K-Tensors: Clustering Positive Semi-Definite Matrices

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Abstract

This poster introduces a novel **self-consistency clustering algorithm (K-Tensors)** designed for positive-semidefinite matrices based on their **eigenstructures**. As positive semi-definite matrices can be represented as **ellipses or ellipsoids** in $\Re^p$, $p \geq 2$, it is critical to maintain their structural information to perform effective clustering. However, traditional clustering algorithms often vectorize the matrices, resulting in a loss of essential structural information. To address this issue, we propose a clustering algorithm involving the following concepts:

- Projection of Positive Semi-Definite Matrix
- Distance Metric Based on Eigenstructure of Positive Semi-Definite Matrices
- Self-Consistency Clustering Algorithms

This innovative approach to clustering positive semi-definite matrices has broad applications in several domains, including financial and biomedical research, such as analyzing functional connectivity data. By maintaining the structural information of positive semi-definite matrices, our proposed algorithm promises to cluster the positive semi-definite matrices in a more meaningful way, thereby facilitating deeper insights into the underlying data in various applications.

Preliminaries: Self-Consistency and Self-Consistency Algorithm

Hastie and Stuetzle [1989] introduced a self-consistent curve or principal curve to provide a curve summary of the data. Let $\boldsymbol{X} \in \Re^p$ be a random vector with density h and finite second moments assuming $\mathcal{E}(\boldsymbol{X}) = 0$. Let $\mathbf{f}$ denote a smooth C^∞ unit-speed curve in $\Re^p$. the projection index $\lambda_{\mathbf{f}} : \Re^p \to \Re^1$ is defined as:

$$\lambda_{\mathbf{f}}(\mathbf{x}) = \sup_{\lambda} \left\{ \lambda : \|\mathbf{x} - \mathbf{f}(\lambda)\| = \inf_{\mu} \|\mathbf{x} - \mathbf{f}(\mu)\| \right\}.$$

The projection index $\lambda_{\mathbf{f}}(\mathbf{x})$ of $\mathbf{x}$ is the value of λ for which $\mathbf{f}(\lambda)$ is closest to $\mathbf{x}$. Then $\mathbf{f}$ is called self-consistent or principal curve of h if $\mathcal{E}(\mathbf{X}|\lambda_{\mathbf{f}}(\mathbf{X})) = \mathbf{f}(\lambda)$ for a.e. λ.

Tarpey [1999] presented the self-consistency algorithm, which can be viewed as a generalization of the K-means algorithm. Let $\mathcal{S} \subset \Re^p$ be a measurable set and define the *domain of attraction* of a point $\mathbf{y} \in \mathcal{S}$, denoted by $\mathcal{D}_{\mathbf{y}}(\mathcal{S})$:

$$\mathcal{D}_{\mathbf{y}}(\mathcal{S}) := \left\{ \mathbf{x} \in \Re^p : \|\mathbf{x} - \mathbf{y}\| < \|\mathbf{x} - \mathbf{z}\|, \mathbf{z} \in \mathcal{S}, \mathbf{z} \neq \mathbf{y} \right\}.$$

This set represents the *domain of attraction* of $\mathbf{y}$ towards the points in $\mathcal{S}$, containing all the points in $\mathcal{S}$ that is closer to $\mathbf{y}$ than to any other point $\mathbf{z}$ in $\mathcal{S}$.

Preliminaries: Common Principal Components

Flury [1984] proposed the concept of common principal components as an extension to principal components analysis. This approach assumes that n groups share the same principal component axes, This method can be formulated as an optimization problem:

$$\underset{\mathbf{B}}{\text{minimize}} \quad \prod_{i=1}^{n} \left(\frac{\det\left(\operatorname{diag}\left(\mathbf{B}^T \boldsymbol{\Psi}_i \mathbf{B}\right)\right)}{\det\left(\mathbf{B}^T \boldsymbol{\Psi}_i \mathbf{B}\right)} \right)$$

$$\text{subject to} \quad \mathbf{B}^T\mathbf{B} = \mathbf{I},$$

Where $\boldsymbol{\Psi}_i$ is covariance matrix of each subpopulation. Different approaches for estimating the common principal components have been proposed by Flury and Gautschi [1986], Vollgraf and Obermayer [2006], and Hallin et al. [2014]. These methods use maximum likelihood estimation (MLE) and S-estimation to estimate the common principal components from the positive semi-definite matrices.

Some Notation

- $\mathcal{V}_q(\Re^p) = \{\mathcal{X} \in \Re^{p\times q} : \mathcal{X}^T\mathcal{X} = \mathbf{I}_q\}$: the set of all orthonormal q-frames in $\Re^p$
- $\mathbf{S}_+^p = \{\mathcal{X} \in \Re^{p\times p} | \mathcal{X} = \mathcal{X}^T, \mathcal{X} \succeq 0\}$: the set of all positive semi-definite matrices in $\Re^{p\times p}$
- $\mathscr{D}_+^p = \{\mathcal{X} \in \Re^{p\times p} | \mathcal{X} = (\mathbf{a}\mathbf{1}^T) \circ \mathbf{I}_p, \mathbf{a} \in \Re^p, \mathbf{a} \succeq 0\}$ the set of all diagonal matrices in $\Re^{p\times p}$ with only non-negative elements

Here, $\mathbf{I}$ is the identity matrix, $\mathbf{1}$ is the vector with all elements equal to 1, and $\circ$ represents Hadamard product.

Projections, Principal Positive Semi-Definite Tensors, and Principal Positive Semi-Definite Matrices

We assume that there exists a random positive semi-definite matrix $\boldsymbol{\Psi} \in \mathbf{S}_+^p$, with a probability density function denoted by $\mathbf{f}$. Additionally, we consider a p-frame orthonormal matrix $\mathbf{B} \in \mathcal{V}_p(\Re^p)$ in $\Re^p$ and define the projection of the random matrix $\boldsymbol{\Psi}$ onto $\mathbf{B}$ as follows:

$$\mathcal{P}_{\mathbf{B}}(\boldsymbol{\Psi}) = \mathbf{B}\boldsymbol{\Lambda}_{\mathbf{B}}(\boldsymbol{\Psi})\mathbf{B}^T,$$

where $\boldsymbol{\Lambda}_{\mathbf{B}}(\boldsymbol{\Psi}) = (\mathbf{B}^T\boldsymbol{\Psi}\mathbf{B}) \circ \mathbf{I} \in \mathscr{D}_+^p$ is a diagonal matrix that depends on the random matrix $\boldsymbol{\Psi}$, given a fixed $\mathbf{B}$. This projection allows us to determine the proportion of the random positive semi-definite matrix $\boldsymbol{\Psi}$ that can be explained by the orthonormal frame $\mathbf{B}$.

Domain of Attraction to an Orthonormal Basis

Let $\mathcal{A} \subset \mathbf{S}_+^p$ be a subset of all positive semi-definite matrices. We define $\mathcal{D}_{\mathbf{B}}(\mathcal{A})$ the *domain of attraction* of $\mathbf{B}$ with respect to the subset of positive semi-definite matrices $\mathcal{A}$ as follow:

$$\mathcal{D}_{\mathbf{B}}(\mathcal{A}) := \left\{ \boldsymbol{\Psi} \in \mathbf{S}_+^p, : \|\boldsymbol{\Psi} - \mathcal{P}_{\mathbf{B}}(\boldsymbol{\Psi})\|_F^2 \leq \inf_{\mathbf{A}} \|\boldsymbol{\Psi} - \mathcal{P}_{\mathbf{A}}(\boldsymbol{\Psi})\|_F^2, \mathbf{A} \neq \mathbf{B}, \mathbf{A} \in \mathcal{V}_p(\Re^p) \right\},$$

where $\|\cdot\|_F^2$ is the squared Frobenius norm. The *domain of attraction* toward an orthonormal basis matrix $\mathbf{B}$ is defined as the matrices that can be better diagonalized by orthonormal matrix $\mathbf{B}$ compared to any other orthonormal matrix $\mathbf{A}$. $\mathcal{P}_{\mathbf{B}}(\boldsymbol{\Psi})$ is another representation of principal or self-consistent positive semi-definite tensors. We are able to identify the *domain of attraction* of $\mathbf{B}$ by analyzing the differences between $\boldsymbol{\Psi}$ and its corresponding slice on the principal positive semi-definite tensor.

K-Tensors: Algorithm for Clustering Positive Semi-Definite Matrices

Algorithm 1: K-Tensors: Clustering Positive Semi-Definite Matrices

Set i $= 0$.
Start with an initial K partition of the data: $\mathcal{D}_{\mathbf{B}_k^0}(\mathcal{A})$
while $i > 1$ *and* ***Loss***$^i \neq$ ***Loss***$^{i-1}$ **do**
  for $1 \leq k \leq K$ **do**
    estimate common principal components for each group and update $\mathbf{B}_{k^i}$ by

$$\mathbf{B}_{k^i}^* = \sup_{\|\mathbf{B}_k\|_F^2} \left\{ \mathbf{B}_k : \left\|\boldsymbol{\Psi} - \mathcal{P}_{\mathbf{B}_k}(\boldsymbol{\Psi})\right\|_F^2 = \inf_{\mathbf{B}_k} \left\|\boldsymbol{\Psi} - \mathcal{P}_{\mathbf{B}_r}(\boldsymbol{\Psi})\right\|_F^2 \middle| \mathbf{B}_r \in \mathcal{V}_p(\Re^p), \mathbf{B}_k \neq \mathbf{B}_r \right\}$$

    obtain the new assignment for each observation and update $\mathcal{D}_{\mathbf{B}_{k^i}}(\mathcal{A})$ by

$$\mathcal{D}_{\mathbf{B}_{k^i}} = \left\{ \boldsymbol{\Psi} \in \mathbf{S}_+^p, : \left\|\boldsymbol{\Psi} - \mathcal{P}_{\mathbf{B}_k}(\boldsymbol{\Psi})\right\|_F^2 \leq \inf_{\mathbf{B}_r} \left\|\boldsymbol{\Psi} - \mathcal{P}_{\mathbf{B}_r}(\boldsymbol{\Psi})\right\|_F^2, \mathbf{B}_r \neq \mathbf{B}_k, \mathbf{B}_r \in \mathcal{V}_p(\Re^p) \right\}$$

    calculate the loss of this iteration by **Loss**$^i = \sum_{i=1}^n \sum_{k=1}^K \|\boldsymbol{\Psi}_i - \mathcal{P}_{\mathbf{B}_{k^i}^*} \mathbb{I}(i \in k)\|_F^2$
  end
end

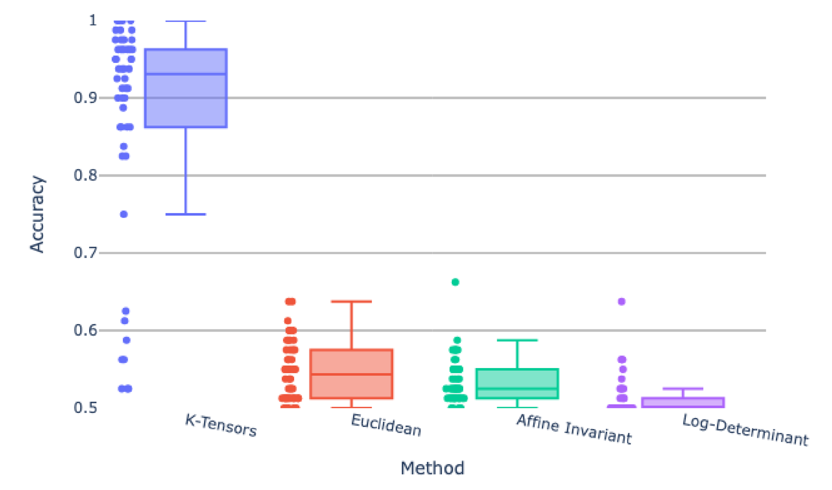
Definition: Principal Semi-Positive Tensors

Define a mapping from a diagonal matrix to a positive semi-definite matrix for a given $\mathbf{B} \in \mathcal{V}_p(\Re^p)$: $\mathcal{U}_{\mathbf{B}}(\boldsymbol{\Lambda}) = \mathbf{B}\boldsymbol{\Lambda}\mathbf{B}^T : \mathscr{D}_+^p \to \mathbf{S}_+^p$. We call $\mathcal{U}_{\mathbf{B}}(\boldsymbol{\Lambda})$ the principal, or self-consistency positive semi-definite tensors of $\mathbf{f}$ if $\mathcal{U}_{\mathbf{B}}(\boldsymbol{\Lambda}) = \mathcal{E}(\boldsymbol{\Psi}|\mathbf{B}(\boldsymbol{\Psi}) = \mathbf{B}, \boldsymbol{\Lambda}(\boldsymbol{\Psi}) = \boldsymbol{\Lambda})$ for a.e. $\boldsymbol{\Lambda}$.

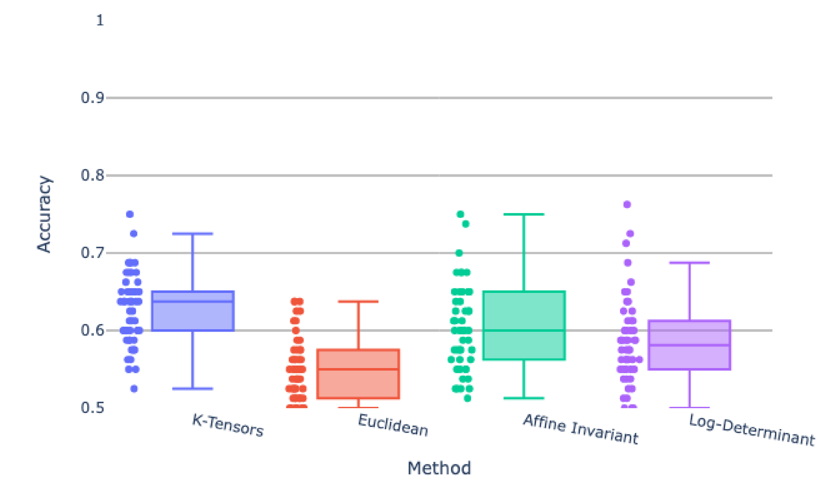
Simulation Studies

We evaluate the performance of our K-tensors algorithm in two simulation settings. In the first setting, we follow the structure proposed in Cook and Forzani [2008], where each functional connectivity matrix $\boldsymbol{\Psi}_i$ is modeled as $\boldsymbol{\Psi}_{i\in C_k} = \mathbf{U}_k\boldsymbol{\Lambda}_i\mathbf{U}_k^T + \mathbf{E}_i$. Here, $\boldsymbol{\Psi}_i$ and $\mathbf{E}_i$ are positive semi-definite matrices, $\boldsymbol{\Lambda}_i$ is a diagonal matrix, and $\mathbf{U}_k$ is an orthonormal matrix representing the latent subpopulations.

In the second simulation setting, we consider the Wishart distribution with degree of freedom from 10 to 45. In both settings, we assume 2 underlying true clusters, with each cluster consisting of 50 observations.



(a) Cook and Forzani [2008] Settings
$\mathcal{E}\|\mathbf{E}_i\|$ from 0.1 to 0.6



(b) Wishart Distribution Settings
df from 10 to 45

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