**"A Supervised Singular Value Decomposition for Independent Component Analysis of fMRI"**

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Supplementary Report

This document summarizes two sets of supplementary materials for the paper.

# 1 A Simulation Study with Boxcar-type Temporal Components

This section reports a simulation study where the temporal components are boxcar-type stepwise periodic functions. The simulation results suggest that, for the purpose of detecting regions of interest, the frequencies of the temporal components are the most important factors, while the exact shapes of the temporal components are less crucial. Our proposed SSVD-ICA technique makes use of the frequency information, while approximates the temporal components using sine functions. Although not exact, the technique still works well for stepwise periodic functions, and much better than the conventional SVD-ICA.

## 1.1 Data Description

According to the ICA decomposition model, to simulate an $M \times N$ fMRI data matrix $\mathbf{X}$, we first simulate the $M \times r$ spatial component matrix $\mathbf{A}$ and the $r \times N$ time series matrix $\mathbf{S}$ separately. The data matrix $\mathbf{X}$ is then obtained as $\mathbf{X} = \mathbf{AS}$.

In this study, we set $r = 5$, $M = 30 \times 30 \times 10$ and $N = 240$. Basically, there are 5 underlying independent components; each column of $\mathbf{A}$ is a spatial map that consists of 10 slices and each slice contains $30 \times 30$ voxels; while each row of $\mathbf{S}$ is a time series of length 240 that corresponds to the relevant spatial component in $\mathbf{A}$.

The first four time components are simulated using simple boxcar functions (*instead of sine functions*), plus Uniform noises randomly generated between $[-0.05,\ 0.05]$. The components are plotted in Figure 1. The amplitudes of the first four components are 0.5, 0.45, 0.35 and 0.4,

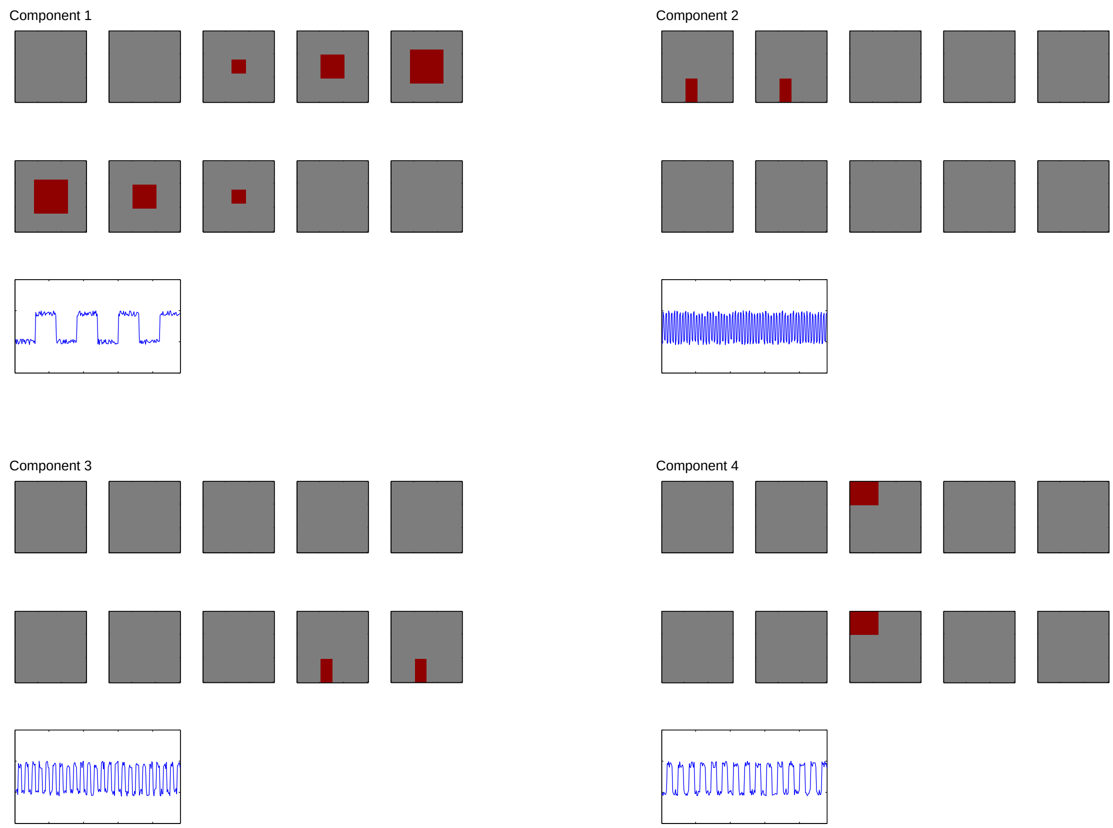



Figure 1: The first four components used in the simulation. In each panel, the first 10 images are the spatial component maps (one column of $\mathbf{A}$), and the dark red areas stand for activated voxels. The solid line in the subsequent plot is the corresponding time series (one row of $\mathbf{S}$).

respectively. The corresponding frequencies are chosen as 1/18Hz, 1/1.2Hz, 1/3Hz and 1/4.8Hz. The last time component is pure noise sampled uniformly between $-0.05$ and 0.05.

The voxels in $\mathbf{A}$ are assigned a binary number of 0 or 1. In each component, the voxels with value 1 correspond to the regions that are activated by the corresponding time stimulus, and they are plotted as dark red areas in Figure 1. The spatial components are the same as the ones used in the paper's simulation study.

To simulate spikes in the data, we randomly select 10% of the entries in the simulated $\mathbf{X}$, and replace them with uniform noises between 1 and 6. The range is chosen such that the simulated spikes are indeed outliers, judged by the 1.5-Inter-Quartile-Range rule of thumb.

## 1.2 Analysis

Following the standard practice in ICA, we first normalized the contaminated data matrix **X** by column centering and row standardization (Hastie and Tibshirani, 2002). Both ICA and SSVD-ICA were then applied to the normalized matrix. Note that SSVD-ICA assumes the temporal components as sine functions. For computing, we employed the fastICA algorithm (Hyvärinen, Karhunen and Oja, 2001), because of its fast computation and popularity .

To effectively display the activated voxels in the spatial maps, the values in each map were standardized to z-scores (McKeown et al., 1998a) by subtracting the component mean and then dividing the component standard deviation. The voxels with $|z| \geq 1$ were then identified as those activated, and they were assigned value 1 when plotting; while the other voxels (with $|z| < 1$) were assigned 0.

## 1.3 Results

The results from SSVD-ICA are shown in Figure 2. Although the method approximates the stepwise temporal components using sine functions, all four spatial components can be recovered reasonably well. (Dark red areas again indicate the activated voxels.) This suggests that the frequencies are the most important factors. Note that the recovered spatial components are re-arranged afterwards to follow the same order as those in Figure 1, because default components extracted by ICA do not follow any particular order.

Figure 3 shows the results from the conventional ICA that uses SVD for dimension reduction. We requested ICA to extract 10 components; however, only seven could be successfully extracted. Among them, only the first and the fourth spatial components could be partially recovered; even so, the result is more blurred than the corresponding ones from SSVD-ICA. The conventional ICA has trouble identifying the other components. One can also see the temporal components detected by ICA are spiky, reflecting the effect of the spikes.

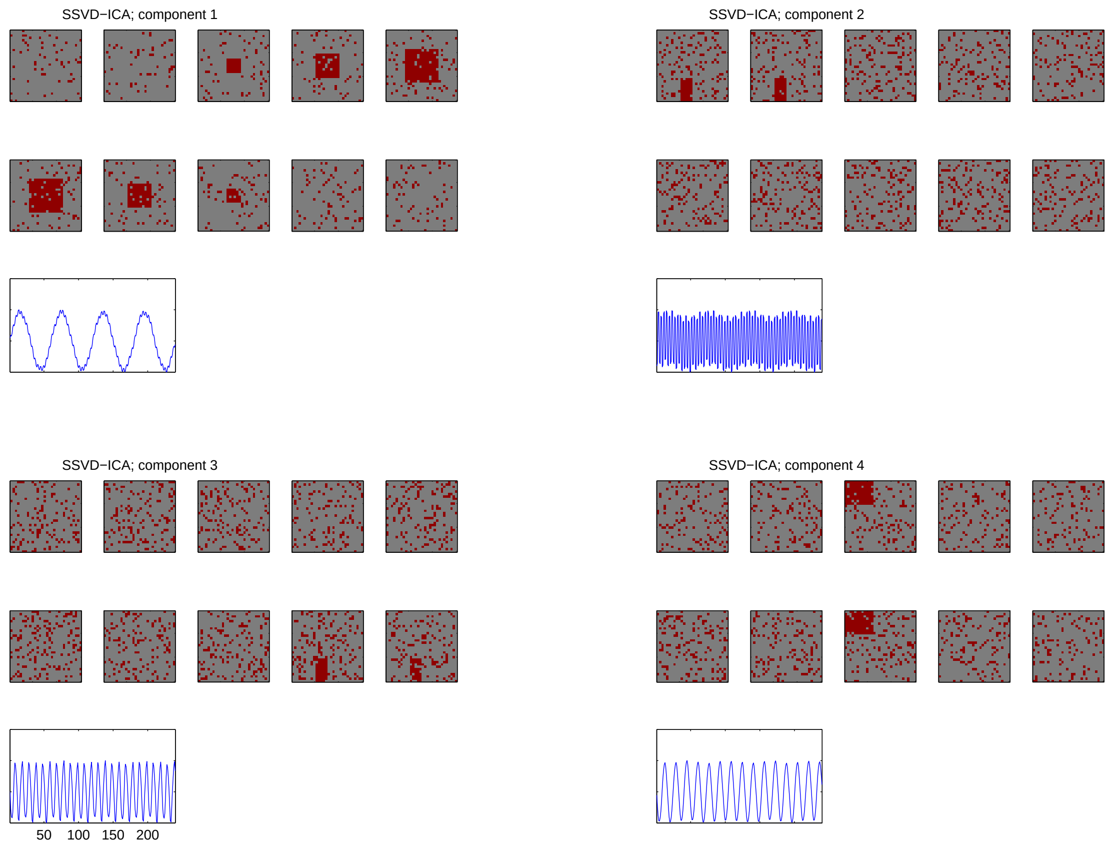



Figure 2: The first four components detected by the proposed SSVD-ICA.




Figure 3: The seven components detected by the conventional ICA.

# 2 Some Discussion about the Robust Singular Value Decomposition of Liu et al. (2003)

In addition to being robust, another advantage of our Supervised SVD approach is its computational efficiency as we now discuss.

We initially started our research by implementing an existing robust SVD procedure proposed by Liu et al. (2003). Gabriel and Zamir (1979) described an alternating least squares algorithm for computing SVD. To make SVD more robust, Liu et al. (2003) replaced the least-squares regression by outlier-resistant regression methods such as $L_1$ regression or least trimmed squares regression. Their robust SVD is implemented in *PowerArray*, available at `http://www.niss.org/PowerArray/`.

The following simulation study shows that their numerical procedure performs well for simulated data. However, our experience suggests that the procedure is prohibitively hard to compute in real fMRI data analysis. Hence, we did not pursue further with their approach. Instead, we started to study the supervised SVD, which is the subject of our paper.

## 2.1 Data Description

For simplicity, we consider a simulation study with $r = 5$ components, $M = 30 \times 30 \times 1$ voxels, and $N = 240$ time points. We simulated the data based on a simple rest-activate block design. Each rest or activate period holds 30 scans. There are 4 rest-activate periods altogether. The repetition time (TR) is set as 0.3 seconds. Hence each rest-activate period lasts for $60 \times 0.3 = 18$ seconds.

All the voxels are given a numerical value of either 0 or 1. The voxels with value 1 are those that are activated by the corresponding stimulus. The time components are assumed as simple sinusoidal functions. The first component stands for the stimulus of the experiment, hence it is a delayed and blurred version of the block design with the same periodicity. The second and third time series are for the heart beat and breath, with frequencies 1Hz and 0.3Hz respectively. The fourth one is for an artifact effect with frequency 0.7Hz. And the last is for pure noise. The five components have different magnitudes.

We then randomly selected 5% cells from the matrix $\mathbf{X}$ simulated above, and replaced them with randomly generated outliers.

## 2.2 Analysis Results

The panel (a) of Figure 4 presents the results obtained by the ICA procedure with conventional SVD. FastICA algorithm is used and only three components can be extracted. The forth and fifth components cannot converge at all. Even in the three extracted components, only the component for the experiment stimulus is strong enough to be appreciated and the other two contain lots of noise.

Instead, when applying ICA with the robust SVD proposed by Liu et al. (2003), the results are much better as shown in the panel (b) of Figure 4. Both the spatial components and the temporal frequencies can be recovered, although not perfect.

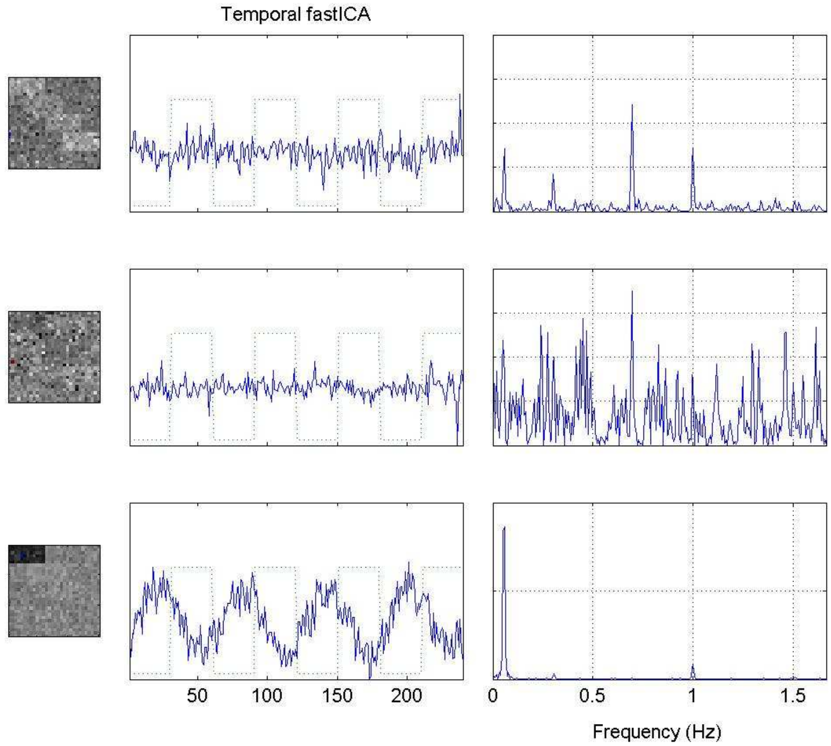
## 2.3 Discussion

Although the robust SVD numerical procedure performs well in simulation, it turns out that the procedure is prohibitively hard to compute when analyzing real fMRI data. Hence, we gave up pursuing further with that approach, and started to study the supervised SVD, which results in our current paper. A careful look at the extracted spatial components also suggests that the extraction is not as clean as the results obtained by our Supervised SVD approach.

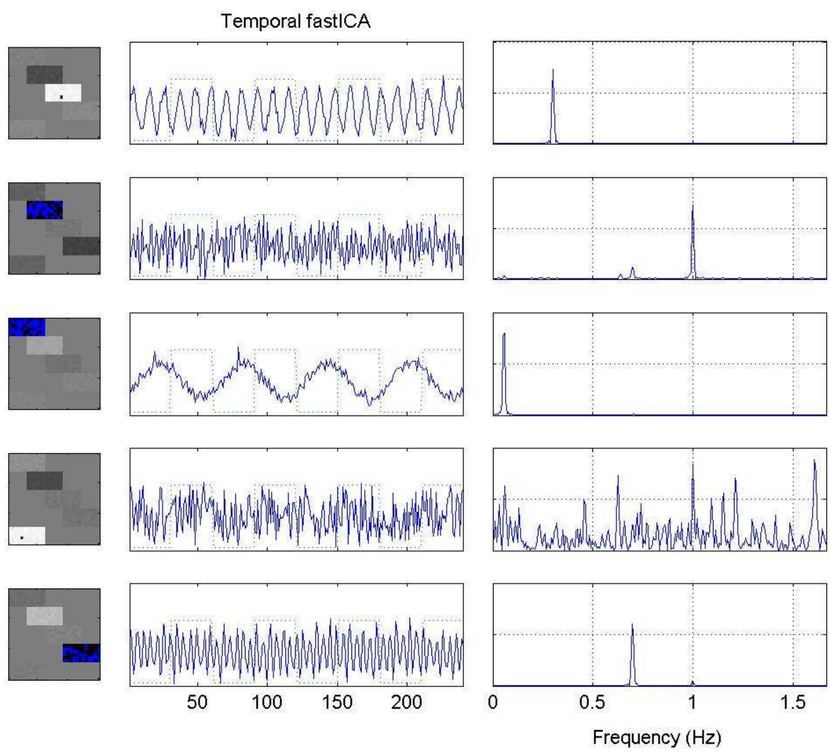
**References**

Gabriel, K. R. and Zamir, S. (1979). Lower rank approximation of matrices by least squares with any choice of weights. *Technometrics* **21**, 489–498.

Liu, L., Hawkins, D. M., Ghosh, S. and Young, S. S. (2003). Robust singular value decomposition analysis of microarray data. *PNAS* **100**, 13167–13172.




**(a) conventional ICA**




**(b) ICA with robust SVD**

Figure 4: Comparison of conventional ICA and ICA with robust SVD.