Multi-Subject fMRI Analysis via Combined Independent Component Analysis and Shift-Invariant Canonical Polyadic Decomposition

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Abstract

Background

Canonical polyadic decomposition (CPD) may face a local optimal problem when analyzing multi-subject fMRI data with inter-subject variability. Beckmann and Smith proposed a tensor PICA approach that incorporated an independence constraint to the spatial modality by combining CPD with ICA, and alleviated the problem of inter-subject spatial map (SM) variability.

New Method

This study extends tensor PICA to incorporate additional inter-subject time course (TC) variability and to connect CPD and ICA in a new way. Assuming multiple subjects share common TCs but with different time delays, we accommodate subject-dependent TC delays into the CP model based on the idea of shift-invariant CP (SCP). We use ICA as an initialization step to provide the aggregating mixing matrix for shift-invariant CPD to estimate shared TCs with subject-dependent delays and intensities. We then estimate shared SMs using a least-squares fit post shift-invariant CPD.

Results

Using simulated fMRI data as well as actual fMRI data we demonstrate that the proposed approach improves the estimates of the shared SMs and TCs, and the subject-dependent TC delays and intensities. The default mode component illustrates larger TC delays than the task-related component.

Comparison with Existing Method(s)

The proposed approach shows improvements over tensor PICA in particular when TC delays are large, and also outperforms SCP with SM orthogonality constraint and SCP with ICA-based SM initialization.

Conclusions

TCs with subject-dependent delays conform to the true situation of multi-subject fMRI data. The proposed approach is suitable for decomposing multi-subject fMRI data with large inter-subject temporal and spatial variability.

Keywords: Canonical polyadic decomposition (CPD); Independent component analysis (ICA); Multi-subject fMRI data; Inter-subject variability; Tensor PICA; Shift-invariant CP (SCP)

1. Introduction

Functional magnetic resonance imaging (fMRI) has provided an efficient way for studying the brain, and group fMRI analysis is essential for expressing data as spatial patterns modulated by time/subject/trial via multilinear decompositions. As brain function is still poorly understood, and fMRI data are noisy, data-driven approaches exhibit great potential in extracting spatial and temporal components from fMRI data with little to no prior information about the brain. Among others, independent component analysis (ICA) (McKeown et al., 1998; Vigario and Oja, 2008; Calhoun et al., 2001; Guo and Pagnonib, 2008; Du and Fan, 2013; Lee et al., 2008; Michael et al., 2014; Risk et al., 2014) and tensor decomposition (TD) (Andersen and Rayens, 2004; Beckmann and Smith, 2005; Mørup et al., 2008; Cichocki et al., 2009; Cichocki et al., 2014; Mørup et al., 2011), two key approaches of blind source separation (BSS), have provided promising results in multi-subject fMRI analysis.

When comparing ICA and TD, ICA emphasizes statistical independence whereas TD stresses multiway data structure. Typical ICA approaches to group fMRI analysis include group ICA (Calhoun et al., 2001; Erhardt et al., 2011; Calhoun and Adali, 2012; Du and Fan, 2013; Afshin-Pour et al., 2014) and independent vector analysis (IVA) (Dea et al., 2011; Lee et al., 2008; Michael et al., 2014). Group ICA performs ICA on the multi-subject fMRI data concatenated in time or in space to obtain common spatial maps (SMs) and individual time courses (TCs) or common TCs and individual SMs. In contrast, IVA carries out joint ICA of multiple datasets by exploiting source dependence across multiple datasets, resulting in individual SMs independent for each subject but dependent among different subjects. Since inter-subject variability can be derived from the individual SMs or TCs, both group ICA and IVA are suitable for capturing inter-subject variability (Allen et al., 2012; Erhardt et al., 2011). Considering that fMRI data possess multiway data structure in terms of space, time, and subject (or trial), TD is attractive due to its capability of retaining multiway linkages and interactions presented in the data (Andersen and Rayens, 2004). Among others, canonical polyadic decomposition (CP decomposition, or CPD), also

called CANDECOMP, or parallel factor analysis (PARAFAC), decomposes multiway data into a linear combination of a series of outer product of rank-one tensors. CPD is a popular TD method as it is not only able to provide a unique decomposition under mild conditions, but also provides useful results for fMRI data (Andersen and Rayens, 2004; Beckmann and Smith, 2005; Stegeman, 2007; Mørup et al., 2008; Mørup et al., 2011; Helwig and Hong, 2012). When applied to multi-subject fMRI analysis, CPD is able to obtain shared SMs, shared TCs, and subject-specific intensities (Beckmann and Smith, 2005; Stegeman, 2007; Kuang et al., 2013).

However, CPD may fall into a local optimal solution when the multiway data are noisy, as is fMRI data. On one hand, the contrast-to-noise ratio (CNR) of fMRI data is usually very low; on the other hand, there naturally exists inter-subject variability along both spatial modality and temporal modality. In order to enhance the robustness of CPD with respect to noise and to facilitate physical interpretation, some additional properties have been efficiently incorporated into CPD as modality constraints (Kolda and Bader, 2009; Cichocki et al., 2014). Beckmann and Smith proposed such a solution termed tensor PICA (Beckmann and Smith, 2005) (we use this name, though the PICA algorithm can be replaced by other ICA algorithms), which treated multi-subject fMRI data as a three-way tensor, and placed the statistical independence constraint on the spatial modality by combining ICA with CPD. More precisely, ICA was first used to estimate the shared SMs, CPD was then employed to estimate the shared TCs and the subject-specific intensities via rank-1 eigenvalue decomposition (Beckmann and Smith, 2005). There are also other methods combining ICA and CPD. One similar method to tensor PICA is BSS-CPD (Zhou and Cichocki, 2012), in which a standard BSS algorithm was first used to extract one factor matrix, CPD was then employed to compute the remainder components via a series of rank-1 singular value decompositions (SVD). Another typical method is ICA-CPD (De Vos et al., 2012). It imposed independence constraints on CPD, and implemented an algebraic CP structure and the property of statistical independence simultaneously (vs. tensor PICA and BSS-CPD implemented sequentially).

There are two problems that may limit performance of the combined ICA/BSS-CPD method when applied to multi-subject fMRI data analysis. One is that, in addition to the inter-subject SM variability, there is also inter-subject TC variability. Because different subjects may generate different responses due to variation in response time or in their hemodynamic delay, the inter-subject TC variability naturally exists for multi-subject fMRI data, and this is a consistent issue with all TD models that do not account for time-shifts. It is thus possible to extract more robust and interpretable components by adding this TC property into the CP model. Although the inter-subject TC changes have not been introduced into CPD of multi-subject fMRI data, both time-domain and frequency-domain shifted CP algorithms have been previously proposed (Hong and Harshman, 2003; Mørup et al., 2008). The time-domain algorithm would be time consuming when many time delays were involved, as the time delays were determined by exhaustively searching (Mørup et al., 2008). Mørup et al. proposed a frequency-domain shift-invariant CP algorithm (SCP) which allowed for arbitrary shifts along one modality in the CP model. SCP successfully coped with variable latencies in the actual multi-trial fMRI data of a subject by accommodating inter-trial TC shift variant into CPD (Mørup et al., 2008). This indeed provides a valuable reference for incorporating inter-subject TC variability into the CP model.

The second problem is that the ICA/BSS and CPD solutions can diverge from one another due to the different objectives if there are iterations between BSS and CPD (De Vos et al., 2012; Helwig and Hong, 2012); on the contrary, the estimates of ICA/BSS and CPD are completely independent when there is no connection between BSS and CPD (Zhou and Cichocki, 2012). As such, the CPD and ICA/BSS approaches should be connected in a new way in order to maximize the benefit.

In this study, we extend tensor PICA in two aspects. First, we assume that multiple subjects share common TCs but with different time delays, and accommodate the subject-dependent TC delays into the CP model based on the idea of SCP. Secondly, we connect the CPD and ICA/BSS approaches in a new way: ICA is utilized as an initialization step of shift-invariant CPD to provide an aggregating mixing matrix estimate; from which the shift-invariant CPD extracts the shared TCs with the subject-dependent

time delays and the subject-specific intensities. Finally, as a post-processing step of the shift-invariant CPD, the shared SMs are estimated via a least-squares fit with the reconstructed aggregating mixing matrix. Due to the ICA initialization and the shift-invariant CPD, the shared TC and SM estimates of our proposed algorithm benefit from both the spatial constraint of SM independence and the temporal constraint of TC delays. Simulated fMRI data as well as actual fMRI data are utilized to evaluate the proposed approach.

2. Method

In this study, italic lower-case letters (e.g., a) denote scalars, bold lower-case letters (e.g., $\mathbf{a}$) denote vectors, bold upper-case letters (e.g., $\mathbf{A}$) denote matrixes, and underlined bold capitals (e.g., $\underline{\mathbf{A}}$) denote tensors. Assuming $\underline{\mathbf{X}} = \{x_{ijk}\} \in \mathbb{R}^{I \times J \times K}$ represents three-way (voxel $\times$ time $\times$ subject) multi-subject fMRI data, K is the number of subjects, J is the number of time points from a single subject, I is the total number of brain voxels obtained by flattening the volume image data, and $i=1, \dots, I$, $j=1, \dots, J$, $k=1, \dots, K$. The standard CP model is as follows:

$$\underline{\mathbf{X}} = \sum_{n=1}^N \mathbf{s}_n \circ \mathbf{b}_n \circ \mathbf{c}_n + \underline{\mathbf{E}} \quad (1)$$

where $\mathbf{S} \triangleq [\mathbf{s}_1, \dots, \mathbf{s}_N] = \{\mathbf{s}_{in}\} \in \mathbb{R}^{I \times N}$, $\mathbf{B} \triangleq [\mathbf{b}_1, \dots, \mathbf{b}_N] = \{\mathbf{b}_{jn}\} \in \mathbb{R}^{J \times N}$, $\mathbf{C} \triangleq [\mathbf{c}_1, \dots, \mathbf{c}_N] = \{\mathbf{c}_{kn}\} \in \mathbb{R}^{K \times N}$ consist of shared SMs, shared TCs, and subject-specific intensities, respectively, N is the number of components, $n=1, \dots, N$, $\circ$ denotes the outer product, and $\underline{\mathbf{E}} = \{e_{ijk}\} \in \mathbb{R}^{I \times J \times K}$ is the residual including the effect of inter-subject SM and TC variability.

By incorporating time delays into the temporal modality of the CP model, the SCP model yields (Mørup et al., 2008):

$$x_{ijk} = \sum_{n=1}^N s_{in} b_{jn(k)} c_{kn} + e_{ijk} \quad (2)$$

where $b_{jn(k)}$ denotes b_{jn} with the time-delay of subject k .

Let $\mathcal{T} = \{\tau_{kn}\} \in \mathbb{R}^{K \times N}$ represent subject-dependent TC delays for the shared TCs, the transpose of frontal slices of the above SCP model becomes:

$$(\mathbf{X}^{(k)})^T = \mathcal{T}_k(\mathbf{B}) \mathbf{D}_k(\mathbf{C}) \mathbf{S}^T + (\mathbf{E}^{(k)})^T \quad (3)$$

where $\mathbf{X}^{(k)} \in \mathbb{R}^{I \times J}$ is the fMRI data of subject k , $k = 1, \dots, K$; $\mathbf{D}_k(\mathbf{C}) = \text{diag}[\mathbf{C}(k, :)] \in \mathbb{R}^{N \times N}$ is a diagonal matrix generated by the k^{th} row of $\mathbf{C}$; $\mathcal{T}_k(\mathbf{B}) = [\mathbf{b}_{1(k)}, \mathbf{b}_{2(k)}, \dots, \mathbf{b}_{N(k)}]$ is a shift function which shifts $\mathbf{b}_n$ ($n = 1, \dots, N$) of subject k with time delays τ_{kn} , τ_{kn} is the time delay of the n^{th} TC component $\mathbf{b}_n$ for subject k ; $\mathbf{b}_{n(k)}$ is obtained by left shifting $\mathbf{b}_n$ τ_{kn} points when $\tau_{kn} > 0$, otherwise right shifting $\mathbf{b}_n$ τ_{kn} points; $\mathbf{E}^{(k)}$ is the k^{th} frontal slices of $\mathbf{E}$. Note the spatial maps $\mathbf{S}$ are independent to the time shifts $\mathcal{T}$.

By temporally concatenating K subjects of fMRI data, we have the ICA model as follows:

$$\mathbf{X} = \begin{bmatrix} (\mathbf{X}^{(1)})^T \\ (\mathbf{X}^{(2)})^T \\ \vdots \\ (\mathbf{X}^{(K)})^T \end{bmatrix} = \begin{bmatrix} \mathcal{T}_1(\mathbf{B}) \mathbf{D}_1(\mathbf{C}) \\ \mathcal{T}_2(\mathbf{B}) \mathbf{D}_2(\mathbf{C}) \\ \vdots \\ \mathcal{T}_K(\mathbf{B})^T \mathbf{D}_K(\mathbf{C}) \end{bmatrix} \mathbf{S}^T + \begin{bmatrix} (\mathbf{E}^{(1)})^T \\ (\mathbf{E}^{(2)})^T \\ \vdots \\ (\mathbf{E}^{(K)})^T \end{bmatrix} = \mathbf{M} \mathbf{S}^T + \mathbf{E} \quad (4)$$

where $\mathbf{X} \in \mathbb{R}^{JK \times I}$ and $\mathbf{E} \in \mathbb{R}^{JK \times I}$ are the unfolded and transposed matrices; $\mathbf{M} \in \mathbb{R}^{JK \times N}$ is the aggregating mixing matrix containing the shared TCs, the subject-dependent delays and intensities with the following unfolding form:

$$\mathbf{M} = \begin{bmatrix} \mathbf{b}_{1(1)} c_{11} & \mathbf{b}_{2(1)} c_{12} & \cdots & \mathbf{b}_{N(1)} c_{1N} \\ \mathbf{b}_{1(2)} c_{21} & \mathbf{b}_{2(2)} c_{22} & \cdots & \mathbf{b}_{N(2)} c_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{b}_{1(K)} c_{K1} & \mathbf{b}_{2(K)} c_{K2} & \cdots & \mathbf{b}_{N(K)} c_{KN} \end{bmatrix} \quad (5)$$

where c_{kn} is the element of $\mathbf{C}$.

We first estimate the aggregating mixing matrix $\mathbf{M}$ using ICA, referring to equation (4), the SM independence constraint is included. From the $\mathbf{M}$ estimate, we then estimate the shared TCs and the subject-dependent delays and intensities using the shift-invariant rank-one approximation, these estimates further incorporate the TC delay constraint in addition to the SM independence constraint. Finally, we employ the shift-invariant CPD estimates to reconstruct a new $\mathbf{M}$ according to equation (5), and determine the least-squares fit of the shared SMs $\mathbf{S}$ under the ICA model given in equation (4); in this case, the estimated shared SMs also benefit from the spatial and temporal constraints, respectively.

In summary, the proposed approach consists of three stages as listed below: ICA stage, shift-invariant rank-one approximation, and estimation of the shared SMs.

2.1. ICA stage

In the following, we assume the component number is N . Prior to ICA, we perform similar data preprocessing as tensor PICA to reduce noise and to reduce the data dimensionality of $\mathbf{X}$ in equation (4). More precisely, the voxel-wise variance is normalized to eliminate noise effects, and dimensionality reduction and data whitening is carried out by two-stage PCA (Beckmann and Smith, 2005; Erhardt et al., 2011). Suppose that $\mathbf{V} \in \mathbb{R}^{N \times JK}$ is the obtained matrix for reducing and whitening, by applying $\mathbf{V}$ to the data $\mathbf{X}$, we have the mixture signals $\mathbf{Z}$ for ICA to decompose:

$$\mathbf{Z} = \mathbf{V}\mathbf{X} \quad (6)$$

where $\mathbf{Z} \in \mathbb{R}^{N \times I}$. As we know, ICA is able to find an unmixing matrix $\mathbf{W} \in \mathbb{R}^{N \times N}$ to recover the source signals $\mathbf{S}$ given in equation (4) as follows:

$$\mathbf{S}_0^T = \mathbf{W}\mathbf{Z} \quad (7)$$

where $\mathbf{S}_0$ is the estimate of $\mathbf{S}$. Note this is the estimate of shared SMs for tensor PICA, but not for the proposed method. Based on the $\mathbf{S}_0$ estimate and equation (4), it is readily to obtain the least-squares estimate of the aggregating mixing matrix $\mathbf{M}$:

$$\mathbf{M}_0 = \mathbf{X}(\mathbf{S}_0^T)^\dagger \quad (8)$$

As mentioned above, $\mathbf{M}_0 \in \mathbb{R}^{JK \times N}$ consists of the shared TCs, the subject-dependent delays, and the subject-specific intensities, which we estimate at the following stage.

2.2. Shift-invariant rank-one approximation

Referring to equation (5), each column of the aggregating mixing matrix $\mathbf{M}$ includes one component of shared TCs, and its subject-dependent delays and intensities. We seek to estimate these factors component by component, thus we perform the shift-invariant rank-one approximation on each column of $\mathbf{M}_0$. The n^{th} ($n=1, \dots, N$) column vector of $\mathbf{M}_0$ is

$$\mathbf{m}_n = \begin{bmatrix} \mathbf{b}_{r(1)}c_{1r} + \boldsymbol{\epsilon}_{r(1)} \\ \mathbf{b}_{r(2)}c_{2r} + \boldsymbol{\epsilon}_{r(2)} \\ \vdots \\ \mathbf{b}_{r(K)}c_{Kr} + \boldsymbol{\epsilon}_{r(K)} \end{bmatrix} \quad (9)$$

where $\mathbf{m}_n \in \mathbb{R}^{JK}$. Compared with the original aggregating mixing matrix $\mathbf{M}$, the ICA estimate $\mathbf{M}_0$ exists permutation and scaling ambiguity. Here we assume the n^{th} column vector $\mathbf{m}_n$ of $\mathbf{M}_0$ provides estimates for the r^{th} component ($\mathbf{b}_r$, $\boldsymbol{\tau}_r$, and $\mathbf{c}_r$) due to permutation ambiguity, but we omit the scaling factor in equation (9) since it can be absorbed by normalizing the estimate of the subject-specific intensity $\mathbf{c}_r = [c_{1r}, \dots, c_{Kr}]^T$, see equation (14). Additionally, $\boldsymbol{\epsilon}_{r(k)}$ denotes the crosstalk from the other components.

Defining $\mathcal{M}_n = [\mathbf{m}_{n1}, \dots, \mathbf{m}_{nK}] \in \mathbb{R}^{J \times K}$, and its k^{th} column vector $\mathbf{m}_{nk} = (\mathbf{m}_n)_{(k-1)J+1:kJ} \in \mathbb{R}^J$, we can reshape $\mathbf{m}_n$ in equation (9) as

$$\mathcal{M}_n = \begin{bmatrix} \mathbf{b}_{r(1)}c_{1r} + \boldsymbol{\epsilon}_{r(1)} & \mathbf{b}_{r(2)}c_{2r} + \boldsymbol{\epsilon}_{r(2)} & \cdots & \mathbf{b}_{r(K)}c_{Kr} + \boldsymbol{\epsilon}_{r(K)} \end{bmatrix} \quad (10)$$

As $\mathbf{b}_{r(1)}, \mathbf{b}_{r(2)}, \dots, \mathbf{b}_{r(K)}$ share the common TC component $\mathbf{b}_r$ but with different time delays, $\mathcal{M}_n$ is a rank-one matrix in the frequency domain.

Given $\mathcal{M}_n = [\mathbf{m}_{n1}, \dots, \mathbf{m}_{nK}]$, we next iteratively learn the r^{th} shared TC component $\mathbf{b}_r = [b_{1r}, \dots, b_{Jr}]^T$, the subject-dependent delays $\boldsymbol{\tau}_r = [\tau_{1r}, \dots, \tau_{Kr}]^T$, and the subject-specific intensities $\mathbf{c}_r = [c_{1r}, \dots, c_{Kr}]^T$. Specifically, $\mathbf{b}_r$ is estimated by using the frequency-domain method (Mørup et al., 2007a; Mørup et al., 2007b; Mørup et al., 2008). Transforming equation (10) into the frequency domain via a discrete Fourier transform, we have $\tilde{\mathcal{M}}_n = [\tilde{\mathbf{m}}_{n1}, \dots, \tilde{\mathbf{m}}_{nK}]$, and

$$\tilde{\mathbf{m}}_{nk} = \tilde{\mathbf{b}}_r c_{kr} \exp \left[-\iota 2\pi \frac{f-1}{J} \tau_{kr} \right] + \tilde{\boldsymbol{\epsilon}}_{r(k)} \quad (11)$$

where $\exp[\cdot]$ is the exponential function, $\iota = \sqrt{-1}$. Referring to equations (10) and (11), the frequency-domain solution $\tilde{\mathbf{b}}_r$ of $\mathbf{b}_r$ can be obtained by minimizing $\sum_{k=1}^K \|\tilde{\boldsymbol{\epsilon}}_{r(k)}\|^2$, in detail

$$\tilde{\mathbf{b}}_r = \arg \min_{\tilde{\mathbf{b}}_r} \sum_{k=1}^K \left\| \tilde{\mathbf{m}}_{nk} - \tilde{\mathbf{b}}_r c_{kr} \exp \left[-\iota 2\pi \frac{f-1}{J} \tau_{kr} \right] \right\|^2 \quad (12)$$

The least-squares solution for $\tilde{\mathbf{b}}_r$ and $\mathbf{b}_r$ is as follows:

$$\begin{aligned} \tilde{\mathbf{b}}_r &\leftarrow \tilde{\mathcal{M}}_n (\mathbf{c}_r \exp \left[-\iota 2\pi \frac{f-1}{J} \boldsymbol{\tau}_r \right])^{T\dagger} \\ \mathbf{b}_r &= \tilde{\mathbf{b}}_r / \|\tilde{\mathbf{b}}_r\| \end{aligned} \quad (13)$$

The update of subject-dependent delays $\boldsymbol{\tau}_r$ includes two cases. When the time delays are assumed to be integers, e.g., for those generated for the simulated data, $\boldsymbol{\tau}_r$ is estimated by maximizing $|\tilde{m}_{nk,f}^* \tilde{b}_{r,f}|$ of cross-correlation; when the time delays are non-integers, e.g., for actual fMRI data, $\boldsymbol{\tau}_r$ is estimated by minimizing $\sum_{k=1}^K \|\tilde{\mathbf{m}}_{nk} - \tilde{\mathbf{b}}_r c_{kr}\|^2$ with Newton-Raphson method. Refer to Mørup et al. (2007a) and Mørup et al. (2007b) for details.

Next, by minimizing $\sum_{k=1}^K \|\mathbf{m}_{nk} - \mathbf{b}_r c_{kr}\|^2$, we update $\mathbf{c}_r = [c_{1r}, \dots, c_{Kr}]^T$ as

$$\begin{aligned} c_{kr} &\leftarrow (\mathbf{m}_{nk})^T (\mathbf{b}_{r(k)})^{T^\dagger}, \quad k=1, \dots, K \\ \mathbf{c}_r &= \mathbf{c}_r / \|\mathbf{c}_r\| \end{aligned} \quad (14)$$

Iterating $\mathbf{b}_r$, τ_r , and $\mathbf{c}_r$ until convergence or the maximal iteration number is reached.

2.3. Estimation of the shared SMs

Based on the shared TCs $\mathbf{b}_n$ ($n=1, \dots, N$), the subject-dependent delays τ_n , and the subject-specific intensities $\mathbf{c}_n$ estimated by the above rank-one approximation, we first form a new aggregating mixing matrix $\hat{\mathbf{M}}$ based on equation (5). Since $\mathbf{b}_n$ and $\mathbf{c}_n$ are normalized, refer to equation (13) and (14), there is no scaling ambiguity among different components of $\hat{\mathbf{M}}$. Then, under the ICA model given in equation (4), the shared SMs are estimated by minimizing the least squares:

$$\hat{\mathbf{S}}^T = \arg \min_{\mathbf{S}} \|\mathbf{X} - \hat{\mathbf{M}}\mathbf{S}^T\|^2 \quad (15)$$

Finally, the resulting shared SMs are updated as follows:

$$\hat{\mathbf{S}} = (\hat{\mathbf{M}}^\dagger \mathbf{X})^T \quad (16)$$

3. Experimental Methods

We compared the proposed approach to tensor PICA and SCP on simulated and actual multi-subject fMRI data for estimating the shared SMs (in brief SMs), the shared TCs (in brief TCs), the subject-dependent TC delays, and the subject-specific intensities. In order to enhance the SCP stability under the inter-subject SM variability, we enforce spatial independence within the SCP model in two ways: one is to impose an orthogonality constraint (linear independence) on the least-squares estimation of the SMs (Bro, 1997):

$$\mathbf{S} = \mathbf{X}\mathbf{M}(\mathbf{M}^T \mathbf{X}^T \mathbf{X}\mathbf{M})^{-0.5} \quad (17)$$

We call it the SCP_O algorithm. Another is to use the SM estimates of ICA with higher-order spatial independence to initialize the alternating least squares iterations in the original SCP algorithm, and this is called the SCP_I algorithm. For both our approach and tensor PICA, two-level PCA was performed for data preprocessing. We used the fastICA algorithm (Hyvärinen et al., 1999) in deflation mode; the selected nonlinearity function was *tanh*, and the stop criterion was set to less than 10^{-6} or maximum iteration 1000. Regarding the two SCP algorithms SCP_O and SCP_I and our shift-invariant rank-one approximation, we estimated integer time shifts for the simulated fMRI data but non-integer time delays for the actual fMRI data, and set the stop criterion to less than 10^{-6} or maximum iteration 1000.

When analyzing the actual fMRI data, we show that our approach will work for non (or less)-task related components in addition to the task-related components. Considering the default mode network (DMN) is one of the most widely studied resting state networks (Raichle et al., 2001; Smith et al., 2009), we selected DMN as an example of the non-task related components to compare among the four algorithms.

3.1. Simulated data

We used the simulation toolbox SimTB at <http://mialab.mrn.org/software/simtb> (Allen et al., 2012; Erhardt et al., 2012) to generate the simulated multi-subject fMRI data. There were a total of 20 ‘subjects’ ($K = 20$). We generated 30 components ($N = 30$) that are identical for all subjects, each consisting of a SM and a corresponding TC (i.e., the shared SM and TC). The SM contained 100×100 voxels, and the TC included 260 time-points in length with a repetition time of 2 s/sample. A task-related component shown in Fig. 2 was generated by convolving a block design (40 seconds on, 30 seconds off) with a hemodynamic response function. After removing the voxels out of the brain and flattening the volume image data, we obtained a three-way data of size $7688 \times 260 \times 20$. In addition, Gaussian noise was added to generate the simulated data with different CNR, defined as $20\lg(\hat{\sigma}_s/\hat{\sigma}_n)$ dB, where $\hat{\sigma}_s$ is the temporal standard deviation of the source signal and $\hat{\sigma}_n$ is that of the Gaussian noise, for details see Allen et al. (2012).

In order to simulate the actual fMRI data with spatial and temporal variability, we further changed the above-generated ideal SMs and TCs by adding various spatial changes and different time delays for each subject. For all components of each subject, the SM activations were changed with translation, rotation and spread in terms of the uniform distribution $\mathcal{U}$. Specifically, the x and y translation changes conformed to $\mathcal{U}(-\Delta s, \Delta s)$, meaning that the maximal horizontal translation was Δs voxels to the left or to the right, and the maximal vertical translation was Δs voxels up or down. Likewise, the rotation changes were with $\mathcal{U}(-10\Delta s, 10\Delta s)$, resulting in a maximal $10\Delta s$ degrees rotation in a counter-clockwise or clockwise direction; the spread or size was changed according to $\mathcal{U}(1 - 0.04\Delta s, 1 + 0.04\Delta s)$ to have $\pm 0.04\Delta s$ expansion or contraction. We set $\Delta s = 0, 1, 2, 3, 4, 5$, thus the range of SM changes was within 5 voxels of x and y translation, 50 degrees of rotation, and 0.2 of spread, as compared with the original SM.

The TC changes were set similarly. The time shifts were picked up from a uniform distribution $\mathcal{U}(-2\Delta t, 2\Delta t)$ with $\Delta t = 0, 1, 2, 3, 4, 5$, thus the maximum shift to left or to right is 10 points. Taking all of the spatial and temporal changes into account, there are totally 36 cases of combined SM and TC changes.

As the exact component number (here $N = 30$) is usually unknown, we retained 50 principal components (PCs) in the first-level PCA and 20 ~ 40 PCs in the group-level PCA. As a result, the range of component number was $N = 20 \sim 40$.

3.2. Actual fMRI data

The fMRI dataset were collected from 16 subjects performing a finger-tapping motor task, while receiving auditory instructions. The paradigm conformed to a block design with alternating periods of 30 seconds on (finger tapping) and 30 seconds off (rest). Each participant was collected with 165 whole head fMRI images. The experiments were performed on a 3T Siemens TIM Trio system with a 12-channel radio frequency (RF) coil. The fMRI experiment used a standard Siemens gradient-echo EPI sequence

modified to store real and imaginary data separately. The following parameters were used: field-of-view = 24 cm, slice thickness = 3.5 mm, slice gap = 1 mm, number of slices = 32, matrix size = 64×64 , TE = 29 ms, TR = 2 s, flip angle = 70 degrees. Preprocessing of the data was performed using the SPM software package (<http://www.fil.ion.ucl.ac.uk/spm/software/spm/>). Data were co-registered using INRIAAlign (Freire and Mangin 2001; Freire, et al. 2002) to compensate for movements in the fMRI time series images. Images were then spatially normalized into the standard Montreal Neurological Institute space. Following spatial normalization, the data (originally acquired at $3.75 \times 3.75 \times 4.5 \text{ mm}^3$) were slightly sub-sampled to $3 \times 3 \times 3 \text{ mm}^3$, resulting in $53 \times 63 \times 46$ voxels. Then, the images were spatially smoothed with a $10 \times 10 \times 10 \text{ mm}^3$ full width at half-maximum Gaussian kernel.

After removing the voxels out of the brain and flattening the volume image data, the three-way actual fMRI data were of size $59610 \times 165 \times 16$. We retained 50 PCs in the first-level PCA and 35 PCs in the group-level PCA, i.e., $N = 35$. The component number N was also changed from 20 to 50 to show its effect on the four algorithms.

3.3. Performance index

For the simulated fMRI data, we compute the absolute Pearson correlation coefficients $|\rho_c|$ between an estimate and its ground truth. Results presented either $|\rho_c|$ or $(1 - |\rho_c|)$ averaged over 50 runs. To obtain a fair comparison of the TC estimates, we utilized the maximal $|\rho_c|$ values for each separate run by calculating $|\rho_c|$ between the shifted TC estimates and its ground truth.

When analyzing the actual fMRI data, we also want to compute $|\rho_c|$ for the estimates of the task-related component and the non-task-related component DMN. As GLM (Friston et al., 1995) is a standard method directly using the paradigm of the fMRI data, we employ group GLM (a one sample t-test was performed on the single-subject GLM results, and $p < 0.05$) to estimate a task-related SM, and then utilize this GLM estimate as an SM reference (the ground truth) of the task-related SM estimate (Yu et al., 2015).

In addition, we utilize model TC (obtained by convolving the stimuli with the canonical SPM hemodynamic response function) as the ground truth of the task-related TC estimate. Regarding the non-task-related component DMN, we utilize the DMN component extracted from the resting fMRI data by Smith et al. (2009) as the SM reference. Note the other DMN components found in task or resting-state fMRI data (Damoiseaux et al., 2006; De Luca, et al., 2006; Laird et al., 2011; Lin et al., 2010; Allen, et al., 2011) could also be used. DMN is active during rest states but typically shows reduced activity during tasks, and its TC tends to be negatively correlated with the task-related TC (Broyd et al., 2009), we thus also use the model TC as a TC reference of DMN. We calculated the $|\rho_c|$ value from a separate run each time and then averaged the results over 50 runs.

In addition, we calculate a 95% confidence interval (CI) on 50 runs of $|\rho_c|$ estimates. Since the standard deviation σ of the $|\rho_c|$ estimates needs to be estimated, here we use the t distribution. Given the sample size of each $|\rho_c|$ is 50 (i.e., degrees of freedom=49), the t -value for the 95% interval is 2.0096, thus the margin of error is $2.0096\sigma/\sqrt{50}$, and the CI is $|\rho_c| \pm 2.0096\sigma/\sqrt{50}$. We also performed a paired t -test between the average $|\rho_c|$ of our method and those of tensor PICA, SCP_O and SCP_I, respectively, in an effort to show the significant difference between our method and the other three algorithms.

4. Results

4.1. Simulated data

The simulated data were used to evaluate the effects of the spatial and temporal changes, the noise, and the number of components on the proposed approach, tensor PICA, SCP_O and SCP_I. The task-related component was taken as an example to show the results.

4.1.1. Effects of spatial changes, temporal changes, and noise

Here we used the true component number $N = 30$. The absolute Pearson correlation coefficient deviations $1 - |\rho_c|$ and the margin of error were utilized as the performance index. We compared the four algorithms under the 36 cases of combined SM and TC changes, and took $\text{CNR} = 10\text{dB}$, 0dB , and -10dB as examples to demonstrate the noise effects. Fig. 1 shows the results. The proposed approach yielded the lowest $1 - |\rho_c|$ for all cases, followed by tensor PICA, SCP_I, and SCP_O (the three algorithms have variant $1 - |\rho_c|$ under different cases), and SCP_I always exhibited lower $1 - |\rho_c|$ than SCP_O. More specifically, for the top row of $\text{CNR} = 10\text{dB}$, see Fig. 1(a), the SM estimates of the four algorithms demonstrated visible degradation with the increase of the SM changes Δs ($\Delta s = 0, 1, 2, 3, 4, 5$), but illustrated slight degradation with the increase of the TC changes Δt ($\Delta t = 0, 1, 2, 3, 4, 5$). When the SM changes became larger (e.g., $\Delta s \geq 3$), SCP_I outperformed tensor PICA. As for the TC estimates, the four algorithms exhibited quite different results. Tensor PICA showed slight degradation with the increase of Δs but visible degradation with the increase of Δt . SCP_O exhibited visible degradation with the increase of the SM changes, and could outperform tensor PICA for the cases with much larger TC changes but smaller SM changes (e.g., $\Delta t \geq 4, \Delta s \leq 3$). In contrast, the proposed approach and SCP_I illustrated slight degradation not only with the increase of Δs but also with the increase of Δt . SCP_I got better than tensor PICA when the TC changes became larger (e.g., $\Delta t \geq 3$). The improvements of the proposed approach over tensor PICA become significant when the SM changes or the TC changes are larger.

When decreasing CNR to $\text{CNR} = 0\text{dB}$ and -10dB , see the middle row and the bottom row, the proposed algorithm and tensor PICA were slightly impacted when estimating the SMs, whereas the two SCP algorithms illustrated sensitive performance to the noise. SCP_I and SCP_O showed significantly decreased performance, and much larger SM changes were needed for SCP_I to outperform tensor PICA, e.g., $\Delta s \geq 4$ for $\text{CNR} = 0\text{dB}$ and $\Delta s \geq 5$ for $\text{CNR} = -10\text{dB}$. However, the TC estimates showed difference: tensor PICA exhibited obvious reduction of performance while our approach yielded almost the same

results as those for CNR=10dB. SCP_I and SCP_O showed smaller $1-|\rho_c|$ changes for the TC estimates than for the SM estimates, and both became better than tensor PICA when $\Delta t \geq 4$.

Observing all margin of error indexes shown in Fig. 1, we found that the proposed method and tensor PICA achieved similar performance – the margin of error was much smaller and stabler than SCP_I and SCP_O for all cases. SCP_O demonstrated the greatest sensitivity to noise in that their margin of error dramatically increased with the decrease of CNR under the cases with larger SM changes. Table 1 includes the paired t -test results between the average $|\rho_c|$ of our method and those of tensor PICA, SCP_I and SCP_O, respectively. The t -values ranged from 7.46 ($p < 10^{-8}$) to 55.05 ($p < 10^{-34}$). This verifies that the proposed method significantly improves the SM and TC estimates compared to tensor PICA, and the two SCP algorithms.

Fig. 2 shows two cases of comparison of the four approaches in terms of the SMs, the TCs, the subject-dependent TC time shifts, and the subject-specific intensities. One case is with higher CNR and smaller spatial and temporal changes (CNR = 10dB, $\Delta s=1$, $\Delta t=1$), and the other is with lower CNR and larger spatial and temporal changes (CNR = -10dB, $\Delta s=3$, $\Delta t=3$). The proposed approach provided the best estimates of SM and TC according to the SM image, the TC waveform and the $|\rho_c|$ values, see the first two rows of Fig. 2. Tensor PICA also achieved good estimates followed by SCP_I. SCP_O had the worst performance. When comparing the estimated subject-dependent TC time shifts, as shown in the third row of Fig. 2, the proposed approach achieved an accuracy of 55% ~ 70%, SCP_I had 40% ~ 55%, whereas SCP_O was 35% ~ 45% (note we did not present the subject-dependent time shift results of tensor PICA, as the time shifts were not its direct outputs). As for the subject-specific intensity, see the bottom row of Fig. 2, the proposed approach yielded better estimates matching to the ground truth than tensor PICA, followed by SCP_I and SCP_O (e.g., for the case of CNR = 10dB, $\Delta s=1$, $\Delta t=1$, the correlation coefficients with the ground truth were 0.989, 0.968, 0.951, and 0.894, respectively).

Finally, we presented the noise influence (CNR = -20dB to 20dB) on the SM and TC estimates without ($\Delta s=0$, $\Delta t=0$) and with spatial and temporal changes (taking $\Delta s=3$, $\Delta t=3$ as an example) in Fig. 3. The proposed approach and tensor PICA showed robustness except for CNR < -18dB. The advantage of the proposed approach over tensor PICA was clearly illustrated under a relatively larger spatial and temporal changes ($\Delta s=3$, $\Delta t=3$), as shown in Fig. 3B(1) and 3B(2). SCP_O exhibited significantly decreased $|\rho_c|$ when CNR < -14dB even when there were no spatial and temporal changes. SCP_I achieved higher and stabler $|\rho_c|$ as compared to SCP_O, and this even significantly outperformed tensor PICA for estimating the TCs when CNR $\geq$ 2dB. The CI results in Fig. 3 also demonstrated that the proposed algorithm and tensor PICA had much better stability than SCP_I and SCP_O. When observing the paired t -test results displayed in Table 2, we also found that the minimal t -value was 6.17 ($p < 10^{-5}$), Therefore, the proposed algorithm can achieve significant improvement over the other three methods.

4.1.2. Effects of the component number

As the true number of the components N (here $N = 30$) is unknown in the real situation, we next test how the four algorithms are impacted by changing N from 20 to 40 under different CNR and spatial and temporal changes. Specifically, we displays in Fig. 4 the $|\rho_c|$ values for the SM and TC estimates in cases of CNR = 10dB, $\Delta s=0$, $\Delta t=0$ and CNR = -10dB, $\Delta s=3$, $\Delta t=3$, and the specific results for $N = 20$ and $N = 40$ including the SM images, the TC waveforms, and their $|\rho_c|$ values. We observed that the proposed approach exhibited nearly constant performance within the wide range of component number, while tensor PICA showed fluctuation when estimating the TCs under lower CNR and larger spatial and temporal changes (CNR=-10dB, $\Delta s=3$, $\Delta t=3$). For the two cases, SCP_O was much sensitive to the component number compared to SCP_I, but both SCP algorithms obtained relatively better performance when using the true number $N = 30$. When examining the CI results included in Fig. 4 and the paired t -test results ($t \geq 12.38$, $p < 10^{-6}$) presented in Table 3, it is further confirmed that the improvements of the proposed method over tensor PICA, SCP_I and SCP_O are significant.

4.2. Actual fMRI data

The actual fMRI data naturally included inter-subject variability across both SM modality and TC modality, though the data were collected from subjects under the same stimuli. Comparison of the four approaches in Fig. 5 and Fig. 6 verified this fact.

4.2.1. Task-related component

Fig. 5 shows the SMs, the TCs, the subject-dependent TC delays, the subject-specific intensities estimated by the four approaches, in addition to the reference SM estimated by group GLM, and a table including the $|\rho_c|$ values between the SM estimates and the GLM reference. As there was no prior information about the real TC delays, we computed the largest $|\rho_c|$ values between the shifted TC estimates of ICA and the model TC to give reference TC delays, see the black bars in Fig. 5(4). Note that the task-related TC delays are not large (the largest delay is about -2.5 point) for the actual fMRI data used in this study.

We observed from Fig. 5(1) that the SM estimates of the four algorithms were all in agreement with the GLM reference, while the proposed approach yielded the best results in terms of the contiguity of the task-related activations, the interference of other components, and the $|\rho_c|$ values given in Fig. 5(2). Similar to the results of the simulated data, the proposed approach also estimated the best TC, see Fig. 5(3), and the higher accuracy of TC delays, see Fig. 5(4). As for the subject-specific intensities, as displayed in Fig. 5(5), the proposed approach and tensor PICA yielded consistent estimates (correlation was 0.997). SCP_I followed this intensity trend (correlation with the proposed was 0.858), whereas SCP showed a visible deviation (correlation with the proposed was 0.734).

4.2.2. DMN component

Fig. 6 presents the estimated DMN results of the four algorithms, including the SMs, the TCs, the subject-dependent TC delays, the subject-specific intensities, the DMN reference provided by Smith et al. (2009), and a table of the $|\rho_c|$ values between the SM estimates and the DMN reference. The same method as

above (refer to subsection 4.2.1) was utilized to generate reference TC delays for DMN, see the black bars in Fig. 6(4). Note the DMN TC delays are larger than the task-related one (the largest DMN delay is about -3.5 point).

The proposed approach and tensor PICA obtained the SM estimates in good agreement with the DMN reference, while the proposed approach showed relatively higher intensity, fewer missing voxels, and larger $|\rho_c|$ values, see Fig. 6(1) and Fig. 6(2). SCP_I also provided a similar SM estimation but with some extra voxels at the edge of brain, compared to the reference DMN. In contrast, SCP_O did not estimate a satisfying SM (with more edge and missing voxels). When comparing the TC estimates shown in Fig. 6(3), the proposed approach yielded the highest (negative) $|\rho_c|$ values with the model TC. SCP_I yielded a slightly better TC estimate than tensor PICA (-0.572 vs. -0.564). This verifies the simulation results that SCP_I can outperform tensor PICA for estimating TC when the TC delays are larger. Examining the estimates of the subject-dependent TC delays illustrated in Fig. 6(4), we found that the proposed approach achieved higher accuracy than SCP_I and SCP_O, in particular when the time delays were larger. Finally, the proposed approach and tensor PICA yielded similar estimates for the subject-specific intensities (correlation was 0.980), while SCP_I and SCP_O showed difference (correlations were 0.710 and 0.669, respectively), see Fig. 6(5).

4.2.3. Effects due to the selected number of components

We changed the component number N from 20 to 50 to investigate its effects on the four algorithms, Fig. 7 shows the results for the task-related component. The proposed algorithm exhibited very stable performance in terms of the $|\rho_c|$ values and CI for estimating both SMs and TCs. Tensor PICA also showed stable estimates for TCs, but the performance decreased for SMs when $N < 30$, see Fig. 7(1) and Fig. 7(2). SCP_I and SCP_O were more sensitive to the changes of N , as compared to our method and tensor PICA, e.g., both algorithms showed obvious degradation for $N < 30$. For details, we specifically presented the SM images, the TC waveforms and their $|\rho_c|$ values with the GLM reference and the model

TC for $N = 20$ and $N = 50$, see Fig. 7(3) ~ Fig. 7(6). It is not hard to find that the four algorithms all achieved relatively better performance for $N = 35$. As such, we used $N = 35$ in the above experiments.

We also performed the paired t -test to evaluate the difference between the average $|\rho_c|$ values of the proposed approach and tensor PICA, SCP_O and SCP_I, respectively, for the task-related component (referring to Fig. 7) and DMN, the results ($t \geq 4.81$, $p < 0.003$) are shown in Table 4. As expected, the proposed method shows significant difference from tensor PICA, SCP_I and SCP_O.

5. Discussion

In this study, we proposed a combined approach of ICA and shift-invariant CPD in order to utilize both the multiway structure and the statistical information of the multi-subject fMRI data, and to deal with the inter-subject spatial and temporal variability simultaneously. We extended tensor PICA by incorporating the TC delays into the CP model and by connecting ICA and shift-invariant CPD in a new way. Using the simulated fMRI data as well as the actual fMRI data, we demonstrate that the proposed approach yields improved estimates of the shared SMs, the shared TCs with subject-dependent time delays, and the subject-specific intensities.

CPD has great potential in finding common SM and TC components that retain spatial, temporal and subject linkages and interactions presented in the data (Andersen and Rayens, 2004), but may fall into a local optimal solution when analyzing the noisy fMRI data with inter-subject spatial and temporal variability. Tensor PICA addresses inter-subject spatial variability by incorporating a spatial constraint of SM independence. We extend tensor PICA by further accommodating a temporal constraint of TC delays consistent with what is observed in real data. It is thus not surprising that the proposed approach shows improvements over tensor PICA. Tensor PICA provides good estimates when the TC changes are small but shows degradation when the TC changes become larger. SCP_I always illustrates better performance than SCP_O, and even outperforms tensor PICA when estimating the SMs with larger SM changes or when estimating the TCs with larger TC changes. This indicates that the SM independence is a better

constraint than the SM orthogonality (linear independence) for SCP to deal with inter-subject spatial variability. Nevertheless, SCP_I is inferior to the proposed approach and tensor PICA in terms of the quality of SM and TC estimates and the robustness to noise. This may be due to the mutual interference between unsatisfying TCs and SMs estimates that is introduced by the iterative learning of SCP.

When adding the temporal constraint in addition to the spatial constraint, we aim to maximize the benefit from one another. The aggregating mixing matrix, see equations (4) and (8), has been estimated by ICA under the spatial constraint of SM independence; thus, when using aggregating mixing matrix to estimate the shared TCs with subject-dependent time delays and the subject-specific intensities at the shift-invariant CPD stage, these factors benefit from the temporal constraint as well as the spatial constraint. Along this line, the least-squares estimates of the shared SMs also accommodate the positive effect of both the temporal and spatial constraints by using the shift-invariant CPD results. Compared with tensor PICA that employed iterative connection between CPD and ICA with different objectives (De Vos et al., 2012; Helwig and Hong, 2012), our integration of CPD and ICA is in a CPD-centered way and immune from the risk of divergence. In addition, the proposed approach achieves robustness with respect to the noise and the changes of component number by virtue of the temporal and spatial constraints that can better describe the temporal and spatial characteristics of the actual multi-subject fMRI data.

According to the results of the simulated fMRI data, the larger the inter-subject temporal variability is, the higher the accuracy of the TC delay estimation is, and the bigger the benefit of the CPD-ICA connection is. The results of the actual fMRI data suggest that the temporal variability of the DMN component is larger than that of the task-related component, and the proposed approach shows significant improvements for estimating the DMN component. Therefore, the proposed approach may find promising application in analysis of the resting fMRI data, as the inter-subject temporal variability from the resting fMRI data is usually larger than from the task-related fMRI data. Note the proposed method could also improve the analysis of the event-related task fMRI data that do not have periodic TC components, and the periodicity can be enforced by introducing a temporal windowing function (Mørup et al., 2008).

The proposed approach can extract the shared SMs and the shared TCs from multiple-subject fMRI data. In the meantime, it provides the subject-dependent time delays and the subject-specific intensities, which are indeed inter-subject variability that could find utility in brain study (Caffo, et al., 2010; Li, et al., 2012; Calhoun et al., 2001; Calhoun and Adali, 2012; Allen, et al., 2011). For example, the subject-specific intensities have been utilized as predictors of disease risk in numerous studies across a wide-variety of illnesses (Caffo, et al., 2010; Li, et al., 2012; Calhoun et al., 2004; Calhoun et al., 2009; Tursich et al., 2015; Weiland et al., 2015). Note we did not consider TC shape variability (Mørup et al., 2011) across multiple subjects, future work on this extension might provide additional and valuable inter-subject variability.

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Tables

Table 1. The t -values and p -values of the paired t -test for evaluating the difference between the average $1-|\rho_c|$ values of the proposed approach and tensor PICA/SCP_O/SCP_I, for the influence of SM and TC changes and noise on the task-related SM and TC estimates, as displayed in Fig. 1.

		10dB		0dB		-10dB	
		t -values	p -values	t -values	p -values	t -values	p -values
Proposed vs. Tensor PICA	SM	13.02	5.57e^{-15}	13.77	1.07e^{-15}	11.91	17.26e^{-14}
	TC	8.71	2.74e^{-10}	37.38	8.34e^{-30}	8.22	1.10e^{-9}
Proposed vs. SCP_O	SM	55.05	1.37e^{-35}	22.15	3.53e^{-22}	33.42	3.79e^{-28}
	TC	16.94	1.94e^{-18}	7.46	9.92e^{-9}	21.14	1.62e^{-21}
Proposed vs. SCP_I	SM	17.45	7.59e^{-19}	18.74	7.89e^{-20}	16.13	8.94e^{-18}
	TC	26.47	9.79e^{-25}	17.52	6.74e^{-19}	17.47	7.32e^{-19}

Table 2. The t -values and p -values of the paired t -test for evaluating the difference between the average $|\rho_c|$ values of the proposed approach and tensor PICA/SCP_O/SCP_I, for the noise influence on the task-related SM and TC estimates, as displayed in Fig. 3.

		$\Delta s=0, \Delta t=0$		$\Delta s=3, \Delta t=3$	
		t -values	p -values	t -values	p -values
Proposed vs. Tensor PICA	SM	12.20	1.02e^{-10}	17.60	1.22e^{-13}
	TC	7.01	8.41e^{-7}	21.41	2.94e^{-15}
Proposed vs. SCP_O	SM	20.94	4.47e^{-15}	21.92	1.86e^{-15}
	TC	6.17	5.01e^{-6}	7.61	2.48e^{-7}
Proposed vs. SCP_I	SM	6.84	1.21e^{-6}	6.57	2.13e^{-6}
	TC	6.29	3.84e^{-6}	11.59	2.50e^{-10}

Table 3. The t -values and p -values of the paired t -test for evaluating the difference between the average $|\rho_c|$ values of the proposed approach and tensor PICA/SCP_O/SCP_I, for the component number effects on the task-related SM and TC estimates, as displayed in Fig. 4.

		CNR=10dB, $\Delta s=0$, $\Delta t=0$		CNR=-10dB, $\Delta s=3$, $\Delta t=3$	
		t -values	p -values	t -values	p -values
Proposed vs. Tensor PICA	SM	51.86	1.72e^{-13}	26.72	1.25e^{-10}
	TC	27.24	1.03e^{-10}	41.54	1.57e^{-12}
Proposed vs. SCP_O	SM	19.30	3.04e^{-9}	27.67	8.82e^{-11}
	TC	34.34	1.04e^{-11}	22.80	5.95e^{-10}
Proposed vs. SCP_I	SM	20.43	1.74e^{-9}	47.12	4.47e^{-13}
	TC	12.38	2.17e^{-7}	74.96	4.36e^{-15}

Table 4. The t -values and p -values of the paired t -test for evaluating the difference between the average $|\rho_c|$ values of the proposed approach and tensor PICA/SCP_O/SCP_I, for the component number effects on the SM and TC estimates of the task-related component and DMN from actual fMRI data.

		Task-related		DMN	
		t -values	p -values	t -values	p -values
Proposed vs. Tensor PICA	SM	5.01	2.43e^{-3}	13.04	1.25e^{-5}
	TC	13.77	9.12e^{-6}	12.97	1.29e^{-5}
Proposed vs. SCP_O	SM	8.33	1.62e^{-4}	35.37	3.41e^{-8}
	TC	14.53	6.67e^{-6}	7.49	2.93e^{-4}
Proposed vs. SCP_I	SM	4.81	2.99e^{-3}	15.88	3.96e^{-6}
	TC	12.84	1.38e^{-5}	7.17	3.70e^{-4}

Figure Captions

Figure 1. Comparison of the proposed approach, tensor PICA, SCP_O and SCP_I in terms of the absolute Pearson correlation coefficient deviations ($1 - |\rho_c|$) between the task-related SM and TC estimates and their ground truth with margin of error under 36 cases of combined SM and TC changes ($\Delta s = 0, 1, 2, 3, 4, 5$, and $\Delta t = 0, 1, 2, 3, 4, 5$) with CNR = -10dB (a), 0dB (b), and -10dB (c). The lower the ($1 - |\rho_c|$) values are, the better the performance is. The true component number $N = 30$ of the simulated fMRI data was utilized.

Figure 2. Comparison of the proposed approach, tensor PICA, SCP_O and SCP_I under (A) CNR = 10dB, $\Delta s = 1$, $\Delta t = 1$ and (B) CNR = -10dB, $\Delta s = 3$, $\Delta t = 3$. (1) The task-related SM estimates ($|Z| > 1$) and the $|\rho_c|$ values with the ground truth. (2) The task-related TC estimates and the $|\rho_c|$ values with the ground truth. (3) The subject-dependent TC time shifts estimated by the proposed approach, SCP_O and SCP_I, and the accuracy of estimation with respect to the ground truth. (4) The estimated subject-specific intensities and the $|\rho_c|$ values with the ground truth. The true component number $N = 30$ of the simulated fMRI data was utilized.

Figure 3. Comparison of the noise influence (CNR = -20dB to 20dB) on the proposed approach, tensor PICA, SCP_O and SCP_I in terms of $|\rho_c|$ and CI of the task-related SM and TC estimates without and with spatial and temporal changes. (A) $\Delta s = 0$, $\Delta t = 0$. (B) $\Delta s = 3$, $\Delta t = 3$. The true component number $N = 30$ of the simulated fMRI data was utilized.

Figure 4. Comparison of the component number N (from 20 to 40) effects on the proposed approach, tensor PICA, SCP_O and SCP_I in terms of $|\rho_c|$ and CI of the task-related SM and TC estimates under two cases of CNR and spatial and temporal changes: (A) CNR = 10dB, $\Delta s = 0$, $\Delta t = 0$; (B) CNR = -10dB, $\Delta s = 3$, $\Delta t = 3$, and the specific SM images, TC waveforms, and their $|\rho_c|$ values for $N = 20$ and $N = 40$ (note the true component number is 30).

Figure 5. Results of the task-related component estimated by the proposed approach, tensor PICA, SCP_O and SCP_I from actual fMRI data with $N = 35$. (1) The GLM reference and the SM estimates ($|Z| > 2.5$). (2) The $|\rho_c|$ values between the SM estimates and the GLM reference. (3) The TC estimates and the $|\rho_c|$ values with the model TC. (4) The subject-dependent TC delays estimated by the proposed approach, SCP_O and SCP_I. The reference time delays shown as the black bars are generated by the largest $|\rho_c|$ values between the shifted TC estimates of ICA and the model TC. (5) The subject-specific intensities.

Figure 6. Results of default mode network (DMN) estimated by the proposed approach, tensor PICA, SCP_O and SCP_I from actual fMRI data with $N = 35$. (1) The DMN reference and the SM estimates ($|Z| > 2.5$). (2) The $|\rho_c|$ values between the SM estimates and the DMN reference. (3) The TC estimates and the $|\rho_c|$ values with the model TC. (4) The subject-dependent TC delays estimated by the proposed approach, SCP_O and SCP_I. The reference time delays shown as the black bars are formed by the largest $|\rho_c|$ values between the shifted TC estimates of ICA and the model TC. (5) The subject-specific intensities.

Figure 7. Effects of the component number N (from 20 to 50) on the proposed approach, tensor PICA, SCP_O and SCP_I when estimating the task-related component from the actual fMRI data. (1) The $|\rho_c|$ values and CI of the SM estimates. (2) The $|\rho_c|$ values and CI of the TC estimates. (3) The SM images and the $|\rho_c|$ values for $N = 20$. (4) The SM images and the $|\rho_c|$ values for $N = 50$. (5) The TC waveforms and the $|\rho_c|$ values for $N = 20$. (6) The TC waveforms and the $|\rho_c|$ values for $N = 50$.

Figure 1

Figure 2

Figure 3

Figure 4

A. CNR=10dB, $\Delta s = 0$, $\Delta t = 0$

(1) $|\rho_d|$ of SM

(2) $|\rho_d|$ of TC

(3) SM and TC for $N = 20$

(4) SM and TC for $N = 40$

B. CNR=-10dB, $\Delta s = 3$, $\Delta t = 3$

(1) $|\rho_d|$ of SM

(2) $|\rho_d|$ of TC

(3) SM and TC for $N = 20$

(4) SM and TC for $N = 40$

Figure 5

(1) SM($|Z|>2.5$)

(a) DMN Reference

(b) Proposed

(c) Tensor PICA

(d) SCP-O

(e) SCP-I

(2) $|\rho_c|$ between SM estimates and GLM reference

	Proposed	Tensor PICA	SCP_O	SCP_I
$ \rho_c $	0.513	0.498	0.425	0.455

(3) TC

(4) Time delay

(5) Subject intensity

Figure 6

(1) SM($|Z|>2.5$)

(a) DMN Reference

(b) Proposed

(c) Tensor PICA

(d) SCP-O

(e) SCP-I

(2) $|\rho_c|$ between SM estimates and DMN reference

	Proposed	Tensor PICA	SCP_O	SCP_I
$ \rho_c $	0.713	0.658	0.500	0.578

(3) TC

(4) Time delay

(5) Subject intensity

Figure 7