Joint Estimation of Activity Signal and HRF in fMRI using Fused LASSO

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***Abstract*—In this paper, we propose a novel voxel-based method for joint estimation of underlying activity signal and hemodynamic response function (HRF) in functional magnetic resonance imaging (fMRI). In the proposed two stage iterative framework, fused-least absolute shrinkage and selection operator (Fused LASSO) penalty is utilized for activity detection and HRF estimation. Conditions of smoothness and sparsity are imposed on HRF for its estimation. The validity of the proposed method is demonstrated on both synthetic and real fMRI data.**

***Keywords*-functional MRI, Hemodynamic Response Function, fused LASSO, l^1 minimization.**

I. Introduction

Functional Magnetic Resonance Imaging (fMRI) is being used extensively for neuroscience research and clinical applications [1]. fMRI is a non-invasive method that measures blood oxygen-level dependent (BOLD) signals in the brain where BOLD signal is the convolution of an activity signal (or stimulus) with hemodynamic response function (HRF) that is characteristic of the brain region [2].

To infer meaningful information in fMRI data, statistical methods play a crucial role [3]. Conventional, general linear model (GLM) framework in fMRI relies on apriori knowledge of experimental paradigm and hence, the extrinsic activity signal (or stimulus) [4, 5]. In addition, studies also assume a predefined shape of HRF [6]. Thus, typically each voxel's BOLD time series is regressed on constructed or known temporal regressors, and region activation is detected using this predefined information. However, we may not have knowledge of activity signal when it is intrinsic stimulus such as during discharges in epilepsy, resting state, etc. [7-8]. In addition, the shape of HRF may also be different in different regions of the brain as well as in patients with neuro-disorders [9]. Thus, there is a need for developing a methodology for joint estimation of underlying activity signal and the shape of HRF.

Although methods have been proposed for the estimation of activity signal [10-14], these methods assume apriori a canonical shape of HRF. For example, in [10] fixed canonical HRF is assumed along with spatio-temporal priors on the underlying activity signal to estimate the activity signal. In addition to the limitation of a fixed apriori HRF shape, region based estimation is assumed while voxels may have different HRFs within a region of interest (ROI). Recently, in [11], voxel based canonical HRF is used to design finite rate innovation sampling kernel to estimate the underlying activation signal. In [12-14], sparsity constraint is imposed on underlying activity signal in the GLM framework, but again assuming apriori canonical HRF shape.

Thus, the above methods have drawbacks because HRF may vary across different regions of the brain and across different subjects. Since HRF modeling can play a crucial role in the estimation of the underlying activity signal, we propose a method for the joint estimation of HRF and the activity signal. To take care of HRF variability across ROI, we use massive univariate approach, i.e., voxel-based estimation framework. This framework takes care of spatio temporal variability of the HRF. In the joint estimation framework, we use a two-stage iterative procedure. First, we estimate the underlying activity signal via fused least absolute shrinkage and selection operator (fused LASSO) constraint on activity signal assuming some initial shape of HRF. Next, we refine the HRF estimate using the estimated activity signal at each voxel. This procedure is iterated until the shapes of HRF and the activity signal converge. The proposed method has been tested on both the synthetic and the real fMRI data.

This paper is organised as follows. Section 2 describes the fMRI time series model. Section 3 describes the proposed method for joint estimation of HRF and activity signal. Simulation results on both simulated and real fMRI data are presented in Section 4. In the end, conclusions are presented in section 5.

II. FMRI time series model

This section presents a brief background on fMRI signal time series. Let us consider that M no. of brain volumes, at time instants t_j where $j = 1, 2, \ldots, M$, have been captured during an fMRI experiment. The BOLD signal intensity at a particular voxel V_i in the scanned brain volumes can be represented as a time series $\mathbf{y}_i = [y_{i,1}, y_{i,2}, ..., y_{i,M}]$.

In general, an fMRI signal is comprised of a) hemodynamic signal modeled as convolution of activity signal with HRF and b) noise that is correlated in time generally modeled as autoregressive noise of order 1 (AR (1)) [15]. Thus, the BOLD signal at a voxel V_i is represented as [3]:

$$\mathbf{y}_i = \mathbf{s}_i \otimes \mathbf{h}_i + \xi_i, \qquad (1)$$

where $\mathbf{s}_i$ is a vector of length M representing activity signal, $\mathbf{h}_i$ is the amplitude of L-length HRF at voxel V_i, and ξ_i is the vector of M-length representing colored AR(1) noise $\xi_i \in N(0, \mathbf{\Gamma})$, where $\mathbf{\Gamma}$ is a symmetric positive definite covariance matrix of size MxM with its l^{th} element $\rho^{|l|}$. Equation (1) has two unknown functions: the HRF $\mathbf{h}_i$ and the activity signal $\mathbf{s}_i$.

III. Proposed Joint estimation framework

In this section, we present the proposed joint estimation framework of HRF and activity signal. We carry out estimation as a two-stage iterative method wherein we first estimate the activity signal $\mathbf{s}_i$ followed by estimation of HRF $\mathbf{h}_i$.

A. Stage-1: Estimation of activity signal

The model in (1) can be rewritten as

$$\mathbf{y}_i = \mathbf{H}_i \mathbf{s}_i + \xi_i. \tag{2}$$

where $\mathbf{H}_i$ is a Toeplitz convolution matrix of dimension MxM. The first column of $\mathbf{H}_i$ is filled with HRF padded with M-L zeros at the end.

In this paper, we limit the method to the estimation of block related designs. In this scenario, the activity signal will be sparse and the first difference will be more sparse. Thus, we impose a fused least absolute shrinkage and selection operator (LASSO) penalty to the activity signal. Fused LASSO which is introduced in [16], encourages sparsity in both coefficients and their successive first difference. It has been used in many applications, such as image denoising, time varying networks, prostate cancer analysis, etc [17-19].

Using the above motivation, we formulate the problem of estimation of activity signal as below:

$$\hat{\mathbf{s}}_i = \underset{\mathbf{s}_i}{argmin} \left\| \mathbf{R}_v(\mathbf{y}_i - \mathbf{H}_i \mathbf{s}_i) \right\|_2 + \lambda_0 \left\| \mathbf{s}_i \right\|_1 + \lambda_1 \sum_{j=2}^{M} | \, s_{i,j} - s_{i,j-1} \, |, \tag{3}$$

where $\mathbf{R}_v$ is the decorrelation or the noise whitening matrix resulting from the Cholesky factorization of the inverse of noise covariance matrix $\mathbf{\Gamma}$ ($\mathbf{\Gamma}^{-1} = \mathbf{R}_v^T \mathbf{R}_v$) [20]. λ_1 is the regularisation parameter. This problem is difficult to solve because fused LASSO penalty is non-smooth and nonseparable. Thus, this estimation problem can be reformulated in matrix form as below:

$$\hat{\mathbf{s}}_i = \underset{s_i}{argmin} \left\| \mathbf{R}_v(\mathbf{y}_i - \mathbf{H}_i \mathbf{s}_i) \right\|_2 + \lambda_0 \left\| \mathbf{s}_i \right\|_1 + \lambda_1 \left\| \, \mathbf{T}\mathbf{s}_i \, \right\|_1, \tag{4}$$

where $\mathbf{T}$ is the first difference matrix operator as given below:

$$\mathbf{T} = \begin{bmatrix} -1 & 1 & 0 & . & . & 0 & 0 \\ 0 & -1 & 1 & 0 & . & . & 0 \\ 0 & 0 & -1 & 1 & 0 & . & . \\ 0 & 0 & . & . & . & . & . \\ . & . & . & . & . & . & 0 \\ 0 & . & . & . & 0 & -1 & 1 \\ 0 & 0 & . & 0 & 0 & 0 & -1 \end{bmatrix}$$

This optimization problem can be solved easily. However, in (4), $\mathbf{H}_i$ is unknown. Thus, we start with an initialization of HRF using the canonical shape of HRF.

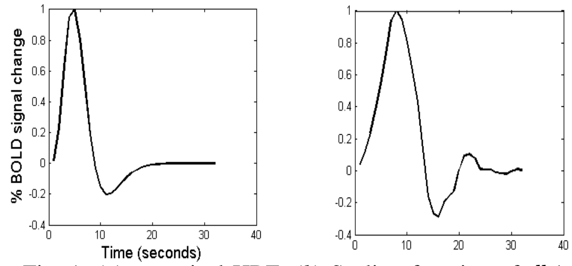

Fig. 1: (a) canonical HRF; (b) Scaling function of $db4$

B. Stage-2: Estimation of HRF

This subsection describes the estimation of HRF in the joint iterative estimation framework. The model in equation (1) can also be written as:

$$\mathbf{y}_i = \mathbf{S}_i \mathbf{h}_i + \xi_i. \tag{5}$$

where $\mathbf{S}_i$ is a MxL Toeplitz convolution matrix consisting of lagged stimulus estimated covariates at voxel V_i.

In our recent work [21], we have drawn following assumptions on HRF:

B1) HRF is a smooth function over time. Thus, we incorporated this knowledge into our formulation and apply the Tikhonov regularisation technique for imposing a smoothness constraint on the HRF [22]. This smoothing constraint is imposed by the second difference matrix operator $\mathbf{D}$ which is defined as

$$\mathbf{D} = \begin{bmatrix} 2 & -1 & 0 & . & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & . & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & . & . \\ 0 & 0 & . & . & . & . & . \\ . & . & . & . & 2 & -1 & 0 \\ 0 & . & . & . & -1 & 2 & -1 \\ 0 & 0 & . & 0 & 0 & -1 & 2 \end{bmatrix}$$

We minimize l^2 norm of $\mathbf{D}\mathbf{h}_i$.

B2) In [21], we noted that the shape of the scaling function corresponding to the orthogonal wavelet *Daubechies*-4 (or *db*4) (refer to Fig. 1(b)) is quite similar to the theoretical HRF shape generally assumed (refer to Fig. 1(a)). Thus, HRF analyzed via $db4$ will be sparse in the wavelet domain. Using this argument, we imposed sparsity on $\mathbf{W}\mathbf{h}_i$, where $\mathbf{W}$ is the matrix operator corresponding to $db4$ [21].

Using the above assumptions, we formulate the problem of estimation of HRF mathematically using Lagrangian multiplier method as below:

$$\hat{\mathbf{h}}_i = \underset{h_i}{argmin} \left\| \mathbf{R}_v(\mathbf{y}_i - \mathbf{S}_i \mathbf{h}_i) \right\|_2 + \lambda_2 \left\| \mathbf{D}\mathbf{h}_i \right\|_2 + \lambda_3 \left\| \mathbf{W}\mathbf{h}_i \right\|_1 \tag{6}$$

where λ_2 and λ_3 are the Lagrangian multipliers or the regularization parameters.

C. Complete Algorithm

The above procedure of subsections *A* and *B* are repeated iteratively until the shapes of $\hat{\mathbf{s}}_i$ and $\hat{\mathbf{h}}_i$ converge. The pseudo code for the joint iterative estimation is provided in Table-1.

Table-1

Pseudo Code for the Iterative Joint Estimation framework

Input Parameters

Tikhonov regularisation matrix **D** (size *L* x *L*)

Fused LASSO matrix **T** (size *M* x *M*)

Daubechies-4 matrix **W** (size *L* x *L*)

Initialize HRF matrix $\mathbf{H}_i$(size *M* x *M*)

Lagrangian multipliers λ_1, λ_2, and λ_3 (scalars)

Noise covariance matrix $\boldsymbol{\Gamma}$

Input Data

Measured voxel V_i's time series stacked in a column $\mathbf{r}_i$ (size *M* x 1)

Start

Step-1 $\mathbf{y}_i$=detrend($\mathbf{r}_i$)

Step-2 Compute estimate of activity signal $\hat{\mathbf{s}}_i$

$$\hat{\mathbf{s}}_i = \arg\min_{\mathbf{s}_i} \left\| \mathbf{R}_v(\mathbf{y}_i - \mathbf{H}_i\mathbf{s}_i) \right\|_2 + \lambda_0 \left\|\mathbf{s}_i\right\|_1 + \lambda_1 \left\|\mathbf{T}\mathbf{s}_i\right\|_1$$

Step-3 Compute estimate of HRF $\hat{\mathbf{h}}_i$ using $\hat{\mathbf{s}}_i$

$$\hat{\mathbf{h}}_i = \arg\min_{\mathbf{h}_i} \left\| \mathbf{R}_v(\mathbf{y}_i - \mathbf{S}_i\mathbf{h}_i) \right\|_2 + \lambda_2 \left\|\mathbf{D}\mathbf{h}_i\right\|_2 + \lambda_3 \left\|\mathbf{W}\mathbf{h}_i\right\|_1$$

Repeat Step-2 and Step-3 until the shapes of $\hat{\mathbf{s}}_i$ and $\hat{\mathbf{h}}_i$ converge.

Output $\hat{\mathbf{h}}_i$ and $\hat{\mathbf{s}}_i$

IV. Validation of the Proposed Method

This is to note that the goal of the paper is to estimate the underlying stimulus along with HRF. Thus, it is important that the ground truth is known for the purpose of method validation. In this work, we test the proposed method on the synthetic data constructed with a known HRF and known activity signal with varying duration and varying onset times. For the real fMRI data, block activity signal is used as the ground truth. This implies that we know some ground truth on the activity signal (or stimulus) in the real data too for the purpose of validation of the proposed method, although HRF is unknown in the real data.

A. Results on Synthetic fMRI Data

We generated synthetic fMRI time series by convolving activity signal with the canonical HRF. We designed canonical HRF of length $L = 32$ using the difference of two gamma functions [24]. The shape of this HRF is shown in Fig. 1(a).

In order to assess the proposed framework, we test our algorithm on the above synthetic data where activity signal is generated with 5 ON periods of duration 6s, 5s, 10s, 3s, and 1s with onsets at 10s, 40s, 100s, 140s, 180s, respectively. We generated 200 time points of the synthetic BOLD fMRI signal as below:

$$\mathbf{y} \equiv y[n] = s[n] \otimes h[n] + \xi[n] \tag{7}$$

For the sake of simplicity, noise is assumed to be white. Additive white Gaussian noise is generated with variances 0.75, 0.5, 0.25, 0.1, and 0.05. Thus, $\mathbf{R}_v$ in (3) and (6) is the identity matrix of size MxM. For computing the mean square error (MSE), 500 Monte Carlo cycles have been performed over voxel time-series (i.e., considering 500 different realizations of noise time-series). MSE between the canonical and estimated HRF is calculated as below:

$$MSE = \frac{1}{500}\sum_{k=1}^{500}\left[\frac{1}{L}\sum_{n=0}^{L-1}(\hat{h}_k[n] - h_k[n])^2\right] \tag{8}$$

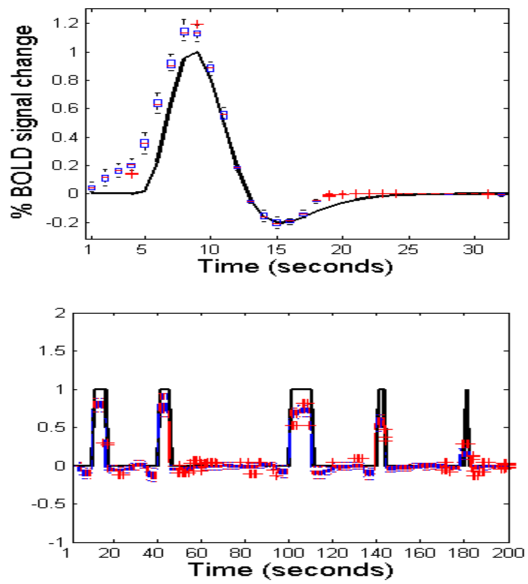

Fig. 2: (a): Estimated HRF; (b) Estimated Activity Signal

Table-2: MSE calculated between estimated and the actual HRF (that is used in the synthetic data)

	Noise Variance σ^2				
	0.05	0.1	0.25	0.5	0.75
MSE using the Proposed method	0.0151	0.0159	0.0171	0.0183	0.0220

The estimated HRF and the estimated activity signal for noise variance of $\sigma^2 = 0.1$ and the regularization parameters of $\lambda_0 = 0.001, \lambda_1 = 0.3, \lambda_2 = 1$, and $\lambda_3 = 0.7$ are shown in Fig. 2(a) and Fig. 2(b), respectively. These parameters are determined empirically where the MSE is minimum. Voxel time series is generated using canonical HRF and the algorithm was initialized using the shape of *Daubechies*-4 (or *db*4) scaling function (Refer to Fig. 1(b)). From Fig. 2(b), we observe that the proposed method is able to extract stimuli sequences or the activity signal with variable onset and duration. The MSE results on the estimated HRF using the proposed algorithm are tabulated in Table-2. Fig. 3 shows the receiver operating characteristics (ROC) curve on the estimated activity signal. It is observed that the performance of the proposed method is satisfactory on the synthetic data.

B. Results on Real fMRI Data

In this section, we present results on real fMRI data acquired from one subject performing a right hand sense task in 3-T MR

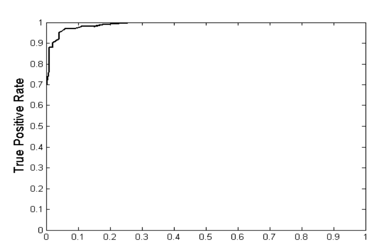

Fig. 3: ROC curve for single voxel time series with σ^2=0.25

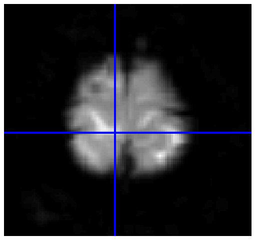

Fig. 4: Seed voxel at (40, 43, 66)

scanner. This dataset consists of an acquisition of 36 contiguous slices with 128x128x36 voxels of voxel size 4x4x4 mm^3. 100 brain volumes with repetition time of 3s are acquired. The task involved is an example of block design paradigm starting with 10 volumes of rest followed by 10 volumes of activity, and so on. Data is preprocessed using SPM8 toolbox [25]. Pre-processing steps include realignment (with the first scan for removal of motion artefact), slice time correction (with the first slice of each volume), and normalisation (with the MNI atlas). Resultant fMRI data had 100 scan points of 79x95x68 voxels each. We did not use smoothing in preprocessing as our algorithm inherently enhances signal to noise ratio (SNR). We discarded first 12 dummy scans, resulting in 88 brain volumes. We also did detrending of real fMRI data prior to extraction of underlying activity signal. This helps in removing the trend from fMRI data and brings it to baseline.

First, we present result on the seed voxel which lies in somatosensory region of the brain and is supposed to be active in right hand sense task. In general, Brodmann regions 1, 2, 3 are found to be associated with somatosensory region [26]. Union of these Broadmann regions is extracted using the WFU Pickatlas Tool in Matlab [27]. Then, seed voxel was extracted in this region using our recent work [21]. The coordinates of the seed voxel were found to be (40, 43, 66). Fig. 4 depicts this seed voxel on the corresponding axial brain slice.

Next, we follow the procedure outlined in Table-1 and estimate both the HRF and the activity signal. We start our algorithm with the canonical HRF shape as shown in Fig. 1(a). The regularization parameters are set to the same values as that used in the synthetic fMRI experiment. Values of ρ in the range of 0 to 1 are tested for an initialization of $\mathbf{R}_v$. Empirically ρ =0.1 is selected for whitening of AR(1) noise on voxel time series. Optimization is carried out in CVX, a package for specifying and solving convex programs [28]. Fig. 5 shows the estimated HRF and the estimated activity signal using the proposed method. The estimated activated signal in Fig. 5(b) is having a block nature. Since first 12 scans were dummy, we observe estimated signal to start from activity (block) followed by the rest block. Although the applied stimulus is in uniform blocks of 10 rest and 10 activity, the estimated activity signal represents the perceived activity stimulus by brain and hence, has a slightly varied shape. This is to note that, in [21], we proposed a method for seed voxel detection using known activity signal. Thus, estimated activity signal at that voxel should closely resemble the applied stimuli which is indeed the case as observed from Fig. 5b. This experiment

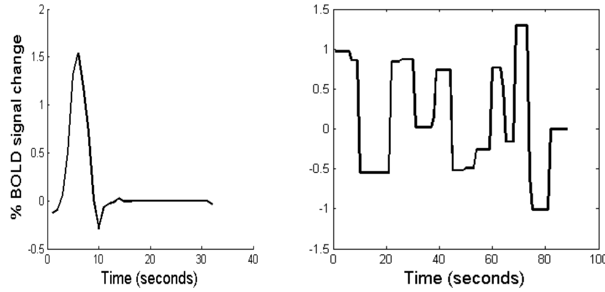

Fig. 5: (a): Estimated HRF; (b) Estimated Activity Signal at voxel (40, 43, 66) using the proposed method

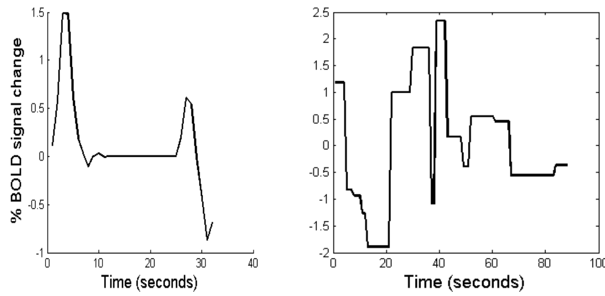

Fig. 6: (a): Estimated HRF; (b) Estimated Activity Signal at voxel (41, 45, 66) using the proposed method

shows that our framework of joint estimation in this paper is robust and reliable.

Next, for the sake of completeness, we test our algorithm on other active voxels. Voxel with coordinates [41, 45, 66] is extracted based on highest norm of voxel time-series lying in somatosensory region. Fig. 6 shows the estimated HRF and the estimated activity signal using the proposed method. We note that on this voxel, the perceived activity stimulus by brain differs from applied stimuli in a greater manner compared to the seed voxel.

In future, we will extend the proposed method to resting state data for the detection of intrinsic activity signal in order to build robust resting state networks.

V. Conclusions

In this paper, we have introduced a joint iterative framework for the estimation of hemodynamic response function (HRF) and the underlying activity signal. This estimation is based on two-stage iterative method. The proposed framework estimates voxel-wise HRF via imposing constraints of sparsity in the wavelet-domain and smoothness in time-domain on HRF. The activity signal is estimated using fused LASSO penalty which imposes sparsity on coefficients as well as on first difference of the activity signal. The proposed method is observed to perform satisfactorily.

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