Weight Adjusted Tensor Method for Blind Separation of Underdetermined Mixtures of Nonstationary Sources

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***Abstract*—In this paper, a novel algorithm to blindly separate an instantaneous linear underdetermined mixture of nonstationary sources is proposed. It means that the number of sources exceeds the number of channels of the available data. The separation is based on the working assumption that the sources are piecewise stationary with a different variance in each block. It proceeds in two steps: 1) estimating the mixing matrix, and 2) computing the optimum beamformer in each block to maximize the signal-to-interference ratio of each separated signal with respect to the remaining signals. Estimating the mixing matrix is accomplished through a specialized tensor decomposition of the set of sample covariance matrices of the received mixture in each block. It utilizes optimum weighting, which allows statistically efficient (CRB attaining) estimation provided that the data obey the assumed Gaussian piecewise stationary model. In simulations, performance of the algorithm is successfully tested on blind separation of 16 speech signals from nine linear instantaneous mixtures of these signals.**

***Index Terms*—Blind source separation, Cramér–Rao lower bound, multilinear models, nonstationary processes, tensor decomposition, underdetermined mixture.**

I. Introduction

In recent years, a lot of attention has been paid to blind separation of underdetermined mixtures of signals, in which the number of original sources is higher than that of the observed signals. Unlike the "(over)determined" case, when the number of the mixtures is equal to or exceeds the number of the sources, the estimation of the mixing transformation (matrix) is not equivalent to the estimation of the original signals.

Most of the proposed methods rely on the sparsity of signals in a domain, e.g., the time-frequency one [1], [2], [11]. The mixing matrix is identified by localizing points where several sources are active at the same time so that the mixture is locally overdetermined there. This type of searching usually requires exhaustive computations, which limits the applicability of these methods to a lower number of observation channels and sources.

Many algebraic methods for the underdetermined BSS utilize various decompositions of different data structures such as cumulant, correlation and cross-correlation matrices or tensors. The original signals are assumed to be mutually independent, so the task corresponds to independent component analysis [6], and either the non-Gaussianity, nonwhiteness, or nonstationarity of the signals is taken into account [8], [10], [12]. A good survey of the related literature can be found in [12]. These methods primarily estimate the mixing matrix, leaving the retrieval of the original signals to another step.

In this paper, a novel underdetermined separation method is proposed, which is suitable for separation of signals that are non-stationary, having time-varying variances, such as speech signals or some biomedical signals. The signals are assumed to be piecewise stationary with a different variance in each block. This signal model was advocated e.g., by Pham and Cardoso [21]. Recently, this signal model and a related separation algorithm called "Block Gaussian SEParation" (BGSEP) [25] was used in a time-domain blind audio separation method called "Time Audio Blind separation with Complete Decomposition of the observation space" (TABCD) [14]. In TABCD, several other ICA algorithms can be used to decompose the observation space as well, but BGSEP was often the method of the choice because of its nearly best achievable performance (compared to other methods) and very low computational complexity. A good performance of BGSEP compared to other ICA methods in separating linear mixtures of speech signals was shown in [15].

Performance of BGSEP can be tuned up by a proper selection of the block length. The method is not overly sensitive to the selection of the length, but in general it should follow the rate of the variability of the signal parameters (variances). In speech processing, stationarity of the signal is assumed in block of the length 20–30 ms. In biomedical applications, the length of blocks should be related to a duration of important events that the data may contain; for example, it is a duration of one eye blink in electroencephalogram (EEG) or one hearth beat in electrocardiogram (ECG). The assumption about equal length of

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This paper has supplementary downloadable multimedia material available at http://ieeexplore.ieee.org provided by the authors. This includes a Matlab p-code of the algorithm, 16 channel speech data, and a 9 channel mixture. This material is 16.4 MB in size.

Color versions of one or more of the figures in this paper are available online at http://ieeexplore.ieee.org.

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the blocks is used for simplicity of the presentation and usage of the proposed method. The assumption can be relaxed after a minor modification of the method, assuming the partitioning of the signal to be known in advance. Numerical experiments show that the method produces good separation results although the partitioning does not match the true model, or if there is no true piecewise stationary model exactly valid, as in the case of the speech.

The algorithm proposed in this paper can be regarded as an extension of BGSEP to underdetermined mixtures. It is called UDSEP for easy reference. It is based on a canonical polyadic decomposition (sometimes called "parallel factor decomposition," PARAFAC, in the sequel abbreviated as "CP") of a three-way tensor composed of covariance matrices of the mixture in the blocks. It is an extension of the algorithm "Second Order Blind Identification of Underdetermined Mixtures" (SOBIUM) [12]. In SOBIUM, as well as in other CP methods, high-order tensors are approximated by low-rank ones, which reveal the structure of the data [3], [9], [27]. The error of the approximation is measured as a weighted mean of squared deviations in individual tensor entries.

Traditionally, like in the weighted tensor decomposition method proposed by Paatero *et al.* [20], the weights of the tensor entries are proposed to be inversely proportional to the variance of the entries to achieve the optimum performance. In other words, it is assumed that the tensor entries are mutually independent noisy observations of some true tensor elements, and that their variances are known. By contrast, what we propose is a more sophisticated weighting of the mean-square error (MSE), which reflects possible correlations between errors in different entries. The weighting is derived for the case when the tensor is formed of covariance matrices of the given signal (the mixture) in different non-overlapping time blocks, and the separated signals are modelled as piecewise temporarily white Gaussian processes. The weighting was derived from the maximum likelihood principle. If the statistical model of the data is different, probably it will need another weighting.

For the tensor decomposition itself it is proposed to adapt the algorithm of Paatero *et al.* [20]. This is a specific modification of the damped Gauss–Newton or Levenberg–Marquardt method [19]. The algorithm is initialized by the outcome of SOBIUM [12].

Once the mixing matrix is estimated, it can be used for the separation of the original signals. Many techniques have already been proposed in the literature, especially those based on the sparsity of signals [2], [17], [18]. Owing to the piecewise stationary model of signals assumed here, we consider the optimum beamformer in each block, which maximizes the signal-to-interference ratio of each separated signal with respect to the remaining signals. We show in the paper that the method allows, for example, to separate 16 speech sources out of nine linear instantaneous mixtures of the length 8 s sampled at 16 kHz with the output signal-to-interference ratio (SIR) of 0–5 dB. The separated speech signals are understandable.

The number of the sources may not always be known in advance. In biomedical applications, it is typically not known. It would be desirable to have an automatic method of estimating the number of active sources. One possibility considered in the paper is the use of the minimum description length (MDL) criterion. Basically, it is equal to the value of the log-likelihood function of the corresponding signal model plus a penalty term that expresses complexity of the signal model. The number of active sources might be estimated as the one leading to the minimum MDL criterion.

This paper is organized as follows. Section II introduces the signal model and tensor of the covariance matrices. In Section III, a novel weighted criterion for fitting the tensor is proposed. Sections IV and V contain details of the weighted CP optimization. Section VI presents a method of estimating the separated signals based upon the estimate of the mixing matrix. Section VII contains details of computing the Cramér–Rao lower bound on the variances of elements of the mixing matrix, in order to show that the proposed method is asymptotically statistically efficient. Section VIII details how we compute the MDL criterion, Section IX contains simulations, and Section X concludes the paper.

II. Signal Model

Assume that the received signal $\mathbf{X}$ can be written as

$$\mathbf{X} = \mathbf{AS} \qquad (d \times N) \tag{1}$$

where the mixing matrix $\mathbf{A}$ has the size $d \times r$, $r > d$, and the source matrix $\mathbf{S}$ contains r independent sources, stored in rows. Next, assume that the signals can be partitioned into M blocks (epochs). In each block, the separated sources have zero mean and a fixed variance. Let D_{kf}—that is, the (k, f)th element of a matrix $\mathbf{D}$—denote the variance of the fth signal in the kth block. The length of each block is $N_1 = N/M$ and we assume, for simplicity, that it is an integer. Let $\mathbf{R}_k$ denote the theoretical covariance matrix of the mixture in the kth block. Then

$$\mathbf{R}_k = \sum_{f=1}^{r} D_{kf}\mathbf{A}_{:,f}\mathbf{A}_{:,f}^T = \mathbf{A}\mathrm{diag}(\mathbf{D}_{k,:})\mathbf{A}^T \tag{2}$$

where $\mathbf{A}_{:,f}$ is the fth column of the matrix $\mathbf{A}$, and $\mathbf{D}_{k,:}$ is the kth row of $\mathbf{D}$. The set of the M covariance matrices represents a three way tensor of the dimension (d, d, M) with the elements

$$\mathcal{R}_{kij}(\boldsymbol{\theta}) = \sum_{f=1}^{r} A_{if}A_{jf}D_{kf}. \tag{3}$$

Here, $\boldsymbol{\theta}$ represents a parameter vector that consists of all elements of the matrices $\mathbf{A}$ and $\mathbf{D}$. Symbolically,

$$\mathcal{R}(\boldsymbol{\theta}) = \mathcal{I} \times_1 \mathbf{A} \times_2 \mathbf{A} \times_3 \mathbf{D} \tag{4}$$

where $\mathcal{I}$ is the identity tensor of the dimension (r, r, r), and $\times_i$ denotes a matrix multiplication in the mode i, $i = 1, 2, 3$. The tensor $\mathcal{R}(\boldsymbol{\theta})$ is written as a sum of r rank-one tensors and by definition, the tensor rank is equal at most r. There are three modes, two of which are equal to $\mathbf{A}$, and the third mode $\mathbf{D}$ has nonnegative elements.

III. CP/INDSCAL Decomposition

Identifiability of the CP tensor decomposition has been studied by several authors, most notably Kruskal [16]. The

decomposition is called *Indscal*, if the first two factors are identical. A *sufficient* condition requires that $2k_{\mathbf{A}} + k_{\mathbf{D}} \geq 2r + 2$, where $k_{\mathbf{A}}$ and $k_{\mathbf{D}}$ is the Kruskal rank of $\mathbf{A}$ and $\mathbf{D}$, respectively. In the best case, $k_{\mathbf{A}} = d$ and $k_{\mathbf{D}} = r$ provided that $M \geq r$. Then, the Kruskal condition requires that

$$r \leq 2d - 2. \tag{5}$$

A tighter *sufficient* (but not necessary) condition on the maximum tensor rank admitting an essentially unique decomposition was derived in [24], see also [13].[1] The condition for the Indscal problem in the real domain is

$$\frac{r(r-1)}{2} \leq \frac{d(d-1)}{4}\left[\frac{d(d-1)}{2}+1\right] - \binom{d}{4} 1_{d\geq 4} \tag{6}$$

where $1_{d\geq 4}$ is the indicator of the event $d \geq 4$, and the matrix $\mathbf{D}$ must have a full column rank.

Note that in our model, the number of the free tensor elements, is $Md(d+1)/2$ due to symmetry of the covariance matrices, and the number of free parameters of the decomposition is $r(d + M - 1)$. For $d = 2$ and $r = 3$, the latter number exceeds the former one for any M. This fact indicates that separation of three sources from two mixtures might be problematic in this tensor method.[2] However, (6) indicates possibility to separate four sources from three mixtures. The number of sources that can yet be separated grows quadratically with the number of mixtures.

Traditional tensor decomposition methods seek for the decomposition of the tensor by minimizing the mean-square fit

$$\mathcal{Q}_1(\boldsymbol{\theta}) = \left\| \widehat{\mathcal{R}} - \mathcal{R}(\boldsymbol{\theta}) \right\|^2 = \sum_{i,j,k} \left(\widehat{\mathcal{R}}_{kij} - \mathcal{R}_{kij}(\boldsymbol{\theta}) \right)^2. \tag{7}$$

However, in our statistical model, the estimated tensor elements are mutually correlated, and the minimization of the criterion in (7) is not statistically optimum. We prove in Appendix A that the asymptotically optimum criterion which should replace (7) is

$$\mathcal{Q}_2(\boldsymbol{\theta}) = \sum_{k=1}^{M} \mathrm{tr}\left[\widehat{\mathbf{R}}_k^{-1} \left(\widehat{\mathbf{R}}_k - \mathbf{R}_k(\boldsymbol{\theta}) \right) \widehat{\mathbf{R}}_k^{-1} \left(\widehat{\mathbf{R}}_k - \mathbf{R}_k(\boldsymbol{\theta}) \right) \right] \tag{8}$$

where $\mathrm{tr}(\cdot)$ denotes the trace of a matrix, assuming that the covariance matrices $\mathbf{R}_k$ are invertible. More generally, we can write

$$\mathcal{Q}_3(\boldsymbol{\theta}) = \sum_{k=1}^{M} \mathrm{tr}\left[\mathbf{C}_k \left(\widehat{\mathbf{R}}_k - \mathbf{R}_k(\boldsymbol{\theta}) \right) \mathbf{C}_k \left(\widehat{\mathbf{R}}_k - \mathbf{R}_k(\boldsymbol{\theta}) \right) \right] \tag{9}$$

where the matrices $\mathbf{C}_k$ are chosen as $\mathbf{C}_k = (\widehat{\mathbf{R}}_k + \varepsilon \mathbf{I})^{-1}$ with a suitable small positive constant ε to maintain regularity of the criterion under all circumstances. Note that in the special case $\mathbf{C}_1 = \ldots = \mathbf{C}_M = \mathbf{I}$ the criteria (7) and (9) coincide. For numerical purposes it is thus convenient to initialize the optimization by the outcome of a standard parallel factor analysis algorithm, choose a large initial ε, and decrease it gradually towards zero.

Note that each of the optimization problems (7)–(9) has the same scale uncertainty, which basically says that the change of scale in one mode of any factor can be compensated by appropriate change in scale of the same factor in one of the other two modes. Therefore, it is possible to assume, without any loss in generality, that all columns of $\mathbf{A}$ have unit norm, or to fix (exclude from the minimization) one element in each column of the matrix $\mathbf{D}$.

IV. Nonnegativity Constraint on $\mathbf{D}$

If the SOBIUM algorithm is applied to the tensor $\mathcal{R}$, it may occur that some entries of the estimated matrix $\mathbf{D}$ are negative, because this algorithm does not impose any constraint on the signs of the factor matrices' elements. It would not give a meaningful model of the data, because the variances of the separated signals have to be nonnegative by definition.

A vast literature exists on a nonnegative tensor decomposition—see, e.g., the partial overview in [4]. Since we wish to use the Levenberg–Marquardt method for the minimization of the criterion, it seemed natural to adopt the method from [20] which consists of augmenting the target criterion by a suitable barrier function. Following [20], we propose subtracting a scaled sum of logarithms of the factor elements. Such a barrier function is easy to differentiate. In our case, however, the criterion would not be invariant with respect to the scale uncertainty, because only one mode is constrained to be nonnegative, not all. Bearing this in mind, we propose the criterion

$$\mathcal{Q}_4(\boldsymbol{\theta}) = \mathcal{Q}_3(\boldsymbol{\theta}) - \alpha \sum_{f=1}^{r} \left[\sum_{k=1}^{M} \log D_{kf} + M \log \left(\sum_{k=1}^{d} A_{kf}^2 \right) \right]. \tag{10}$$

The criterion in (10) has the advantage that if a column in mode $\mathbf{A}$ is multiplied by a constant and the corresponding column in $\mathbf{D}$ is divided by the same constant squared, the criterion is not affected.

In (10), α is a positive parameter which starts from an initial value (e.g., 1) and is decreased gradually towards zero during the optimization. In each fifth iteration, parameter α is multiplied by a factor smaller than 1, say 0.5. It is important that at the end of the optimization, α should be close to zero so that the barrier function does not influence position of the minimum of the criterion. The barrier should only maintain nonnegativity of elements of $\mathbf{D}$.

Note that the presence of the barrier function makes the criterion function smoother in the sense that it removes some local minima of the function. Thus, for larger α the function is easier to minimize. Gradual decrease of α increases probability of the optimization process not to be stacked in local minima. Alternative optimization strategies also exist: e.g., an *interior-point trust-region-based method* [5].

V. Optimization Details

Optimization of the criterion in (10) can proceed using the following steps.

1) Initialize the algorithm by the outcome of SOBIUM by De Lathauwer [12].

[1]The condition (6) applies with probability one if the matrix $\mathbf{A}$ is drawn randomly from a continuous distribution.

[2]Some other methods such as ALESCAF [7] using higher order statistics and higher than three-way tensors allow identification of three or more non-Gaussian sources from two mixtures.

TABLE I
LEVENBERG–MARQUARDT METHOD

begin
$i := 0; \quad \nu := 2; \quad \boldsymbol{\theta} := \boldsymbol{\theta}_0;$
$\boldsymbol{\Psi} := \boldsymbol{\Psi}(\boldsymbol{\theta}); \quad \boldsymbol{\xi} := \boldsymbol{\xi}(\boldsymbol{\theta});$
$found := (\|\boldsymbol{\xi}\|_\infty \leq \varepsilon_1); \quad \mu := \tau * \max(\mathrm{diag}(\boldsymbol{\Psi}));$
while (**not** $found$) **and** $(i < i_{max})$
$i := i + 1; \quad \Delta\boldsymbol{\theta} := (\boldsymbol{\Psi} + \mu\mathbf{I})^{-1}\boldsymbol{\xi}$
if $\|\Delta\boldsymbol{\theta}\| \leq \varepsilon_2(\|\boldsymbol{\theta}\| + \varepsilon_2)$
$found := \mathbf{true}$
else
$\boldsymbol{\theta}_{new} := \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$
$\rho := [\mathcal{Q}(\boldsymbol{\theta}) - \mathcal{Q}(\boldsymbol{\theta}_{new})]/[\Delta\boldsymbol{\theta}^T(\boldsymbol{\xi} + \mu\Delta\boldsymbol{\theta})]$
if $\rho > 0$ {step accepted}
$\boldsymbol{\theta} := \boldsymbol{\theta}_{new}; \quad \boldsymbol{\Psi} := \boldsymbol{\Psi}(\boldsymbol{\theta}); \quad \boldsymbol{\xi} := \boldsymbol{\xi}(\boldsymbol{\theta});$
$found := (\|\Delta\boldsymbol{\theta}\|_\infty \leq \varepsilon_1);$
$\mu := \mu * \max\{\frac{1}{3}, 1 - (2\rho - 1)^3\}; \quad \nu := 2;$
else
$\mu := \mu * \nu; \quad \nu := 2 * \nu$
end

2) Make the elements of the factor matrix $\mathbf{D}$ positive (take an absolute value or add a constant).
3) Iterate (until convergence is achieved) the LM algorithm

$$\Delta\boldsymbol{\theta} = (\boldsymbol{\Psi} + \mu\mathbf{I})^{-1}\boldsymbol{\zeta}$$

where $\boldsymbol{\Psi}$ is the Hessian of the criterion (10), $\boldsymbol{\zeta}$ is its gradient, and μ is a positive parameter that is gradually modified by the technique described in [19], see also Table I. After each five steps of the LM algorithm, decrease ε in (9) and α in (10) to one half of their current respective values.

The closed form of the Hessian and the gradient are derived in Appendix B. This method usually requires 50–100 iteration steps to converge. Note that the part of $\boldsymbol{\Psi}$ that corresponds to the estimated elements of $\mathbf{D}$ is block diagonal and therefore it can be inverted more effectively. The main block of $\boldsymbol{\Psi}$ to be inverted has the size $dr \times dr$. The inversion is computationally the most complex part of the algorithm. The complexity of each iteration is thus $O(d^3r^3)$.

VI. ESTIMATION OF THE SEPARATED SIGNALS

Assume that the mixing matrix $\mathbf{A}$ and the variances of the separated signals on each interval are already estimated or that they are known *a priori*. In terminology of the sensor array processing, columns of $\mathbf{A}$ represent directions of arrivals of waves that are additively combined on the array sensors to form the received signals, i.e., rows of the matrix $\mathbf{X}$. Although it is not possible to find an inverse of $\mathbf{A}$ which has, by assumption, more columns than rows, we show that it is still possible to estimate the original signals. The separation can be interpreted as finding beamformers, one for each separated source and each block. The beamformers are represented by some to-be-determined d- dimensional vectors $\mathbf{w}_j$, $j = 1, \ldots, r$, such that

$$\widehat{\mathbf{S}}_{j,:} = \mathbf{w}_j^T\mathbf{X} = \mathbf{w}_j^T\mathbf{A}\mathbf{S} \tag{11}$$

is an estimate of the jth source, the jth row of $\mathbf{S}$. The expression (11) can be rewritten as

$$\widehat{\mathbf{S}}_{j,:} = \sum_{\ell=1}^{r} \mathbf{w}_j^T\mathbf{A}_{:,\ell}\mathbf{S}_{\ell,:} = \mathbf{w}_j^T\mathbf{A}_{:,j}\mathbf{S}_{j,:} + \sum_{\ell\neq j} \mathbf{w}_j^T\mathbf{A}_{:,\ell}\mathbf{S}_{\ell,:}. \tag{12}$$

Therefore the SIR of the jth estimated source in the kth block, where variances of the individual sources are $D_{k\ell}$, $\ell = 1, \ldots, r$, is

$$\mathrm{SIR}_{kj}(\mathbf{w}_j) = \frac{\left(\mathbf{w}_j^T\mathbf{A}_{:,j}\right)^2 D_{kj}}{\sum_{\ell\neq j}\left(\mathbf{w}_j^T\mathbf{A}_{:,\ell}\right)^2 D_{k\ell}}. \tag{13}$$

The SIR is varying from block to block, as well as the beamformer that maximizes it. Note that (13) can be written as

$$\mathrm{SIR}_{kj}(\mathbf{w}_j) = \frac{\mathbf{w}_j^T\mathbf{M}_1\mathbf{w}_j}{\mathbf{w}_j^T\mathbf{M}_2\mathbf{w}_j} \tag{14}$$

where $\mathbf{M}_1 = D_{kj}\mathbf{A}_{:,j}\mathbf{A}_{:,j}^T$ and $\mathbf{M}_2 = \mathbf{R}_k - D_{kj}\mathbf{A}_{:,j}\mathbf{A}_{:,j}^T$. It readily follows that the beamformer maximizing the SIR is the so-called MVDR beamformer, (up to an arbitrary multiplicative constant) equal to the principal generalized eigenvector of the matrix pencil $(\mathbf{M}_1, \mathbf{M}_2)$. The beamformer can be further shown to be equal to

$$\arg\max_{\mathbf{w}_j} \mathrm{SIR}_{kj}(\mathbf{w}_j) = \gamma\mathbf{R}_k^{-1}\mathbf{A}_{:,j} \tag{15}$$

where γ is an arbitrary constant. It is convenient to set $\gamma = D_{kj}$ so that the proposed jth beamformer at the kth block is

$$\mathbf{w}_{jk} = D_{jk}\mathbf{R}_k^{-1}\mathbf{A}_{:,j}. \tag{16}$$

Let $\mathbf{X}^{(k)}$ denote the kth block of the data (the mixture) and $\widehat{\mathbf{S}}^{(k)}$ be the separated sources in the kth block. With the choice (16) it holds that

$$\mathbf{X}^{(k)} = \mathbf{A}\widehat{\mathbf{S}}^{(k)} = \sum_{j=1}^{r} \mathbf{A}_{:,j}\mathbf{w}_{jk}^T\mathbf{X}^{(k)} \tag{17}$$

because

$$\sum_{j=1}^{r} \mathbf{A}_{:,j}\mathbf{w}_{jk}^T = \sum_{j=1}^{r} \mathbf{A}_{:,j}\left(D_{kj}\mathbf{R}_k^{-1}\mathbf{A}_{:,j}\right)^T = \left[\sum_{j=1}^{r} D_{kj}\mathbf{A}_{:,j}\mathbf{A}_{:,j}^T\right]\mathbf{R}_k^{-1} = \mathbf{I} \tag{18}$$

thanks to (2). In other words, the choice (16) ensures the fit between the mixture of the separated signals and the original mixture.

An estimated optimum beamformer is obtained by replacing the theoretical matrices $\mathbf{R}_k$, $k = 1, \ldots, M$, $\mathbf{A}$ and $\mathbf{D}$ by their sample estimates. Note that unlike the determined case $r \leq d$, the SIR of the separated signals will not grow to infinity with increasing data length, but only approach the SIR of the optimal beamformer. The optimal SIR of the jth estimated source in the

kth block can be written, after a straightforward computation, as

$$\mathrm{SIR}_{jk}^{(\mathrm{opt})}(\mathbf{w}_{jk}) = \frac{D_{kj}\mathbf{A}_{:,j}^T\mathbf{R}_k^{-1}\mathbf{A}_{:,j}}{1 - D_{kj}\mathbf{A}_{:,j}^T\mathbf{R}_k^{-1}\mathbf{A}_{:,j}}. \tag{19}$$

The total optimum SIR (for known $\mathbf{A}$ and $\mathbf{D}$) of the jth separated source in all blocks together is

$$\begin{aligned}\mathrm{SIR}_j^{(\mathrm{opt})}&\left(\{\mathbf{w}_{jk}\}\right)\\ &= \frac{\sum_{k=1}^M \left(\mathbf{w}_{jk}^T\mathbf{A}_{:,j}\right)^2 D_{kj}}{\sum_{k=1}^M \mathbf{w}_{jk}^T\left(\mathbf{R}_k - D_{kj}\mathbf{A}_{:,j}\mathbf{A}_{:,j}^T\right)\mathbf{w}_{jk}}\\ &= \frac{\sum_{k=1}^M D_{kj}^3\left(\mathbf{A}_{:,j}^T\mathbf{R}_k^{-1}\mathbf{A}_{:,j}\right)^2}{\sum_{k=1}^M D_{kj}^2\mathbf{A}_{:,j}^T\mathbf{R}_k^{-1}\mathbf{A}_{:,j}\left(1 - D_{kj}\mathbf{A}_{:,j}^T\mathbf{R}_k^{-1}\mathbf{A}_{:,j}\right)}.\end{aligned} \tag{20}$$

Note that if the jth signal were estimated with *the same* beamformer in all blocks, the resulting SIR would be *worse*, in general. Such optimum joint beamformer would be equal to

$$\mathbf{w}_j^{(\mathrm{one})} = \left(\sum_{k=1}^M \mathbf{R}_k\right)^{-1}\mathbf{A}_{:,j} \tag{21}$$

and its SIR would be

$$\mathrm{SIR}_j^{(\mathrm{one})} = \frac{\left(\mathbf{A}_{:,j}^T\mathbf{w}_j^{(\mathrm{one})}\right)^2\sum_{k=1}^M D_{kj}}{\sum_{k=1}^M\left(\mathbf{w}_j^{(\mathrm{one})}\right)^T\left(\mathbf{R}_k - D_{kj}\mathbf{A}_{:,j}\mathbf{A}_{:,j}^T\right)\mathbf{w}_j^{(\mathrm{one})}}. \tag{22}$$

After some simplifications,

$$\mathrm{SIR}_j^{(\mathrm{one})} = \frac{\mathbf{A}_{:,j}^T\left(\sum_{k=1}^M \mathbf{R}_k\right)^{-1}\mathbf{A}_{:,j}\sum_{k=1}^M D_{kj}}{1 - \mathbf{A}_{:,j}^T\left(\sum_{k=1}^M \mathbf{R}_k\right)^{-1}\mathbf{A}_{:,j}\sum_{k=1}^M D_{kj}}. \tag{23}$$

VII. Cramér–Rao Lower Bound

Cramér–Rao lower bound (CRLB) is a tool to verify whether an algorithm achieves the best achievable performance, measured in terms of the mean square estimation error of the mixing matrix $\mathbf{A}$. In most practical cases, the CRLB is asymptotically equal to the covariance matrix of the error of the maximum likelihood estimate.

The mixture data in the kth block are represented by a zero mean Gaussian random vector with the covariance matrix $\mathbf{R}_k$ defined in (2). By taking all the available samples into account, the whole model is parameterized by the elements of the matrices $\mathbf{A}$ and $\mathbf{D}$ that are yet to be estimated. Yet, there is a scale ambiguity which has to be fixed; otherwise, the Fisher information matrix (FIM) would not be invertible. Without loss of generality, we assume that the scale of the original sources is one, which means $\sum_{k=1}^M D_{kf} = 1$, $f = 1,\ldots,r$. Therefore, we fix the variance of the signals in the first block so that

$$D_{1f} = 1 - \sum_{k=2}^M D_{kf}, \quad f = 1,\ldots,r. \tag{24}$$

Consequently, there are $(d + M - 1)r$ parameters to be estimated; let $\boldsymbol{\vartheta}$ denote the truncated parameter vector $\boldsymbol{\theta}$ containing only these parameters.

The pqth element of the FIM of the mixed signals at any time instant in the kth block is given by [22, p. 134, Theorem 5.1]

$$\mathbf{F}_{pq}^{(k)} = \frac{1}{2}\mathrm{tr}\left[\mathbf{R}_k^{-1}\frac{\partial\mathbf{R}_k}{\partial\vartheta_p}\mathbf{R}_k^{-1}\frac{\partial\mathbf{R}_k}{\partial\vartheta_q}\right] \tag{25}$$

where the partial derivatives are applied element-wise. Now the whole FIM can be computed numerically by using the rules derived in Appendix C. Since samples of the mixed signals at different time instants are independent, the FIM of the entire data set is

$$\mathbf{F} = N_1\sum_{k=1}^M \mathbf{F}^{(k)}. \tag{26}$$

Finally, the CRLB of the covariance of any unbiased estimator $\hat{\boldsymbol{\vartheta}}$ of $\boldsymbol{\vartheta}$ reads as

$$\mathrm{cov}[\hat{\boldsymbol{\vartheta}}] \geq \mathbf{F}^{-1}. \tag{27}$$

The CRLB can be used to derive a Cramér–Rao induced lower bound (CRIB) of the mean-square angular deviation[3] between columns of the mixing matrix $\mathbf{A}$ and its estimates, as follows.

Let $\mathbf{A}_{:,k}$ be the kth column of $\mathbf{A}$, and $\hat{\mathbf{A}}_{:,k}$ be its sample estimate. Let $\mathrm{CRLB}(\mathbf{A}_{:,k})$ be the submatrix of $\mathbf{F}^{-1}$ which bounds the mean square error in estimating $\mathbf{A}_{:,k}$. The angle ω between $\mathbf{A}_{:,k}$ and $\hat{\mathbf{A}}_{:,k}$ is defined through its cosine as

$$\cos\omega_k = \frac{\mathbf{A}_{:,k}^T\hat{\mathbf{A}}_{:,k}}{||\mathbf{A}_{:,k}||||\hat{\mathbf{A}}_{:,k}||} = \frac{x + \varepsilon}{\sqrt{x(x + 2\varepsilon + \nu)}} \tag{28}$$

where $x = \mathbf{A}_{:,k}^T\mathbf{A}_{:,k}$, $\varepsilon = \mathbf{A}_{:,k}^T\Delta\mathbf{A}_{:,k}$, $\nu = \Delta\mathbf{A}_{:,k}^T\Delta\mathbf{A}_{:,k}$, and $\Delta\mathbf{A}_{:,k} = \hat{\mathbf{A}}_{:,k} - \mathbf{A}_{:,k}$. Taking the second-order Taylor series expansion on both sides of (28) and neglecting all higher-order terms of ω, ε and ν we get

$$1 - \frac{1}{2}\omega_k^2 = 1 + \frac{1}{2}\frac{\varepsilon^2}{x^2} - \frac{1}{2}\frac{\nu}{x}. \tag{29}$$

Therefore

$$\omega_k^2 = \frac{x\nu - \varepsilon^2}{x^2} = \frac{1}{x^2}\left[x\Delta\mathbf{A}_{:,k}^T\Delta\mathbf{A}_{:,k} - \mathbf{A}_{:,k}^T\Delta\mathbf{A}_{:,k}\Delta\mathbf{A}_{:,k}^T\mathbf{A}_{:,k}\right] \tag{30}$$

and consequently

$$\begin{aligned}\mathrm{E}\left[\omega_k^2\right] &= \frac{1}{x^2}\left\{x\mathrm{E}\left[\Delta\mathbf{A}_{:,k}^T\Delta\mathbf{A}_{:,k}\right]\right.\\ &\qquad\left. - \mathbf{A}_{:,k}^T\mathrm{E}\left[\Delta\mathbf{A}_{:,k}\Delta\mathbf{A}_{:,k}^T\right]\mathbf{A}_{:,k}\right\}\\ &= \frac{1}{x^2}\left\{x\mathrm{E}\left[\mathrm{tr}\left(\Delta\mathbf{A}_{:,k}\Delta\mathbf{A}_{:,k}^T\right)\right]\right.\\ &\qquad\left. - \mathbf{A}_{:,k}^T\mathrm{E}\left[\Delta\mathbf{A}_{:,k}\Delta\mathbf{A}_{:,k}^T\right]\mathbf{A}_{:,k}\right\}.\end{aligned} \tag{31}$$

[3]Note that the deviation may or may not be interpreted as an angular error of direction-of-arrival of the signal on the sensor array.

If $\hat{\mathbf{A}}_{:,k}$ is the maximum likelihood estimate of $\mathbf{A}_{:,k}$, it holds asymptotically that $\mathrm{E}[\Delta\mathbf{A}_{:,k}\Delta\mathbf{A}_{:,k}^T] = \mathrm{CRLB}(\mathbf{A}_{:,k})$. It follows that the CRIB on the mean-square angle deviation of $\hat{\mathbf{A}}_{:,k}$ can be defined as

$$\begin{aligned}\mathrm{CRIB}(\mathbf{A}_{:,k}) &= \frac{\mathrm{tr}\,[\mathrm{CRLB}(\mathbf{A}_{:,k})]}{\|\mathbf{A}_{:,k}\|^2} - \frac{\mathbf{A}_{:,k}^T\mathrm{CRLB}(\mathbf{A}_{:,k})\mathbf{A}_{:,k}}{\|\mathbf{A}_{:,k}\|^4} \\ &= \frac{1}{\|\mathbf{A}_{:,k}\|^2}\mathrm{tr}\left[\Pi_{A_{:,k}}^{\perp}\mathrm{CRLB}(\mathbf{A}_{:,k})\right] \qquad (32)\end{aligned}$$

where

$$\Pi_{A_{:,k}}^{\perp} = \mathbf{I} - \mathbf{A}_{:,k}\mathbf{A}_{:,k}^T/\|\mathbf{A}_{:,k}\|^2 \qquad (33)$$

is the projection operator to the orthogonal complement of $\mathbf{A}_{:,k}$. It easily follows that the CRIB is always non-negative.

VIII. Estimating the Number of the Sources

In many applications, e.g., in biomedical signal processing—EEG in particular—the number of the sources may not be known in advance. It would be highly desirable to have a method of estimating the model order. In this paper, we propose one possible approach—using the MDL [23].

The MDL can be written as a sum of two terms: a log-likelihood function of the model achieved at the given data, and a penalty term that accounts for the model complexity. The log-likelihood function of the data model for given number of sources (tensor rank) was derived in Appendix A. The number of free parameters in the model is $r(d+M-1)$. The resultant MDL criterion is then

$$\begin{aligned}\mathrm{MDL}(r) = \frac{N_1}{2}\sum_{k=1}^{M}\left[\log\det\mathbf{R}_k + \mathrm{tr}\left(\mathbf{R}_k^{-1}\widehat{\mathbf{R}}_k\right)\right] \\ +r(d+M-1)\log N_1. \qquad (34)\end{aligned}$$

It is believed that minimization of the MDL criterion gives an asymptotically unbiased estimate of the dimension of the model, if the number of data in each block grows to infinity. In practice, it appears that if the signal does not exactly fit the assumed model (such as speech signals), minimization of the MDL slightly overestimates the number of the sources.

IX. Simulations

A. Artificial Data Obeying the Model

Four artificial signals of the length $N = 10\,000$ partitioned into $M = 10$ epochs (blocks) of equal length were generated as independent zero mean Gaussian random variables with variances D_{mk}, where m is the index of the epoch and k is the index of the signal. The variances versus m and k were taken as variables in Fig. 1. The variances were normalized so that $\sum_m D_{mk} = 1$ for all k. Note that three of the variances were set close to zero at some epoch, but it need not be assumed that some signals are not active, as some other methods require.

The data were mixed in three observed channels via a mixing matrix with columns $\mathbf{A}_{:,k} = [1, \cos(\phi_k), \sin(\phi_k)]^T$, where $(\phi_1, \phi_2, \phi_3, \phi_4) = (0, \pi/4, \pi/2, 3\pi/4)$.

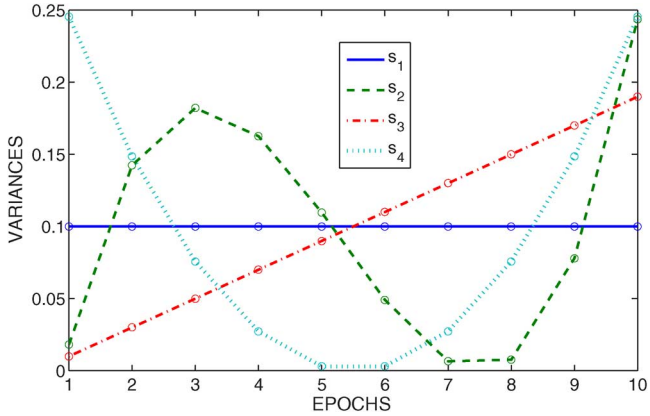

Fig. 1. Variances of the artificial signals in the ten epochs.

TABLE II
Mean-Square Angular Error of Columns of $\mathbf{A}$ [dB]

component no.	1	2	3	4
UDSEP	-28.0	-29.4	-26.4	-34.8
SOBIUM	-24.8	-23.7	-21.4	-32.5
CRIB	-25.7	-27.3	-22.4	-34.2

The data were generated repeatedly in 500 independent trials, mixed together and analyzed by the proposed algorithm. The outcome of the algorithm was sorted to fit the orders and the signs of the original signals. Quality of the separation was measured by the mean-square angular error (MSAE) of columns of the estimated mixing matrix from their true counterparts. The MSAE of the proposed algorithm, the MSAE of SOBIUM, and the corresponding CRIB (32) are summarized in Table II. We note that the performance of UDSEP significantly (by 2.3–5.7 dB) exceeds the performance of SOBIUM, and it even exceeds the CRIB in the case of the second and the third signal. The estimator is thus superefficient.

We believe that the superefficiency is caused by the very small variance of the original signals in some of the epochs. Since the variances are estimated as well, and they cannot be negative, their restricted range is in conflict with the assumed unbiasedness of the estimator. The assumption of nonnegativity of some parameters may also be interpreted as a prior knowledge about the parameter, which improves the ratability of the parameters (all of them) in general, but it is not underpinned by the Cramér–Rao theory.

The hypothesis is confirmed by the following test. All variances are increased by some value, say v, the same for all signals and epochs. Performance of the algorithms is studied for varying v. With growing v the dynamics of variance profiles of the signals are reduced, and, consequently, the separation accuracy is lowered. Results are shown in Fig. 2. If the value of v exceeds 0.1, the estimation errors of the second and the third column of $\mathbf{A}$ follow the CRIB. The estimation of the first and last columns of $\mathbf{A}$ tends to follow the bound as well, but for $v \geq 0.2$ there are 1%–4% of trials which spoil the plain average angular error. If these trials are excluded, the coincidence between the CRIB and the estimation error is very good again.

The estimated matrix $\mathbf{A}$ was used to build beamformers that separate the individual sources, described in Section VI. It was

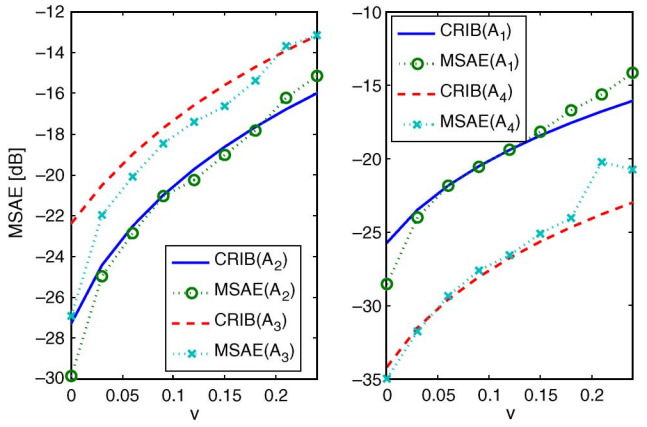

Fig. 2. Mean-square angular errors in estimating columns of the mixing matrix $\mathbf{A}$ plus corresponding Cramér–Rao induced bound versus the increment v added to all variances in Fig. 1.

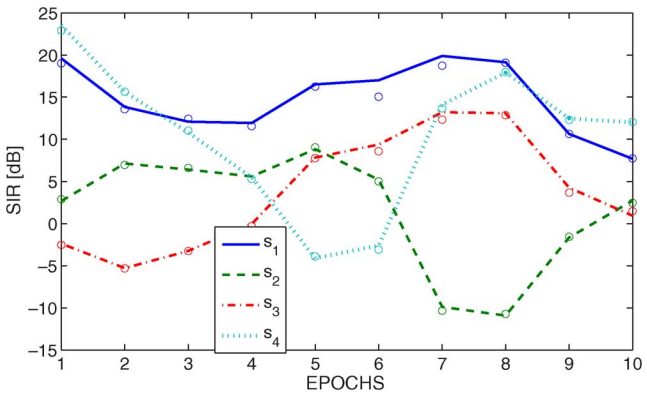

Fig. 3. SIR of the optimum separating beamformers obtained for the true mixing matrix $\mathbf{A}$ (solid, dashed, dot-dashed and dotted line) and those obtained through the estimated $\mathbf{A}$ (circles).

TABLE III
SIR OF THE SEPARATED SIGNALS [dB]

component no.	1	2	3	4
UDSEP	12.92	4.21	4.17	13.02
SOBIUM	12.43	3.24	3.59	12.65
SIR_{opt}	13.36	5.07	5.89	13.62
SIR_{one}	11.02	1.28	1.28	11.02

found that the output SIR differs a little from the SIR of the optimum beamformer that would be obtained by using the original (correct) matrix $\mathbf{A}$. This is shown in Fig. 3. For each signal, the periods of the low output SIR correspond to periods where the input SIR is low as well (cf. Fig. 1). Finally, the overall SIR of the separated signals obtained by UDSEP and SOBIUM, and SIR of the optimum beamformer (20) and (23) are presented in Table III. Again, UDSEP outperforms SOBIUM, and is close to the performance of the optimum beamformer, which assumes knowledge of the mixing matrix.

B. Robustness Against Mismodeling

This subsection presents two examples that demonstrate robustness of the proposed algorithm against exact validity of the assumed data model. The data are generated in the same way as in the previous subsection in 100 independent trials. In the first experiment, the algorithm is run with tentatively wrong partitioning of the data. The data are partitioned into 5 to 20 segments. Results are summarized in Fig. 4, which shows the mean square angular error in estimating the columns of $\mathbf{A}$, and also total SIR obtained by the estimated separating beamformer. We note that the differences in performance due to the incorrect number of epochs are surprisingly minor. The second experiment (Fig. 5) shows robustness of the algorithm against an additive noise, which is included in the data but not in the assumed model. Here, the correct partitioning into $M = 10$ is used.

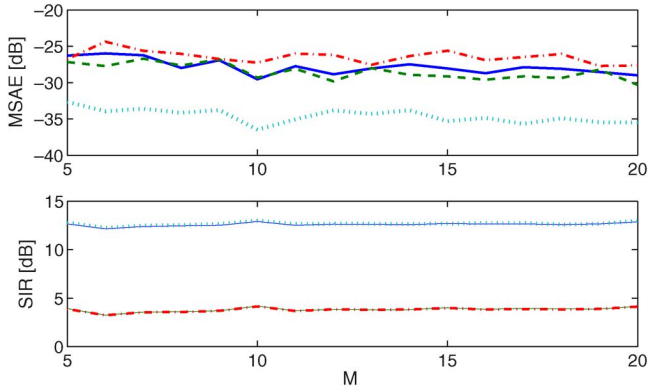

Fig. 4. Average angular error in estimating columns of the mixing matrix (upper diagram) and SIR of the separated signals (lower diagram) versus the number of epochs in the incorrectly partitioned signal.

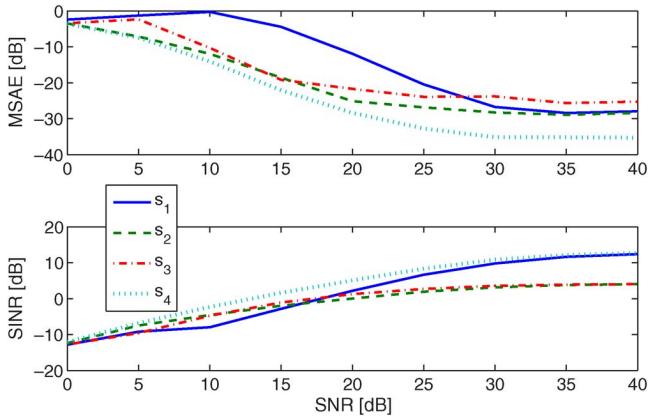

Fig. 5. Average angular error in estimating columns of the mixing matrix (upper diagram) and signal-to interference and noise (SINR) of the separated signals (lowed diagram) versus the input SNR, defined as $-10\log_{10}$ of the variance of the additive noise.

C. Crossing Sources (Colinear Factors)

The experiment from the Section IX-A was repeated with the difference that the first source had a changing position. In particular, the first column of the DOA matrix $\mathbf{A}$ was parameterized as $\mathbf{A}_{:,1} = [1; \cos\phi_1; \sin\phi_1]^T$ again, but the angle ϕ_1 was changing from 0 to π. In this interval, ϕ_1 crossed the angles of the other three sources. The result is shown in Fig. 6. It can be noticed that if ϕ_1 lies in vicinity of each of ϕ_2, ϕ_3 and ϕ_4, estimates of all columns of $\mathbf{A}$ have an increased variance. On the

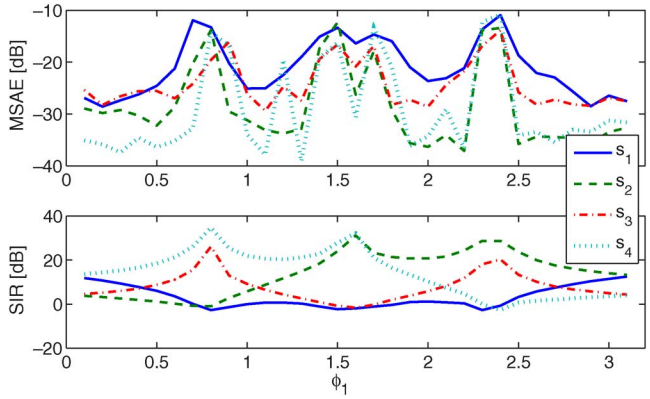

Fig. 6. Average angular error in estimating columns of the mixing matrix (upper diagram) and SINR of the separated signals (lowed diagram) versus varying parameter ϕ of the first source. At $\phi = k\pi/4$, $k = 1, 2, 3$, the first column of $\mathbf{A}$ is identical to the second, the third, and the fourth column, respectively.

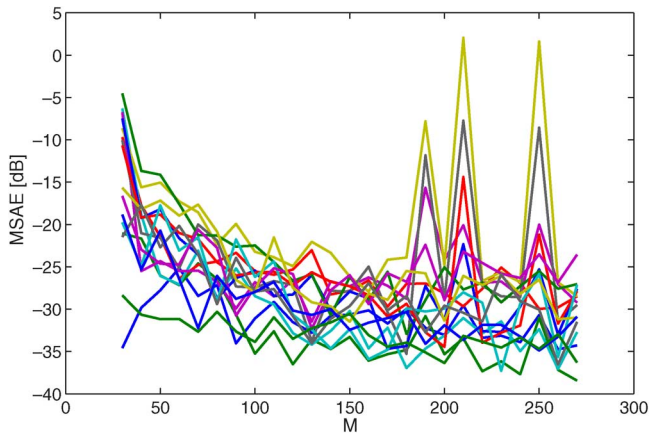

Fig. 7. Squared angular errors in estimating columns of the mixing matrix for UDSEP versus varying number of epochs.

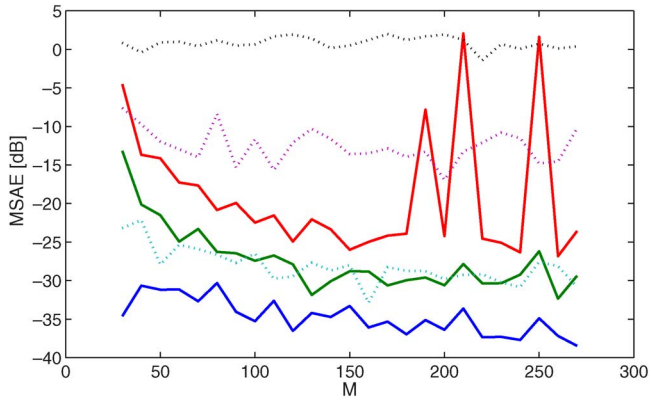

Fig. 8. Maximum, median and minimum average angular error in estimating columns of the mixing matrix for UDSEP (solid lines), and for SOBIUM (dotted lines) versus varying number of epochs.

other hand, the SIR of the separated signals is good for the other two sources, that are not crossed.

D. Acoustic (Speech) Data Separation

In this subsection, the set of 16 speech utterances of the length 8.375 s sampled at 16 kHz, normalized to have zero mean and unit variance, are taken as the original sources $\mathbf{S}$. The 9×16 mixing matrix is defined as by its columns of the form $\mathbf{A}_{:,k} = [1, \cos\phi_k, \cos 2\phi_k, \ldots, \cos 8\phi_k]^T$, where ϕ_k are auxiliary angles $\phi_k = k\pi/17$, $k = 1, \ldots, 16$. Note that all columns of $\mathbf{A}$ have the same norm. The structure of the matrix $\mathbf{A}$ is not used for the separation.[4] The SIR of the original signals in the mixture vary between -10 and -20 dB. The mixture $\mathbf{X} = \mathbf{AS}$ is processed by UDSEP with M blocks, where M was changing between 30 and 270. This means that the length of each block was from 279 to 31 ms. Angular errors of columns of the mixing matrix for UDSEP are plotted in Fig. 7. We note that for $M = 190$, 210 and 250, the algorithm has converged to a wrong local minimum. Three of the sixteen sources were not separated, accuracy of the other sources was not affected. A possible remedy to this problem is to let the algorithm run from several initial point, and select the result that leads the best fit of the tensor for the given rank. (It was not implemented, yet.) A comparison with performance of SOBIUM is presented in Fig. 8, where the minimum, maximum, and median angular error is shown for both of the methods. It is shown that UDSEP performs, indeed, much better. The same conclusion follows from comparison of the SIR of the separated signals, presented in Fig. 9. The algorithm does not seem to be very sensitive to the selection of the

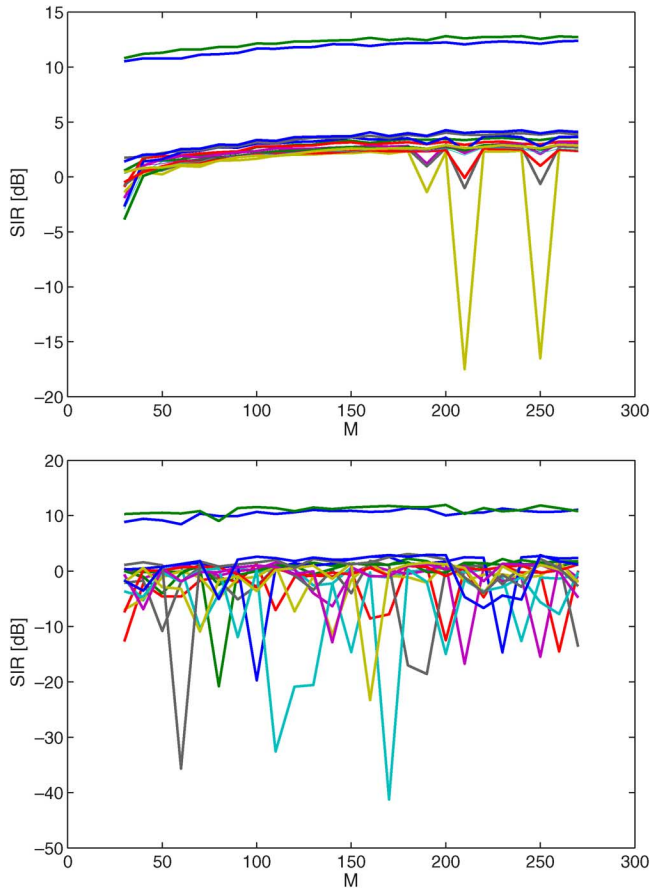

Fig. 9. SIR of the separated signals for UDSEP (upper diagram) and SOBIUM (lower diagram).

[4]We have also tried to generate $\mathbf{A}$ at random; Separation results were usually similar. The fixed $\mathbf{A}$ is used to avoid random large errors.

number of the epochs. The optimum is achieved for approximately 150 epochs, i.e., the length of each one was cca 56 ms.

Finally, we have studied usefulness of the MDL criterion, presented in Section VII. It appeared to overestimate the number of the sources. For example, for $M = 500$, it monotonically decreased with increasing expected number of sources until $d = 19$, and $d = 19$ is not the global minimum. It was observed, however, that if the number of the sources is overestimated, most of the truly existing sources are separated with a good accuracy and have larger estimated separation SIR than the fictitious (not really existing) sources. Design of a reliable method of estimating the number of the sources may be subject of a further research.

The mixture, the separated signals, and p-code of the separating procedure were posted on the Internet [26].

X. Conclusion

We have presented a novel blind algorithm to separate underdetermined instantaneous mixtures of nonstationary signals. The algorithm is based on a specifically weighted tensor decomposition of the set of covariance matrices of the received signal (mixture) in partitioning the signal in epochs. The tensor decomposition weighting is tailored to the signal model which assumes that the original (to be separated) signals are stationary inside the epochs but have variances which are different epoch to epoch. Performance of the algorithm significantly exceeds that of the general tensor decomposition method in SOBIUM. In simulations, the algorithm exceeds the corresponding Cramér–Rao bound, if variances of some of the signals at some of the epochs are close to zero. Experiments with separation of speech signals show that the algorithm performs very well, even when the signals do not obey the assumed model. It largely outperforms SOBIUM and is not much sensitive to the chosen length of the blocks. The algorithm may have potential applications in biomedical signal processing and in speech processing.

Appendix A

Derivation of the weighted criterion (8).

The criterion is derived from the maximum likelihood principle. The joint likelihood function of the data is

$$f(\mathbf{X}) = \prod_{k=1}^{M} (2\pi \det \mathbf{R}_k)^{-N_1/2} \exp\left[-\frac{1}{2}\sum_{t=1}^{N_1} \mathbf{X}_{k,:,t}^T \mathbf{R}_k^{-1} \mathbf{X}_{k,:,t}\right]$$

where $\mathbf{X}_{k,:,t}$ is the tth d dimensional sample of kth block of the mixture, and N_1 is the number of samples in each block. The log likelihood function is then

$$-\log f(\mathbf{X}) = \text{const} + \sum_{k=1}^{M} \frac{N_1}{2}\left[\log\det \mathbf{R}_k + \operatorname{tr}\left(\mathbf{R}_k^{-1}\widehat{\mathbf{R}}_k\right)\right] \tag{35}$$

where

$$\widehat{\mathbf{R}}_k = \frac{1}{N_1}\sum_{t=1}^{N_1} \mathbf{X}_{k,:,t}\mathbf{X}_{k,:,t}^T \tag{36}$$

The maximum likelihood estimate of a vector parameter $\boldsymbol{\theta}$ is obtained by inserting the model covariance $\mathbf{R}_k(\boldsymbol{\theta})$ in place of the theoretical matrices $\mathbf{R}_k$ in (35), and minimizing the resultant expression with respect to $\boldsymbol{\theta}$.

In place of the true log-likelihood function, one can minimize its suitable approximation, obtained by a second order Taylor series expansion as a function of $\mathbf{R}_k$ in a neighborhood of $\mathbf{R}_k = \widehat{\mathbf{R}}_k$. Neglecting the third and higher order terms in $\Delta\mathbf{R}_k = \mathbf{R}_k - \widehat{\mathbf{R}}_k$ it holds

$$\log\det \mathbf{R}_k \approx \log\det \widehat{\mathbf{R}}_k + \operatorname{tr}\left(\widehat{\mathbf{R}}_k^{-1}\Delta\mathbf{R}_k\right) - \frac{1}{2}\operatorname{tr}\left(\widehat{\mathbf{R}}_k^{-1}\Delta\mathbf{R}_k\widehat{\mathbf{R}}_k^{-1}\Delta\mathbf{R}_k\right)$$

and

$$\operatorname{tr}\left(\mathbf{R}_k^{-1}\widehat{\mathbf{R}}_k\right) \approx \operatorname{tr}(\mathbf{I}) - \operatorname{tr}\left(\widehat{\mathbf{R}}_k^{-1}\Delta\mathbf{R}_k\right) + \operatorname{tr}\left(\widehat{\mathbf{R}}_k^{-1}\Delta\mathbf{R}_k\widehat{\mathbf{R}}_k^{-1}\Delta\mathbf{R}_k\right).$$

Consequently,

$$-\log f(\mathbf{X}) \approx \text{const}' + \frac{N_1}{4}\sum_{k=1}^{M} \operatorname{tr}\left(\widehat{\mathbf{R}}_k^{-1}\Delta\mathbf{R}_k\widehat{\mathbf{R}}_k^{-1}\Delta\mathbf{R}_k\right). \tag{37}$$

This concludes the proof that the minimization of (8) is approximately equivalent to computation of the maximum likelihood estimate of the parameter $\boldsymbol{\theta}$.

Appendix B

This Appendix presents details of computation of the gradient and the Hessian of the weighted criterion (9). (Derivatives of the barrier function in (10) are simpler and are omitted to save space.)

$$\begin{aligned}\mathcal{Q}_3(\boldsymbol{\theta}) &= \sum_{k=1}^{M} \operatorname{tr}\left[\mathbf{C}_k\Delta\mathbf{R}_k(\boldsymbol{\theta})\mathbf{C}_k\Delta\mathbf{R}_k(\boldsymbol{\theta})\right] \\ &= \sum_{k,\alpha,\beta,\gamma,\delta} C_{k\alpha\beta}\Delta R_{k\beta\gamma}C_{k\gamma\delta}\Delta R_{k\delta\alpha}\end{aligned} \tag{38}$$

where $C_{k\alpha\beta}$ is the $(\alpha\beta)$th element of $\mathbf{C}_k$ and $\Delta R_{k\alpha\beta}$ is the $(\alpha\beta)$th element of $\Delta\mathbf{R}_k(\boldsymbol{\theta}) = \mathbf{R}_k(\boldsymbol{\theta}) - \widehat{\mathbf{R}}_k$ for $k = 1, \ldots, M$ and $\alpha, \beta = 1, \ldots, d$. The gradient and the Hessian of the criterion have the elements

$$\begin{aligned}\frac{\partial\mathcal{Q}_3(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}_i} &= 2\sum_{k=1}^{M} \operatorname{tr}\left[\mathbf{C}_k\Delta\mathbf{R}_k(\boldsymbol{\theta})\mathbf{C}_k\frac{\partial\Delta\mathbf{R}_k(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}_i}\right] \\ \frac{\partial^2\mathcal{Q}_3(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}_i\partial\boldsymbol{\theta}_j} &= 2\sum_{k=1}^{M} \operatorname{tr}\left[\mathbf{C}_k\frac{\partial\Delta\mathbf{R}_k(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}_i}\mathbf{C}_k\frac{\partial\Delta\mathbf{R}_k(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}_j}\right] \\ &\quad + 4\sum_{k=1}^{M} \operatorname{tr}\left[\mathbf{C}_k\Delta\mathbf{R}_k(\boldsymbol{\theta})\mathbf{C}_k\frac{\partial^2\Delta\mathbf{R}_k(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}_i\partial\boldsymbol{\theta}_j}\right]\end{aligned} \tag{39}$$

for $i, j = 1, \ldots, \dim(\boldsymbol{\theta}) = r(d + M)$. It can be shown that the first term on the right-hand side of (39) represents an element of a matrix which is always positive definite (or at least

positive semidefinite), provided that the matrices $\mathbf{C}_k$ are positive definite. The latter part of the Hessian might be indefinite, in general. Moreover, the latter term is negligible if the fitting error $\Delta\mathbf{R}_k(\boldsymbol{\theta})$ is small. Note that for convergence of the Gauss-Newton algorithm or L-M algorithm it is desired that the Hessian is positive definite. Therefore, we shall neglect the latter term in the rest of the paper. Since

$$\Delta R_{k\beta\gamma} = \sum_{f=1}^{r} D_{kf} A_{\beta f} A_{\gamma f} - (\widehat{\mathbf{R}}_k)_{\beta\gamma} \tag{40}$$

its derivatives with respect to elements of $\boldsymbol{\theta}$, i.e., A_{ij} and D_{mg}, $i = 1, \ldots, d$, $j, g = 1, \ldots, r$, and $m = 1, \ldots, M$ read

$$\frac{\partial \Delta R_{k\beta\gamma}}{\partial A_{ij}} = \delta_{i\beta} D_{kj} A_{\gamma j} + A_{\beta j} D_{kj} \delta_{\gamma i} \tag{41}$$

$$\frac{\partial \Delta R_{k\beta\gamma}}{\partial D_{mg}} = \delta_{km} A_{\beta g} A_{\gamma g}. \tag{42}$$

Replacing in (39) according to (41) and (42) we get, after some simplifications,

$$\frac{\partial^2 \mathcal{Q}_3(\boldsymbol{\theta})}{\partial A_{ij} \partial A_{mg}} = 4 \sum_{k=1}^{M} (V_{jmk} V_{gik} + \widetilde{W}_{jgk} C_{mik}) \tag{43}$$

$$\frac{\partial^2 \mathcal{Q}_3(\boldsymbol{\theta})}{\partial A_{ij} \partial D_{mg}} = 4 W_{gjm} V_{gim} D_{mj} \tag{44}$$

$$\frac{\partial^2 \mathcal{Q}_3(\boldsymbol{\theta})}{\partial D_{ij} \partial D_{mg}} = 2 \delta_{im} W_{gjm} W_{gjm} \tag{45}$$

where

$$V_{jmk} = D_{kj} \left(\mathbf{A}^T \mathbf{C}_k^{-1} \right)_{jm} \tag{46}$$

$$W_{jgk} = \left(\mathbf{A}^T \mathbf{C}_k^{-1} \mathbf{A} \right)_{jg} \tag{47}$$

$$\widetilde{W}_{jgk} = D_{kj} D_{kg} \left(\mathbf{A}^T \mathbf{C}_k^{-1} \mathbf{A} \right)_{jg}. \tag{48}$$

We can summarize the results in matrix form as

$$\boldsymbol{\Psi}_3 = \frac{\partial^2 \mathcal{Q}_3(\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T} = \begin{bmatrix} \boldsymbol{\Psi}_{AA} & \boldsymbol{\Psi}_{AD} \\ \boldsymbol{\Psi}_{AD}^T & \boldsymbol{\Psi}_{\mathrm{DD}} \end{bmatrix} \tag{49}$$

where

$$\boldsymbol{\Psi}_{AA} = \begin{bmatrix} \boldsymbol{\Psi}_{AA}^{11} & \cdots & \boldsymbol{\Psi}_{AA}^{1d} \\ \vdots & & \vdots \\ \boldsymbol{\Psi}_{AA}^{d1} & \cdots & \boldsymbol{\Psi}_{AA}^{dd} \end{bmatrix} \tag{50}$$

$$\boldsymbol{\Psi}_{AD} = \begin{bmatrix} \boldsymbol{\Psi}_{AD}^{11} & \cdots & \boldsymbol{\Psi}_{AD}^{1M} \\ \vdots & & \vdots \\ \boldsymbol{\Psi}_{AD}^{d1} & \cdots & \boldsymbol{\Psi}_{\mathrm{DD}}^{dM} \end{bmatrix} \tag{51}$$

$$\boldsymbol{\Psi}_{\mathrm{DD}} = \begin{bmatrix} \boldsymbol{\Psi}_{\mathrm{DD}}^{11} & \cdots & \boldsymbol{\Psi}_{\mathrm{DD}}^{1M} \\ \vdots & & \vdots \\ \boldsymbol{\Psi}_{\mathrm{DD}}^{M1} & \cdots & \boldsymbol{\Psi}_{\mathrm{DD}}^{MM} \end{bmatrix} \tag{52}$$

$$\boldsymbol{\Psi}_{AA}^{im} = 4 \left(\boldsymbol{V}_i \boldsymbol{V}_m^T + \sum_{k=1}^{M} C_{mik} \widetilde{\mathbf{W}}_k \right) \tag{53}$$

$$\boldsymbol{\Psi}_{AD}^{im} = 4 \mathbf{D}_m \mathbf{W}_m \mathrm{diag}(V_{:,i,m}) \tag{54}$$

$$\boldsymbol{\Psi}_{\mathrm{DD}}^{im} = 2 \delta_{im} \mathbf{W}_m \odot \mathbf{W}_m. \tag{55}$$

$\odot$ is the Hadamard (elementwise) product and $\mathbf{V}_i$ and $\mathbf{W}_i$ are matrices

$$\boldsymbol{V}_i = (V_{:,i,:})_{r \times M} \tag{56}$$

$$\mathbf{W}_i = \mathbf{A}^T \mathbf{C}_i^{-1} \mathbf{A} \qquad (r \times r) \tag{57}$$

$$\widetilde{\mathbf{W}}_i = \mathbf{D}_i \mathbf{A}^T \mathbf{C}_i^{-1} \mathbf{A} \mathbf{D}_i \tag{58}$$

$$\mathbf{D}_i = \mathrm{diag}(\mathbf{D}_{i,:}). \qquad (r \times r). \tag{59}$$

Note that $\boldsymbol{\Psi}_{\mathrm{DD}}$ in (49) and (55) is block diagonal and therefore it is convenient to use a lemma for inversion of partitioned matrices to reduce memory requirements and computational time of the algorithm.

Appendix C

Straightforward computations of the partial derivatives in (25) by the elements of $\boldsymbol{\vartheta}$ give, respectively,

$$\left[\frac{\partial \mathbf{R}_k}{\partial A_{\alpha\beta}} \right]_{ij} = \begin{cases} 2 D_{k\beta} A_{i\beta} & \alpha = i = j \\ D_{k\beta} A_{j\beta} & i = \alpha \wedge j \neq \alpha \\ D_{k\beta} A_{i\beta} & i \neq \alpha \wedge j = \alpha \\ 0 & i \neq \alpha \wedge j \neq \alpha \end{cases}, \tag{60}$$

$$\left[\frac{\partial \mathbf{R}_1}{\partial D_{\kappa\beta}} \right]_{ij} = - A_{i\beta} A_{j\beta}, \tag{61}$$

$$\left[\frac{\partial \mathbf{R}_k}{\partial D_{\kappa\beta}} \right]_{ij} = \delta_{k\kappa} A_{i\beta} A_{j\beta}, \qquad k > 1 \tag{62}$$

where $\alpha = 1, \ldots, d$, $\beta = 1, \ldots, r$, and $\kappa = 2, \ldots, M$.

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