MV-PURE ESTIMATOR OF DIPOLE SOURCE SIGNALS IN EEG

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ABSTRACT

We consider the problem of dipole source signals estimation in electroencephalography (EEG) using beamforming techniques in ill-conditioned settings. We take advantage of the link between the linearly constrained minimum-variance (LCMV) beamformer in sensor array processing and the best linear unbiased estimator (BLUE) in linear regression modeling. We show that the recently introduced reducedrank extension of BLUE, named minimum-variance pseudounbiased reduced-rank estimator (MV-PURE), achieves much lower estimation error not only than LCMV beamformer, but also than the previously derived reduced-rank principal components (PC) and cross-spectral metrics (CSM) beamformers in ill-conditioned settings. The practical scenarios where the considered estimation model becomes ill-conditioned are discussed, then we show the applicability of MV-PURE dipole source estimator under those conditions through realistic simulations.

Index Terms— MV-PURE estimator, reduced-rank estimation, dipole source signal, electroencephalography, sensor array processing

1. INTRODUCTION

In recent years, beamforming techniques have found applications in processing signals originating from electroencephalographic (EEG) and magnetoencephalographic (MEG) sensor arrays. In particular, the celebrated linearly constrained minimum-variance (LCMV) beamformer (recently also called as multiple constrained minimum-variance beamformer in brain signal processing) has often been used as reference for new beamforming methods in EEG/MEG source signal estimation (see e.g. [1–4] and references therein), which is the problem we are interested in this paper. An important aspect of LCMV beamforming is its inter-

An important aspect of LCMV beamforming is its interpretation in terms of the celebrated best linear unbiased estimator (BLUE), also known as the Gauss-Markov estimator [5, 6], which is widely used in linear regression models for the estimation of an unknown deterministic vector of parameters. In this framework, it is well-known that enforcing unbiasedness is inherently inadequate in ill-conditioned and/or highly noisy settings, as it leads to huge variance of the obtained estimate. On the other hand, the reduced-rank approach provides significant gain in performance in such settings, as it introduces a small amount of bias in exchange for large savings in variance [7–10].

Here we show that a model for EEG dipole source signals estimation may be naturally interpreted in the linear regression framework. This opens the possibility of using robust reduced-rank estimators developed for the linear regression model in dipole source estimation. In particular, the numerical simulations contained in this paper indicate that closely positioned and correlated dipole sources which may be located in areas of low sensor sensitivity yield ill-conditioned estimation models, which is in line with known theoretical results (see e.g. [1] and references therein). Thus, there is a great need to introduce efficient reduced-rank estimation methods for such settings in EEG source signals estimation, which is the main contribution of this paper.

The proposed solution for such settings is the recently introduced minimum-variance pseudo-unbiased reduced-rank estimator (MV-PURE), which in terms of linear regression model is defined as a closed form solution of a hierarchical non-convex constrained optimization problem [9, 10]. MV-PURE achieves minimum variance among all solutions of the first stage optimization problem for simultaneously minimizing, under a rank constraint, all unitarily invariant norms of an operator applied to the unknown parameter vector in view of suppressing bias. These properties ensure that, among reduced-rank estimators of a predefined rank, the MV-PURE estimator has minimum variance among those with least possible bias. Moreover, compared with Tikhonov regularization-based methods [11], it does not require sophisticated or application-specific algorithms for finding optimal value of the regularization parameter [12, 13]. Instead, only discrete-valued rank of MV-PURE needs to be determined, and efficient implementation of a rank-selection criterion minimizing unbiased estimate of the predicted-MSE of MV-PURE is proposed in [14].

Therefore, the aim of this work is to show that MV-PURE achieves significantly lower estimation error in reconstructing dipole source signals in EEG for ill-conditioned settings not only than LCMV beamformer, but also than principal components (PC) and cross-spectral metrics (CSM) beamformers, in which rank-reduction is implemented to replace the covariance matrix of the filtered observed signal by its reduced-rank approximations [3]. The numerical examples are performed with realistically simulated EEG measurements obtained through boundary element method (BEM)-based modeling (see [15, Section IV] for in-depth description and derivation of this model) using the Helsinki BEM library [16], and with an uniformly distributed EEG sensor array conforming to the 5-10 sensor placing system, thus ensuring the reproducibility of the results.

The paper is organized as follows: in Section 2 we introduce the EEG measurement model considered, and we demonstrate its close relation with linear regression model. Then, in Section 3 we show how MV-PURE estimator can be interpreted in terms of the EEG model, then we discuss its benefits in such settings. In Section 4 we show the applicability of MV-PURE through numerical examples using realistically simulated EEG data. We close with Section 5 where conclusions are drawn and areas of future research are discussed.

2. PRELIMINARIES

We consider the case of measuring potentials over the scalp produced by L dipole sources using an array of m sensors. We assume that the sources change in time, but remain at the same position θ during the measurement period t = 1, 2, ..., N. This assumption holds in practice for evoked response and event-related experiments [3, 17]. Then, the $m \times N$ spatiotemporal data matrix Y for a given trial can be modeled as

$$Y = A(\theta)Q + E,\tag{1}$$

where $A(\theta)$ is the $m \times 3L$ array response matrix, Q is the $3L \times N$ matrix of dipole moments, and E is the noise matrix of spatially correlated background activity approximated by zero-mean random dipoles representing spontaneous brain activity [18]. The array response matrix can be calculated through BEM in the case where the head is approximated with a realistic geometry and for a known θ . This forward solution of generating EEG measurements has already been implemented in the Helsinki BEM library [16].

In this paper we consider the problem of dipole source signals estimation with fixed dipole locations, and look into beamforming methods which use two elements to estimate Qbased on Y: the array response matrix $A(\theta)$ which is available by design of the EEG forward problem, and the noise covariance matrix R, which is generally unknown but can be estimated from the observed data. We assume that the total time samples N is larger than the number of sensors m which ensures that the covariance matrix is positive definite.

Model (1) represents, from a statistical modeling viewpoint, a linear regression model used for estimation of an unknown deterministic parameter Q in the presence of additive noise E, then the aim is to estimate Q based on observations Y in a linear fashion:

$$\widehat{Q} := \Phi Y, \tag{2}$$

where we call the constant matrix $\Phi \in \mathbb{R}^{3L \times m}$ an estimator, and \widehat{Q} denotes an estimate of Q. In fact, (1) can be seen as a linear regression model where $A(\theta)$ corresponds to its *model matrix* of full column rank 3L.

Under those conditions, the BLUE estimator (denoted by Φ_{BLUE}) minimizes the variance of its estimate subject to the condition $\Phi_{BLUE}A(\theta) = I_{3L}$ and is defined as the solution of the following optimization problem [5, 6, 9, 10]:

$$\begin{cases} \text{minimize} & tr \left[\Phi R \Phi^T \right] \\ \text{subject to} & \Phi A(\boldsymbol{\theta}) = I_{3L}, \end{cases}$$
(3)

with the corresponding solution given by

$$\Phi_{BLUE} := (A(\boldsymbol{\theta})^T R^{-1} A(\boldsymbol{\theta}))^{-1} A(\boldsymbol{\theta})^T R^{-1}.$$
 (4)

In array signal processing, the optimization problem (3) with its unique solution (4) for a linear model (1) is equivalent to the LCMV beamformer, whose spatial filtering properties for localization and estimation of brain electrical activity have been previously demonstrated [1–4]. However, it can be easily observed that requirement of a unit response in the pass band, which corresponds to the condition $\Phi A(\theta) = I_{3L}$ in (3), leads to huge variance $tr [\Phi R \Phi^T]$ if $A(\theta)^T R^{-1}A(\theta)$ is ill-conditioned, i.e., if it possesses some vanishingly small singular values (which, in our settings, are equal to the eigenvalues as $A(\theta)^T R^{-1}A(\theta)$ is positive definite). Unsurprisingly, this is also a recurrent problem in estimation in linear

regression, as the equality $\Phi A(\theta) = I_{3L}$ leads to uniform unbiasedness of the estimate, which is inherently inadequate in ill-conditioned settings. From the point of view of either the array signal processing or the estimation in linear regression, the same core problem is observed: if we set an eigenvalue decomposition (EVD) of $A(\theta)^T R^{-1} A(\theta)$ as

$$EVD\{A(\boldsymbol{\theta})^T R^{-1} A(\boldsymbol{\theta})\} = V \Sigma V^T, \qquad (5)$$

such that the eigenvalues are organized in nonincreasing order, then inserting (4) into (3) reveals that the variance of BLUE estimator (and hence, LCMV beamformer) is expressed as

$$tr\left[\Phi_{BLUE}R\Phi_{BLUE}^{T}\right] = \sum_{i=1}^{3L} \frac{1}{\sigma_i},\tag{6}$$

where σ_i , i = 1, ..., 3L are eigenvalues of $A(\theta)^T R^{-1} A(\theta)$. Thus, if the trailing eigenvalues $\sigma_{r+1}, ..., \sigma_{3L}$ for some r < 3L are vanishingly small, the resulting variance (6) will be huge.

In terms of model (1) considered in this paper, illconditioning occurs when the dipole sources are close to each other, specially when they are located far from electrodes, which is consistent with theoretical results (see e.g. [1] and references therein). Therefore, there is great need to introduce a solution that improves the performance compared to classical LCMV approach in such settings, and we propose such a solution next.

3. MV-PURE ESTIMATOR FOR DIPOLE SOURCE SIGNALS ESTIMATION IN EEG

The reduced-rank approach has been in continuous use since early seminal papers [7, 8], and it has been employed in linear estimation under linear regression model to combat illconditioning by introducing small amount of bias (induced by rank-reduction) in exchange for huge savings in variance. Recently, the minimum-variance pseudo-unbiased reducedrank estimator (MV-PURE) has been introduced as the optimal extension of BLUE approach (3) to the reduced-rank case [9, 10]. Namely, the MV-PURE estimator (without linear constraints) is defined as the solution of the following optimization problem, for a given rank constraint $r \leq 3L$:

$$\begin{cases} \text{minimize} \quad tr \left[\Phi_r R \Phi_r^T\right] \\ \text{subject to} \quad \Phi_r \in \bigcap_{\iota \in \mathfrak{I}} \mathcal{P}_r^{\iota}, \end{cases}$$
(7)

with

 $\mathcal{P}_{r}^{\iota} = \arg\min_{\Phi_{r} \in \mathcal{X}_{r}^{3L \times m}} \| \Phi_{r} A(\boldsymbol{\theta}) - I_{3L} \|_{\iota}^{2}, \ \iota \in \mathfrak{I}, \quad (8)$

and

$$\mathcal{X}_{r}^{3L \times m} := \{ \Phi_{r} \in \mathbb{R}^{3L \times m} : rank(\Phi_{r}) \le r \le 3L \}, \quad (9)$$

where \mathfrak{I} is the index set of all *unitarily invariant* norms, i.e., norms satisfying $|| UXV ||_{\iota} = || X ||_{\iota}$ for all orthogonal $U \in \mathbb{R}^{k \times k}$, $V \in \mathbb{R}^{n \times n}$ and all $X \in \mathbb{R}^{k \times n}$ [19]. Then, the solution to problem (7) for a given rank constraint $r \leq 3L$ is given by [10]

$$\Phi_{MV-PURE}^r = V_r V_r^T \Phi_{BLUE},\tag{10}$$

where $V = (v_1, \ldots, v_{3L})$ with $V_r = (v_1, \ldots, v_r)$ with the resulting projection matrix $V_r V_r^T$, and where Φ_{BLUE} is of the form (4).

In comparison to the full-rank case, it is not possible to enforce unit response in the pass band, as the equality $\Phi_r A(\theta) = I_{3L}$ cannot be achieved if r < 3L. Nevertheless, the closest approximation may be obtained in the reducedrank case by minimizing (8) simultaneously in terms of all unitarily invariant norms, as it is done for the MV-PURE estimator. Then, the minimum-variance solution is chosen among those satisfying conditions (8), which results in a natural extension of the full-rank approach (3) to the reducedrank case (7). The benefits of the reduced-rank approach by MV-PURE estimator in ill-conditioned settings can be observed as follows: let us assume that last 3L - r eigenvalues $\sigma_{r+1}, \ldots, \sigma_{3L}$ of $A(\theta)^T R^{-1}A(\theta)$ are vanishingly small. Then, by choosing MV-PURE estimator of rank r it can be easily verified that its variance is equal to

$$tr\left[\Phi_{MV-PURE}^{r}R(\Phi_{MV-PURE}^{r})^{T}\right] = \sum_{i=1}^{r} \frac{1}{\sigma_{i}},\qquad(11)$$

which is much smaller than of the full rank BLUE estimator, as it completely avoids the impact of the trailing 3L - reigenvalues which are an issue in (6). The penalty paid for the possibly huge savings in variance results in a minimum possible deviation from unit response in the pass band (among the estimators of rank r) thanks to condition (8).

Therefore, the same motivation for the use of MV-PURE works in the case of spatial filtering in array signal processing, in particular for dipole source signals estimation in EEG under model (1), as well as in estimation under linear regression model [9, 10]. We believe thus that MV-PURE could be established as a highly competitive solution also in such settings, and we demonstrate the validity of this claim through numerical examples in the next section.

4. NUMERICAL EXAMPLES

In the following simulations, we consider the solution through BEM of the forward problem in EEG using a realistic head model, then we evaluate the performance of LCMV and MV-PURE beamformers. In our simulations, we estimated R by its finite sample estimate. The EEG data was generated using an array of m = 87 sensors uniformly distributed over surface of the head model.

Furthermore, we considered the case of two dipoles located at positions $p_1 = [8.7, -87.0, 28.9]^T$ mm and $p_2 = [29.3, -37.1, 67.9]^T$ mm, with a common interferer located between them at $p_3 = [14.0, -74.9, 48.9]^T$ mm, then our problem corresponded to the estimation of L = 3 sources. The dipole source components were defined as Q = Xq(t), where $X \in \mathbb{R}^{9\times 3}$ is of the form

$$X = \begin{pmatrix} 0.7 & 0 & 0 \\ 0 & 0.7 & 0 \\ 0 & 0 & 0 \\ 0 & 0.3 & 0 \\ 0 & 0 & 0 \\ 0.7 & 0 & 0 \\ 0 & 0 & 0.7 \\ 0 & 0 & 0 \\ 0 & 0 & 0.5 \end{pmatrix},$$
(12)

where $q(t) = [q_1(t), q_2(t), q_3(t)]^T$ contains dipole basis

functions allowed to change in time according to

$$q_{1}(t) = 10 \exp\left(-\frac{(t-100)^{2}}{11^{2}}\right) - 5 \exp\left(-\frac{(t-80)^{2}}{17^{2}}\right)$$

$$q_{2}(t) = 5 \exp\left(-\frac{(t-80)^{2}}{8^{2}}\right) - 10 \exp\left(-\frac{(t-100)^{2}}{11^{2}}\right)$$
(13)
$$q_{3}(t) = 10 \sin(0.06\pi t)$$

with units of [nA m] and t in milliseconds. Note that from (12) and (13) we obtain the source components of two correlated dipoles plus a common interferer, which are given by $[0.7 q_1(t), 0.7 q_2(t), 0]^T$, $[0.3 q_2(t), 0, 0.7 q_1(t)]^T$, and $[0.7 q_3(t), 0, 0.5 q_3(t)]^T$, and are located at positions p_1 , p_2 , and p_3 , respectively. The signals were sampled every 0.33 ms for duration of 100 ms, thus obtaining N = 300 samples. Similar models have been used in previous research (see e.g. [3] and references therein) as they approximate a typical evoked response.

Next, the EEG measurements were generated using the Helsinki BEM library with a head model composed by three tesselated meshes which were nested one inside the other in order to approximate the geometry of the scalp, skull, and brain. Each volume was given a homogeneous conductivity of 0.33, 0.0041, and 0.33 S/m, respectively. Finally, to approximate realistic spatially correlated noise, we generated 400 random dipoles in order to model spontaneous brain activity [18]. The signal-to-noise ratio (SNR) was defined as

$$SNR[dB] = 10 \log_{10} \frac{\|AQ\|_F}{\|E\|_F},$$
 (14)

and the noise power was set in order to obtain SNR[dB] levels of 3,5,7,9. We averaged the results over 1000 independent noise realizations.

Under these conditions, we were able to simulate an illconditioned estimation problem, with large condition number of the matrix $A(\theta)^T R^{-1}A(\theta)$ for a given estimate of noise covariance matrix R. In particular, the average spread of singular values of $A(\theta)^T R^{-1}A(\theta)$ suggested that we may obtain a significant gain in performance by lowering the rank of MV-PURE to r = 8 from the full rank 3L = 9.

In order to compare the performance of the proposed method, we included the evaluation of LCMV beamformer implemented as generalized sidelobe canceller of full-rank (GSC), PC and CSM beamformers as indicated in [3]. Furthermore, using the fact that in this particular example third coefficient of first dipole, second coefficient of second dipole, and second coefficient of third dipole are all zero for duration of trial, we introduced the linearly constrained version of MV-PURE estimator which used this particular information in the estimation process (see [10] for the closed form expression of this version of MV-PURE estimator).

The performance of the solutions considered in the above described settings were evaluated using the squared estimation error, i.e.

$$\operatorname{error} = \parallel Q - \widetilde{Q} \parallel_{F}^{2}, \tag{15}$$

which was averaged over 1000 independent noise realizations. The rank of the correlation matrix approximation was set as 7r for PC and CSM beamformers. The results are shown in Figure 1, where it is seen that the MV-PURE estimator offers a larger gain in performance for lower SNR, which is in line with theoretical analysis and numerical simulations in [10]. Note that the GSC (full-rank) is in our settings simply a different implementation of Φ_{BLUE} in (4), thus their performances overlap in the figure.



Fig. 1. Estimation error as a function of SNR for the different estimators considered. The dotted line corresponds to the linearly constrained (lc) version of the MV-PURE.

An example of the performance of the MV-PURE estimator (without linear constraints) and PC beamformer (which achieves the lowest estimation error apart from MV-PURE estimators in Figure 1) is shown in Figure 2. It is seen that the estimation variance of MV-PURE estimator is much lower than the variance in the PC beamformer for certain coefficients.

5. CONCLUDING REMARKS

We have presented an efficient solution to dipole source signals estimation in EEG under ill-conditioned settings. The gain in performance was motivated by theoretical considerations and demonstrated afterwards by means of realistic numerical simulations.

We would also like to emphasize that the gain in performance of MV-PURE estimator does not come at the expense of computational cost. Indeed, an efficient recursive computation method which is inherently parallel and does not require any matrix inversions for estimation of wide-sense stationary processes (such as those considered in this paper) is available for the MV-PURE estimator of the form (10) in [20]. Therefore, the results here presented highlight flexibility of the MV-PURE framework, and encourage us to expand its usage in brain signal processing by further theoretical research and experiments with real data in the direction initiated in this paper.

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Fig. 2. Estimated signal components for SNR[dB] \approx 3.

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