Constrained Spatiotemporal Independent Component Analysis and Its Application for fMRI Data Analysis

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Abstract

In general, Independent component analysis (ICA) is a statistical blind source separation technique, used either in spatial or temporal domain. The spatial or temporal ICAs are designed to extract maximally independent sources in respective domains. The underlying sources for spatiotemporal data (sequence of images) can not always be guaranteed to be independent, therefore spatial ICA extracts the maximally independent spatial sources, deteriorating the temporal sources and vice versa. For such data types, spatiotemporal ICA tries to create a balance by simultaneous optimization in both the domains. However, the spatiotemporal ICA suffers the problem of source ambiguity. Recently, constrained ICA (c-ICA) has been proposed which incorporates a priori information to extract the desired source. In this study, we have extended the c-ICA for better analysis of spatiotemporal data. The proposed algorithm, i.e., constrained spatiotemporal ICA (constrained st-ICA), tries to find the desired independent sources in spatial and temporal domains with no source ambiguity. The performance of the proposed algorithm is tested against the conventional spatial and temporal ICAs using simulated data. Furthermore, its performance for the real spatiotemporal data, functional magnetic resonance images (fMRI), is compared with the SPM (conventional fMRI data analysis tool). The functional maps obtained with the proposed algorithm reveal more activity as compared to SPM.

Key words : Independent component Analysis (ICA), Spatiotemporal ICA, Constrained ICA, Statistical parametric mapping (SPM), Functional magnetic resonance imaging (fMRI).

I. INTRODUCTION

Independent component Analysis (ICA), a blind source separation (BSS) method based on higher order statistics, decomposes the linear memory-less observations into their underlying maximally independent sources and their corresponding mixing weights [1,2]. There are two conventional modalities in which ICA can be used to decompose the spatiotemporal data into a set of spatial or temporal ICs i.e., spatial ICA and temporal ICA. Spatial ICA finds underlying independent spatial sources and the mixing matrix contains corresponding set of time sequences; temporal ICA finds independent temporal sequences and the obtained mixing matrix gives the corresponding set of spatial modes. With the success of ICA in medical signal processing there is a strong

interest in ICA for the analysis of spatiotemporal data e.g., fMRI images. fMRI is a non-invasive technique used to study spatiotemporal brain functions in both research and clinical areas [3]. It can measure small changes in the MR signal caused by small changes in blood oxygenation level, when specific areas of brain are performing the given task [4]. By acquiring successive images from multiple slices of head in time, image intensity variation at each voxel represent the blood oxygenated level dependent (BOLD) response to a given task. Therefore, it is possible to determine active brain regions for a given task by correlating each voxel signal in MR image sequences to the experimental paradigm. The spatial resolution in fMRI images can go up to 1mm, making it a preferred technique for accurate source localization.

In 1998, McKeown et al. [5] for the first time introduced ICA for fMRI data analysis, with the assumption that fMRI data is a mixture of spatially independent components. Biswal and his colleagues [6] applied the ICA in the temporal domain for fMRI un-mixing. So far, most of the applications of ICA for fMRI are based on ICA using the spatial mode (Spatial ICA). However the choice of spatial or temporal ICA is

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controversial: Comparison and discussion on the underlying assumptions for the use of spatial and temporal ICA is given in [7]. Some authors have also applied ICA on the fMRI data in the complex domain [8] considering that the phase information which is normally discarded in usual ICA application provides vital information. ICA has been successful in the identification of various source signals in fMRI [9] which are considered challenging for the second order techniques such as correlation and regression analysis.

The foremost assumption for ICA application is that the underlying sources should be independent. However, for spatiotemporal data like fMRI image sequences it is difficult to fulfill this independence criterion for both the spatial and temporal domains (i.e., independent sources in spatial domain as well as independent sources in temporal domain). In such cases, spatial or temporal ICA tries to find a set of maximally independent sources in one domain at the cost of their corresponding unconstrained set of sources in the other domain. Lately, Spatiotemporal ICA [10] has been proposed to create a balance by jointly optimizing the sources in spatial and temporal domains. Stone and his colleagues [10] suggested that skew symmetric source distribution is more realistic assumption for fMRI studies. Suzuki et. al. [11] also assumed a skew symmetric distribution in his study. In 2002, Seifritz and his team used a combination of spatial and temporal ICA to analysis the spatiotemporal data [12]. They first used the spatial ICA to locate a region of interest and finally temporal ICA to find the temporal response of human auditory cortex. However, for the higher dimensional data like fMRI, spatiotemporal ICA gives large number of independent components making the subsequent analysis very complicated and subjective. In other words, there exists source ambiguity for ICAs in the conventional spatial, temporal, and spatiotemporal modes.

The existing ICA models are blind source separation methods; they do not take advantage from the a priori

information that might be available about the desired source. In the case of fMRI data, the paradigm information is vital. The conventional ICAs use this information for sorting the ICs found instead of utilizing it in the un-mixing process. Recently, Lu and Rajapakse introduced an algorithm, constrained ICA, [13] that can incorporate a priori information in the un-mixing process. In temporal mode, this algorithm has been applied for fMRI data analysis [13]. Constrained ICA has also been applied for artifact removal from EEG signals [14]. However constrained ICA, which is the same as the spatial or temporal ICA except that it includes the constraints in the cost function, also suffers from the same disadvantage as of spatial or temporal ICA i.e., the maximal independent component in one domain and deteriorated components in the corresponding domain.

As mentioned above, there exists a problem of source ambiguity in the case of spatiotemporal ICA. In case of, constrained ICA source identification problem is solved by incorporating the a priori information. However, the performance of earlier for spatiotemporal data is better than the later. In this study, considering the spatiotemporal nature of fMRI data, we extend constrained ICA into constrained spatiotemporal ICA (constrained st-ICA) that finds independent, yet desired temporal and spatial sources thus solving the source ambiguity problem for spatiotemporal data. The proposed method is based on the singular value decomposition (SVD) and cascade of two simplified one unit ICA-R blocks as shown in the schematic diagram Fig. 1. The performance of the algorithm against the conventional ICAs is tested using the simulated data. To analyze the performance for real spatiotemporal data, it is applied to fMRI data and its results are compared to those of the conventional fMRI data analysis tool i.e., Statistical Parametric Mapping (SPM). The functional maps obtained with the proposed algorithm reveal more active brain regions compared with the SPM. Based on the results we strongly believe that the proposed algorithm could be used for
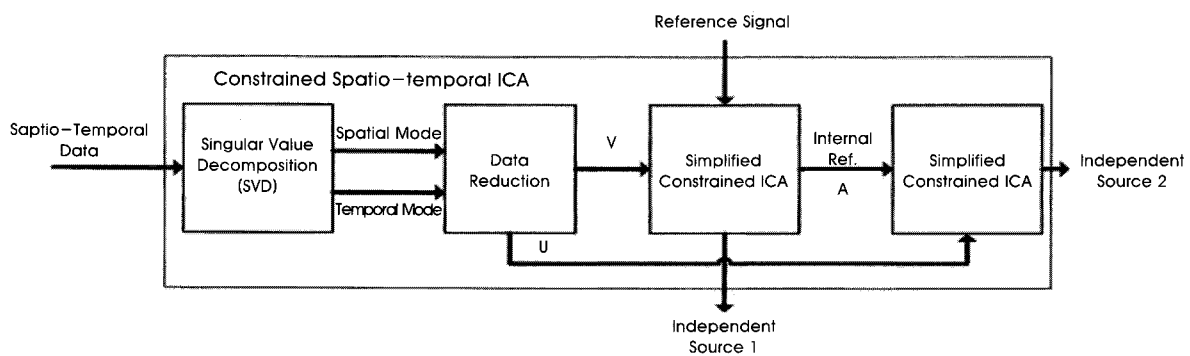

Fig. 1. The schematic diagram of the constrained spatiotemporal ICA.

spatiotemporal data analysis.

II. INDEPENDENT COMPONENT ANALYSIS

Independent component Analysis (ICA) assumes that a linear memory-less observation matrix $X = (x_1, ..., x_m)^t$ can be decomposed into underlying set of independent sources $S = (s_1, ..., s_n)^t$ such that,

$$X = SA \quad \text{or} \quad \hat{S} = XW \tag{1}$$

where A is the $m \times n$ mixing matrix and W is the un-mixing matrix.

General implementations of ICA can be found in the literature [1,2]. If the observation matrix contains image sequence, Equation 1 can be written as $X = SAT^t$ where $S = (s_1, ..., s_k)^t$ represent the independent spatial sources, $T = (t_1, ..., t_k)^t$ the corresponding independent time courses, and Λ the diagonal scaling parameters.

A. Spatial and Temporal ICA

The observation matrix X can be decomposed into $X = UDV^t$ using singular value decomposition (SVD) where U is an $m \times m$ Eigen image matrix, V a $n \times n$ matrix of corresponding Eigen sequences, and D a $m \times n$ diagonal matrix of singular values. By retaining the k singular value we can reduce the rank of the matrix.

$$X \approx \hat{X} = \hat{U}\hat{D}\hat{V}^t \tag{2}$$

Spatial ICA assumes that the $m \times k$ Eigen image matrix $\hat{U}$ can be decomposed into the k spatially independent components. $S = (s_1, ..., s_k)^t$ The corresponding time courses can be obtained as follows.

$$\hat{X} = SA_s \hat{D}\hat{V}^t = ST_s \tag{3}$$

where the rows of $T_s = A_s \hat{D}\hat{V}^t$ contain corresponding time courses. On the other hand, temporal ICA assumes that $n \times k$ Eigen sequence matrix can be decomposed into the k independent temporal components $T = (t_1, ..., t_k)^t$. The corresponding spatial modes can be obtained as follows.

$$\hat{X} = \hat{U}\hat{D}A_t^t T^t = S_t T^t \tag{4}$$

where each column of $S_t = \hat{U}\hat{D}A_t^t$ is the spatial mode.

B. Spatiotemporal ICA

The Spatiotemporal ICA (stICA) [8] is based on the assumption that sometimes underlying spatial and temporal sources are not completely independent. In these cases, spatial or temporal ICA will not produce good results in their corresponding temporal and spatial domains respectively. stICA treats the spatial and temporal domains equally by maximizing the following cost function:

$$h_{st}(W_s, \Lambda) = \alpha H(Y_s) + (1 - \alpha)H(Y_t) \tag{5}$$

where W_s is the spatial un-mixing matrix, Λ the scaling matrix, α the relative weighting factor, $H(Y_t)$ the temporal entropy, $Y_t = \sigma_t y_t$ the cdfs of temporal signals, $y_t = \hat{V}W_t$ extracted temporal signals, $H(Y_s)$ the spatial entropy, $Y_s = \sigma_s y_s$ the cdfs of spatial signals, and $y_s = \hat{U}W_s$ the extracted spatial signals.

C. Constrained ICA

When a priori information about the desired source is available, we can incorporate this information in the constrained ICA (cICA) algorithm [13]. These constraints (or references) guide the algorithm in the direction of only desired independent sources during the optimization process. Variant of unit cICA algorithm can be found in [15]. We will discuss the in detail the one unit cICA algorithm, which is the integral part of our proposed constrained spatiotemporal ICA, with simplifications/modifications that come naturally in our implementation in the next section.

III. CONSTRAINED SPATIOTEMPORAL ICA

The spatiotemporal data where the underlying independence criterion is difficult to establish; the conventional ICA algorithms have some weaknesses, i) spatial or temporal ICA tries to find the maximally independent components in the spatial or temporal domains respectively affecting the components in the corresponding domains, ii) ordering of the output sources are random (source ambiguity), iii) the number of sources found for the high dimensional data are very large (such as sequences of fMRI images), making the subsequent analysis laborious and highly subjective. The stICA tries to overcome the first above mentioned disadvantage of conventional ICA by simultaneously optimizing the spatial and temporal domains. However, it suffers from source ambiguity and large number of derived sources for high dimensional data; same as that of conventional ICAs. The

cICA finds only a specific or a subset of sources and also solves a source ambiguity problem by incorporating a priori information. However, the cICA being exactly the same as that of conventional ICA (same contrast function, same optimization procedure) else than it includes some constrains into the contrast function suffers from the above mentioned first disadvantage of the conventional ICA. In the proposed constrained st-ICA we have tried to collect the advantages of stICA and cICA to overcome the above mentioned disadvantages of conventional ICA.

In this algorithm, we exploited the salient features of SVD along with the one unit cICA algorithm. The SVD: (i) decompose the observed spatiotemporal data into a set of spatial and temporal modes, (ii) the modes are orthonormal and (iii) the rank reduction can be done by selecting an appropriate number of k vectors. Based on these properties, corresponding underlying sources in the two domains can be found independently if some a priori information about the desired source is available. As shown in fig. 1 there are two simplified/fast cICA blocks, we first explain the cICA and the simplifications/modifications that come naturally with our proposed constrained spatiotemporal ICA algorithm then at the end complete algorithm will be explained.

Let there are 'n' independent source signals $s(t) = [s_1(t), s_2(t), \dots, s_n(t)]^t$ and 'm' the number of observed mixtures $x(t) = [x_1(t), x_2(t), \dots, x_m(t)]^t$. The a priori information, which represents some traces of the desired independent source, can be represented in terms of the reference signal $r(t)$. The information in the signal $r(t)$ may be incorporated as closeness constraint onto the ICA contrast function. The closeness constraint for single IC can be written as

$$g(w) = \varepsilon(w^t x, r) - \xi \leq 0 \qquad (6)$$

where ε is some closeness measure (e.g. Mean square error or correlation). The closeness threshold parameter is denoted by ξ. Various ICA algorithms use different contrast functions depending on the application area in which they are used. However the ICA contrast function based on negentropy is very reliable and flexible. In the original one unit cICA algorithm there are two constrains i.e., equality constraints and the inequality constraints. Equality constraints are to keep the unity variance and the inequality constraints are to incorporate the a priori information. In our case, the input data has inherently unit variance because both the modes are orthonormal; we don't need the equality constraints. Therefore the optimization equation for the constrained spatiotemporal ICA is as follows.

$$maximize:\ J(y) \approx \rho[E\{G(y)\} - E\{G(v)\}]^2$$
$$Subject\ to: g(w) \leq 0\ or\ \hat{g}(w) = g(w) + b^2 = 0 \qquad (7)$$

where $J(y)$ denotes the one-unit ICA contrast function introduced by [2], ρ a positive constant, v a zero mean, unit variance Gaussian variable. $G(\cdot)$ is a non-quadratic function as defined in [2], $g(w)$ the closeness constraint mentioned in Equation 5, and b the slack variable. By explicitly manipulating for the optimum b^* the equation 7 can be solved through the use of an augmented Lagrangian function.

$$C(w, \mu) = J(y) + \mu^t \hat{g}(w) + \frac{1}{2} \| \hat{g}(w) \|^2$$
$$C(w, \mu) = J(y) - \frac{1}{2\gamma}[\max^2\{\mu + \gamma g(w), 0\} - \mu^2] \qquad (8)$$

where C represents the new contrast function to be optimized, μ is the Lagrange multiplier and γ is the scalar penalty parameter. Learning of the weights can be achieved through Newton like learning process.

$$w_{k+1} = w_k - \eta R_{xx}^{-1}(C'')^{-1}C'$$
where
$$R_{xx} = E\{xx^t\} = I$$
therefore
$$w_{k+1} = w_k - \eta(C'')^{-1}C'$$
$$w \leftarrow \frac{w}{|w|} \qquad (9)$$
and
$$C' = \bar{\rho}E\{x\,G'_y(y)\} - \frac{1}{2}\mu E\{x g'_y(w)\}$$
$$C'' = \bar{\rho}E\{x\,G''_{y^2}(y)\} - \frac{1}{2}\mu E\{x g''_{y^2}(w)\}$$

The optimum multipliers can be found by iteratively applying the gradient ascent method.

$$\mu_{k+1} = \max\{0,\ \mu_k + \gamma g(w_k)\} \qquad (10)$$

The presented cICA algorithm is simple and fast compared to cICA presented by Lu [13]. There are no equality constrains and matrix inversion (R_{xx}^{-1}) at each iteration is avoided to achieve speed.

Given the spatiotemporal data, the spatial and temporal modes can be obtained via SVD. Appropriate data reduction is also done. A priori information and the appropriate SVD mode (spatial or temporal) after data reduction are given to the first cICA block. The outputs will be the independent source and

the mixing vector of that domain. From the mixing vector reference signal for the corresponding independent source in the other domain can be generated as given in Equation 11. This reference signal and the other reduced SVD mode are presented to the second cICA block. The output will be the independent component of this domain, corresponding to the previously extracted independent component. Constrained st-ICA, fMRI data as a specific example, can be described as follows:

Step 0: The observation matrix X contains the fMRI image sequence.

Step 1: Reduce the dimension of the observation matrix X using SVD. Find $\hat{U}$ and $\hat{V}$ according to Equation 2. The matrix $\hat{U}$ contains spatial mode and $\hat{V}$ contains temporal modes.

Step 2: Generate reference signal from a priori information; inverted fMRI experiment protocol.

Step 3: Zero mean and normalize the reference signal.

Step 4: Call the simplified cICA with $\hat{V}$ and reference as the inputs. Upon convergence the output will be the independent source in the time domain.

Step 5: To determine the corresponding independent spatial source generate the reference signal (a priori information) for the spatial source according to the following equation:

$$r = \hat{X}((\hat{V}w_t)^t)^{-1} \ or \ r = X(T^t)^{-1} \qquad (11)$$

where w_t is un-mixing vector and T is the independent time source recovered at Step 4.

Step 6: Zero mean and normalize the reference.

Step 7: Call the cICA with $\hat{U}$ and reference found at the Step 6. Upon convergence output will be independent spatial source corresponding to the independent time source found in Step 4.

IV. fMRI EXPERIMENT AND DATA ACQUISITION

fMRI data was acquired on a 3.0T MR scanner (Magnum 3.0, Medinus, Korea) using a T2-weighted EPI sequence (TR = 2850ms, TE = 36ms, flip angle =70°, 64 × 64 matrix, FOV = 240 × 240 mm, slice thickness = 4mm, voxel size = 3.75 × 3.75 × 4mm³) with 29 transaxial slices covering the whole brain regions. To minimize motion artifact, we tightly fixed the head using sponge in the head coil.

A well-established protocol for alpha activity modulation for human brain is closing (thus inducing the alpha activity) and opening (thus suppressing the alpha activity) of the eyes
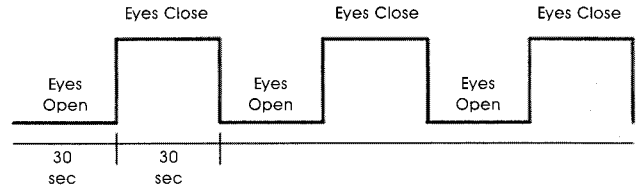

Fig. 2. Experimental protocol for fMRI data collection.

[5]. By adopting this experimental protocol, after several minutes of dark adaptation, we asked each subject (5 male, 26±3 years old) to open his eyes for 30 sec and then close for 30 sec. This cycle was repeated three times to obtain 60 flash image for one complete experiment. Fig. 2 shows experimental protocols.

V. RESULTS

The performance of the proposed constrained st-ICA algorithm was tested using the simulated data. Four temporal and spatial sources were generated as shown in Fig 3(a). Each temporal source is of 100 sample points and each spatial source is of 40 × 40 matrix. As evident in the Fig. 3(a) neither temporal nor spatial sources are independent. These simulated sources are mixed together to create a spatiotemporal data. The results of spatial ICA and temporal ICA on this mixture data set are shown in Fig. 3(b) and (c). Both, the spatial and temporal ICA try to find maximal independent sources in the spatial or temporal domains respectively, deteriorating the sources in the other (corresponding) domain. On the other hand, constrained st-ICA finds independent sources in two stages with minimal inter domain affect. It employs a priori information so that only the desired sources (connected sources) should be extracted from the two domains. The results of constrained st-ICA are shown in Fig. 3(d). The results indicate that the quality of temporal sources obtained with constrained st-ICA is superior to those obtained with spatial ICA and the obtained spatial sources are superior to those obtained with temporal ICA. The reason for this is that the cost function of temporal or spatial ICA are designed to find maximally independent temporal or spatial sources respectively thus effecting the sources in their corresponding domains. However, this is not the case with the proposed constrained st-ICA as explained in detail in the constrained spatiotemporal ICA section. Also, the time consumed by spatial or temporal ICA (Pentium (R) 4 CPU 3.01 GHz, 1GB of Ram) to derive sources is in the range of 5 - 6 Sec. whereas, for the constrained st-ICA the time to extract the desired source is in the range of 3.0 - 3.5 sec.

For real life application, the proposed algorithm is applied for fMRI analysis. The fMRI data collected for each individual is realigned and convolved with a Gaussian filter (8 × 8 × 8) for smoothing. The data from each individual was processed separately on a single volume basis. Each row of an observation matrix X contains an image. The ON-OFF stimulation (inverted) (Fig. 2) was used as the initial reference. Independent spatial and temporal components are recovered according to the algorithm presented above in the constrained spatiotemporal ICA section.

Once a component map is recovered, it is converted to the z-map [5] according to the Equation 12.

$$z_{ij} = \frac{s_{il} - m_i}{\sigma_i} \geq threshold \qquad (12)$$

where i is the row index, j is the column index, S is row and column of the spatial component recovered, m_i the mean, and σ_i the standard deviation of the ith row of S. The threshold value selected for our implementation was 0.6. Details of how to calculate the threshold value can be found in [5].

(a) Simulated temporal and spatial sources

(b) Sources recovered using spatial ICA

(c) Sources recovered using temporal ICA

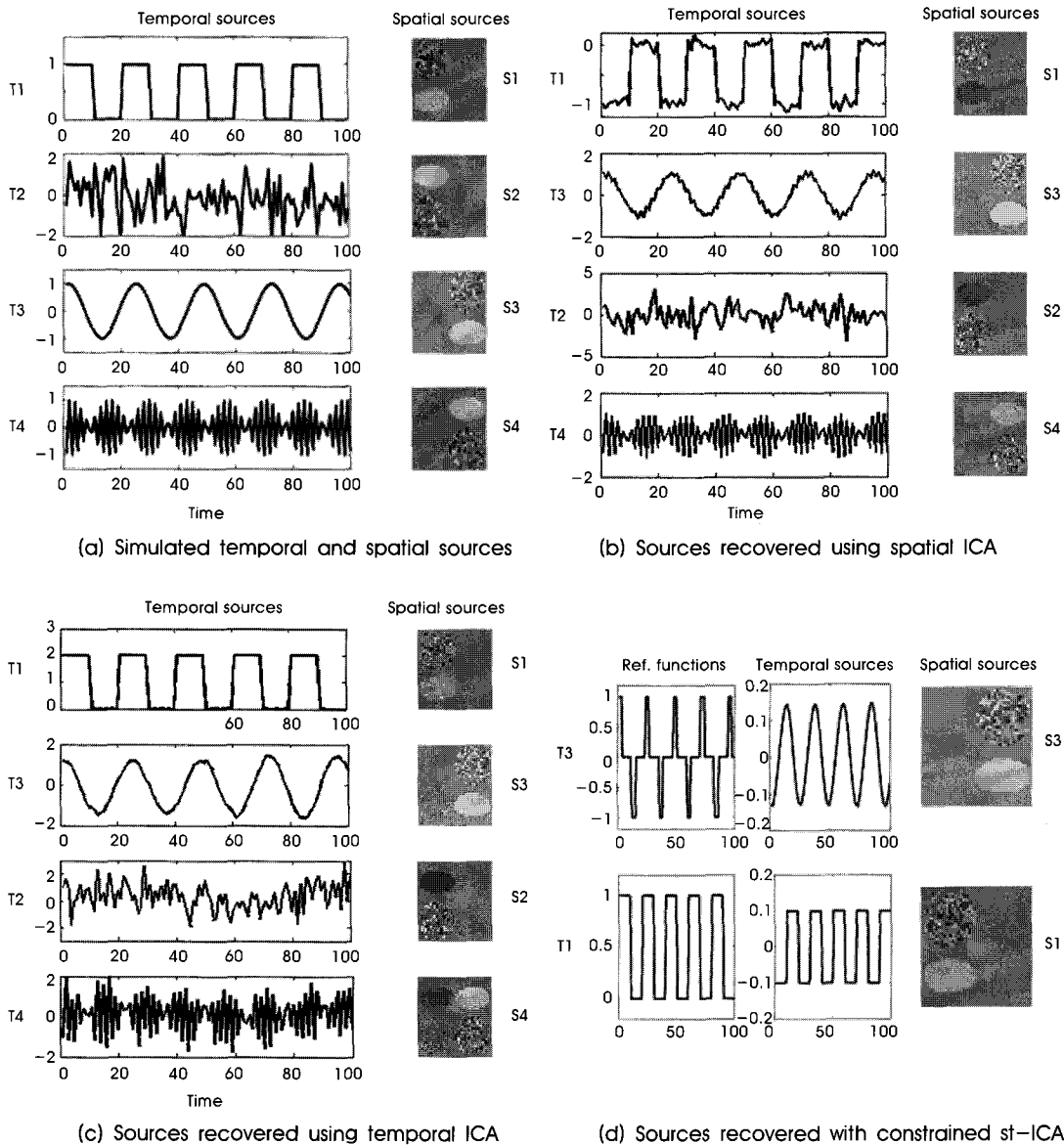(d) Sources recovered with constrained st-ICA

Fig. 3. (a) Simulated Sources (b) The result of spatial and (c) temporal ICA, Deteriorations in the corresponding domain are clearly visible. (d) Constrained st-ICA gives better results compared to other ICAs. In (d) first column are the ref. functions used, centre column are the temporal sources and right column are the spatial sources recovered.
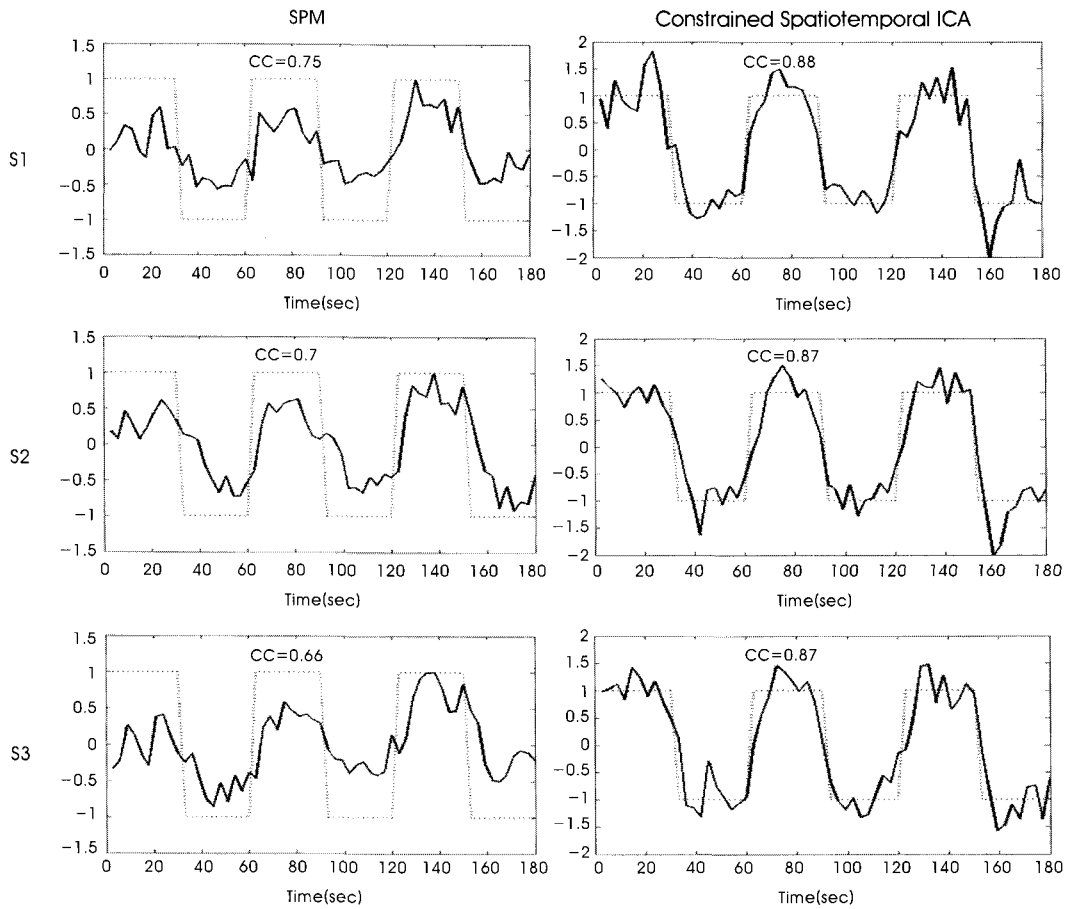
Fig. 4. Time sequences (solid) obtained with constrained st-ICA has higher correlation with the ref. signal (dotted), inverted ON-OFF stimulation sequence, compared with those obtained with SPM.
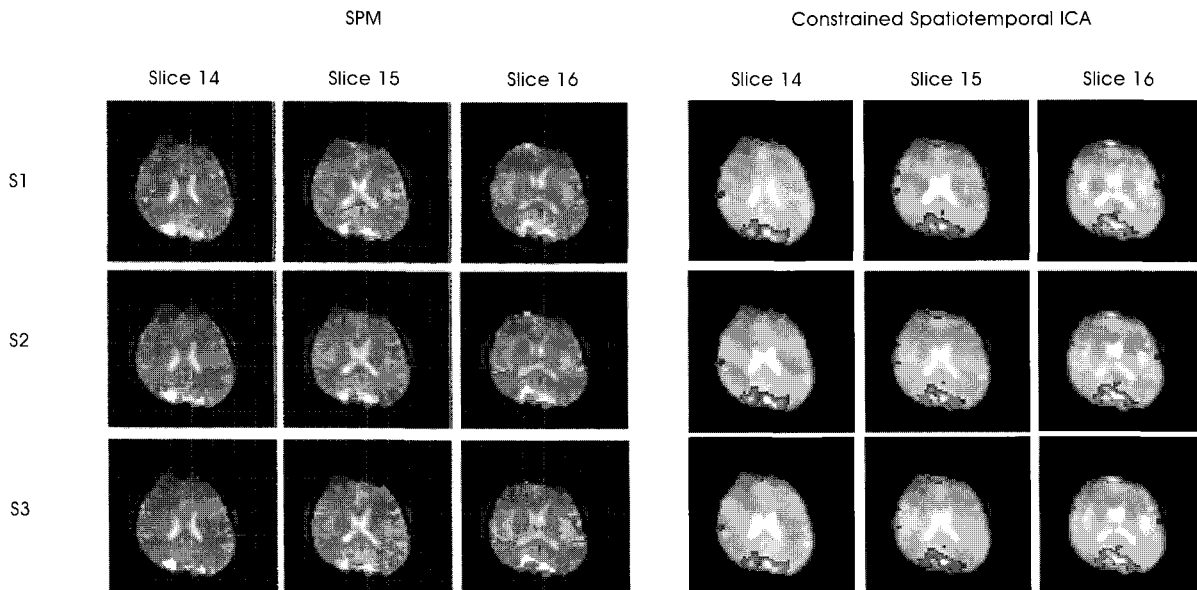

Fig. 5. SPM and constrained spatiotemporal ICA processed fMRI data. Z-score maps obtained with constrained st-ICA shows frontal activity which was missed by SPM in most of the cases.

The time courses (temporal sources) recovered with the constrained st-ICA is shown in Fig. 4. The time courses have higher correlation with the ON-OFF stimulation reference (cc = 0.87 ~ 0.88) compared to SPM (cc = 0.66 ~ 0.75) results.

The functional maps (spatial sources) obtained with constrained st-ICA are compared with those obtained with SPM. The results for the slice 14, 15 and 16 for three different subjects are presented in Fig. 5. In the previous alpha modulation fMRI experiments, the functional maps are known to have activity in the frontal and occipital regions [16]. The functional maps by constrained st-ICA reveal more frontal activities, which is missed by SPM in most of the cases. The results indicate that the proposed constrained st-ICA may be a more effective method for fMRI data analysis.

VI. DISCUSSION AND CONCLUSIONS

In this study a new algorithm, constrained-stICA is proposed. The method tries to find the desired independent spatial and temporal components by separating the input image sequences into spatial and temporal modes that can be analyzed independently by incorporating the a priori information. The conventional ICA algorithms, for data sets like image sequences, try to find maximum independent component without taking into considering the fact that if the extracted IC is not independent how badly the IC in the corresponding domain may be affected. If the conventional ICA is applied separately on spatial and temporal domains obtained with SVD. There is no way that the output of the two ICAs can be connected together as the ordering of the components is random.

In this study, we have validated the performance of the proposed algorithm by comparing the results of simulated data set with the conventional ICAs. Furthermore as a real application, we have applied the algorithm on a set of fMRI data and the compared the results with the SPM, which is the conventional technique for fMRI analysis. The results of the proposed algorithm on the simulated data as well as the fMRI data indicate that the proposed algorithm could be more effective technique for the analysis of spatiotemporal data.

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