

Using Geometry of the Set of Symmetric Positive Semidefinite Matrices to Classify Structural Brain Networks

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Abstract. This paper presents a method of symmetric positive semidefinite (SPSD) matrices classification and its application to the analysis of structural brain networks (connectomes). Structural connectomes are modeled as weighted graphs in which edge weights are proportional to the number of streamline connections between brain regions detected by a tractography algorithm. The construction of structural brain networks does not typically guarantee that their adjacency matrices lie in some topological space with known properties. This makes them differ from functional connectomes - correlation matrices representing co-activation of brain regions, which are usually symmetric positive definite (SPD). Here we propose to transform structural connectomes by taking their normalized Laplacians prior to any analysis, to put them into a space of symmetric positive semidefinite (SPSD) matrices, and apply methods developed for manifold-valued data. The geometry of the SPD matrix manifold is well-known and used in many classification algorithms. Here we expand existing SPD matrix-based algorithms to the SPSPD geometry and develop classification pipelines on SPSPD normalized Laplacians of structural connectomes. We demonstrate the performance of the proposed pipeline on structural brain networks reconstructed from the Alzheimer's Disease Neuroimaging Initiative (ADNI) data.

Keywords: brain networks, Riemannian geometry

1 Introduction

Riemannian geometry offers a powerful approach to process structured data that can be represented by symmetric positive definite (SPD) matrices; these belong to a differentiable manifold, with a corresponding nonlinear structure. Riemannian geometry tools allow us to find geodesics (the shortest differentiable path between two SPD matrices) and calculate its length explicitly to use any distance-based algorithms. Alternatively, SPD matrices may be projected to a tangent space which approximates local structure of the manifold. As this space is Euclidean, projections can be analyzed as usual vectors.

For the last decade, Riemannian-based analytic tools have been used in various medical imaging applications, including DTI-based tensor computing [15] and classifying

brain functional data from electroencephalography (EEG) or functional magnetic resonance imaging (fMRI). EEG covariance matrices are commonly used in brain-computer interface algorithms; these matrices are symmetric positive definite, so methods based on Riemannian geometry can be applied. In EEG-based classification, such methods resulted in state-of-the-art algorithms that outperformed existing benchmarks [1, 2].

Covariance matrices based on fMRI data have attracted particular attention, given the rapid development of connectomics approaches [19]. These matrices can represent macroscale functional brain connectivity (functional connectomes). Recently, several Riemannian geometry-based algorithms have been proposed to classify functional connectomes. Slavakis et al. [18] introduced a novel approach to track time-varying brain connectivity patterns. They used geodesics on a Riemann manifold and tangent spaces of this manifold to cluster their observations, with excellent performance on synthetic data. Ng et al. [14] projected fMRI covariance matrices onto a tangent space of a Riemann manifold of SPD matrices to reduce interrelation of covariance matrix elements; this significantly improved classification accuracy in four task-related fMRI experiments.

Functional activation signals across multiple brain regions may be represented by covariance matrices, allowing us to apply Riemannian geometry to their classification. However, this does not hold for structural connectivity matrices which capture information on anatomical pathways rather than functional interrelations between brain regions. Elements of these matrices represent the number of streamlines between the respective cortical regions estimated using a diffusion-based tractography algorithm. As such, structural connectomes are undirected graphs, and their adjacency matrices are symmetric; importantly as opposed to functional images, they have indefinite connectivity matrices. This difference is crucial for approaches based on Riemannian geometry as by definition these techniques can be used only for symmetric positive definite matrices.

Dodero et al. [6] proposed a method to overcome this limitation. They studied a Riemannian geometry-based algorithm for both functional and structural connectomes. For structural connectomes, they calculated the Laplacians of the original connectivity matrices to obtain symmetric positive semidefinite (SPSD) matrices, and added the identity matrix with a small multiplier to produce SPD matrices and applied the same classification pipeline as for functional connectomes. The experiments on the Autism Spectrum Disorder connectome database demonstrated a classification accuracy of 60.76% and 68% for functional and structural connectomes, respectively.

The Laplacian is a useful transformation for a structural connectivity matrix as it guarantees its positive semi-definiteness. However, Laplacians are not invariant to scaling of the corresponding adjacency matrix, and scaling of structural connectivity matrices is known to affect classification accuracy [16]. Another limitation of Dodero et al.'s method is the regularization of the Laplacians. It serves the purpose of converting SPSPD Laplacians into SPD matrices; but manipulating the Laplacian diagonal elements makes the Laplace operator hard to interpret.

Here, we introduce an approach to overcome the two limitations, scaling and regularization, providing a framework to classify disease in human structural connectivity matrices. First, we use normalized Laplacians to facilitate inter-subject comparability of connectomes to avoid the scaling problem. Second, we introduce a Riemannian met-

ric for SPSPD matrices, a step that allows us to work with network Laplacians directly, without any preliminary regularization.

This paper is organized as follows: Section 2 reviews Riemannian geometry-based methods for classifying SPD matrices. Section 3 introduces the two novel classification algorithms that use the SPSPD normalized Laplacians of the structural matrices. Section 4 demonstrates disease classification results from the structural connectomes derived from the Alzheimer’s Disease Neuroimaging Initiative (ADNI).

2 Notation and elements of Riemannian geometry

Before proceeding to classification approaches, we introduce some notation. We consider a binary classification of SPD matrices, so as input data we have a set of pairs consisting of an input (an SPD matrix) and an output (a class label):

$$\{\mathbf{X}_i, y_i\}, \mathbf{X}_i \in P(n), y_i \in \{0, 1\}, i = 1, \dots, N;$$

where n is the shape of all matrices, $P(n)$ is the space of SPD matrices $\mathbb{R}^{n \times n}$, N is the number of observations.

The set of all SPD matrices - the positive symmetric cone - forms a differentiable manifold \mathcal{M} of $n^* = n(n+1)/2$ dimensions; see [7] for details. Two key requirements for the construction of classification algorithms are the Riemannian distance and a projection of SPD matrices into a Euclidean space.

The Riemannian distance between two SPD matrices is the length of a geodesic curve which is the shortest differentiable path connecting these matrices represented as points on \mathcal{M} . This can be calculated in an explicit way from the following equation

$$\delta_{spd}(\mathbf{X}_i, \mathbf{X}_j) = \left\| \logm \left(\mathbf{X}_i^{-1/2} \mathbf{X}_j \mathbf{X}_i^{-1/2} \right) \right\|_F, \quad (1)$$

where $\logm(\cdot)$ is the matrix logarithm, $\|\cdot\|_F$ is the Frobenius norm.

δ_{spd} takes into account the nonlinear structure of \mathcal{M} and provides a better metric than the usual Euclidean distance between the vectorized upper triangle of the matrices $\mathbf{X}_i, \mathbf{X}_j$ both in terms of theoretical properties as well as the quality of covariance matrices classification [1].

The second useful property of Riemannian geometry is an ability to project SPD matrices on a tangent space which, by definition, approximates the local structure of \mathcal{M} . Let $\tau_{\mathbf{X}}$ be a tangent space of \mathcal{M} at point \mathbf{X} . Then we can project a covariance matrix \mathbf{X}_i onto the tangent plane $\tau_{\mathbf{X}}$ by

$$\tilde{\mathbf{X}}_i = \mathbf{X}^{1/2} \logm(\mathbf{X}^{-1/2} \mathbf{X}_i \mathbf{X}^{-1/2}) \mathbf{X}^{1/2}. \quad (2)$$

3 Classification of SPD matrices

Most SPD matrix-based classification algorithms may be split into two groups:

1. Kernel methods based on a precomputed matrix of pairwise distances between SPD matrices [10, 2, 6].

2. Two-step algorithms, which consist of (1) a projection of all SPD matrices to a tangent space selected appropriately, and (2) a classification of the projected matrices which are vectors now by a linear classification algorithm, such as Linear Discriminant Analysis or Logistic Regression [1, 14, 11].

3.1 Kernel methods

Kernel-based methods are quite popular machine learning methods for connectomics as they can process connectomes as graphs, whereas other methods usually require connectomes to be converted into vectors (i.e., vectors of global graph metrics) [4]. The core idea of kernel-based methods is based on introducing a distance or a distance-like measure between connectomes. For example, a distance based on similarity in structural connectomes partitions into communities was introduced in [13]. Riemannian-based approaches apparently use a metric on \mathcal{M} .

Once the distance $\delta(\mathbf{X}_i, \mathbf{X}_j)$ is selected, the classification algorithm is straightforward. We can build a kernel from a distance by

$$K_{RBF}(\mathbf{X}_i, \mathbf{X}_j) = \exp(-\gamma \delta(\mathbf{X}_i, \mathbf{X}_j)^2), \quad (3)$$

where $\gamma > 0$ is a parameter. As δ is a metric, K_{RBF} is a positive definite kernel [10]. Now we can use a Support Vector Machine [17] to build a classifier based on K_{RBF} .

3.2 Classification in a tangent space

We can now project our SPD matrices to a tangent space $\tau_{\mathbf{X}}$ using (2). As $\tau_{\mathbf{X}}$ is a Euclidean space, any ordinary classification algorithm can be applied to classify the projections. The most essential question is the choice of a reference point \mathbf{X} . It should be close to the training points $\{\mathbf{X}_i, y_i\}_{i=1}^N$ to keep local approximation by $\tau_{\mathbf{X}}$ accurate enough. Usually, the geometric mean of the training points is used as the reference point. An efficient algorithm to compute the mean of a set of SPD matrices was described in [2].

4 The proposed approaches

In this section we consider a binary classification of structural connectome matrices, so as input data we have a set of pairs of input (an adjacency matrix) and output (a class label):

$$\{\mathbf{A}_i, y_i\}, \mathbf{A}_i \in S(n), y_i \in \{0, 1\}, i = 1, \dots, N;$$

where n is the number of nodes in each connectome, $S(n)$ is the space of all symmetric matrices $\mathbb{R}^{n \times n}$, N is the number of observations.

4.1 Converting structural connectomes to SPSD matrices

The first step is to convert a structural connectome to a SPSD matrix; we calculate its normalized Laplacians by:

$$\mathbf{X}_i = \mathbf{D}_i^{-1/2}(\mathbf{D}_i - \mathbf{A}_i)\mathbf{D}_i^{-1/2}, \quad (4)$$

where \mathbf{D}_i is the diagonal matrix of weighted node degrees, $\mathbf{D}_i|_{k,k} = \sum_l \mathbf{A}_i|_{k,l}$.

4.2 Distance for SPSD matrices

Structural connectomes are indefinite matrices, but normalized Laplacians become symmetric positive semidefinite matrices. To use the algorithms in Section 3, we can replace our SPSP matrices by their regularized SPD versions $\mathbf{X}_i + \alpha \mathbf{I}_n$ (α is a small positive number, \mathbf{I}_n is the identity matrix) as in [6].

As an alternative more accurate approach, we propose to use a similarity measure for SPSP matrices of a fixed rank proposed in [3]. This is a generalization of the Riemannian distance δ_{spd} to the SPSP case, and can be computed as follows:

1. Let \mathbf{X}, \mathbf{Z} be two SPSP matrices of rank m ;
2. Find nonzero eigenvalues $\mathbf{S}_x, \mathbf{S}_z$ and corresponding eigenvectors $\mathbf{V}_x, \mathbf{V}_z$ of matrices \mathbf{X} and \mathbf{Z} , respectively. Matrices \mathbf{V}_* have shape n by m ; diagonal matrices \mathbf{S}_* have shape m by m ; $\mathbf{X} = \mathbf{V}_x \mathbf{S}_x \mathbf{V}_x^T$, $\mathbf{Z} = \mathbf{V}_z \mathbf{S}_z \mathbf{V}_z^T$. \mathbf{V}_x and \mathbf{V}_z are matrices that span $range(\mathbf{X})$ and $range(\mathbf{Z})$.
3. Apply Singular Value Decomposition to calculate orthogonal matrices $\mathbf{O}_x, \mathbf{O}_z$ and a diagonal Σ such that $\mathbf{O}_x \Sigma \mathbf{O}_z^T = \mathbf{V}_x^T \mathbf{V}_z^T$.
4. Calculate $\theta_k = \arccos(\sigma_k)$ (where σ_k are diagonal elements of Σ) which are the principal angles between two subspaces defined by \mathbf{V}_x and \mathbf{V}_z .
5. Select the principal vectors as $\mathbf{U}_x = \mathbf{V}_x \mathbf{O}_x$, $\mathbf{U}_z = \mathbf{V}_z \mathbf{O}_z$.
6. Compute the Riemannian distance between the projection of matrices \mathbf{X}, \mathbf{Z} to the common subspace:

$$\delta_{cs}(\mathbf{X}, \mathbf{Z}) = \delta_{spd} \left((\mathbf{U}_x^T \mathbf{X} \mathbf{U}_x)^{1/2}, (\mathbf{U}_z^T \mathbf{Z} \mathbf{U}_z)^{1/2} \right). \quad (5)$$

7. Compute the distance-like measure between matrices \mathbf{X} and \mathbf{Z} :

$$\delta_{spds}^k = (\|\Theta\|^2 + k\delta_{cs}^2)^{0.5}, \quad (6)$$

where $k > 0$ is a parameter and Θ is the vector composed of principal angles θ_k .

k is a parameter of the described family of similarity measures. Theoretical results do not offer recommendations for selecting k , [3], so we investigated this question empirically (Section 5.3).

The measure, δ_{spds} , is not a metric as it does not satisfy the triangle inequality, but it has several useful properties and a vivid geometric interpretation. Considering our SPSP matrices $\mathbf{X}_i, \mathbf{X}_j$ as flat ellipsoids in R^n , we can decompose $\delta_{spds}(\mathbf{X}_i, \mathbf{X}_j)$ into two parts: $\|\Theta\|$, a distance between the subspaces in which the ellipsoids are contained and δ_{cs} , the Riemannian distance between the ellipsoids within a common subspace of SPD matrices $P(m)$. For more detailed explanations see [3, Section 5].

4.3 Algorithm for Kernel SVM based on δ_{spds}

A generalization of kernel-based approaches is straightforward:

1. Calculate matrix of pairwise ‘distances’ δ_{spds} using (6).
2. Use (3) to calculate the RBF kernel.
3. Build an SVM model using the defined kernel.
4. Kernel width γ and δ_{spds} weight k are two hyper-parameters of the algorithm which should be selected using a nested cross-validation procedure.

4.4 Algorithm for dimensionality reduction based classification

An adaptation of tangent space-based methods to the SPSD case is more complex as we cannot build a tangent space at the matrices' geometric mean. To avoid this limitation, we apply Isomap, a nonlinear dimensionality reduction algorithm [21]. The algorithm is based on the idea of geodesic distances on a manifold. To find such distances, it builds a neighborhood graph internally and then computes the shortest path between two nodes which can be considered as a good approximation of the geodesic distance. Then it applies classical multidimensional scaling [12] to find a low-dimensional embedding which preserves the matrix of pairwise geodesic distances.

The original Isomap algorithm works with Euclidian space and uses L2 distance to build neighborhood graph, but we can also use other distances. In particular, the Riemannian distance between EEG covariance SPD matrices was used in conjunction with Isomap in [11]. We propose δ_{psd} as a distance-like measure which can replace L2 in the case of the SPSD matrices space. The algorithm is as follows

1. Calculate matrix of pairwise 'distances' δ_{psd} using (6).
2. Find a d -dimensional embedding using Isomap algorithm based on the precomputed matrix of pairwise 'distances'. This step converts our initials set of SPSD matrices into a set of Euclidean vectors.
3. Apply a standard classification method. In our experiments we used logistic regression with L2 penalty and regularization coefficient λ .
4. The dimensionality d and regularization coefficient λ are two hyper-parameters of the algorithm which should be selected using a nested cross-validation procedure.

5 Experiments

To evaluate the proposed methods we conducted computational experiments using ADNI, one of the largest public neuroimaging database. We estimated quality of phenotypes classification and compare the proposed approaches with two baseline methods as well as investigated the effect of multiplier k which determine the impact each of the two terms of the similarity measure (6).

5.1 Data

We used the ADNI2 database, consisting of 228 individuals (748 scans; mean age at baseline visit 72.9 ± 7.4 y, 96 women). The ADNI2 cohort subdivides people into participants with Alzheimers disease (AD), mild cognitive impairment, and normal controls (NC), including 47 people (135 scans) with AD, 40 (145 scans) NC, and 80 (278) individuals with late-stage and early-stage MCI (LMCI/EMCI), and 61 (190) NC.

T1-weighted (T1w) images were processed with FreeSurfer [8], where we used cortical parcellation based on the Desikan-Killiany atlas [5] of 68 cortical brain regions. In parallel, the average b_0 of the DWI images was registered to the downsampled (2mm isotropic MNI) T1w image, to account for susceptibility artifacts. DWI images were corrected for eddy current and motion related distortions; b-vectors were rotated accordingly. Probabilistic streamline tractography was performed using the Dipy [9]

LocalTracking module with constrained spherical deconvolution (CSD) [20]. Streamlines longer than 5mm with both ends intersecting the cortical surface were retained. Edge weights in the original cortical connectivity matrices were thus proportional to the number of streamlines detected by the algorithm.

5.2 Setup of experiments

We compared four methods:

1. As the simplest baseline method, we used kernel SVM with L_2 distance between matrices \mathbf{A}_i and the RBF kernel (3).
2. Kernel-based approach proposed by Dodero et al. We calculated connectomes Laplacians, then added the identity matrix with coefficient $1e-3$ (the algorithm is robust to selection of this coefficients as suggested by Dodero et al.) and calculated the log-Euclidean distances between the obtained SPD matrices. For details, see [6].
3. RBF Kernel-SVM based on the δ_{spad}^k similarity measure for a set of k values, see section 4.3.
4. Dimensionality reduction for SPSP matrices combined with the L_2 -penalized Logistic Regression classifier in the reduced space, see section 4.4.

For Kernel-based methods, we used a logarithmic grid of α parameters in (3) and varied SVM regularization parameter. For Isomap algorithm we varied the reduced dimensionality d from 2 to 10. For Logistic regression, we used a logarithmic grid of regularization parameters λ . Parameters for all algorithms were selected using group 10-fold cross-validation (we use group K -fold approach to ensure that all scans from a single subjects belongs to a single fold). For the best set of parameters we repeated 10-fold cross-validation with 10 new partitioning of the data to evaluate the performance.

5.3 Results

Table 1 contains all results of our computational experiments. The obtained quality of classification suggests that for the AD versus NC classification problem both the proposed approaches outperform baseline methods whereas the method from Dodero et al [6] shows better performance than the simple approach which ignores the matrix structure of connectomes completely.

Task	Isomap: SPSP	Kernel SVM: SPSP	Kernel SVM: reg. SPD	Kernel SVM: L_2
AD vs NC	0.816 ± 0.006	0.816 ± 0.007	0.800 ± 0.005	0.772 ± 0.010
AD vs LMCI	0.678 ± 0.006	0.686 ± 0.014	0.688 ± 0.015	0.655 ± 0.016
LMCI vs EMCI	0.341 ± 0.059	0.441 ± 0.022	0.478 ± 0.024	0.447 ± 0.029
EMCI vs NC	0.538 ± 0.012	0.571 ± 0.015	0.539 ± 0.016	0.504 ± 0.018

Table 1: Quality of the compared methods on the 4 binary classification problems. Quality was measured as the area under ROC curve estimated by ten repeats of Group 10-fold cross-validation.

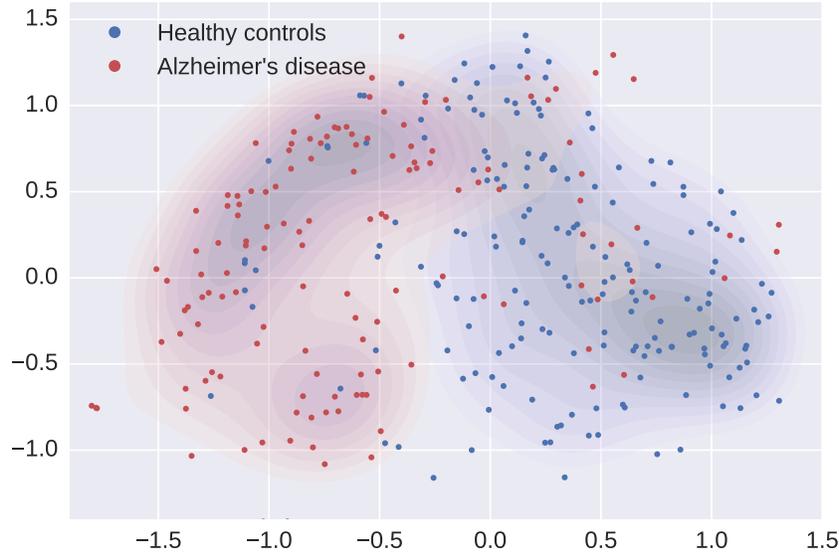


Fig. 1: Structural connectomes for all AD and NC individuals projected to the plane. Blue and red colors depict NC and AD cohorts, respectively. The dots depict MRI scans, the transparent areas depict kernel density estimation for each group

As an additional evaluation of the proposed SPSPD-based dimensionality reduction based approach, we use it to project our data into a 2-dimensional space. **Figure 1** shows the projections of the input matrices for all AD and NC individuals; even 2-D representation is quite informative.

As we mentioned in section 4.2, we need to study the effect of parameter k empirically. **Figure 2** shows the dependency of AD versus NC classification problem quality as a function of k . Notably, the curves are smooth in general, so we can assume that the proposed methods are robust to small variations of the parameter. Interestingly, the optimal values of parameter k are different for the SVM-based method and the dimensionality reduction based one. We assume that the further investigations of this effect are needed.

6 Conclusions

We demonstrated how the powerful framework of Riemannian geometry can be generalized for the analysis and classification of positive semi-definite matrices. We assured positive semi-definiteness of the connectivity matrices of human structural brain networks by taking their normalized Laplacians. We showed that the proposed pipeline outperforms the baselines on the Alzheimers Disease Neuroimaging Initiative dataset which was selected as one of the largest publicly available set of neuroimaging data.

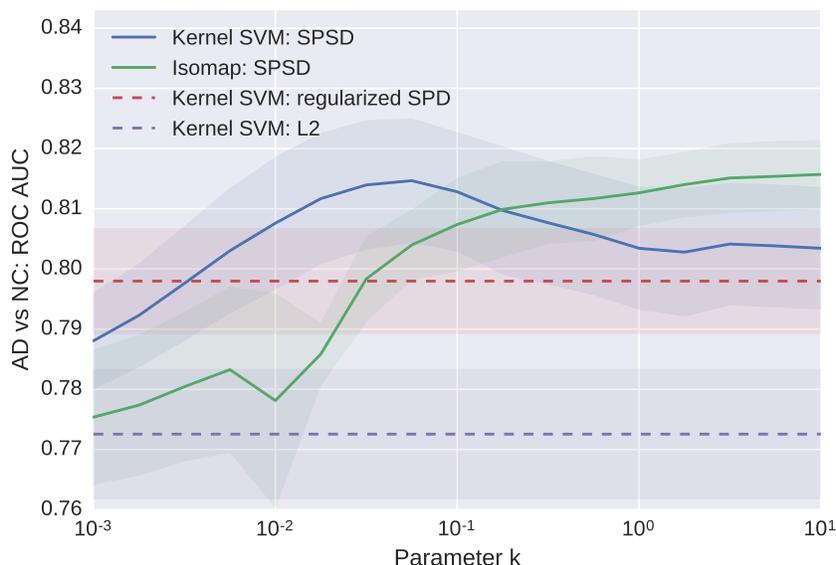


Fig. 2: Quality of classification as a function of similarity measure parameter k . 4 lines depict the mean value of the area under ROC curve estimated by Group 10-fold cross-validation. Transparent areas depicts standard deviation.

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