

1 **Discovering hidden brain network**
2 **responses to naturalistic stimuli via**
3 **tensor component analysis of**
4 **multi-subject fMRI data**

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1 Abstract

2 The study of brain network interactions during naturalistic stimuli facilitates a
3 deeper understanding of human brain function. Intersubject correlation (ISC) analysis
4 of functional magnetic resonance imaging (fMRI) data is a widely used method that
5 can measure neural responses to naturalistic stimuli that are consistent across subjects.
6 However, interdependent correlation values in ISC artificially inflated the degrees of
7 freedom, which hinders the investigation of individual differences. Besides, the
8 existing ISC model mainly focus on similarities between subjects but fails to
9 distinguish neural responses to different stimuli features. To estimate large-scale brain
10 networks evoked with naturalistic stimuli, we propose a novel analytic framework to
11 characterize shared spatio-temporal patterns across subjects in a purely data-driven
12 manner. In the framework, a third-order tensor is constructed from the timeseries
13 extracted from all brain regions from a given parcellation, for all participants, with
14 modes of the tensor corresponding to spatial distribution, time series and participants.
15 Tensor component analysis (TCA) will then reveal spatially and temporally shared
16 components, i.e., naturalistic stimuli evoked networks, their temporal courses of
17 activity and subject loadings of each component. To enhance the reproducibility of the
18 estimation with TCA, a novel spectral clustering method, tensor spectral clustering,
19 was proposed and applied to evaluate the stability of TCA algorithm. We demonstrate
20 the effectiveness of the proposed framework via simulations and real fMRI data
21 collected during a motor task with a traditional fMRI study design. We also apply the
22 proposed framework to fMRI data collected during passive movie watching to illustrate
23 how reproducible brain networks are identified evoked by naturalistic movie viewing.
24

1 Introduction

2 There is growing interest in studying brain function during naturalistic stimuli e.g.
3 film clips, spoken narratives and music as experimental paradigms to investigate
4 human cognition and behavior in “real-world” (Breakspear and Chang, 2020; Hasson
5 et al., 2004; Huth et al., 2016; Nishimoto et al., 2011; Sonkusare et al., 2019; Spiers
6 and Maguire, 2007). Naturalistic stimulus viewing during functional magnetic
7 resonance imaging (fMRI) is emerging as a powerful tool to define brain
8 imaging-based markers of psychiatric illness (Eickhoff et al., 2020), with several
9 advantages in comparison to unconstrained resting state. Namely, studying brain
10 network function during naturalistic stimulus viewing may facilitate a deeper
11 understanding of human brain function since the passive state is better constrained and
12 it reduces participant motion, which greatly increases the quality of the fMRI data.
13 However, new analytical strategies are needed that assess both the shared rapid
14 temporally evolving brain responses evoked by the naturalistic stimuli in participants,
15 as well as the idiosyncrasy in individual participants (Simony and Chang, 2020).

16 The most popular approach for analysis of naturalistic fMRI data is assessment of
17 intersubject correlations (ISC), which quantifies the across-subject consistency of
18 stimulus-driven responses (Hasson et al., 2004). While evoked brain activity using
19 traditional fMRI study designs and stimuli is relatively straightforward to model,
20 naturalistic stimuli are complex and dynamic, and it is much more difficult to generate a
21 model of evoked activity for analyses. Instead, for dynamic complex stimuli such as
22 movies, ISC measures shared information across brains by using each individual’s
23 brain activity measured by fMRI to model another individual’s brain activity. Using
24 this strategy, the shared brain regions that respond to the same time-locked naturalistic
25 stimuli across subjects can be estimated, even with stimuli that reflect complex
26 dynamic real-life contexts (Hasson et al., 2004; Kauppi et al., 2014; Nastase et al.,
27 2019). Modifications to intersubject functional correlation (IFC), temporal intersubject
28 functional correlation (ISFC) has been proposed that consider the timecourse
29 correlations between all possible pair-wise combinations of brain parcels across
30 subjects (Nastase et al., 2019) and spatial ISC is an extension of temporal ISC to
31 multi-voxel pattern analysis (Haxby et al., 2014; Norman et al., 2006). Generally, the
32 ISC is implemented with either a leave-one-out framework, in which one subject’s time
33 course is correlated with the average of all other subjects for each region, or a pairwise
34 framework, in which correlation analysis is performed between each possible pair of
35 subjects (Finn et al., 2020). A limitation of this computational procedure is that the
36 resulting correlations are highly interdependent and violate the assumption of common
37 parametric tests (Nastase et al., 2019), requiring careful attention to the inference
38 method. In addition, multiple cognitive and affective processes emerge in brain
39 response to complex naturalistic stimuli (Bartels and Zeki, 2004; Simony and Chang,
40 2020). ISC reflects similarity in how each brain region encodes the stimulus across

1 participant, not how a brain region(s) may response to different features of the natural
2 stimuli based on the current ISC model. In order to mitigate these limitations, we
3 proposed a novel tensor component analysis (TCA) framework that characterizes
4 shared spatio-temporal patterns as well as idiosyncratic loadings of evoked activity to
5 naturalistic stimuli across subjects in a purely data-driven manner that assesses all brain
6 networks simultaneously.

7 While a matrix is a 2-D array, multidimensional data with more than 2 dimensions
8 are referred to as tensors. TCA is a fundamental model for tensor decomposition, also
9 known as tensor Canonical Polyadic Decomposition (CPD) (Kolda and Bader, 2009),
10 that has been shown to have superior performance in identifying hidden signal sources
11 compared with matrix decomposition, e.g. principle component analysis (PCA) and
12 independent component analysis (ICA), applied to multidimensional data (Williams et
13 al., 2018). Assuming the data meet the assumption of a mixture model, in which
14 signal sources undergo a linear mixing process, TCA can more accurately estimate
15 sources than matrix decomposition algorithms, and without any constraints. fMRI
16 signals are innately multidimensional property and can be naturally represented in
17 tensor form. In this study, a third-order fMRI tensor is organized as space \times time \times
18 subjects (the order of modes does not impact the estimation). Through TCA analysis,
19 the spatial and temporal information regarding brain network activity evoked by
20 different stimuli exists in the first two dimensions. Subject loadings exist in the third
21 dimension, which are used to investigate subject variability.

22 TCA has shown promise in a range of neuroscience researches. In the field of EEG
23 signal analysis, nonnegative constraint TCA was applied on time-frequency domain
24 data to identify event-related (Cong et al., 2015a, 2015b; Wang et al., 2018) and
25 naturalistic stimulus-evoked EEG response (Zhu et al., 2020b). When TCA was applied
26 for fMRI connectivity analysis, Mokhtari et al. (2019) explored the difference in the
27 results of different tensor organizations and Zhu et al. (2020b) have explored the
28 effectiveness of TCA for MEG data analysis. TCA has also been applied for fMRI data
29 analysis (Andersen and Rayens, 2004) and has been adapted for multi-subject fMRI
30 data analysis by placing spatial and temporal constraints to address inter-subject
31 variability (Beckmann and Smith, 2005; Helwig and Hong, 2013; Kuang et al., 2020,
32 2015; Mørup et al., 2008; Zhou and Cichocki, 2012). We advance TCA for analysis of
33 multi-subject fMRI data collected during naturalistic stimuli viewing by proposing a
34 pipeline that does not place any constraints on the data.

35 In order to characterize stable shared spatio-temporal components across subjects
36 with TCA, the reproducibility of TCA components is evaluated using a novel
37 clustering method, tensor spectral clustering and model order (number of extracted
38 components) is selected in terms of algorithm stability. The effectiveness of the
39 proposed framework is demonstrated with simulated and traditional task fMRI in which
40 we know the ground truth stimulation (and hence brain activity) timecourses. Then we
41 apply the proposed framework to fMRI data collected during movie watching, in which

1 there is no *a priori* model of brain activity, to identify spatial brain networks engaged
2 during the task.

3 The rest of the paper is structured as follows. In section 2, Materials and Methods,
4 we present the TCA model that was used to estimate spatio-temporal shared
5 components, the decomposition algorithm used in this paper, the criteria that were used
6 to evaluate the reproducibility of estimated components and the model order selection
7 method, and the test datasets. In section 3, Results, we show the simulation and motor
8 task fMRI results. After establishing the robustness of the proposed framework, we
9 show results from applied our analytic approach to a naturalistic stimuli fMRI dataset
10 from 184 participants, collected by the Human Connectome Project (HCP). In section 4
11 and 5, Discussion and Conclusions, respectively, we discuss our findings and the
12 conclusions from our work. The basic principle of tensor spectral clustering that is
13 used to evaluate the stability of estimated components is introduced in Appendix.

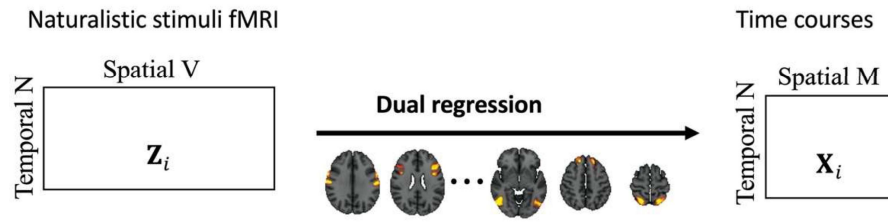
14 **Materials and Methods**

15 **TCA model**

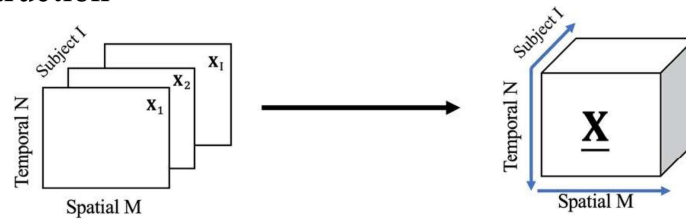
16 The full strategy of TCA for naturalistic stimuli fMRI data consisted of three
17 steps as shown in Fig. 1. Firstly, extract activity timecourses with independent
18 component analysis (ICA) parcellation scheme; then, stack all subjects' timecourses
19 to construct a third-order fMRI tensor; finally, estimate spatio-temporal patterns and
20 corresponding subject loadings with TCA.

21 Rather than applying TCA to voxel-wise fMRI data, a whole brain parcellation
22 scheme is applied to extract node (or region) timecourses for the TCA. This is done for
23 several reasons. First, intensity of BOLD fMRI data is expected to be smooth across
24 neighboring voxels and, with an appropriate parcellation method, node timecourses
25 will have a higher signal noise ratio (SNR) compared with the SNR of timecourses
26 from dense data (Glasser et al., 2016). Using ICA with high model orders (>100 to
27 several hundred) will result in components that feature individual small brain regions,
28 bilateral brain regions, or sparse sub-networks and can thus be considered as nodes for
29 use in network analysis (Smith, 2012). Several studies have demonstrated that time
30 course of spatial independent components can identify intrinsic brain networks (Allen
31 et al., 2014; Jafri et al., 2008; Smith et al., 2012). Other work has also shown that brain
32 parcellation with spatial ICA demonstrates better performance for network modeling
33 compared with other parcellation methods (e.g., anatomical parcellations) and higher
34 model order leads to better performance (Pervaiz et al., 2020). In this study, a brain
35 parcellation scheme derived from ICA of the Human Connectome Project (HCP)
36 resting state fMRI data with model order of 300 (provided by the HCP, Van Essen et al.,
37 (2013)) is used to extract timecourses from nodes for TCA. The timecourses are

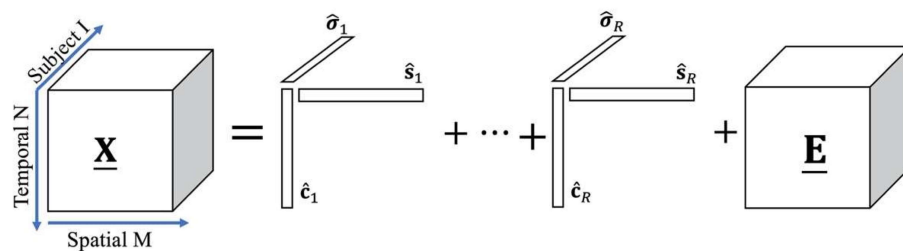
A Time courses estimation with independent components



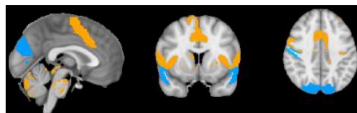
B Tensor construction



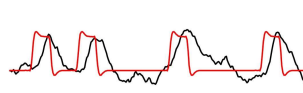
C TCA decomposition



\hat{s} : Spatial distribution



\hat{c} : Time course



\hat{o} : Subject loadings

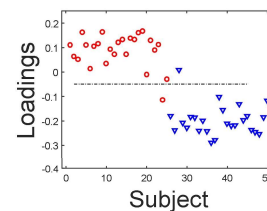


Figure 1 Tensor component analysis pipeline. (A) Estimating node timeseries with dual regression from standard preprocessed dense data. (B) Stacking all subjects' node data to construct a tensor. (C) Extracting tensor components with tensor component analysis. The estimated components of each mode \hat{s} , \hat{c} , \hat{o} correspond to the spatial distribution, time course and subject loadings, respectively.

1 extracted via the first stage of dual regression (Nickerson et al., 2017) in which the full
 2 set of ICA components, \mathbf{S}_{ICA} , are regressed against each participant's 4D fMRI data
 3 (e.g., multivariate spatial regression) to extract the timecourses. This is different from
 4 how conventional binary parcellation masks are used to extract average timecourses
 5 from each node that are then fed into the TCA in that the multivariate spatial regression
 6 accurately handles any potential spatial overlap among the ICA maps due to individual
 7 brain regions participating in more than one brain network (or sub-network)
 8 represented in the ICA maps.

1 Multilinear mixing model

2 For naturalistic stimuli fMRI we assume, similar to ISC model (Finn et al., 2020;
3 Nastase et al., 2019), that time courses $\mathbf{C} \in \mathbb{R}^{N \times J}$ (N is the number of time points, J
4 is the number of patterns) and spatial patterns $\mathbf{S} \in \mathbb{R}^{M \times J}$ (M is the number of nodes,
5 300 in this study) of nodes in the parcellation are stimulus-evoked responses that are
6 consistent across subject. However, in contrast to the ISC model, there may also be J
7 patterns that are shared across subjects that correspond to evoked responses associated
8 with different features of the naturalistic stimuli. Thus, in our TCA-based model, for
9 each pattern j , the loading $\sigma_{i,j}$ for subject i is different from other subjects. In this
10 case, for subject i , the node timecourses $\mathbf{X}_i \in \mathbb{R}^{M \times N}$, can be represented as:

$$11 \quad \mathbf{X}_i = \mathbf{S} \times \mathbf{diag}(\sigma_{i,:}) \times \mathbf{C}^T + \mathbf{Id}_i + \boldsymbol{\varepsilon}_i, \quad (1)$$

12 where \mathbf{Id}_i is the stimulus-evoked response that is idiosyncratic to each subject. $\boldsymbol{\varepsilon}_i$
13 corresponds to the spontaneous and noise component, which may reflect spontaneous
14 neural activity and noise from non-neural physiological and scanner sources.
15 $\mathbf{diag}(\sigma_{i,:})$ is a square matrix of order J with the elements of $\sigma_{i,:}$ on the diagonal and
16 the other elements of the matrix is zero.

19 Tensor construction

20 A tensor is constructed from the multi-subject data, $\underline{\mathbf{X}} \in \mathbb{R}^{M \times I \times N}$, which is the data
21 from each subject's \mathbf{X}_i stacked in the subject dimension. I is the total number of
22 subjects. Although the spatial and the temporal patterns are assumed to be shared across
23 participant, the loadings of the pattern in each participant are different. Of note, the
24 model also does not place any assumption on the distribution of temporal courses or
25 spatial distributions.

26 TCA unmixing model

27 TCA, also known as CPD, is a basic model for tensor decomposition. With
28 different constraints, different algorithms can be derived, including non-negative
29 canonical polyadic decomposition (NCPD) (Zhou et al., 2014) and independent
30 constrained CPD (e.g. tensor-ICA Beckmann and Smith, 2005). In the TCA model, a
31 third-order tensor $\underline{\mathbf{X}}$ can be represented as the sum of several rank-1 tensors and a
32 residual tensor $\underline{\mathbf{E}}$ (Hitchcock, 1927), which is illustrated in Fig.1 (C). The
33 mathematical formula is as follow:

$$34 \quad \underline{\mathbf{X}} = \sum_{r=1}^R \hat{\mathbf{s}}_r \circ \hat{\boldsymbol{\sigma}}_r \circ \hat{\mathbf{c}}_r + \underline{\mathbf{E}} = \sum_{r=1}^R \underline{\mathbf{X}}_r + \underline{\mathbf{E}}, \quad (2)$$

35 where vectors $\hat{\mathbf{s}}_r \in \mathbb{R}^{M \times 1}$, $\hat{\boldsymbol{\sigma}}_r \in \mathbb{R}^{I \times 1}$ and $\hat{\mathbf{c}}_r \in \mathbb{R}^{N \times 1}$ are r^{th} estimated tensor
36 component (TC) spatial distribution \mathbf{S} , subject loadings $\boldsymbol{\sigma}$ and temporal courses \mathbf{C}
37 respectively. The operator \circ represents the outer product of vectors. $\underline{\mathbf{X}}_r$ represents the
38 rank-1 tensor that constructed by the corresponding components of each mode. The
39 idiosyncratic stimulus-evoked responses, spontaneous and noise components are
40 contained in the residual tensor $\underline{\mathbf{E}}$ and R represents the number of extracted patterns.
41
42

1 Ideally, the number of tensor components, or model order, should be equivalent to the
2 number of patterns, J , shared across subjects. However, in real-world applications, the
3 number of patterns in the brain is unknown. In this study, model order is determined
4 according to algorithm stability. For each tensor component, the voxel-level spatial
5 distribution can be back reconstructed as $\mathbf{S}_{ICA} \times \hat{\mathbf{s}}_r$, the time course is $\hat{\mathbf{c}}_r$, which is the
6 same across subjects. Differences of subjects exist at $\hat{\boldsymbol{\sigma}}_r$.

7 **TCA estimation algorithm**

8 The alternating least-squares (ALS) algorithm (Cichocki et al., 2015; Kolda and
9 Bader, 2009) is used to estimate factor matrices \mathbf{S} , \mathbf{C} and $\boldsymbol{\sigma}$. In ALS algorithm, two
10 of the factor matrices are fixed to optimize over the third factor matrix. For example,
11 while time courses \mathbf{C} is being estimated, the spatial distribution \mathbf{S} and subject
12 loadings $\boldsymbol{\sigma}$ should be fixed. The spatial distribution can be updated with the
13 following rules:

14

$$15 \quad \mathbf{C} \leftarrow \operatorname{argmin}_{\hat{\mathbf{C}}} \frac{1}{2} \|\mathbf{X} - \sum_{r=1}^R \hat{\mathbf{s}}_r \circ \hat{\boldsymbol{\sigma}}_r \circ \hat{\mathbf{c}}_r\|_F^2, \quad (3)$$

16

17 where F represents the Frobenius norm. The updating rule can be solved as a linear
18 least-square problem that is convex and has a closed-form solution. The other factor
19 matrices can be solved with the same updating rule. Three factor matrices were
20 alternating updated until one of the stop criteria is met. The stop criteria can be
21 defined as the absolute different value of data fitting of the adjacent two iterations was
22 less than $1e-8$ or the maximum number of iterations was more than 1000. The ALS
23 algorithm can be free accessed from tensor toolbox (<https://www.tensortoolbox.org>).

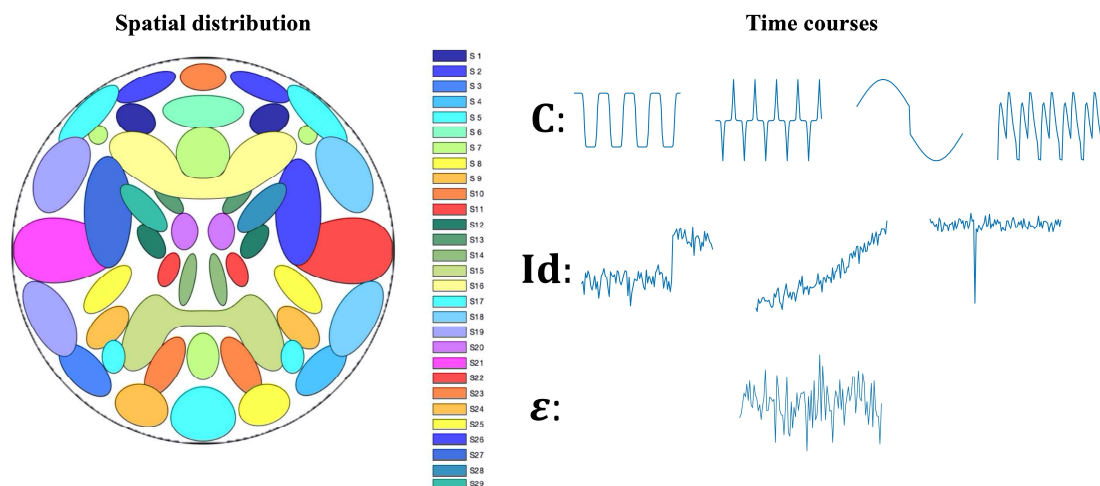
24 **Algorithm stability analysis**

25 Improving the reproducibility of neuroscience research is one of great concern
26 (Poldrack, 2019; Poldrack and Farah, 2015). In this study, in order to assess the
27 reproducibility of estimated rank-1 tensor $\underline{\mathbf{X}}_r = \hat{\mathbf{s}}_r \circ \hat{\mathbf{c}}_r \circ \hat{\boldsymbol{\sigma}}_r$, a novel clustering method,
28 tensor spectral clustering, was proposed. In the stability analysis of TCA algorithms,
29 for the given dataset, the same algorithm with the same parameters will be run K times
30 with different initial conditions. When the number of extracted components is selected
31 as R , for each mode $R \times K$ components can be estimated. Then the similarity
32 matrices across these components of each mode $\mathbf{W}^{(S)}, \mathbf{W}^{(\sigma)}, \mathbf{W}^{(C)} \in \mathbb{R}^{RK \times RK}$ would
33 be fed into tensor spectral clustering, which is a co-clustering method that can fuse
34 and assess the stability information of different modes simultaneously. Details of
35 formulations of tensor spectral clustering can be found in the Appendix. In tensor
36 spectral clustering, the number of clusters is defined as exactly same with the number

1 of extracted components R . The stable component would produce a tight cluster. The
2 stability index is quantified with the average intra-cluster similarities. Ideally, if the
3 estimation of the component is stable, the inner similarity of the corresponding cluster
4 is close to 1. The stability index of unstable components is approach to 0. The
5 algorithm stability is defined as the average of components stability indices.

6 Model order selection

7 Same as ICA, model order (number of extracted components) selection is a
8 significant methodological concern when data driven algorithm is applied for fMRI
9 data analysis (Abou-Elseoud et al., 2010; Beckmann, 2012; Kuang et al., 2018). When
10 the selected model order is appropriate to the tensor to be decomposed, the algorithm
11 would also be stable. In this study, we performed the tensor decomposition algorithm
12 use a range of model orders. The algorithm stability under each model order was
13 evaluated. The components under the model order with the highest algorithm stability
14 index were used for further analysis.
15



16
17 *Figure 2 Ground truth spatio-temporal sources signal used in simulation. The left figure shows the spatial*
18 *distribution of 29 ICA components. The right column shows the time courses to mimic the consistent components*
19 *across subjects (the first row, **C**), the idiosyncratic components (the second row, **Id**) and the spontaneous*
20 *components (the third row, **ε**).*

21 Simulations

22 In this section, we showcase the effectiveness of the proposed framework using
23 numerical experiments which is performed in MATLAB. The spatial distribution of 29
24 ICA components (SimBT (Erhardt et al., 2012) <http://mialab.mrn.org/software>) and
25 time courses $\mathbf{C} \in \mathbb{R}^{100 \times 8}$ (http://mlsp.umbc.edu/simulated_fmri_data.html) are shown
26 in Fig. 2. Four timecourses, as shown in the first row of Fig.2, represent consistent

1 components across subjects. There are also three idiosyncratic components for each
2 subject, which denote the scanner or motion noise consisted in fMRI scanning, as
3 shown in the second row of Fig 2. These components would randomly circle shift for
4 each subject. The timecourse in the third row of Fig 2 represents spontaneous brain
5 activity included in the simulation. The total signal noise ratio (SNR) is controlled to
6 be 2dB. We randomly generated node weight matrix $\mathbf{S} \in \mathbb{R}^{29 \times 8}$ and subject loading
7 matrix $\boldsymbol{\sigma} \in \mathbb{R}^{10 \times 8}$ to generate 10 participants' data. For each subject, the data can be
8 created with equation (1). Then stack all subject data to construct a three-order tensor
9 $\underline{\mathbf{X}}_{\text{Simulation}} \in \mathbb{R}^{29 \times 10 \times 100}$. Then the tensor was decomposed with the model order
10 range from 2 to 10. Under each model order, the TCA algorithm ran 20 times to
11 evaluate the stability of the algorithm. The stability index is calculated with tensor
12 spectral clustering. The correlation coefficient between estimate component and the
13 corresponding ground truth works as a criterion to evaluate the performance of the
14 proposed framework.

15 **Motor task fMRI experiment**

16 The effectiveness of the proposed framework is also demonstrated with traditional
17 motor task fMRI in which we know the ground truth stimulation (and hence brain
18 activity) timecourses. Randomly selected 100 healthy unrelated subjects (22-36 years)
19 were utilized from the WU-Minn Human Connectome Project (HCP; Van Essen et al.,
20 2013). During the motor task, participants are presented with visual cues that ask them
21 to either tap their left or right fingers, or squeeze their left or right toes, or move their
22 tongue to map motor areas. Each block movement type last 12 seconds and is preceded
23 by a 3 second cue. For each subject total 284 scans were collected with TR=0.72s in a
24 3T scanner. Details of motor task of HCP data could be find in Barch et al. (2013).

25 The collected fMRI data went through the standard preprocessing pipeline
26 (motion correction, distortion correction, highpass filtering, and nonlinear alignment
27 to MNI template space (Glasser et al., 2013)) to the standard brain space. Time
28 courses of visual cues for each type of movement were convolved with Hemodynamic
29 Response Function (HRF) and went through a low-pass filtering with a high-frequency
30 cutoff of 0.1Hz. The convolved time courses, as shown red lines in Fig. 4, are used to
31 identify components extracted with TCA. Following the recommendations of previous
32 study (Pervaiz et al., 2020), spatial ICA components were used for brain parcellation.
33 Spatial ICA components are provided by the HCP under number of components of 300
34 and subject-specific time series for each node were derived using dual regression
35 (Nickerson et al., 2017), as shown in Fig. 1 (A). Then time courses were detrended
36 linear, quadratic, and cubic trends, and low-pass filtered with a high-frequency cutoff
37 of 0.1Hz.

38 The data for each subject was then stacked on subject dimension to create a tensor
39 $\underline{\mathbf{X}}_{\text{Motor}} \in \mathbb{R}^{300 \times 100 \times 284}$ to be decomposed. Then the tensor is decomposed with TCA

1 under model order from 2 to 20. And the same decomposition under each model order
2 would be run 20 time to make sure the reproducibility of the estimated components.
3 Then the model order is selected with the proposed model order selection method based
4 on algorithm stability analysis strategy.

5 **Naturalistic stimuli fMRI experiment**

6 The naturalistic fMRI dataset is also from the HCP (Van Essen et al., 2013).
7 Subjects (healthy, 22-35 years) engaged in a movie-watching paradigm (voxel size =
8 1.6mm^3 , $\text{TR}=1\text{s}$) functional MR scanning in a 7T scanner. The sample used here ($n =$
9 184) reflects all available data for this paradigm. Each subject watched four 15-min
10 movie runs (MOVIE1-MOVIE4). Each run comprised five video clips presented in a
11 fixed order. The fMRI data collected during validation clip (the fifth video clip) was
12 used in this study. The validation clip is consisted of a montage of brief (1min 22s)
13 moving scenes depicting people and landscapes. The music that along with movie
14 scene also contains plenty of information that may evoke consistent brain activities
15 across participants (Alluri et al., 2012). Five music features (Fluctuation Centroid,
16 Fluctuation Entropy, Key Clarity, Mode and Pulse Clarity) were extracted using the
17 MIRTtoolbox (Lartillot, O., 2007). With the proposed framework, dynamic temporal
18 alteration of brain networks can also be estimated. These music features facilitate the
19 understanding and interpretation of the estimated tensor components. With the
20 proposed framework, a component that related to social scene is identified. The
21 subject loadings of the component were used to investigate the relationship between
22 behavior data Antisocial Personality Problems Raw Score and brain activities. The
23 behavior data is a score that evaluates the antisocial personality disorder assessed
24 using the Semi-Structured Assessment for the Genetics of Alcoholism (SSAGA;
25 BUCHOLZ et al., 1994; Hesselbrock et al., 1999).

26 All fMRI analyses began with the FIX-denoised data, which includes standard
27 preprocessing (motion correction, distortion correction, high pass filtering, and
28 nonlinear alignment to MNI template space (Glasser et al., 2013)) plus regression of
29 24 framewise motion estimates (six rigid-body motion parameters and their
30 derivatives and the squares of those 12) and regression of confound components
31 identified via independent components analysis (Griffanti et al., 2014;
32 Salimi-Khorshidi et al., 2014). Details of data acquisition and basic data
33 preprocessing can be found in previous studies (Glasser et al., 2013; T. Vu et al., 2016;
34 Van Essen et al., 2012). The tensor organization procedure is exactly same with that
35 of motor task fMRI, as shown in Fig. 1 and the tensor to be decomposed is
36 $\underline{\mathbf{X}}_{\text{Naturalistic}} \in \mathbb{R}^{300 \times 184 \times 82}$.

37 In this experiment, our goals are three-fold. Firstly, apply the proposed
38 framework to all subjects to explore what kinds of brain activity can be evoked with
39 the movie stimuli. All subjects' fMRI data went through the proposed framework.
40 Then the relationship between the estimated components and subjects' behavior data

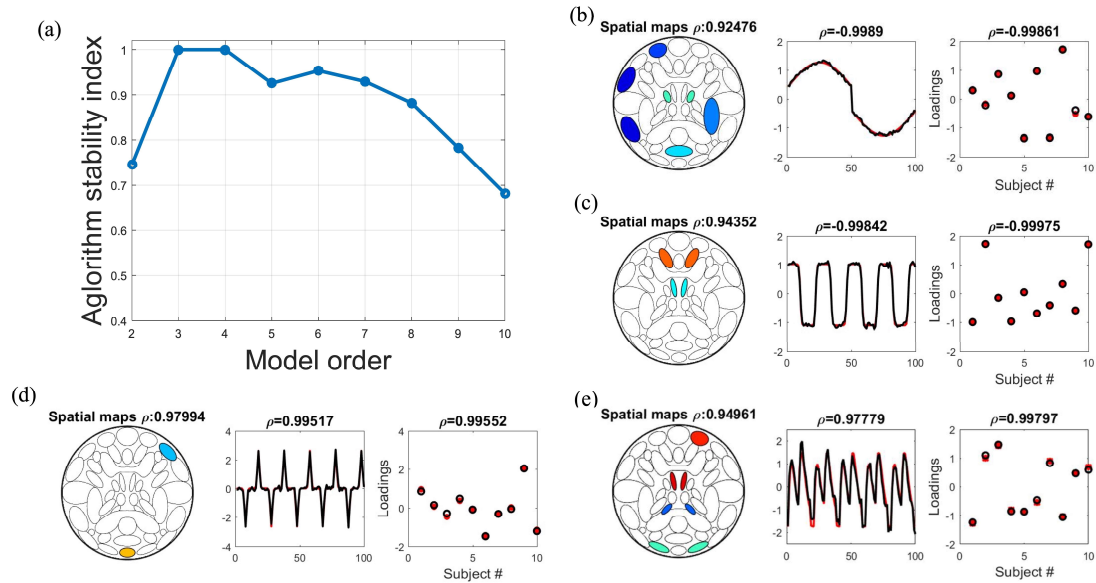
1 as well as music features was further analyzed. Secondly, to investigate the
2 reproducibility of the estimated components, the subjects were randomly and equally
3 divided into two cohorts. And apply the proposed framework on these two cohorts
4 separately. Then evaluate the consistency of the estimated components from these two
5 cohorts. Thirdly, two version of movie files compiled as stimuli were used in
6 MOVIE4. In the posterior movie stimuli, 4 frames were added before the validation
7 clip, the deviation of two version movie is only 167ms, no more than 1 TR. To
8 evaluate the performance of the proposed framework on exploring subjects'
9 difference, 25 subjects of each type of movie stimuli were randomly selected. Then
10 these 50 subjects' fMRI data went through the proposed framework, to probe whether
11 the conditions' difference can be detected in subject loadings. And performance of
12 TCA and ISC are also compared in this experiment in terms of conditions' difference
13 detection. In ISC, leave-one out method, in which one subject's time course is
14 correlated with the average of all other subjects for each region, was applied to
15 calculate the subjects' score.

16 **Results**

17 **Simulations**

18 Fig. 3 shows the simulation results. Fig. 3(a) exhibits algorithm stability indices
19 under different model orders. We could find that the algorithm stability curve reaches
20 its high at the model order of both 3 and 4. Since the model order selected as 4 means
21 one more component can be extracted, the tensor components at the model order of 4,
22 which is exactly same with the number of consistent components across subjects,
23 were further analyzed. Note that the algorithm stability index at the model order is 1,
24 which means all components estimated on the model order from different runs are the
25 same and all these components are repeatable. The spatial distribution, time courses
26 and subject loadings of each component are exhibited in Fig.3 (b-e). Based on the
27 correlation coefficient between estimated components and ground truths, we could
28 find that all four components are successfully estimated. In order to highlight the
29 activated and deactivated brain regions, the spatial distribution of the estimated
30 component was exhibited with proportional threshold (10%, Garrison et al. (2015)). In
31 spatial distribution, warm colors represent activation (relative to global average) while
32 cool colors represent deactivation within each component.

33



1

2

Figure 3 Simulation results. (a) Algorithm stability under different model orders. The algorithm reaches the highest stability at the model order of 4, which is exactly same with the number of consistent components. (b) - (e) estimated components and ground truths. The symbol ρ means the correlation coefficient between estimate component and the corresponding ground truth. In spatial distribution, proportional threshold (10%, Garrison et al. (2015)) was used and warm colors represent activation (relative to components global average) while cool colors represent deactivation (relative to components global average) within each component.

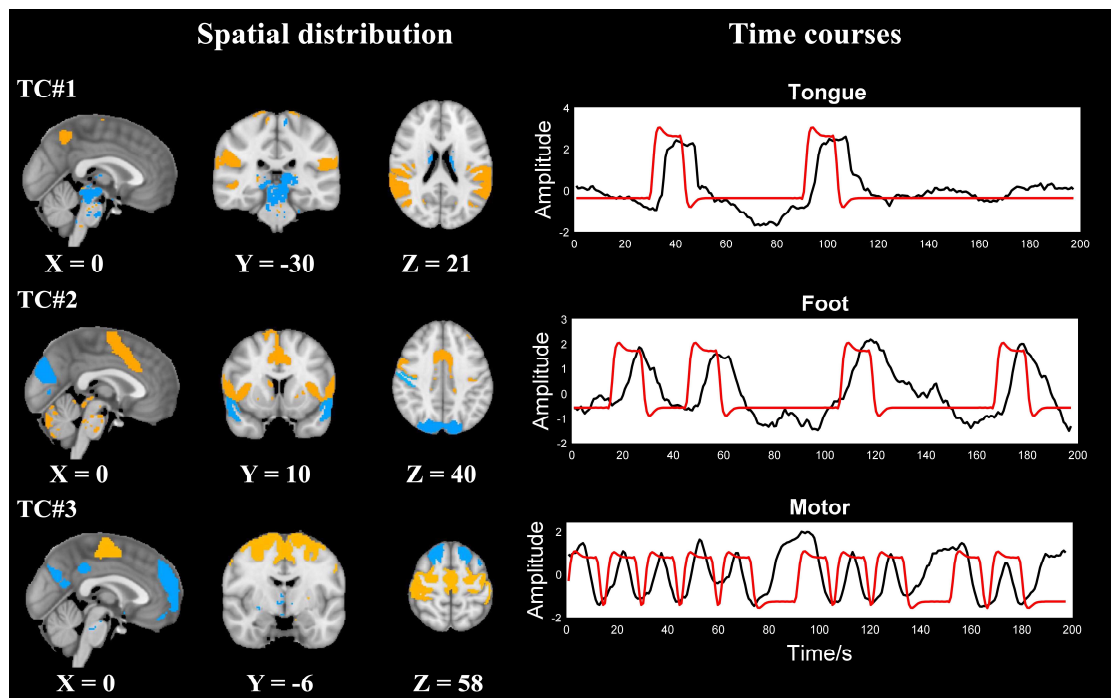
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Figure 4 The spatial distribution (left) and the time courses (right) of estimated components from motor task fMRI (TC: tensor component). In spatial distribution, warm colors represent activation (relative to within-state global average) while cool colors represent deactivation (relative to within-state global average) within each state. In time courses, the black line represents estimated time courses, and the red line represents visual cues after being convolved with hemodynamic response function.

10

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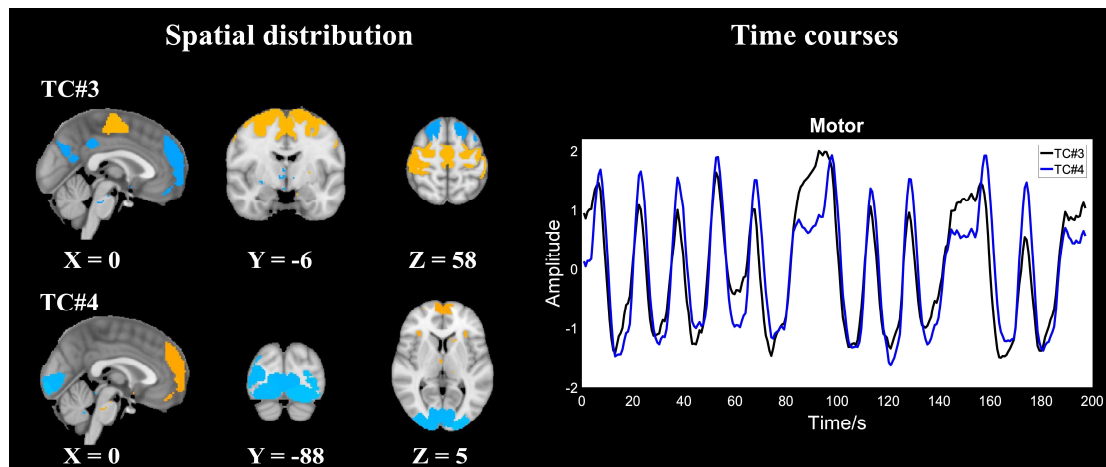
13

1 Motor task fMRI experiment

2 For motor task fMRI data, with the proposed framework, the algorithm stability
3 curve reaches its peak at the model order of 5. Hence, the estimated components at the
4 model order of 5 were further analysis.

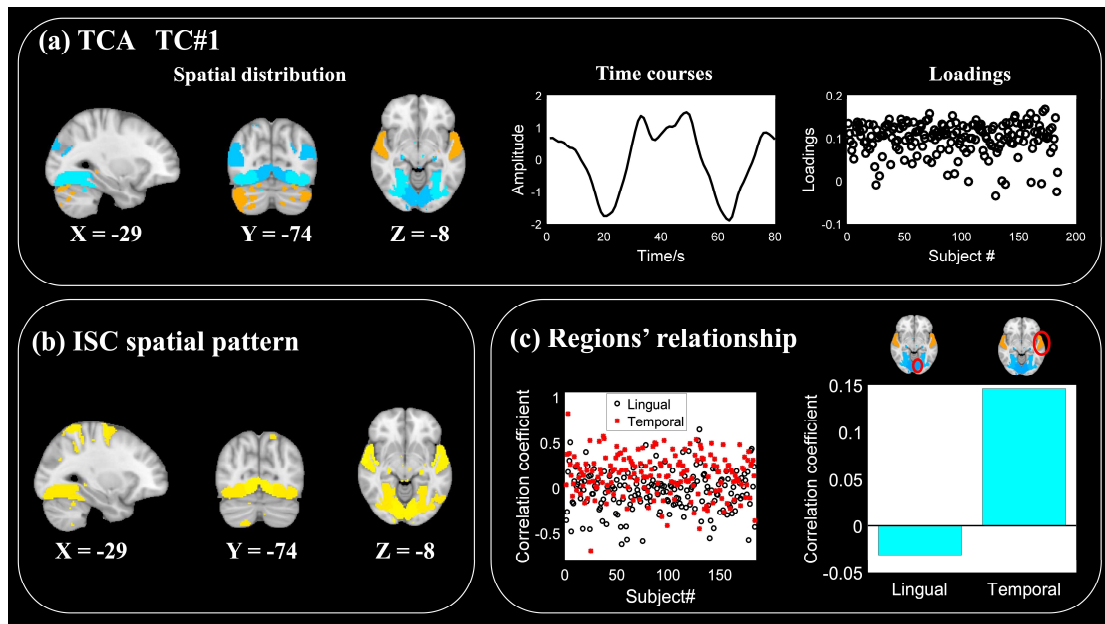
5 The spatial distribution, time courses of the estimated components are
6 demonstrated in Fig. 4. The spatial distribution was also proportional thresholded
7 (10%, Garrison et al. (2015)) and the warm colors represent activation and the cool
8 colors represent deactivation. For each component, after standardization, both
9 stimulus timing and estimated time courses are demonstrated in the same subfigure to
10 identify of the estimated components. In the experiment, the embedded components
11 that correspond to the tongue (TC#1), foot (TC#2) and total movement (TC#3) are
12 successfully estimated. However, the components that corresponding to the hand
13 movement is failed to be detected. For the tensor component that corresponding to the
14 tongue movement (TC#1), the brainstem plays an important role. The postcentral
15 gyrus dominates the movement of foot (TC#2). For total movement tensor component,
16 sensorimotor area is activated (TC#3).

17 Fig. 5 shows the estimated components with similar time course but different
18 spatial distribution. It worth note that, even though the time courses are similar
19 between TC#3 and TC#4, different spatial distribution split them into different
20 components. Compared with TC#4, sensorimotor area is activated in TC#3, while
21 visual area plays more important roles in TC#4. We believe that TC#3 is related to
22 motor decision making and the TC#4 is evoked with stimulus cues.



23

24 *Figure 5 The estimated components with similar time course but different spatial distribution. The TC#3*
25 *corresponding to the motor decision making and the TC#4 represent the brain activity evoked with visual cues.*



1

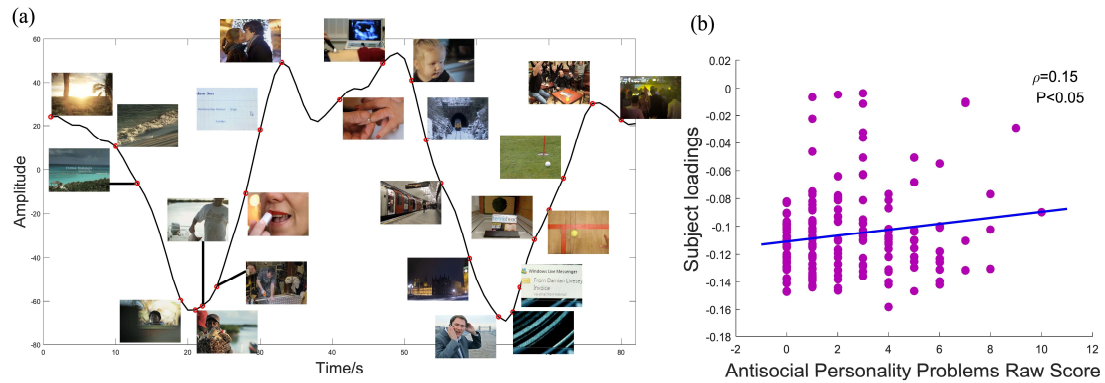
2 *Figure 6 (a) The spatial distribution, the time course, and the subject loadings of the first estimated tensor*
3 *components of naturalistic stimuli fMRI (TC: tensor component). (b) Spatial pattern estimated with ISC. (c) The*
4 *scatter plot (left) shows the correlation coefficient of subject temporal courses of lingual gyrus and temporal gyrus*
5 *with time course estimated with tensor component analysis (TCA). The bar graph (right) shows the average value of*
6 *correlation coefficient.*

7 **Naturalistic stimuli fMRI experiment**

8 For naturalistic stimuli fMRI, the TCA algorithm reaches the highest stability at
9 the model order of 3. The estimated components under the model order are further
10 analyzed.

11 The spatial distribution, time courses and subject loadings of the first tensor
12 component are shown in Fig. 6 (a). Fig. 6 (b) shows the ISC estimated spatial pattern
13 with the same data. Bilateral occipital fusiform gyrus, lingual gyrus and superior
14 temporal gyrus are covered by both TCA component and ISC result. However,
15 bilateral postcentral gyrus and superior parietal lobule and left precentral gyrus are
16 also found in ISC result but not in TCA component. Bilateral cerebellum and lateral
17 occipital cortex only exist in TCA component. Fig. 6 (c) shows the correlation
18 coefficient of subject temporal courses of lingual gyrus and temporal gyrus, which are
19 both covered by TCA component and ISC result, with time course of the first tensor
20 component estimated with tensor component analysis. The bar plot of Fig. 6(c) shows
21 that the time course of lingual gyrus is negative correlated with the estimated time
22 course, but the time course of temporal gyrus is positive correlated with the estimated
23 time course, which demonstrates that under the movie stimuli lingual gyrus and
24 temporal gyrus with opposite activation pattern. TCA component successfully
25 demonstrate it but ISC fails to.

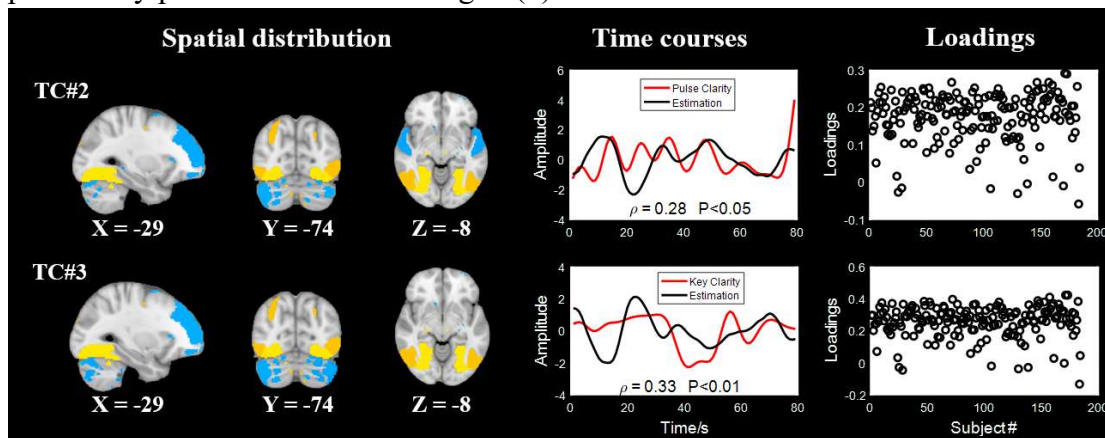
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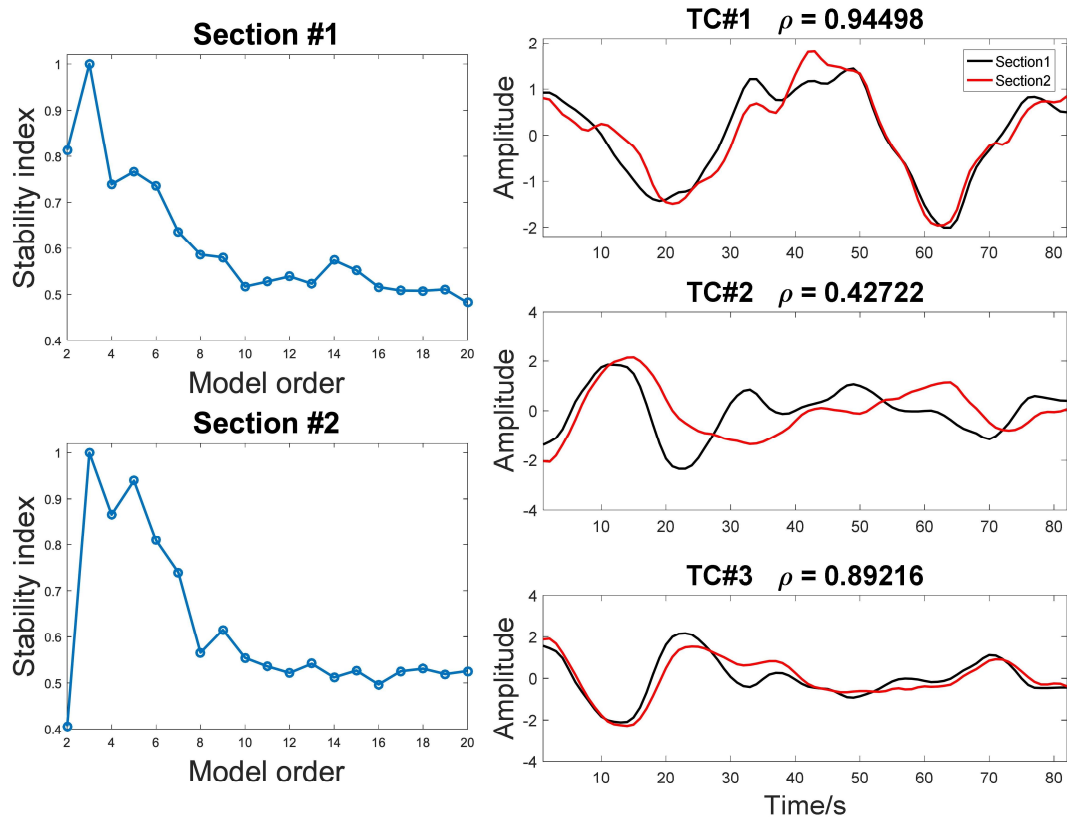
2 *Figure 7 (a) Timeline of the first tensor component and the onset point of each scene. The trends of the timeline with*
 3 *landscape and social related scene are different. (b) The subject loadings of the first tensor component significant*
 4 *(uncorrected) correlated with Antisocial Personality Problems Raw Score (ρ : correlation coefficient).*

5 For the TC#1, the estimated time course and the onset point in the stimuli movie
 6 is matched to show the relationship of them, as shown in Fig. 7 (a). We have a
 7 preliminary feeling that, the landscape scene will lead the curve goes up while the
 8 social related scene will make the curve goes down. Hence, we test the correlation
 9 coefficient between the subject loadings of this component and the social related
 10 behavior data. We found that it is significant correlated with score of antisocial
 11 personality problem as shown in Fig. 7 (b).



12

13 *Figure 8 The second and the third components estimated with tensor component analysis. The red lines in*
 14 *temporal subfigure (medium) show the time course of music features that correlated with estimated time course*
 15 *significantly (ρ : correlation coefficient).*

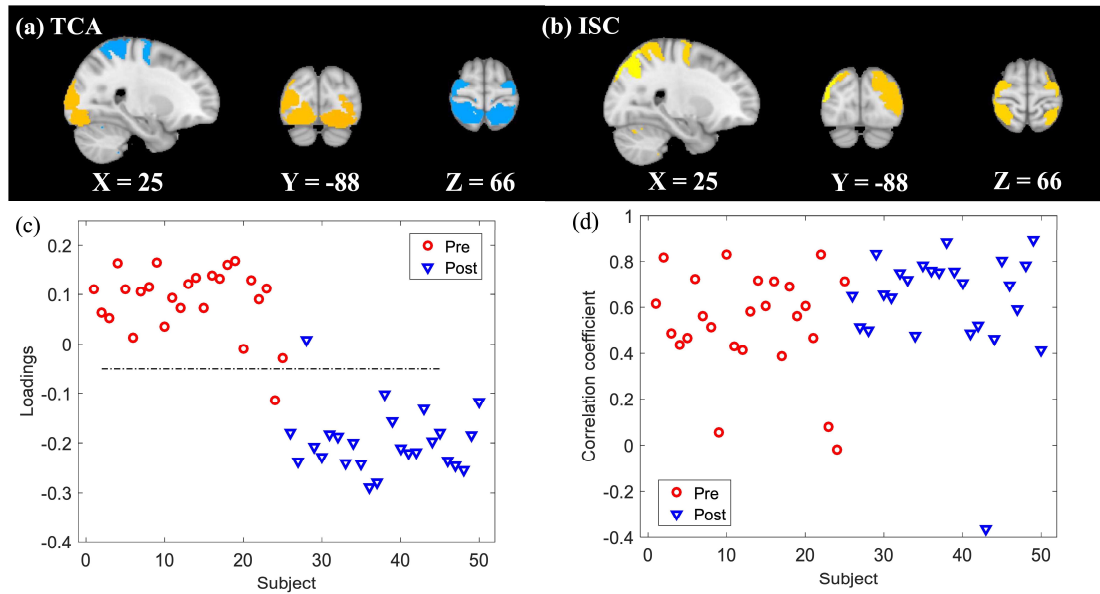


1

2 *Figure 9 Reproducibility of the estimated components. The section#1 and section#2 represent different cohort of*
3 *randomly divided subjects (ρ : correlation coefficient).*

4 Figure 8 shows the second and the third components estimated with tensor
5 component analysis. The red lines in temporal subfigure (medium) show the time
6 course of music features that significantly correlated with estimated time course. The
7 time course of the second tensor component significantly correlated with the music
8 feature Pulse Clarity and the time course of the third tensor component significantly
9 correlated with the music feature Key Clarity. For all three estimated tensor
10 components, bilateral cerebellum, occipital fusiform gyrus, and lateral occipital cortex
11 are involved in. The lingual gyrus is deactivated in the TC#1 but not in TC#2 and
12 TC#3. Different from the TC#1, left frontal pole is deactivated in both TC#2 and
13 TC#3. The bilateral superior temporal gyrus exists in TC#1 and TC#2 but not in
14 TC#3.

15 To test the reproducibility of the estimated component, the subjects were equally
16 divided into two groups. These two groups went through the same TCA framework
17 separately. As shown in Fig. 9, for both group, algorithm reaches the highest
18 algorithm stability at the model order of 3. The right column of Fig. 9 demonstrates
19 the consistency between two decomposition runs. It shows that the TC#1 and TC#3
20 from both cohorts are highly consistent, which means these components are evoked
21 by the stimulus movie. We also observed that the consistency of the corresponding
22 spatial distribution and find that correlation coefficients are also high (not shown in
23 the paper). However, the consistency of the TC#2 of two cohorts is a little bit low.



1
2 *Figure 10 Comparison of TCA and ISC in terms of detection of individual difference. (a) Spatial distribution of the*
3 *first component estimated with TCA. (b) Spatial distribution of ISC estimated consistent map. (c) Subject loadings of*
4 *the first TC exhibit difference of experiment conditions (TC: tensor component). (d) Subjects' score of ISC*
5 *calculated with leave-one out method. The red circles represent loadings of subject of the first version movie stimuli.*
6 *The blue triangles represent loadings of subject of the second version movie stimuli.*

7 We also evaluated the power of the proposed framework in terms of subjects'
8 difference detection. The framework was applied on subjects that went through two
9 with millisecond deviation movie stimuli and view it as two conditions. The results
10 shown that subjects with different conditions are successfully distinguished with the
11 estimated subject loadings, as shown in Fig. 10(c). The subjects at different conditions
12 can be easily distinguished with a threshold value (dash line of Fig. 10(c)). In contrast,
13 even though ISC can also identify spatial distribution (Fig. 10 (b)), which is similar
14 with that of TCA component (Fig. 10(a)), conditions' difference is destroyed by
15 subject correlation (Fig. 10(d)).

16 Discussion

17 In this study, an analysis framework to discover shared spatio-temporal
18 components across subjects from naturalistic stimuli fMRI with TCA was proposed.
19 In the framework, a third-order tensor is constructed from the timeseries extracted from
20 all brain regions from a given parcellation, for all participants, with modes of the tensor
21 corresponding to spatial distribution, time series and participants. TCA will then reveal
22 spatially and temporally shared components, i.e., naturalistic stimuli evoked networks,
23 their temporal courses of activity and subject loadings of each component. The stability
24 of the extracted components is evaluated with a novel clustering method, tensor
25 spectral clustering, to guarantee the reproducibility of the results. Based on the

1 algorithm stability under a range of model orders, the most suitable model order that
2 makes algorithm stable can be recommended. Extensive experiments demonstrate that
3 the framework is feasible, and the interpreted and reproduced components can be
4 extracted.

5 Compared with traditional fMRI study designs, naturalistic stimuli are complex
6 and dynamic, and it is much more difficult to generate a model of evoked activity for
7 analyses. Under the movie stimuli, the timecourses of brain activity across subjects
8 are consistent, which is changing along with movie plots going on. Besides, the
9 specific shared brain network(s) would also be activated for the same kind of
10 information processing. Based on this assumption, a TCA framework that can
11 characterize shared spatio-temporal patterns of evoked activity to naturalistic stimuli
12 across subjects was proposed. fMRI signals have an innate multidimensional property
13 and can be naturally represented in tensor form. Then the tensor can be decomposed
14 with TCA. The estimated components of each mode represent the spatial distribution,
15 time courses and subject loadings, which exhibit participant difference. This work
16 demonstrates that TCA can meet the naturalistic stimuli fMRI's analysis needs and
17 under the proposed framework, the brain activities evoked with naturalistic stimulus
18 were extracted and the patterns that corresponding to different stimuli features is also
19 distinguished (Fig. 6 and Fig. 8).

20 The proposed framework exhibits several merits. Firstly, different from ISC, the
21 proposed framework can estimate subject loadings directly, which can be used to
22 explore participants' difference (Fig. 7(b)) or conditions' difference (Fig. 10).
23 Secondly, the specific brain activities response to features of stimuli can be separated
24 (Fig. 6). Furthermore, the components that with the same time series but different
25 spatial distribution can also be distinguished (Fig. 5). Thirdly, the time courses of
26 estimated components can also be estimated, which facilitate the interpretation of the
27 estimated components. Fourthly, combined with evaluation of algorithm stability,
28 reproducibility of the estimation is promoted (Fig. 9).

29 With the proposed framework, TCA exhibits promising performance. For motor
30 task fMRI, TCA successfully identify networks evoked by tongue, foot and total
31 movement (Fig. 4). Even though the temporal courses are similar between visual
32 stimuli and motor decision, TCA can successfully distinguish them. However, the
33 algorithm fails to identify the components that evoked with hand movement. This
34 may because that hand movement is sophisticated and the variance across subjects
35 makes it difficult to estimate a common spatio-temporal pattern. This also reflects that
36 the proposed framework can only be applied to extract the components that are highly
37 consistent across subjects. More advanced method that can extract misalignment
38 components across participants worth further investigation. Under the naturalistic
39 stimulus, the various across subjects have attracted more and more attention (Finn et
40 al., 2020; Nastase et al., 2019). With the proposed framework, individual difference
41 can successfully be distinguished. Firstly, the component that related to the behavior
42 data Antisocial Personality Problems Raw Score is identified with the proposed

1 framework (Fig.7 (b)). Secondly, TCA successfully identify subjects with millisecond
2 stimuli difference (Fig. 10 (c)). Compared with ISC, TCA can not only distinguish the
3 participants' difference but also the temporal courses of each pattern, which facilitate
4 the interpretation of the estimated pattern. In terms of spatial distribution, TCA can
5 not only estimate the naturalistic stimuli evoked spatial distribution but also the
6 relationship of brain regions that are involved in the same brain network (Fig. 6 (a)
7 and Fig. 6 (b)). This is because ISC only concern about the consistency across
8 subjects but ignore the network spatial configuration.

9 Improving the reproducibility of neuroscience research is one of great concern
10 (Poldrack, 2019; Poldrack and Farah, 2015). To guarantee the stability of the TCA
11 algorithm, a novel spectral clustering algorithm was proposed and applied on the
12 components estimated from multiple runs. In simulation experiment, the model order
13 selected based on algorithm stability is exactly same with the number of consistent
14 components across subject, which demonstrates that with the algorithm stability index
15 appropriate model order can be recommended (Fig. 3(a)). In the naturalistic stimuli
16 fMRI, the results demonstrate that subjects shared spatial-temporal components are
17 reproduced with different individuals (Fig. 9). Actually, we also assessed the
18 test-retest validity of the same subject went through the same naturalistic stimuli.
19 However, the consistency is poor, which may because the neural processing alters
20 with repetitive stimuli.

21 Naturalistic stimuli fMRI is a powerful tool to study brain network interactions
22 during the daily life. Our results demonstrate that with appropriate movie stimuli and
23 our proposed processing framework, the brain activity that significant correlated with
24 Antisocial Personality Problems Raw Score is identified (Fig. 7). This shows the
25 power of the naturalistic stimuli. The subjects with high antisocial score may fake
26 their response when they go through the questionnaire or in abstract stimuli paradigm.
27 However, the brain activity is hard to pretend in the naturalistic stimuli paradigm.
28 Since the movie stimuli applied in this study is not designed for this purpose and the
29 correlation coefficient value (Fig. 7(b)) will not significant after correction, a more
30 suitable movie stimuli to evoke wanted components worth further investigation.
31 Besides, only three shared spatial-temporal components can be estimated in the
32 experiment. Even though naturalistic stimuli contain plenty of features, because of
33 variance of subjects' attention, there are not much brain activities shared across
34 subjects. In the further study, the selection/designation of naturalistic stimuli need pay
35 more attention to.

36 There are some limitations of this study. In this study, brain template comes from
37 ICA with settled dimensionality. Several studies (Allen et al., 2014; Jafri et al., 2008;
38 Pervaiz et al., 2020; Smith et al., 2012) have demonstrate that time course of spatial
39 independent components can identify intrinsic brain networks. The performance of
40 TCA with different templates (Glasser et al., 2016; Janes et al., 2019; Shen et al.,
41 2013) was also compared and ICA template performs best. However, several studies
42 have demonstrated that the model order can greatly impact on the estimated

1 components (Abou-Elseoud et al., 2010; Beckmann, 2012; Kuang et al., 2018). We
2 also tested the back-projection method to get the voxel level spatial distribution.
3 Limited with selected model order, the ICA template is still not pure, which makes the
4 voxel-level spatial distribution hard to be thresholded. Our previous study (Hu et al.,
5 2020) has proposed an effective strategy, Snowball ICA, to address the
6 dimensionality selection issue. In the further study, a more comprehensive template
7 worth being further investigated with Snowball ICA. Even though the paper
8 demonstrate that the proposed framework can distinguish subjects that went through
9 millisecond deviation stimuli, how the framework can be applied on disease diagnosis,
10 coordinate with appropriate naturalistic stimuli, still need further investigation.

11 **Conclusion**

12 The proposed tensor analysis framework is a powerful method that can extract
13 embedded components evoked with naturalistic stimuli. With the proposed framework,
14 meaningful and reproduced tensor components can be extracted and subjects that with
15 different conditions are successfully distinguished. Three experiments (simulation,
16 motor task fMRI, naturalistic stimuli fMRI) demonstrated that the proposed
17 framework is a promising tool to extract brain networks evoked with naturalistic
18 stimuli.

19 **Acknowledgements**

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25 **Appendix: TCA stability analysis with** 26 **tensor spectral clustering**

27 **Background of spectral clustering on graph theory**

28 In this study, a novel tensor spectral clustering algorithm is proposed to evaluate the
29 stability of TCA algorithms. For ease of understanding, background of spectral

1 clustering is demonstrated at here. Spectral clustering is a technique that roots from
 2 graph theory. Consider an undirected weighted graph $G = (V, E)$. V is a set of nodes.
 3 E is a set of edges between nodes. The weighted adjacency matrix of G is denoted as a
 4 symmetric matrix \mathbf{W} . The generalized degree of the vertices of G is defined as $\mathbf{D} =$
 5 $\text{diag}(\mathbf{W}\mathbf{e})$, where \mathbf{e} is an all-ones vector. The combinatorial Laplacian matrix is
 6 defined as $\mathbf{K} = \mathbf{D} - \mathbf{W}$. The *transition matrix* of the graph $\mathbf{P} = \mathbf{W}^T\mathbf{D}^{-1}$ is a column
 7 stochastic matrix. Thus, the matrix could be interpreted as Markov chain. The
 8 stationary distribution of the Markov chain $\pi = \text{diag}(\mathbf{D})$.

9

$$10 \quad \mathbf{P}\text{diag}(\mathbf{D}) = \mathbf{W}^T\mathbf{D}^{-1}\text{diag}(\mathbf{D}) =$$

$$11 \quad \mathbf{W}^T \begin{bmatrix} d_1^{-1} & 0 & 0 & 0 \\ 0 & d_2^{-1} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & d_n^{-1} \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix} = \text{diag}(\mathbf{D}) \quad (\text{A1})$$

12

13 It also means that $\text{diag}(\mathbf{D})$ is an eigenvector of \mathbf{P} and the corresponding eigenvalue is
 14 one (R.Benson et al., 2015).

15 In the partition of a graph, it is assumed that the graph could be separated two parts S
 16 and \bar{S} . Bottleneck of a graph is the boundary of two clusters. The bottleneck ratio of the
 17 set Ψ is defined as:

18

$$19 \quad \Phi(\Psi) = \frac{\text{cut}(\Psi)}{\pi(\Psi)}, \quad (\text{A2})$$

20

21 where $\text{cut}(\Psi) = \sum_{V_i \in \Psi, V_j \in \bar{\Psi}} \mathbf{W}_{ij}$, $\pi(\Psi) = \sum_{V_i \in \Psi} \pi_i$. Small bottleneck ratio indicates
 22 a good partition of the graph (Levin et al., 2007).

23 The indicator vector f over the nodes in G is defined:

24

$$25 \quad f_i = \begin{cases} 0 & V_i \notin \Psi \\ 1 & V_i \in \Psi \end{cases}. \quad (\text{A3})$$

26

27 The property of Laplacian matrix is leveraged as follow:

28

$$29 \quad f^T \mathbf{K} f = \frac{1}{2} \sum_{i,j=1}^n w_{ij} (f_i - f_j)^2$$

$$30 \quad = \sum_{V_i \in \Psi, V_j \in \bar{\Psi}} w_{ij} = \text{cut}(\Psi). \quad (\text{A4})$$

31

32 Since $\pi = \text{diag}(\mathbf{D})$, $\pi(\Psi)$ could be represented as $f^T \mathbf{D} f$. Hence, the objective of
 33 matrix spectral clustering is to find a f to minimize $f^T \mathbf{K} f / f^T \mathbf{D} f$.

1 Both matrices \mathbf{K} and \mathbf{D} are positive definite. According to generalized Rayleigh
2 entropy, the solution is the vector f such that $\mathbf{K}f = \lambda\mathbf{D}f$. We observed that:

$$\begin{aligned} 4 \quad \mathbf{K}f = \lambda\mathbf{D}f &\Leftrightarrow (\mathbf{I} - \mathbf{D}^{-1}\mathbf{W})f = \lambda f \\ 5 \quad &\Leftrightarrow \mathbf{P}^T f = (1 - \lambda)f \end{aligned} \quad (\text{A5})$$

7 So, the problem becomes looking for the eigenvector of \mathbf{P} (Ng et al., 2002).

8 Tensor spectral clustering

9 For multimode tensor spectral clustering, different mode has different *transition*
10 *matrix*. In this appendix, three modes tensor is used as an example for tensor spectral
11 clustering. $\mathbf{P}^{(1)}$, $\mathbf{P}^{(2)}$, $\mathbf{P}^{(3)}$ are three transition matrices for three modes tensor
12 decomposition. They are calculated as follow:

$$14 \quad \mathbf{P}^{(m)} = \mathbf{W}^{(m)T} \mathbf{D}^{(m)-1}, \quad (\text{A6})$$

16 where $\mathbf{D}^{(m)}$ is defined exactly same with matrix spectral clustering. The generalized
17 *transition tensor* $\underline{\mathbf{P}}$ could be defined as:

$$19 \quad \underline{\mathbf{P}} = \underline{\mathbf{I}} \times_1 \mathbf{P}^{(1)} \times_2 \mathbf{P}^{(2)} \times_3 \mathbf{P}^{(3)}, \quad (\text{A7})$$

21 where $\underline{\mathbf{I}} \in \mathbb{R}^{RK \times RK \times RK \times RK}$ is a unit tensor, and the number of modes of $\underline{\mathbf{I}}$ is one more
22 than the number of modes of the tensor to be decomposed.

23 Same to matrix spectral clustering, generalized singular value decomposition (SVD),
24 HOSVD (Lieven et al., 2000), is applied on *transition tensor* $\underline{\mathbf{P}}$. For HOSVD of $\underline{\mathbf{P}}$, the
25 essence of the decomposition of the last mode is eigen value decomposition of
26 covariance matrix of matrix unfolding of tensor $\underline{\mathbf{P}}$ on the last mode. The unfolding of
27 tensor $\underline{\mathbf{P}}$ on the last mode is denoted with $\underline{\mathbf{P}}_{(\text{end})}$, which can be calculated as follow:

$$29 \quad \underline{\mathbf{P}}_{(\text{end})} = \underline{\mathbf{I}}_{(\text{end})} (\mathbf{P}^{(1)} \otimes \mathbf{P}^{(2)} \otimes \mathbf{P}^{(2)})^T. \quad (\text{A8})$$

31 The covariance matrix of $\underline{\mathbf{P}}_{(\text{end})}$ is:

$$\begin{aligned} 33 \quad \underline{\mathbf{P}}_{(\text{end})} \underline{\mathbf{P}}_{(\text{end})}^T &= \underline{\mathbf{I}}_{(\text{end})} (\mathbf{P}^{(1)} \otimes \mathbf{P}^{(2)} \otimes \mathbf{P}^{(3)})^T \\ 34 \quad & \left(\underline{\mathbf{I}}_{(\text{end})} (\mathbf{P}^{(1)} \otimes \mathbf{P}^{(2)} \otimes \mathbf{P}^{(3)})^T \right)^T. \end{aligned} \quad (\text{A9})$$

36 We defined that:

1

$$\mathbf{W}_{\text{TSC}} = \mathbf{W}^{(1)}\mathbf{W}^{(1)} \circledast \mathbf{W}^{(2)}\mathbf{W}^{(2)} \circledast \mathbf{W}^{(3)}\mathbf{W}^{(3)} \quad (\text{A10})$$

$$\mathbf{D}_{\text{TSC}} = \mathbf{D}^{(1)}\mathbf{D}^{(1)} \circledast \mathbf{D}^{(2)}\mathbf{D}^{(2)} \circledast \mathbf{D}^{(3)}\mathbf{D}^{(3)} \quad (\text{A11})$$

$$\mathbf{K}_{\text{TSC}} = \mathbf{D}_{\text{TSC}} - \mathbf{W}_{\text{TSC}} \quad (\text{A12})$$

5

6 \mathbf{W}_{TSC} is a symmetric matrix and represents weighted adjacency matrix of TSC. \mathbf{D}_{TSC}
7 is a diagonal matrix. Both matrices \mathbf{K}_{TSC} and \mathbf{D}_{TSC} are positive definite. Then the
8 equation (A9) could be reduced as:

9

$$\mathbf{P}_{\text{TSC}} = \mathbf{D}_{\text{TSC}}^{-1/2} \mathbf{W}_{\text{TSC}} \mathbf{D}_{\text{TSC}}^{-1/2} = \underline{\mathbf{P}}_{(\text{end})} \underline{\mathbf{P}}_{(\text{end})}^{\text{T}}. \quad (\text{A13})$$

11

12 Same with matrix spectral clustering, the purpose of tensor spectral clustering is to
13 find a f to minimize $f^{\text{T}} \mathbf{K}_{\text{TSC}} f / f^{\text{T}} \mathbf{D}_{\text{TSC}} f$. Based on the generalized Rayleigh
14 entropy and diagonal property of \mathbf{D}_{TSC} , the objective function:

15

$$f^{\text{T}} \mathbf{K}_{\text{TSC}} f / f^{\text{T}} \mathbf{D}_{\text{TSC}} f = f^{\text{T}} (\mathbf{D}_{\text{TSC}} - \mathbf{W}_{\text{TSC}}) f / f^{\text{T}} \mathbf{D}_{\text{TSC}} f \quad (\text{A14})$$

17

18 is equivalent to find a f to minimize $f^{\text{T}} (\mathbf{I} - \mathbf{D}_{\text{TSC}}^{-1/2} \mathbf{W}_{\text{TSC}} \mathbf{D}_{\text{TSC}}^{-1/2}) f = f^{\text{T}} (\mathbf{I} - \mathbf{P}_{\text{TSC}}) f$.

19

20 At this stage, the problem of tensor spectral clustering is reduced to matrix spectral
21 clustering. So, the last mode eigenvector of HOSVD of *transition tensor* $\underline{\mathbf{P}}$ could be
22 used for multimode co-clustering.

22

Given a set of samples that we want to cluster into k subsets, each sample has more
23 than one modality to be considered. The procedure of TSC is as follows:

24

1. Form the weighted adjacency matrices of each modality: $\mathbf{W}^{(1)}, \mathbf{W}^{(2)}, \mathbf{W}^{(3)}, \dots$.

25

2. Define the *transition matrix* of each modality: $\mathbf{P}^{(1)}, \mathbf{P}^{(2)}, \mathbf{P}^{(3)}, \dots$. Then the
26 *transition tensor* $\underline{\mathbf{P}}$ is defined with equation (A7).

27

3. Find the k eigenvectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k$ corresponding to the k largest
28 eigenvalues of the last mode of *transition tensor* $\underline{\mathbf{P}}$ with HOSVD. Form the
29 matrix $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k]$ by concatenating eigenvectors in columns.

30

4. Normalize each row of \mathbf{V} to have unit length $\mathbf{L}_{i,j} = \mathbf{V}_{i,j} / (\sum_j \mathbf{V}_{i,j}^2)^{1/2}$.

31

5. Cluster points, each row of \mathbf{L} , into k clusters via Hierarchical clustering
32 (Gordon, 1987).

33

6. Find the corresponding row i of \mathbf{L} and original sample, assign the original
34 sample to the cluster j that row i assigned.

35

The TSC software is available at

36

https://github.com/GHu-DUT/Tensor_Spectral_Clustering.

37

For the stability analysis of TCA algorithms, for the given dataset, the same
38 algorithm with the same parameters will be run K times. Under the number of
39 extracted components R , for each mode, there are $R \times K$ components. When TSC

1 was applied in the stability analysis of TCA algorithms, the similarity matrices of
2 each mode $\mathbf{W}^{(S)}, \mathbf{W}^{(\sigma)}, \mathbf{W}^{(C)}$ work as weighted adjacency matrices. Furthermore,
3 eigenvector of last mode of *transition tensor* \mathbf{P} would be fed into Hierarchical
4 clustering. The number of clusters is defined as exactly same with the number of
5 extracted components R. The stable component would produce a tight cluster. The
6 stability index is quantified with the average intra-cluster similarities. Ideally, if the
7 extraction of the component is stable, the inner similarity of the corresponding cluster
8 is close to 1. The stability index of unstable components is approach to 0. The
9 algorithm stability is defined as the average of components stability indices. When the
10 selected model order is appropriate to the tensor to be decomposed, the algorithm
11 would also be stable. Hence, the hyperparameter such as model order can be
12 recommended in terms of algorithm stability.

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