

FMRI UNMIXING VIA PROPERLY ADJUSTED DICTIONARY LEARNING

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ABSTRACT

The mapping of the functional networks within the brain is a major step towards a deeper understanding of the brain function. It involves the blind source separation of obtained fMRI data, usually performed via independent component analysis (ICA). Recently, there is an increased interest for alternatives to ICA for data-driven fMRI unmixing and notably good results have been attained with Dictionary Learning (DL) - based analysis. In this paper, the K-SVD DL method is appropriately adjusted in order to cope with the special properties characterizing the fMRI data.

Index Terms— Matrix Factorization, fMRI, Blind Source Separation, Dictionary Learning

1. INTRODUCTION

Functional Magnetic Resonance Imaging (fMRI) [1] is a powerful non-invasive tool for localizing and analyzing brain activity. Most commonly it is based on blood oxygenation level-dependent (BOLD) contrast, which translates to detecting localized changes in the hemodynamic flow of oxygenated blood in activated brain areas. This is achieved by exploiting the different magnetic properties of oxygen-saturated versus oxygen-desaturated hemoglobin.

In the brain, tasks involving action, perception, cognition, etc., are performed via the simultaneous activation of a number of *functional brain networks* (FBN), which are engaged in proper interactions in order to effectively execute the task. Such networks are usually related to low-level brain functions and they are defined as a number of *segregated* specialized small brain regions, potentially distributed over the whole brain. These regions collaborate in order to coherently perform a certain brain function [2]. The segregated brain regions involved in a certain brain network are said to be *integrated*, [2], in the sense that irrespective of their anatomical proximity or remoteness, they exhibit strong anatomical and/or functional connectivity. Functional connectivity is often expressed as strong coherence in the activation time-patterns of these regions. Examples of such brain networks are the visual, sensorimotor, auditory, default-mode, dorsal attention, and executive control networks.

A challenging fMRI experimental procedure is the task-free one, referred to as *resting-state* fMRI. In this case, there is no correlation to previously known activation patterns, induced by external stimulus to the subject, and, hence, the steady-state functional analysis of the brain activity needs to be realized blindly. Independent Component Analysis (ICA) [3], which searches for functionally independent components or “sources” in the recorded fMRI signal is the most commonly used method in this case.

Recently, there is an increased interest for alternatives to ICA for data-driven fMRI unmixing. Notably good results have been attained with Dictionary Learning (DL) - based fMRI analysis, which can be grouped in two major categories. Those dealing with the analysis of the fMRI data of a single subject (e.g. of a certain person)[4, 5] and those that jointly accommodate data of multiple subjects, e.g.,[6–8]. In a different approach [9], DL was applied not on the data matrix itself but on correlations between columns of \mathbf{Y} corresponding to carefully selected Regions of Interest (ROIs). In this paper, we focus on the single subject case and particularly to DL based on the popular K-SVD (K-Singular Value Decomposition) method [10,11]. The K-SVD is properly modified in order to be rendered suitable for the analysis of fMRI data. In particular, a mechanism for the detection and effective joining of FBNs which are incorrectly split by conventional K-SVD is proposed in order to comply with the segregation and integration properties of the FBN. Moreover, extra care is given in order to cope well with machine artifacts.

2. PROBLEM DESCRIPTION

The data is collected during an fMRI experiment from successive 3D brain volume scans. Relying on adequate post-processing, which effectively compensates for possible time-lags [1], it is fairly accurate to assume that each acquisition is performed instantly. Therefore, the outcome of each scan, is a number of, say n , values, quantifying the activation at n points across the brain, at a certain time instance, say i . These points (voxels) are spatially distributed on a 3D grid and their values are collected in vector $\mathbf{y}_i \in \mathbb{R}^n$. Such vectors are also referred to as spatial maps. Considering t successive acquisitions, the full amount of data is collected in a matrix $\mathbf{Y} = [\mathbf{y}_1^T, \mathbf{y}_2^T, \dots, \mathbf{y}_t^T]^T \in \mathbb{R}^{t \times n}$. Hereafter, the notations, $\mathbf{Y}_{i,\cdot}$ and $\mathbf{Y}_{\cdot,j}$ are used to denote the i th and the j th row and column respectively. Moreover, $\mathbf{Y}_{I,J}$, is the submatrix of \mathbf{Y}

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having the rows and columns indexed in vectors I, J . Note that, $\mathbf{Y}_{i,\cdot}$ are the voxel values at time instance i and $\mathbf{Y}_{\cdot,j}$ are the values of the j th voxel along time.

Following the discussion in 1, FBNs networks are characterized by specific regions (clusters of voxels) distributed across the brain, which are activated synchronously. Accordingly, brain networks can be described by spatial maps, $\mathbf{s}_j \in \mathbb{R}^n$, having values different than, essentially, zero at those indices corresponding to activated voxels only. Apparently, vectors \mathbf{s}_j are *sparse*, i.e., they comprise mostly zeros (or very close to zero). Assume that during an fMRI experiment, a number of, say p , FBNs are activated and interact in order to deal with the requested brain task and let these vectors being collected as rows in matrix $\mathbf{S} \in \mathbb{R}^{p \times n}$. If these FBN *interact linearly*, then at any time instance, i , the corresponding fMRI data vector, $\mathbf{Y}_{i,\cdot} = \mathbf{T}_{i,1}\mathbf{S}_{1,\cdot} + \mathbf{T}_{i,2}\mathbf{S}_{2,\cdot} + \dots + \mathbf{T}_{i,p}\mathbf{S}_{p,\cdot}$, where $\mathbf{T}_{i,j}$ expresses the contribution of the j th spatial map in the formation of the i th row of \mathbf{Y} . The rank of \mathbf{Y} equals to p and it can be factorized as $\mathbf{Y} = \mathbf{T}\mathbf{S}$, where $\mathbf{T} \in \mathbb{R}^{t,p}$. The columns $\mathbf{T}_{\cdot,i}$ of matrix \mathbf{T} reveals the time courses associated with the corresponding spatial maps signals $\mathbf{S}_{i,\cdot}$.

The task of fMRI unmixing, is to estimate the spatial maps corresponding to the FBNs, \mathbf{S} , and their evolution in time determined by \mathbf{T} . This is essentially a matrix factorization (MF) problem. There are numerous methods/approaches, which are able to factor \mathbf{Y} as the multiplication of two appropriately sized matrices, $\mathbf{Y} = \mathbf{A}\mathbf{B}$, however this factorization is not unique. Indeed, since \mathbf{Y} is rank deficient, all its column vectors lie on a p dimensional subspace¹. For example, any matrix \mathbf{A} comprising p vectors, which span the column space of \mathbf{Y} , it can serve in the MF task when combined with a proper matrix \mathbf{B} . So for successful fMRI data analysis, *constraints with respect to the structure of the estimated matrices \mathbf{A} and/or \mathbf{B} need to be set in order, among the potentially infinite number of \mathbf{A}, \mathbf{B} combinations, the MF method to return a pair of matrices which is as close as possible to \mathbf{T}, \mathbf{S} . Such constraints stem from a priori known information regarding the true matrices. For example, in this paper matrix \mathbf{B} , which represents the spatial maps, is constrained to be sparse. In non blind fMRI analysis methods, for example in General Linear Model (GLM), \mathbf{A} is predefined and related to Hemodynamic Response Function (HRF) [1].*

3. FMRI UNMIXING VIA DICTIONARY LEARNING

Dictionary learning (DL) is conventionally related to the sparse representation / sparse coding problems. The objective of sparse coding is to chose a few elementary signals, called atoms, drawn from a pre-specified set of such signals, referred to as *dictionary*, which better represents a certain signal \mathbf{y} . Let \mathbf{A} be a dictionary matrix, i.e., having the dictionary atoms as columns. A popular form that sparse coding can take is mathematically described as follows [12, 13]:

$$\min_{\mathbf{b}} \|\mathbf{y} - \mathbf{A}\mathbf{b}\| \text{ s.t. } \|\mathbf{b}\|_0 \leq k, \quad (1)$$

¹The columns have been centered in order to have zero mean

where $\|\cdot\|_0$ is the ℓ_0 pseudo-norm counting the number of nonzero components of the unknown vector \mathbf{b} and k is the number of atoms, which are linearly combined to represent \mathbf{y} . Apparently, the better suited for a certain signal (or class of signals) a dictionary is, the sparser the representations of similar signals will be. Here comes the role of DL. Based on a number of representative/training signals $\mathbf{y}_i, i = 1 \dots n$, DL aims to train a dictionary, i.e., to find a set of atoms, which can sparsely represent the training signals and consequently any other similar signal. In matrix form, DL is described as [10]:

$$\min_{\mathbf{A}, \mathbf{B}} \|\mathbf{Y} - \mathbf{A}\mathbf{B}\|_{\mathbb{F}}^2, \text{ s.t. } \|\mathbf{B}_{\cdot,j}\|_0 \leq k, j = 1 \dots n, \quad (2)$$

where \mathbf{Y} contains the training examples as columns and $\|\cdot\|_{\mathbb{F}}$ is the Frobenious norm. Moreover, a constraint on the dictionary norm is necessary in order to avoid degenerate solutions, with the unit-norm request for each atom being the most popular. Alternative DL forms are also possible, such as regularized versions where the sparsity constraint is not explicitly imposed on the columns of \mathbf{B} [14].

The question that comes first in mind is why DL is potentially suitable for fMRI unmixing. The answer is that as a byproduct of the DL procedure, the produced atoms *capture high level features and intrinsic information* about the batch of training signals itself. Moreover, DL is inherently a constrained MF approach since it aims to factor \mathbf{Y} as the product of \mathbf{A}, \mathbf{B} with the latter having sparse columns. Accordingly, \mathbf{B} is likely to have sparse rows as well. This is a property suitable to the fMRI case since the spatial maps, at least those having a physiological origin, are sparse (see also discussion in 1).

One of the most popular DL methods is the K-SVD, which alternates between two learning stages until convergence. In the first stage, \mathbf{B} is estimated via a series of sparse codings implemented column by column, i.e.

$$\min_{\mathbf{B}_{\cdot,j}} \|\mathbf{Y}_{\cdot,j} - \mathbf{A}\mathbf{B}_{\cdot,j}\| \text{ subject to } \|\mathbf{B}_{\cdot,j}\|_0 \leq k, \quad (3)$$

$\forall j$ and the dictionary \mathbf{A} is fixed to its latest estimate. In the second stage, the dictionary atoms are updated and on the same time, the nonzero values of \mathbf{B} are further refined. Denoting by \mathbf{z}_i and $\bar{\mathbf{z}}_i$ two vectors comprising the indices of the zeros and the nonzeros of $\mathbf{B}_{i,\cdot}$, the second stage is described by the following minimization problem,

$$\min_{\mathbf{A}, \mathbf{B}} \|\mathbf{Y} - \sum_{i=1}^p \mathbf{A}_{\cdot,i} \mathbf{B}_{i,\cdot}\|_{\mathbb{F}}^2 \text{ s.t. } \mathbf{B}_{i,\mathbf{z}_i} = 0, i = 1, \dots, p, \quad (4)$$

where the matrix product, $\mathbf{A}\mathbf{B}$ in the Frobenious norm has been equivalently written as the sum of p rank-1 matrices and the constraint forces the updated matrix \mathbf{B} to keep the same support. Denote by $\mathbf{E}^{(i)}$ the reconstruction error achieved without the participation of the i th dictionary atom, i.e., $\mathbf{E}^{(i)} = \mathbf{E} - \mathbf{A}_{\cdot,i} \mathbf{B}_{i,\cdot}$, where $\mathbf{E} = \mathbf{Y} - \mathbf{A}\mathbf{B}$. The original K-SVD, minimizes (4) in p steps optimizing one dictionary atom and the corresponding row of \mathbf{B} restricted to $\bar{\mathbf{z}}_i$, at a time. In

particular, for the i th dictionary atom, the best 1-rank approximation of $\mathbf{E}_{\bar{z}_i}^{(i)}$, is computed via SVD, i.e. $\mathbf{E}_{\bar{z}_i}^{(i)} = \mathbf{U}\mathbf{D}\mathbf{V}^T$ and then $\mathbf{A}_{\cdot,i} = \mathbf{u}_1$, and $\mathbf{B}_{i,\bar{z}_i} = d_1\mathbf{v}_1^T$, where $\mathbf{u}_1, \mathbf{v}_1$ are the left and right singular vectors that correspond to the larger singular value d_1 .

Although K-SVD has been proved to be one of the most reliable and well performing algorithms in DL specialized applications, it was recently shown that when it is used for MF in the fMRI context, performs inferiorly than potentially faster DL methods. A notable example is the Fast Incoherent Dictionary Learning (FIDL) algorithm, [5], which is using steepest descent iterations in order to update the matrices \mathbf{A} and \mathbf{B} directly rather than in a column by column manner. The enhanced performance that FIDL exhibits is due to the fact that it complies better with the nature of the fMRI data. First, the dictionary atoms are forced to be incoherent something that promotes the integration property of the FBNs and second, the sparsity property is not enforced to each column separately but to the whole matrix \mathbf{B} . In this manner, spatial components, i.e. rows of \mathbf{B} , which are not sparse because, for example are due to artifacts, are easier accommodated than in the K-SVD case.

4. FMRI-SUITED K-SVD

Encouraged by the superior performance attained by the K-SVD in several applications, we here further elaborate on this method in order to render it suitable for fMRI unmixing. Apparently, in order for a DL method to operate well on fMRI data, a careful assessment on how well it complies with the segregation and integration properties of the FBN, is necessary. Moreover, extra care is required in order to cope well with machine artifacts. Apart from the performance front, low computational complexity is definitely a merit due to the massive volume of fMRI data. Next, a modified K-SVD complying with the above recommendations is proposed.

4.1. Detecting and Joining split FBNs

DL on fMRI data often leads to the undesirable behaviour described next: Segregated brain regions corresponding to the same FBN is possible to get split in several time-course/spatial-map vectors. However, due to the fact that all these regions are functionally associated, the corresponding time-course vectors are going to be similar, i.e., correlated. In FIDL, such splits are prevented due to the fact that the dictionary atoms, i.e., the time courses, are forced to be uncorrelated using a properly modified cost function. Although there are K-SVD variants which promotes incoherence among the dictionary atoms, e.g., [15], when they are applied in fMRI are unable to supersede FIDL or fast ICA performance [5]. Following a different route, here we incorporate in K-SVD a different mechanism for detecting and joining together spatial maps, which are likely to correspond to the same FBN.

In particular, after the dictionary update stage, the strictly lower triangular Gram matrix containing the correlations

among the dictionary atoms is computed

$$\mathbf{G}_{i,j} = \begin{cases} \mathbf{A}_{\cdot,i}^T \mathbf{A}_{\cdot,j}, & i > j \\ 0, & \text{otherwise} \end{cases} \quad (5)$$

The larger an entry, in magnitude, $|\mathbf{G}_{i,j}|$ of the Gram matrix is, the more likely for the corresponding time courses $\mathbf{A}_{\cdot,i}$ and $\mathbf{A}_{\cdot,j}$ is to belong to the same FBN.

To this end, a user defined parameter $\mu_A \in [0, 1]$ is introduced. Any pair of dictionary atoms having correlation larger than $\mu_A \in [0, 1]$ are considered to belong to the same FBN. The approach followed for detecting and joining together two or more spatial maps is described next. The Gram matrix is searched for at least one entry larger, in magnitude, than μ_A . If such entry does not exist, then the algorithm proceeds to the next K-SVD iteration. If exists, then the leftmost column of the Gram matrix having such an entry, say this is the \bar{m} th one, provides all the necessary information about the spatial maps that need to be merged. Denote as \mathbf{m} a vector containing the index \bar{m} plus the indices in which $|\mathbf{G}_{\cdot,\bar{m}}|$, is larger than μ_A . Then the spatial maps at the rows of $\mathbf{B}_{\mathbf{m},\cdot}$ as well as the corresponding time courses, $\mathbf{A}_{\cdot,\mathbf{m}}$ need to be merged because they correspond to the same FBN. Denote by, $\bar{\mathbf{b}}$ and $\bar{\mathbf{a}}$ the spatial map and the time course that results from the merging. In this paper, $\bar{\mathbf{b}}$ and $\bar{\mathbf{a}}$ are chosen to be those optimizing

$$\min_{\bar{\mathbf{a}}, \bar{\mathbf{b}}} \|\mathbf{A}_{\cdot,\mathbf{m}} \mathbf{B}_{\mathbf{m},\cdot} - \bar{\mathbf{a}} \bar{\mathbf{b}}^T\|_{\text{F}}^2. \quad (6)$$

Note that $\mathbf{A}_{\cdot,\mathbf{m}} \mathbf{B}_{\mathbf{m},\cdot}$ is the overall contribution of those spatial maps indexed in \mathbf{m} in explaining the data matrix \mathbf{Y} . Having decided that all these maps are parts of the same FBN, then they should be replaced by a single time-course/spatial map pair. This is what (6) attempts to. The solution of the above minimization task is given by the best rank-1 approximation of $\mathbf{A}_{\cdot,\mathbf{m}} \mathbf{B}_{\mathbf{m},\cdot}$. It can be computed via SVD similarly to the dictionary update stage of the original K-SVD.

The estimated FMN replaces one of the involved spatial maps, say the \bar{m} , i.e. $\mathbf{A}_{\cdot,\bar{m}} = \bar{\mathbf{a}}$ and $\mathbf{B}_{\bar{m},\cdot} = \bar{\mathbf{b}}$. The rest of those involved in the merging, i.e. those with indices in \mathbf{m} have their corresponding time courses replaced with randomly selected columns of the error matrix \mathbf{E} . This choice is justified by the fact that \mathbf{E} represents the residual which have not been represented by the estimated matrices \mathbf{A} and \mathbf{B} , yet. The associated rows of \mathbf{B} will be filled by the sparse coding stage in the next K-SVD iteration.

In a similar fashion, spatial maps which are found to be highly correlated, i.e. corresponding to values in the Gram matrix larger than a user defined value μ_B , are also being merged. The physical reason for that is that it has been observed that different FBNs do not overlap much, spatially. Accordingly, spatial maps which are highly correlated, meaning that they have similar supports, is highly likely to correspond to the same FBN, which have been duplicated, by mistake, in the DL process. Such a condition is usually takes place whenever, a time-course has been split in two or more parts.

4.2. Coping with machine induced artifacts

Real fMRI data do not only comprise of signals related to the brain activity, known as signals of interest, but they also con-

tain signals related to machine-induced artifacts. The latter include motion-related signals due to head movement, respiration, cardiac pulsation, etc. There are also signals related to noise artifacts from scanner drifts (slowly rising), electronic interferences, etc. In most cases, these artifacts exhibit low localization and are usually spread over wider brain areas rendered, in this way, dense. Here, we exploit this property, which need to be properly incorporated into the first stage of the K-SVD, in order to impose the formation of a certain number of, say r , dense rows in the spatial map matrix \mathbf{B} . Parameter r is user defined and it should be roughly equal to the number of components due to artifacts, which are expected.

Without loss of generality, the first r rows of \mathbf{B} will be forced to be dense. In the sparse coding stage of K-SVD, the request for the first r components of $\mathbf{B}_{:,i}$, $\forall i$, to be nonzeros is translated to a typical case of sparse reconstruction with partly known support (PKS) [16]. In this paper, for the sparse coding stage we use a low cost Orthogonal Matching Pursuit (OMP) algorithm, [17], properly modified in order to comply with the request above. In particular, the PKS-OMP can directly initiate from iteration r , setting the nonzero support set accordingly.

4.3. Low computational complexity implementation

A critical issue related to fMRI unmixing is that of computational complexity which might be proved infeasible for several techniques due to the large data matrices involved. For this reason, in the proposed K-SVD variant the techniques which have been proposed in [17] for the efficient implementation of the original K-SVD have been adjusted to fit the fMRI-suited K-SVD. Accordingly, the Batch-OMP is used incorporating the fact that the support is partially known, i.e. the first r components are fixed to be nonzero.

From the discussion above it was pointed out that many rank-1 approximations are required not only in the dictionary updating stage but also when potential merging of spatial maps is required. For this reason the SVD, even though gives the exact solution to the problem, it had been replaced with the approximate scheme proposed in [17].

5. PERFORMANCE EVALUATION

In this study, the synthetic albeit realistic fMRI data set used in [18] was used. These data result from the mixture of eight main sources depicted in the upper row of Fig. 1). The time course for each component (lower row of Fig. 1) defines the temporal characteristics of the corresponding source, namely one task-related (S1), two transiently task-related (S2, S6) and several artifact types (S3, S4, S5, S7, S8), including respiration, cardiac pulsation, scanner drift, background noise, etc. These sources can be considered as spatial maps that are activated according to their time course and mixed linearly to produce the final (simulated) fMRI data.

The source signals in the upper row of Fig. 1 are vectorized and mixed according to the corresponding time courses producing a data matrix $\mathbf{Y} \in \mathbb{R}^{100 \times 3600}$. Four methods are fed with this data matrix in order to separate the 8 sources

Dsize=12	Ca	Cm	Cam
fastICA	0.776 (0.917)	0.849 (0.971)	0.812 (0.944)
FIDL	0.833 (0.961)	0.801 (0.921)	0.817 (0.941)
sparse GLM	0.702 (0.764)	0.714 (0.800)	0.708 (0.782)
Proposed	0.846 (0.950)	0.853 (0.950)	0.850 (0.950)

Table 1. Performance with Dictionary size 12

Dsize=20	Ca	Cm	Cam
fastICA	0.776 (0.917)	0.849 (0.971)	0.812 (0.944)
FIDL	0.836 (0.960)	0.792 (0.895)	0.814 (0.927)
sparse GLM	0.798 (0.914)	0.697 (0.793)	0.747 (0.853)
Proposed	0.862 (0.972)	0.861 (0.952)	0.861 (0.962)

Table 2. Performance with Dictionary size 20

blindly. That is, the fast ICA [19], the FIDL [5], the sparse GLM [4] and the proposed method. In order for the performance evaluation to be statistically reliable, the final results are the outcome of the ensemble average of 20 independent runs, where each run correspond to a different, randomly chosen initialization of the algorithms.

The performance results are tabulated in the Tables 1 and 2, corresponding to dictionary sizes 12 and 20 respectively. In particular, Ca is the mean absolute correlation over the 20 runs for the best-matched time courses, Cm is the mean absolute correlation over the 20 runs for the corresponding activation maps and Cam is the mean of Ca and Cm. The mean absolute correlation is a proper performance measure whenever the ground truth is known [18], such as in the current study. Two values are shown for each case. One in parenthesis and one plain. In the latter, the mean correlation of all the 8 sources have been taken, whether in the parenthesis the mean concerns only the three sources directly related to brain activations, i.e. sources S1, S2 and S6. For fastICA, the best configuration included 'symmetric' approach and 'skew' non-linearity ('pow3' for brain-only sources experiments), with stabilized algorithm in all cases. For FIDL the set up given in section 4.2 in [5] was adopted since it concerns very similar data to the ones in this study. Notable improvements with different parameter configurations were not observed apart from parameter k_{max} . For best performance it was set to 50 and 10 for dictionary sizes 12 and 20, respectively.

For the proposed algorithm the free parameters were set up to the following values: $\mu_A = 0.8$, $\mu_B = 0.7$, the sparsity level in the sparse coding stage $k = 8$, i.e. equal to the rank of the data matrix and the number of nonsparse rows, $r = 3$. Note that both r and k are not the true values in the specific data set which have four nonsparse rows and the number of nonzeros per column varies from 4 to 6. Moreover, for the approximate SVD, 20 iterations have been used.

The proposed algorithm, with limited exceptions, outperforms the rest of the evaluated algorithms. Two observations are worthy to emphasize. First, the modifications which are made in order to deal better in the fMRI context, led to significant performance improvement over the sparse GLM, which in fact is the K-SVD without the proposed extensions. Second, both ICA and FIDL favor either the spatial maps (ICA) or the time courses (FIDL). On the contrary the proposed

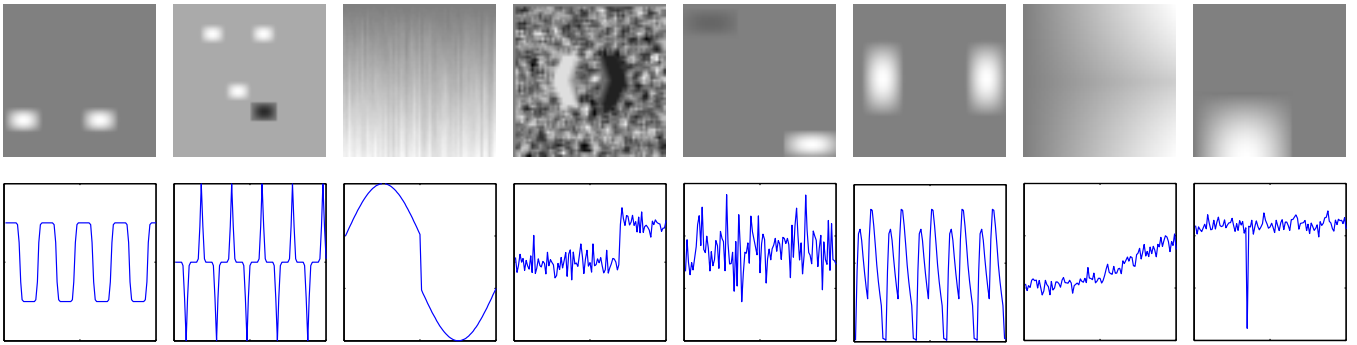


Fig. 1. Spatial-aps and the corresponding time-courses

method exhibits similar performance with respect to both Ca and Cm. This results a clear improvement when the average Cam is considered.

With respect to computational complexity, although the original K-SVD is quite heavy, the Batch-OMP and approximate SVD simplifications used here reduces it considerably. It turns out that the proposed method has the same order of complexity with FIDL, however, it converges much faster leading to lower overall computational burden. In particular, the results shown corresponds to 10 iterations of the proposed algorithm whereas FIDL requires about 50 to converge (see Fig. 2). In detail, the computational complexity analysis will be presented elsewhere.

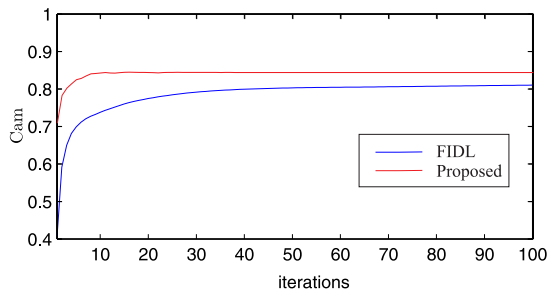


Fig. 2. Convergence speed of the proposed method over FIDL

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