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A critique of Tensor Probabilistic Independent Component Analysis: Implications and recommendations for multi-subject fMRI data analysis

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ABSTRACT

Tensor Probabilistic Independent Component Analysis (TPICA) is a popular tool for analyzing multi-subject fMRI data (*voxels* × *time* × *subjects*) because of TPICA's supposed robustness. In this paper, we show that TPICA is not as robust as its authors claim. Specifically, we discuss why TPICA's overall objective is questionable, and we present some flaws related to the iterative nature of the TPICA algorithm. To demonstrate the relevance of these issues, we present a simulation study that compares TPICA versus Parallel Factor Analysis (Parafac) for analyzing simulated multi-subject fMRI data. Our simulation results demonstrate that TPICA produces a systematic bias that increases with the spatial correlation between the true components, and that the quality of the TPICA solution depends on the chosen ICA algorithm and iteration scheme. Thus, TPICA is not robust to small-to-moderate deviations from the model's spatial independence assumption. In contrast, Parafac produces unbiased estimates regardless of the spatial correlation between the true components, and Parafac with orthogonality-constrained voxel maps produces smaller biases than TPICA when the true voxel maps are moderately correlated. As a result, Parafac should be preferred for the analysis multi-subject fMRI data where the underlying components may have spatially overlapping voxel activation patterns.

1. Introduction

Beckmann and Smith (2005) proposed the Tensor Probabilistic Independent Component Analysis (TPICA) model for the analysis of multi-subject functional magnetic resonance imaging (fMRI) data of the form *voxels* × *time* × *subjects*. According to Beckmann and Smith (2005), the TPICA model is a three-way extension of the PICA model (Beckmann and Smith, 2004), analogous to how the Parallel Factor Analysis model (Parafac; Harshman, 1970) is a three-way extension of the standard Principal Component Analysis model (Hotelling, 1933; Pearson, 1901). In their seminal paper, Beckmann and Smith (2005) provide an iterative two-stage algorithm to estimate the TPICA model's parameters, and state that this algorithm will decompose multi-subject fMRI data "into a set of independent spatial maps together with associated time courses *and* estimated subject modes" (p. 295). Furthermore, Beckmann and Smith (2005) state that "[c]ompared to a Parafac decomposition, the [T]PICA estimation shows... an increased robustness against deviation from the model assumptions" (p. 309). Since the introduction of TPICA, numerous studies have used the approach to analyze multi-subject neuroimage data (e.g., Hermans et al., 2011; Ibarretxe-Bilbao et al., 2011; Jeong and Kubicki, 2010; Leech et al., 2011; Lesage et al., 2010; O'Muircheartaigh et al., 2011; Poudel et al., 2010; Sala-Llonch et al., 2010; Sauvage et al., 2011; Wolf et al., 2010).

In this paper, we show that TPICA does not necessarily perform as Beckmann and Smith (2005) claim it does. Specifically, we provide an explicit formulation of Beckmann and Smith's proposed TPICA algorithm, and we point out some fundamental flaws of the approach. The first flaw relates to TPICA's overall objective (i.e., enforcing independence on the estimated voxel maps in trilinear fMRI data), which is only appropriate when the true components have voxel maps with non-overlapping activation patterns. The second flaw relates to the TPICA algorithm's iterative nature, and can be corrected with a simple adjustment to the estimation procedure. To demonstrate the implications of these flaws, we present the results of a simulation study comparing the quality of a TPICA solution versus a Parafac solution when analyzing simulated multi-subject fMRI data. The simulation manipulates the number of active voxels that are shared between the components (as well as the data signal-to-noise ratio), in attempt to examine how varying degrees of spatial correlation (i.e., overlapping voxel activity) between the components affect the quality of the TPICA and Parafac component estimates.

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The remainder of this paper is organized as follows. First, the general ideas of ICA and PICA are presented. Then, the Parafac and TPICA models are presented, highlighting the distinctions between the two models' assumptions. Next, the benefits of Parafac and TPICA for multi-subject fMRI data analysis are compared, and some limitations of TPICA are discussed. We then present a simulation study comparing TPICA and Parafac for the analysis of multi-subject fMRI data. Finally, we discuss the implications of our findings for neuromiage data analysis, as well as the potential of Parafac for the analysis of multi-subject neuromiage data.

2. Theory

2.1. Notation

Scalars will be denoted by lower-case italic Roman letters, vectors by lower-case boldface Roman letters, and matrices by upper-case boldface Roman letters. This rule will be broken when writing generic indices (e.g., $j = 1, \ldots, J$). For a given matrix $\mathbf{A} \equiv \{a_{ij}\}_{I\times J}$, the transpose will be denoted by $\mathbf{A}'$, and the inverse by $\mathbf{A}^{-1}$. The Kronecker product of $\mathbf{A} \equiv \{a_{ij}\}_{I\times J}$ and $\mathbf{B} \equiv \{b_{kl}\}_{K\times L}$ will be denoted using $\otimes$, such as $\mathbf{A} \otimes \mathbf{B} \equiv \{a_{ij}\mathbf{B}\}_{KI\times LJ}$. Similarly, the Khatri-Rao product (i.e., columnwise Kronecker product) of $\mathbf{A} \equiv \{a_{ik}\}_{I\times K}$ and $\mathbf{B} \equiv \{b_{jk}\}_{J\times K}$ will be denoted using $\odot$, such as $\mathbf{A} \odot \mathbf{B} \equiv \{\mathbf{a}_k \otimes \mathbf{b}_k\}_{JI\times K}$, where $\mathbf{a}_k$ and $\mathbf{b}_k$ denote the kth columns of $\mathbf{A}$ and $\mathbf{B}$, respectively. Functions will be denoted using lower-case Greek letters such as ϕ, and a function's first and second derivatives will be denoted using accents of one and two dots, respectively, such as $\dot{\phi}$ and $\ddot{\phi}$. Finally, all scalars, vectors, matrices, and arrays that are assumed to be random variables will be underlined.

2.2. Overview of ICA and PICA

2.2.1. ICA model

Suppose that $\underline{\mathbf{x}} \equiv \{\underline{x}_j\}_{J\times 1}$ is an observable random vector that takes values in $\mathbb{R}^J$ (the set of all real-valued J-dimensional vectors).[1] The ICA model (see Comon, 1994; De Lathauwer et al., 2000) assumes that the *observed signals* $\underline{\mathbf{x}}$ have the form

$$\underline{\mathbf{x}} = \mathbf{M}\underline{\mathbf{a}} + \underline{\mathbf{e}} \tag{1}$$

where $\underline{\mathbf{a}} \equiv \{\underline{a}_f\}_{F\times 1}$ is a vector of latent random variables (referred to as *source signals*) that are assumed to be mutually independent of one another, $\mathbf{M} \equiv \mathbf{SR}$ is the $J \times F$ unobservable *mixing matrix* that linearly transforms (i.e., mixes) the source signals to produce the observed signals, $\mathbf{S} \equiv \{s_{jf}\}_{J\times F}$ is the long (i.e., $J > F$) portion of the mixing matrix related to the covariance structure of $\underline{\mathbf{x}}$, $\mathbf{R} \equiv \{r_{f_1 f_2}\}_{F\times F}$ is an orthogonal rotation matrix, and $\underline{\mathbf{e}} \equiv \{\underline{e}_j\}_{J\times 1}$ is a vector of latent *noise signals*. In addition, it is assumed that (a) at most, one element of $\underline{\mathbf{a}}$ is Gaussian, while the remaining elements are non-Gaussian, (b) $\underline{\mathbf{a}}$ and $\underline{\mathbf{e}}$ are independent of one another, and (c) the variables $\underline{\mathbf{x}}$, $\underline{\mathbf{a}}$, and $\underline{\mathbf{e}}$ each have zero mean vectors and finite covariance matrices. Given realizations of $\underline{\mathbf{x}}$, the goal of ICA is to estimate the mixing matrix and/or the corresponding realizations of the source signals.

Without making any additional assumptions about the distribution of $\underline{\mathbf{e}}$, the decomposition proposed in Eq. (1) is an ill-posed problem, because there is not enough information to distinguish the source signals from the noise signals. However, if the covariance matrix of $\underline{\mathbf{e}}$ is assumed to have the form $\mathrm{E}(\underline{\mathbf{e}}\,\underline{\mathbf{e}}') = t^2\mathbf{T}$ (where E denotes the statistical expectation and $\mathbf{T} \equiv \{t_{j_1 j_2}\}_{J\times J}$ is some positive definite, symmetric matrix), then $\underline{\mathbf{x}}$ can be *prewhitened* to produce a reformulated ICA model with white noise:

$$\underline{\mathbf{x}}_{\mathrm{p}} = \mathbf{S}_{\mathrm{p}}\mathbf{R}\underline{\mathbf{a}} + \underline{\mathbf{e}}_{\mathrm{p}} \tag{2}$$

where $\underline{\mathbf{x}}_{\mathrm{p}} = \mathbf{T}^{-1/2}\underline{\mathbf{x}}$ is the prewhitened observed vector, $\mathbf{S}_{\mathrm{p}} = \mathbf{T}^{-1/2}\mathbf{S}$ is the prewhitened structure portion of the mixing matrix, $\underline{\mathbf{e}}_{\mathrm{p}} \equiv \mathbf{T}^{-1/2}\underline{\mathbf{e}}$ is the prewhitened noise vector, $\mathbf{T}^{-1/2} \equiv \mathbf{VD}^{-1/2}\mathbf{V}'$, and $\mathbf{VDV}'$ is the full-rank eigenvalue decomposition of $\mathbf{T}$. After prewhitening, the covariance matrix of the noise vector has the form $\mathrm{E}(\underline{\mathbf{e}}_{\mathrm{p}}\,\underline{\mathbf{e}}_{\mathrm{p}}') = t^2\mathbf{I}_J$ (where $\mathbf{I}_J$ represents the $J\times J$ identity matrix), and the covariance matrix of $\underline{\mathbf{x}}_{\mathrm{p}}$ has the form $\mathrm{E}(\underline{\mathbf{x}}_{\mathrm{p}}\,\underline{\mathbf{x}}_{\mathrm{p}}') = \mathbf{S}_{\mathrm{p}}\mathbf{S}_{\mathrm{p}}' + t^2\mathbf{I}_J$. This assumes that the elements of $\underline{\mathbf{a}}$ have unit variance, which can be assumed (without loss of generality) because the scales of the source signals and the mixing vectors are undetermined in the ICA model.

For a random data matrix $\underline{\mathbf{X}} \equiv \{\underline{x}_{ij}\}_{I\times J}$ that consists of I samples measured on J random variables, the ICA model can be written as

$$\underline{\mathbf{X}} = \underline{\mathbf{A}}\,\mathbf{R}'\,\mathbf{S}' + \underline{\mathbf{E}} \tag{3}$$

where the rows of $\underline{\mathbf{A}} \equiv \{\underline{a}_{if}\}_{I\times F}$ and $\underline{\mathbf{E}} \equiv \{\underline{e}_{ij}\}_{I\times J}$ contain samples of the random vectors $\underline{\mathbf{a}}$ and $\underline{\mathbf{e}}$ from Eq. (1). Defining the prewhitened data matrix as $\underline{\mathbf{X}}_{\mathrm{p}} \equiv \underline{\mathbf{X}}\mathbf{T}^{-1/2}$, the covariance structure of the prewhitened data matrix is assumed to follow the same form as that of the prewhitened vectors: $\mathrm{E}(I^{-1}\underline{\mathbf{X}}'_{\mathrm{p}}\,\underline{\mathbf{X}}_{\mathrm{p}}) = \mathbf{S}_{\mathrm{p}}\mathbf{S}_{\mathrm{p}}' + t^2\boldsymbol{I}_J$. Letting the singular value decomposition (SVD) of $\underline{\mathbf{X}}_{\mathrm{p}}$ be denoted by $\underline{\mathbf{U}}\mathbf{DV}'$, the covariance matrix of the prewhitened data can be written as $\mathrm{E}(I^{-1}\underline{\mathbf{X}}'_{\mathrm{p}}\,\underline{\mathbf{X}}_{\mathrm{p}}) = I^{-1}\mathbf{VD}^2\mathbf{V}'$. Note that the matrix $\mathbf{V}(I^{-1}\mathbf{D}^2 - t^2\mathbf{I}_J)\mathbf{V}'$ will be equivalent to $\mathbf{S}_{\mathrm{p}}\mathbf{S}_{\mathrm{p}}{}'$ and can be used to determine the source signal subspace (i.e., the range of $\mathbf{S}_{\mathrm{p}}$). Furthermore, assuming that the ICA model is correct, we have that $\mathbf{S}_{\mathrm{p}} = \mathbf{V}_F(I^{-1}\mathbf{D}_F^2 - t^2\mathbf{I}_F)^{1/2}$, where $\mathbf{V}_F$ and $\mathbf{D}_F$ denote the first F singular vectors and values of $\underline{\mathbf{X}}_{\mathrm{p}}$, respectively.

Letting $\underline{\mathbf{U}}_F\,\mathbf{D}_F\mathbf{V}_F'$ denote the rank-F SVD of $\underline{\mathbf{X}}_{\mathrm{p}}$, the prewhitened data can be projected onto the signal subspace and *quasiwhitened*, such as

$$\underline{\mathbf{X}}_{\mathrm{q}} = \underline{\mathbf{A}}\,\mathbf{R}' + \underline{\mathbf{E}}_{\mathrm{q}} \tag{4}$$

where $\underline{\mathbf{X}}_{\mathrm{q}} \equiv \underline{\mathbf{X}}_{\mathrm{p}}\,\mathbf{V}_F(I^{-1}\mathbf{D}_F^2 - t^2\mathbf{I}_F)^{-1/2}$ is the $I \times F$ matrix of quasiwhitened data, and $\underline{\mathbf{E}}_{\mathrm{q}} \equiv \underline{\mathbf{E}}_{\mathrm{p}}\mathbf{V}_F(I^{-1}\mathbf{D}_F^2 - t^2\mathbf{I}_F)^{-1/2}$ is the corresponding error term. Note that we refer to this as *quasi*whitening because the residuals in the quasiwhitened model are no longer whitened: $\mathrm{E}(I^{-1}\underline{\mathbf{X}}'_{\mathrm{q}}\,\underline{\mathbf{X}}_{\mathrm{q}}) = \mathbf{I}_F + t^2(I^{-1}\mathbf{D}_F^2 - t^2\mathbf{I}_F)^{-1}$. So, postmultiplying by $\mathbf{R}$

$$\underline{\mathbf{X}}_{\mathrm{q}}\,\mathbf{R} = \underline{\mathbf{A}} + \underline{\mathbf{E}}_{\mathrm{q}}\,\mathbf{R} \tag{5}$$

we see that the residuals are correlated: define $\underline{\mathbf{Z}} \equiv \underline{\mathbf{X}}_{\mathrm{q}}\mathbf{R}$ and note that $\mathrm{E}(I^{-1}\underline{\mathbf{Z}}'\,\underline{\mathbf{Z}}) = \mathbf{I}_F + t^2\mathbf{R}'(I^{-1}\mathbf{D}_F^2 - t^2\mathbf{I}_F)^{-1}\mathbf{R}$. Thus, the matrix $\underline{\mathbf{Z}}$ is not whitened (or even uncorrelated), and the extent of the correlation between the columns of $\underline{\mathbf{Z}}$ will depend on the magnitudes of the elements of $\mathbf{D}_F^2$ and t^2, which depend on the signal-to-noise ratio (SNR) in the data.

Given realizations of the observed signals, the general goal in ICA is to estimate the mixing matrix. Thus, assuming the quasiwhitened ICA model given in Eq. (4), the goal is to find the orthogonal rotation matrix $\hat{\mathbf{R}}$ such that the source signal estimates

$$\underline{\hat{\mathbf{A}}} = \underline{\mathbf{X}}_{\mathrm{q}}\,\hat{\mathbf{R}} \tag{6}$$

are as independent as possible. See Section 1 of the Supplementary Online Material (SOM) that accompanies this article for descriptions of Hyvärinen's (1999) FastICA algorithm and Cardoso and Souloumiac's (1993, 1996) JADE algorithm.

2.2.2. PICA model

As formulated by Beckmann and Smith (2004), the PICA model has the same form as the ICA model given in Eqs. (1) and (3);

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[1] ICA can also be formulated for complex-valued vectors, but only real-valued vectors will be considered in this paper.