sources $R \leq J - 1 + K/2$.

The standard way to compute PARAFAC, is by means of an ‘‘Alternating Least Squares’’ (ALS) algorithm [13]. 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 w.r.t. the remaining unknowns, followed by fixing an other subset of parameters, and optimizing w.r.t. the complimentary set, etc. (Like for matrices, the squared Frobenius norm of a tensor is the sum of the squared moduli of its entries.) More specifically, one optimizes the cost function

$$f(\mathbf{U}, \mathbf{V}, \mathbf{D}) = \|\mathcal{C} - \sum_{r=1}^R \mathbf{u}_r \circ \mathbf{v}_r^* \circ \mathbf{d}_r\|^2. \quad (7)$$

Due to the multi-linearity 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{D} . After updating \mathbf{U} and \mathbf{V} , their columns are rescaled to unit length, to avoid under- and overflow. Although during the iteration the symmetry of the problem is broken, one supposes that eventually \mathbf{U} and \mathbf{V} both converge to \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 $[\mathbf{u}_r \ \mathbf{v}_r]$, $r = 1, \dots, R$. The rank of \mathcal{C} is estimated by trial-and-error. In [16] an exact line search is proposed to enhance the convergence of the ALS algorithm.

4 Case 2: $R \leq K$

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 2 is satisfied. This implies in particular that $R < J^2$.

We stack the entries of tensor \mathcal{C} in a $(J^2 \times K)$ matrix \mathbf{C} as follows:

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

Eq. (4) can be written in a matrix format as:

$$\mathbf{C} = (\mathbf{A} \odot \mathbf{A}^*) \cdot \mathbf{D}^T, \quad (8)$$

in which \odot denotes the Khatri-Rao or column-wise Kronecker product, i.e., $\mathbf{A} \odot \mathbf{A}^* \equiv [\mathbf{a}_1 \otimes \mathbf{a}_1^*, \dots, \mathbf{a}_R \otimes \mathbf{a}_R^*]$. If $R \leq \min(J^2, K)$, then $\mathbf{A} \odot \mathbf{A}^*$ and \mathbf{S} are generically full rank [10]. This 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:

$$\mathbf{C} = \mathbf{U} \cdot \mathbf{\Sigma} \cdot \mathbf{V}^H, \quad (9)$$

in which $\mathbf{U} \in \mathbb{C}^{J^2 \times R}$ and $\mathbf{V} \in \mathbb{C}^{K \times R}$ are column-wise orthonormal matrices and in which $\mathbf{\Sigma} \in \mathbb{R}^{R \times R}$ is positive diagonal. We deduce from (8) and (9) that there exists an a priori unknown matrix $\mathbf{F} \in \mathbb{C}^{R \times R}$ that satisfies:

$$\mathbf{A} \odot \mathbf{A}^* = \mathbf{U} \cdot \mathbf{\Sigma} \cdot \mathbf{F}. \quad (10)$$

If we would know \mathbf{F} , then the mixing matrix \mathbf{A} would immediately follow. Stack the entries of the columns \mathbf{m}_r of $\mathbf{A} \odot \mathbf{A}^*$ in $(J \times J)$ matrices \mathbf{M}_r as follows: $(\mathbf{M}_r)_{ij} \equiv (\mathbf{m}_r)_{(i-1)J+j}$, $i, j = 1, \dots, J$. Then \mathbf{M}_r is theoretically a rank-one matrix: $\mathbf{M}_r = \mathbf{a}_r \mathbf{a}_r^H$. 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 \mathbf{M}_r , $r = 1, \dots, R$.

We will now explain how the matrix \mathbf{F} in (10) can be found. Let \mathbf{E}_r be a $(J \times J)$ matrix in which the r th column of matrix $\mathbf{U}\mathbf{\Sigma}$ is stacked as above. We have

$$\mathbf{E}_r = \sum_{k=1}^R (\mathbf{a}_k \mathbf{a}_k^H) (\mathbf{F}^{-1})_{kr}. \quad (11)$$

This means that the matrices \mathbf{E}_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 [3, 10].

Theorem 1. Consider the mapping $\Phi: (\mathbf{X}, \mathbf{Y}) \in \mathbb{C}^{J \times J} \times \mathbb{C}^{J \times J} \mapsto \Phi(\mathbf{X}, \mathbf{Y}) = \mathcal{P} \in \mathbb{C}^{J \times J \times J \times J}$ 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.

From the matrix $\mathbf{U}\mathbf{\Sigma}$ in the SVD (9) we construct the set of R^2 tensors $\{\mathcal{P}_{rs} \equiv \Phi(\mathbf{E}_r, \mathbf{E}_s)\}_{r,s \in [1,R]}$. It can now be proved [3, 10, 11] that generically there exist exactly R linearly independent symmetric matrices $\mathbf{B}_r \in \mathbb{C}^{R \times R}$ that satisfy:

$$\sum_{t,u=1}^R \mathcal{P}_{tu}(\mathbf{B}_r)_{tu} = 0. \quad (12)$$

Moreover, these matrices can all be diagonalized by \mathbf{F} :

$$\begin{aligned} \mathbf{B}_1 &= \mathbf{F} \cdot \mathbf{\Lambda}_1 \cdot \mathbf{F}^T \\ &\vdots \\ \mathbf{B}_R &= \mathbf{F} \cdot \mathbf{\Lambda}_R \cdot \mathbf{F}^T \end{aligned} \quad (13)$$

in which $\mathbf{\Lambda}_1, \dots, \mathbf{\Lambda}_R$ are diagonal. Eqs. (12) and (13) provide the means to find \mathbf{F} . Eq. (12) is just a linear set of equations, from which the matrices \mathbf{B}_r may be computed. Note that, in the absence of noise, \mathbf{F} already follows from the Eigenvalue Decomposition (EVD)

$$\mathbf{B}_1 \cdot \mathbf{B}_2^{-1} = \mathbf{F} \cdot (\mathbf{\Lambda}_1 \cdot \mathbf{\Lambda}_2^{-1}) \cdot \mathbf{F}^{-1}.$$

In practice, it is more reliable to take all matrices in (13) into account. The set can be simultaneously diagonalized by means of the algorithms presented in [9, 13, 20, 21].

5 Simulations

We conduct a Monte-Carlo experiment consisting of 100 runs. In each run, signal values are drawn from a standardized complex Gaussian distribution and subsequently passed through a filter of which the coefficients are rows of a (16×16) Hadamard matrix. (More specifically, rows 1, 2, 4, 7, 8 and 13 are considered.) The resulting sources are mixed by means of a matrix of which the entries are also drawn from a standardized complex Gaussian distribution and additive Gaussian noise is added.

In the first experiment, we assume $J = 4$ observation channels and $R = 5$ sources. Covariance matrices are computed for $\tau = 0, \dots, 3$. This problem is quite difficult since two of the (4×4) submatrices of \mathbf{D} have a condition number of about 30, which indicates some lack of “diversity” for these submatrices. The number of samples $T = 10000$. The mixing matrix is computed by means of the ALS algorithm described in Section 3. In Fig. 1 we plot the mean relative error $E\{\|\mathbf{A} - \hat{\mathbf{A}}\|/\|\mathbf{A}\|\}$, in which the norm is the Frobenius-norm. (The columns of \mathbf{A} are normalized to unit length and $\hat{\mathbf{A}}$ represents the optimally ordered and scaled estimate.)

In the second experiment, we compute 12 covariance matrices ($\tau = 0, \dots, 11$). This makes the problem better conditioned. We consider $R = 5$ or 6 sources.

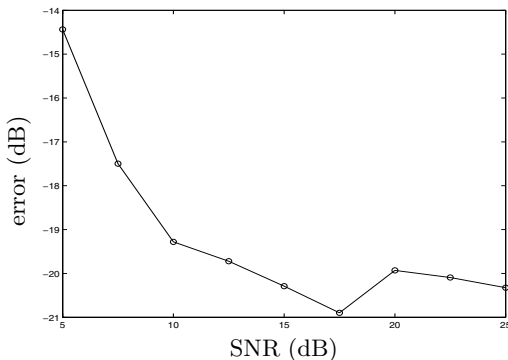


Fig. 1. Relative error in the first experiment ($K = 4$)

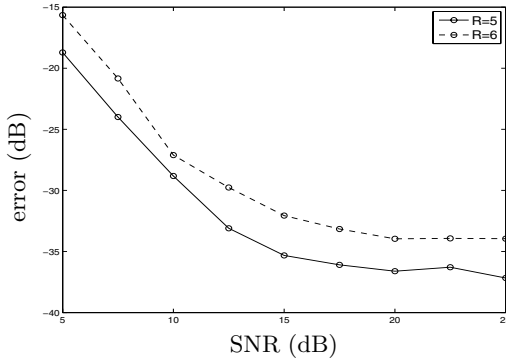


Fig. 2. Relative error in the second experiment ($K = 12$)

The number of samples $T = 5000$. The mixing matrix is computed by means of the algorithm described in Section 4, where we used the algorithm derived in [20] for the simultaneous diagonalization. The mean relative error is shown in Fig. 2. Note that the mixing matrix is estimated with an accuracy of two digits.

To have a reference, we also computed the solution by means of the AC-DC algorithm proposed in [21]. In neither experiment, AC-DC yielded a reliable estimate of the mixing matrix.

6 Conclusion

In this paper we exploited differences in autocovariance to solve the underdetermined ICA problem. The joint decomposition of a set of spatial covariance matrices was interpreted as the decomposition in rank-one terms of the third-order tensor in which these matrices can be 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 $K > R$, the noise-free solution can be obtained by means of an EVD. The same approach can be used for nonstationary sources, by considering spatial covariance matrices at different time instances, sets of spatial time-frequency distributions, etc.

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