Functional alignment by the "light" approach of the von Mises-Fisher-Procrustes model

Allineamento funzionale tramite l'approccio "light" del modello von Mises-Fisher-Procrustes

Angela Andreella, and Livio Finos

Abstract Procrustes-based methods involve the singular value decomposition of a square matrix, leading to polynomial time complexity, and requiring a considerable memory for large-scale problems. Procrustes-based methods are used as functional alignment for fMRI data in multi-subjects analysis. A high-dimensional matrix expresses the subject's neural activation, and Procrustes-based methods are infeasible (computationally). The alignment can be conducted only on regions of interest of the brain. We proposed a "light" version of the Procrustes-based methods. A semi-orthogonal transformation reduces the matrices' dimension before applying the Procrustes alignment, maintaining the variability of the matrix that enters in the decomposition step. fMRI application shows a low decrease in predictive performance.
Abstract *I metodi di Procuste prevedono la decomposizione ai valori singolari di matrici quadrate, portando ad una complessità temporale polinomiale e richiedendo una memoria considerevole per problemi su larga scala. I metodi di Procuste sono utilizzati come allineamento funzionale per i dati fMRI nell'analisi multi-soggetto. Una matrice ad alta densità descrive l'attivazione neurale del singolo soggetto. L'allineamento può dunque essere effettuato solo su determinate zone del cervello. Si propone un approccio "light" del metodo di Procuste. Una trasformazione semi-ortogonale riduce la dimensione delle matrici prima di applicare l'allineamento funzionale, mantenendo la variabilità della matrice che entra nella fase della decomposizione ai valori singolari e mantenendo dunque le prestazioni predittive.*

Key words: Procrustes method, von Mises-Fisher-Procrustes model, semi-orthogonal matrix, fMRI data

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1 Introduction

Procrustes methods are common in various fields such as neuroimaging [4]. However, dealing with high-dimensional data is critical since the Procrustes transformation must perform the Singular Value Decomposition (SVD), which is hugely time-consuming and employs a sizeable storing memory.

This paper proposes a "light" approach to Procrustes methods using the thin SVD. The Procrustes transformation is computed in a lower-dimensional manifold extracted by a semi-orthogonal transformation from the thin SVD of the reference matrix used in the Procrustes algorithm. The original fat matrix is reduced to a lower-dimensional square matrix having dimension equals the rank. Procrustes methods are then applied to these lower-dimensional matrices. Finally, the semi-orthogonal transformation's inverse is used on the aligned matrices to project the objects in the original high-dimensional space.

In practice, the "light" approach is useful in functional Magnetic Resonance Imaging (fMRI) data analysis. High-dimensional matrix, e.g., with dimensions $200 \times 200,000$, represents the neural activation of a subject during some stimuli, where the rows represent the time points and the columns the units of the fMRI image, i.e., the voxels. The Procrustes-based functional alignment is applied to perform multi-subjects fMRI data analysis since the matrices' columns are not in correspondence across subjects. It requires the SVD of a large square matrix with dimension equal to the number of voxels, e.g., roughly $200,000$. Since the runtime is inadmissible, fMRI data's functional alignment can be performed only in Region Of Interest (ROI) of the brain, instead of the whole brain [4]. Thanks to the "light" approach, the time complexity becomes equal to $O(n^3)$, where n is the number of time points. It speeds up the ROI analysis and permits the whole-brain analysis.

The paper is organized as follows. Section 2 analyzes the choice of the semi-orthogonal transformation. Section 3 applies the "light" approach to the von Mises-Fisher-Procrustes (vMFP) model proposed in [2]. Finally, the method is applied to fMRI data and evaluated by multi-subjects inference analysis in Section 4. We used the programming language Python, and in particular the `PyMVPA` package [3].

2 Semi-orthogonal transformation

Let $\{X_i \in \mathrm{I\!R}^{\mathrm{n\times m}}\}_{\mathrm{i=1,\dots,N}}$ be a set of rank n matrices, and $M = \sum_{i=1}^{N} X_i/N$. We have N independent observations to be aligned, e.g., subjects, taking values in $\mathrm{I\!R}^{\mathrm{n\times m}}$, where m is the number of variables, e.g., voxels, and n the observations, e.g., time points. The matrices X_i are projected into a lower-dimensional space by a semi-orthogonal transformation [1] defined below.

Definition 1. We call $Q \in \mathrm{I\!R}^{\mathrm{m\times n}}$ a semi-orthogonal matrix if Q is a non-square matrix having orthonormal columns. So, $Q^\top Q = I_n$, it is a partial isometry of the Euclidean space, i.e., rotation or reflection applied from the left.

Instead of the matrices X_i, and M in the Procrustes analysis, we consider the transformations $X_i^\star = X_i Q$, and $M^\star = MQ$, taking values in $\mathbb{R}^{\mathrm{n}\times\mathrm{n}}$. Definition 1 could be rephrased considering the thin SVD with $Q \in \mathbb{R}^{\mathrm{m}\times\mathrm{k}}$, where $k \leq n$. We choose $k = n$ to have a minimal loss of information, and to have unique solutions of the Procrustes-based problem [2, Lemma 1]. The semi-orthogonal matrix Q rotates X_i into a new coordinates system having n uncorrelated dimensions.

The next Theorem is the main result of the paper.

Theorem 1. *Let X_1, X_2 be matrices in $\mathbb{R}^{\mathrm{n}\times\mathrm{m}}$ with rank equals n, $LSQ^\top$ be the thin SVD of X_2, where $Q \in \mathbb{R}^{\mathrm{m}\times\mathrm{n}}$, then:*

$$\mathrm{tr}(X_2^\top X_1) = \mathrm{tr}(Q^\top X_2^\top X_1 Q). \tag{1}$$

Thus, the variability of $X_2^\top X_1$ is also maintained after semi-orthogonal transformation. The “light” approach concentrates the similarity transformation around the first n eigenvectors instead of the full set of data.

3 “Light” von Mises-Fisher-Procrustes model

The vMFP model under the “light” approach is defined as:

$$X_i Q = \alpha_i (MQ + E_i) R_i^{\top\star}, \tag{2}$$

where $E_i \sim \mathscr{MN}_{n,n}(0, \sigma^2 I_n, I_m)$, and $R_i^\star$ distributed as the von Mises-Fisher distribution with location parameter $F^\star \in \mathbb{R}^{\mathrm{n}\times\mathrm{n}}$ and concentration parameter $k \in \mathbb{R}^+$. For further details about the vMFP model’ assumptions, please refers to [2].

W.l.o.g., let $\alpha_i = 1$, and consider the following maximization:

$$\hat{R}_i^\star = \arg\max_{R_i^\star \in \mathscr{O}(n)} \Big\{ -||(X_i Q)^\top - R_i^\star Q^\top M^\top||_F^2 + k\sigma^2 \mathrm{tr}(F^{\top\star} R_i^\star) \Big\}. \tag{3}$$

Following the idea of [2], $R_i^\star$ must combine the columns of $X_i Q$ by exploiting some data prior feature, e.g., spatial closeness. $F^\star$ can be defined as the identity matrix, or by some lower rank approximation of the similarity euclidean distance.

The trace difference between the vMFP model and the “light” one equals $m-n$:

$$\arg\max_{R_i^\star \in \mathscr{O}(n)} (< Q^\top X_i^\top MQ + kF^\star + \frac{m-n}{n} I_n, R_i^\star >_F), \tag{4}$$

since $F^\star$ is a matrix with 1 on the diagonal. The following theorem expresses Theorem 1 in the vMFP model framework.

Theorem 2. *Let consider $X_i, M \in \mathbb{R}^{\mathrm{n}\times\mathrm{m}}$ with rank n, where $i = 1, \ldots, N$, and the thin SVD of M be $LSQ^\top$, where $Q \in \mathbb{R}^{\mathrm{m}\times\mathrm{n}}$, then:*

$$\mathrm{tr}(X_i^\top M + F) = \mathrm{tr}(Q^\top X_i^\top MQ + F^\star + \frac{m-n}{n} I_n). \tag{5}$$

The algorithm presented in [2] must be modified: Q is applied on the data before the functional alignment by the vMFP model decomposing $X_i^{\star\top} M^\star + k^\star F^\star + \frac{m-n}{n} I_n$, instead of $X_i^\top M + k^\star F$, where the term $\frac{m-n}{n} I_n$ enters in the tuning parameter $k\sigma^2$.

4 Functional Magnetic Resonance Imaging data application

Procrustes-based functional alignment methods require the eigendecomposition of a square matrix. In the case of fMRI data, this square matrix has dimensions equals to the number of voxels, i.e., roughly $200,000$. Procrustes-based methods are then unsuitable for aligning the whole brain, it can be applied only on ROIs. In contrast, the "light" version of the vMFP model permits to align the whole subjects' brains and then perform the subsequent analysis on the entire dataset.

The vMFP model and its "light" approach are applied to the *Auditory* data collected by [6]. The neural activations of 18 subjects passively listening to vocal, i.e., speech, and non-vocal sounds are analyzed. The data are preprocessed by a standard procedure using the FMRIB Software Library (FSL) [5]. The prior location matrix is defined as the euclidean similarity distance of the matrix of the voxels' three-dimensional coordinates multiplied by Q.

The aim is to test the group-level activation for each voxel under the null hypothesis of no activation. Let consider the model $\hat{\beta}_{ij} = \mu_j + \varepsilon_{ij}$, where $\hat{\beta}_{ij}$ are the parameter estimates involving brain activation differences under the two stimuli, for each subject i and each voxel $j = 1, \dots, m$, μ_j is the unknown parameter of interest representing the between-subject mean activation, and ε_{ij} are the error terms $\sim (0, \Sigma)$. The one-sample t-test is performed to make inference on μ_j:

$$T_j = \frac{\hat{\mu}_j}{\sqrt{\hat{\sigma}_j{}^2/18}}, \tag{6}$$

where $\hat{\mu}_j = \sum_{i=1}^{18} \hat{\beta}_{ij}/J$ and $\hat{\sigma}_j{}^2 = \sum_{i=1}^{18} (\hat{\beta}_{ij} - \hat{\mu}_j)^2/17$. So, we have m statistical tests, i.e., $H_0^j : \mu_j = 0$, that create a statistical parametric mapping (SPM).

4.1 Region of interest analysis

We perform the group-level activation analysis by considering the Superior Temporal Gyrus (STG) as ROI being responsible for the sensation of sound. The neural activations are expressed by 310×10233 matrices, one for each subject. Figures 1 represent the SPM (6) having data aligned by the vMFP model with and without the "light" approach. The anatomical structure is also maintained if the Q transformation is used. The "light" approach returns a value of $|T_j|$ 46.63% higher than those computed by the original vMFP model, with baseline 50%.

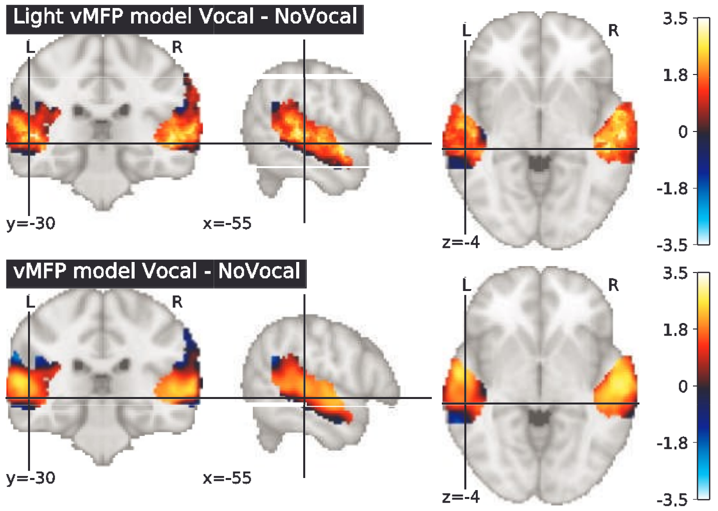

Fig. 1 SPM using STG images aligned by the vMFP model with and without Q transformation.

4.2 Whole-brain analysis

The inferential analysis is performed on the whole brain. The “light” vMFP model is compared with the anatomical alignment, being the only method applicable to the entire brain. Figures 2 show the T_j’s map using data aligned by the vMFP model and the anatomical alignment. The “light” approach returns brain maps with delineated boundaries between positive and negative t-tests preserving the anatomical structure. The functional region of the STG considering the top of Figure 2 seems more blurred than the one calculated using the vMFP model (bottom of Figure 2). The “light” version returns a value of $|T_j|$ 65.67% higher than those returned by the anatomical alignment, with again baseline 50%.

5 Discussion

The “light” version to the vMFP model permits to speed up the computation time in performing the SVD step of the estimation process, and at the same time, permits to apply the functional alignment on high-dimensional data.

The loss of information appears to be negligible in fMRI applications, since the trace of the data does not change if the semi-orthogonal transformation is applied. In the ROI’s analysis, we found a minimal loss of power with respect to the vMFP model [2]. In addition, the alignment using the “light” approach takes approximately 5 minutes while one hour was required to run the original vMFP model. In the whole-brain analysis, the improvement with respect to the anatomical alignment is

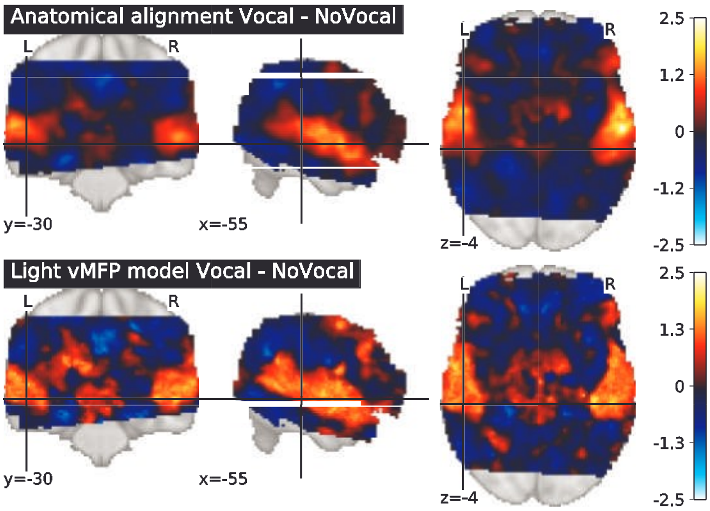

Fig. 2 SPM using brain images aligned by the anatomical alignment and "light" vMFP model.

noticeable, and the computational effort remains affordable (approximately 2 hours on a 1.8 GHz CPU processor with 16 GB of RAM).

The fMRI analysis is focused on understanding the neural activity in ROIs or whole brain. The hypothesis tested in the ROI analysis regards a particular region. In contrast, the whole-brain analysis tests which brain areas show task-related brain activity. Thanks to the "light" approach presented, both analyses can be performed after the functional alignment pre-processing step.

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