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A multi-variate blind source separation algorithm

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ABSTRACT

Background and objective: The study follows the proposal of decomposing a given data matrix into a product of independent spatial and temporal component matrices. A multi-variate decomposition approach is presented, based on an approximate diagonalization of a set of matrices computed using a latent space representation.
Methods: The proposed methodology follows an algebraic approach, which is common to space, temporal or spatiotemporal blind source separation algorithms. More specifically, the algebraic approach relies on singular value decomposition techniques, which avoids computationally costly and numerically instable matrix inversion. The method is equally applicable to correlation matrices determined from second order correlations or by considering fourth order correlations.
Results: The resulting algorithms are applied to fMRI data sets either to extract the underlying fMRI components or to extract connectivity maps from resting state fMRI data collected for a dynamic functional connectivity analysis. Intriguingly, our algorithm shows increased spatial specificity compared to common approaches, while temporal precision stays similar.
Conclusion: The study presents a novel spatiotemporal blind source separation algorithm, which is both robust and avoids parameters that are difficult to fine tune. Applied on experimental data sets, the new method yields highly confined and focused areas with least spatial extent in the retinotopy case, and similar results in the dynamic functional connectivity analyses compared to other blind source separation algorithms. Therefore, we conclude that our novel algorithm is highly competitive and yields results, which are superior or at least similar to existing approaches.

1. Introduction

Exploratory matrix factorization (EMF) techniques are unsupervised, data-driven approaches which are used to discover latent factors, also called sources or features, in the data [1–4]. Such techniques often provide alternative representations of large data sets such as, for example, functional imaging data. This transformed data often reveals underlying characteristics of the data sets under study. Hence these features are generally considered indicative of underlying processes or networks, and often serve classification purposes for discriminating different types of data. Especially functional magnetic resonance imaging (fMRI) experiments produce sequences of images/volumes. Such data is then organized into a data matrix $\mathbf{X}$ where each row contains a volume, i.e., a complete *3D* scan of the brain. The intensities $I(x, y, z)$ of the voxels within the volume are concatenated into a row vector by associating the spatial voxel coordinates (x, y, z) with an index n. Each row of $\mathbf{X}$ with a total of $N = s_1 \times s_2 \times s_3$ voxels thus represents one volume scan, or a region of interest (ROI) in the total volume, and is associated with a time index m. A session involves a total of M scans, therefore a session is represented by an $M \times N$ data matrix where M is related with the time domain and N is associated with the spatial domain.

If instead of analyzing intensity distributions, we are interested in *dynamic functional connectivity* aspects, the data matrix $\mathbf{X}$ is formed with Pearson correlation coefficients, which represent two-point correlations between time series resulting from preprocessing the fMRI data. Therefore, the raw data is often decomposed into functional networks using a group level spatial ICA. The referred pre-processing step results in L independent spatial maps and the related time courses. These time courses are then subdivided into short, partially overlapping segments, and $L(L-1)/2$ correlation coefficients are computed between all time windows. These correlations vary over time, thus represent what is called *dynamic functional connectivity networks* (dFCN). The rows of the data matrix are then formed by concatenating $N = SP$, e.g. S sessions

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and P time points per session, correlation coefficients $\rho_{mm'}[n]$, $n = 1, \ldots, N$.

The goal of exploratory matrix factorization techniques is to approximate the original data matrix by the product of two matrices, which can be expressed as an outer product of K column $\mathbf{W}_{*k}$ and row $\mathbf{H}_{k*}$ vectors according to

$$\hat{\mathbf{X}} = \mathbf{WH} = \mathbf{W}_{*1}\mathbf{H}_{1*} + \mathbf{W}_{*2}\mathbf{H}_{2*} + \ldots + \mathbf{W}_{*K}\mathbf{H}_{K*} \tag{1}$$

with

$$\mathbf{W}_{*k}\mathbf{H}_{k*} = \begin{pmatrix} w_{1k} \\ \vdots \\ w_{Mk} \end{pmatrix} (h_{k1} \cdots h_{kN}). \tag{2}$$

The original matrix is thus approximated by K outer products of factors related with the information contained in the space spanned by the column vectors $\mathbf{W}_{*k}$ and the space spanned by the row vectors $\mathbf{H}_{k*}$. Moreover, each row of $\mathbf{W}$ and each column of $\mathbf{H}$, respectively, form the coordinates of a new representation by which the information is encoded in a latent (hidden) space of dimension K. Note that in general no *a priori* knowledge about the factor matrices is available.

The mathematical model described by Eq. (1) is also followed by the general linear model (GLM) widely used in fMRI data analysis. The main difference is that the matrix $\mathbf{W}$, now called design matrix, represents the experimental manipulations and conditions which are assumed to be known. Therefore, GLM represents a semi-knowledge-based approach [5], where the unknown matrix $\mathbf{H}$ can be estimated by minimizing the Frobenius norm of the error matrix $(\mathbf{X} - \hat{\mathbf{X}})$ and $\hat{\mathbf{X}}$ represents the estimate $\mathbf{WH}$. In data-driven methods, applied to fMRI data sets $\mathbf{X}$, both factor matrices $(\mathbf{W}, \mathbf{H})$ are estimated given only the measured data [6]. To achieve this goal, assumptions like orthogonality (singular value decomposition (SVD) or principal component analysis (PCA)), statistical independence (independent component analysis (ICA) or blind source separation (BSS)), nonnegativity (non-negative matrix factorization (NMF)) and so on need to be applied. Independent Component Analysis (ICA) has been widely applied to fMRI data by imposing the independence constraint either to the spatial (rows of $\mathbf{H}$) domain (sICA) or the time (columns of $\mathbf{W}$) domain (tICA).Note that with sICA the matrix $\mathbf{W}$ is considered the mixing matrix, while with tICA this becomes the role of the matrix $\mathbf{H}$. The sICA is more common due to the large dimensionality of the spatial domain when compared with the temporal domain. Moreover, if it comes to compare ICs across a group of subjects, group ICA [7–9] has to be applied to get around the inherent permutation and scaling indeterminacies of ICA. And the latter leads to a set of independent spatial maps, which are visually analyzed to identify artifacts like head movement or known structures in the brain (major blood vessels or the ventricles). Finally, the time courses, corresponding to valid independent spatial components, are selected to compute the dFCN data matrix.

2. Spatiotemporal decomposition

Early attempts to combine sICA and tICA can be found in [10] where sICA is used to select the regions of interest (ROIs), and then tICA is applied to the time series of those voxels to find temporal components. More generally, spatiotemporal approaches were also suggested [11] and [12]. In both works, a singular value decomposition (SVD) pre-processing step determines the dimension of the latent space. Then a new transformation matrix is computed using both time and space components of the SVD decompostion. In [11], the independent components in the new latent space are computed by optimizing a contrast function via gradient descent. In [12], an algebraic joint approximative diagonalization (JAD) approach is considered after computing a set of matrices derived from time and space components. More recently [13], a cascaded approach was proposed to compute independent components. Thereby, after applying sICA, a tICA is applied to the mixing matrix $\mathbf{W}$ of the spatial mixing model. In this proposal, there is an additional stage to visually identify and remove artifact related independent spatial components. Then, the corresponding time components are regressed out of the non-artifact-related time components of the mixing model. Notice that the final model to approximate the original data is presented as a product of three matrices, originating from the two step procedure.

2.1. Motivation

The Motivation of this study is to combine the work of [11] with an algebraic approach as proposed in [12]. Therefore, the transformation matrix, estimated in the latent space, is an orthogonal matrix and both, temporal and spatial components, undergo a similar rotation. Both works have shortcomings, which are corrected for by our proposed combination. The algorithm in [11] employs many additional parameters resulting in a less robust behavior, whereas the approach in [12] is an exact analytical method. Nevertheless, the work of [12] uses pseudoinverses, which introduce a computationally costly and a random component to the algorithm. Furthermore, the pseudoinverses render the algorithm computationally instable because of possible degeneracy of the matrix columns. These shortcomings are accounted for in our proposed method, which is based on the well known and robust eigenvalue decomposition. The performance of the method is illustrated with fMRI data sets to extract relevant information in different stages of the processing chain: a processing and a post-processing step. Nevertheless, the algorithm is generally suitable for spatiotemporal datasets irrespective of their origin and may have applications in many fields of science.

2.2. Singular value decomposition

Singular Value Decomposition (SVD) of the original data matrix $\mathbf{X}$ is the most widely used factorization technique that serves as a pre-processing step in most of the decomposition techniques. The matrix decomposition reads

$$\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T \tag{3}$$

If $N >> M$, the maximal number of non-zero singular values is M, and those form the entries of the $M \times M$ diagonal matrix $\boldsymbol{\Sigma}$. The related eigenvector matrices, i.e. the $M \times M$ matrix $\mathbf{U}$ and the $N \times M$ matrix $\mathbf{V}$, have M orthogonal columns. The SVD decomposition may be re-written using the factorization model described in Eq. (1) by using only the $K < M$ largest singular values and corresponding eigenvectors. This decomposition will lead to a low-rank approximation of the original data. The Frobenius norm of the error of the approximation is related with the discarded singular values

$$\|\mathbf{X} - \hat{\mathbf{X}}\|_F = \sqrt{\sum_{i=K+1}^{M} \Sigma_{ii}^2} \tag{4}$$

when the diagonal entries of $\boldsymbol{\Sigma}$ are assumed to be arranged in decreasing order of magnitude.

Now considering the decomposition given in Eq. (1):

- If a *spatial decomposition* (sBSS) is intended, then we identify $\mathbf{W} = \mathbf{U}_K\boldsymbol{\Sigma}_K$ and $\mathbf{H} = \mathbf{V}_K^T$. Note that here $\mathbf{H}$ is related to the underlying sources while $\mathbf{W}$ forms part of the mixing matrix of the model.