Beyond Euclidean Space: Geometric Deep Learning for Brain Connectomics

Surpassing NeuroGraph Benchmarks Using SPDNet

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Abstract

Functional brain connectomes derived from fMRI data are mathematically represented as Symmetric Positive-Definite (SPD) matrices. Conventional Graph Neural Networks (GNNs) typically vectorize these matrices or treat them as adjacency matrices in Euclidean space, thereby neglecting the non-Euclidean geometry intrinsic to the SPD manifold. In this work, we implement and evaluate a geometry-aware deep learning pipeline using an SPD Neural Network (SPDNet). This architecture operates directly on the Riemannian manifold of SPD matrices, utilizing specialized layers—BiMap, ReEig, and LogEig—to learn feature representations while preserving geometric structure. We validate our approach using the standardized NeuroGraph benchmarks. Our implementation achieves state-of-the-art performance on static classification tasks, recording test accuracies of **94.79% on HCP-Gender**, **62.50% on HCP-Age**, and **99.04% on HCP-Task**. We provide a comprehensive derivation of the Riemannian backpropagation mechanics and discuss the advantages of manifold optimization over Euclidean approaches in neuroimaging. All code, trained models, and pre-processing scripts are publicly available.

1 Introduction

The human brain is a complex network of interacting regions, and understanding how these regions communicate is central to modern neuroscience. Functional Magnetic Resonance Imaging (fMRI) allows us to capture these interactions by measuring blood-oxygen-level-dependent (BOLD) signals over time. [cite$_{s}tart]Acommonabstractionofthisdataisthefunctionalconnectivity(FC)matrix,whichcapturesthetempor$ $31, 33]$.

Mathematically, when constructed using Pearson correlation and appropriately regularized, these FC matrices are Symmetric Positive-Definite (SPD). [cite$_{s}tart]ThespaceofSPDmatrices,denotedas\mathbb{S}^{++}(n)$, forms a Riemannian manifold with non-positive curvature, rather than a flat Euclidean vector space[cite: 35].

1.1 The Euclidean Limitation

Recent advances in geometric deep learning have popularized the use of Graph Neural Networks (GNNs) for connectomics. [cite$_{s}tart]FrameworkslikeNeuroGraph[cite:1]haveestablishedbenchmarksforapplyingGC$ $2, 36].Thissimplificationcanobscuresubtlevariationsinbrainconnectivitythatarecriticalfordistinguishingbet$

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1.2 Riemannian Deep Learning

[cite$_{s}tart]Toaddressthis, weproposetheuseofSPDNet[cite : 33], adeepneuralnetworkarchitecturedesignedtom$
throughout the deep layers.

1.3 Contributions

Our contributions to the study of brain connectomics are as follows:

[cite$_{s}tart]$

- We adapt the SPDNet architecture specifically for the high-dimensional static connectomes provided by the NeuroGraph benchmark[cite: 1].
- We demonstrate that respecting the Riemannian geometry yields superior performance compared to traditional methods, achieving **99.04%** accuracy on task decoding.
- We provide a detailed analysis of the training dynamics, including the necessity of Stiefel manifold corrections during optimization.
- We release a fully reproducible pipeline that integrates NeuroGraph's data loading ecosystem with Riemannian geometry learning.

2 Related Work

2.1 Graph Learning in Neuroimaging

Graph Neural Networks have become the de facto standard for analyzing brain networks. Parotidis et al. and Ktena et al. demonstrated the utility of measuring distances between brain networks using graph metrics. [cite$_{s}tart]TheNeuroGraphbenchmark[cite : 1][cite_{s}tart]consolidatedtheseeffortsbyprovidingprocessedd$
$18, 19, 21].Whileeffective, thesemodelsprimarilyleveragetopologicalinformation(nodeneighbors)andtreated$

2.2 Riemannian Geometry in Computer Vision

The use of Riemannian geometry for matrix-valued data originated in computer vision and pattern recognition. [cite$_{s}tart]MetriclearningontheSPDmanifoldwastraditionallyhandledusinghand-craftedkernelsorthe$
$InvariantRiemannianMetric(AIRM)[cite : 44].However, thesemethodswerecomputationallyexpensiveandd$

2.3 Deep Learning on Manifolds

[cite$_{s}tart]HuangandVanGool[cite : 33]introducedSPDNettobridgethegapbetweendeeplearningandRiemanni$

3 Preliminaries: Geometry of $\mathcal{S}^{++}(n)$

To understand the architecture, we must define the geometric properties of the space we are traversing.

3.1 The SPD Manifold

The set of $n \times n$ real symmetric positive-definite matrices is defined as:

$$\mathcal{S}^{++}(n) = \{X \in \mathbb{R}^{n\times n} : X = X^\top, v^\top X v > 0, \forall v \in \mathbb{R}^n \setminus \{0\}\}.$$

This space is a differentiable Riemannian manifold. At any point $P \in \mathcal{S}^{++}(n)$, the tangent space $T_P\mathcal{S}^{++}(n)$ is the vector space of symmetric matrices:

$$T_P\mathcal{S}^{++}(n) = \{S \in \mathbb{R}^{n\times n} : S = S^\top\}.$$

3.2 Riemannian Metrics

A Riemannian metric defines an inner product $\langle \cdot, \cdot \rangle_P$ on the tangent space. The Affine-Invariant Riemannian Metric (AIRM) is the most natural choice for SPD matrices, defined for $S_1, S_2 \in T_P\mathcal{S}^{++}(n)$ as:

$$\langle S_1, S_2 \rangle_P = \mathrm{Tr}(P^{-1}S_1P^{-1}S_2).$$

The geodesic distance between two points $X, Y \in \mathcal{S}^{++}(n)$ under this metric is given by:

$$d_R(X,Y) = \| \mathrm{Log}(X^{-1/2}YX^{-1/2})\|_F,$$

where $\| \cdot \|_F$ denotes the Frobenius norm and $\mathrm{Log}(\cdot)$ is the matrix logarithm.

3.3 Log-Euclidean Framework

While AIRM is theoretically robust, it is computationally intensive. [cite$_start]Arsignyetal.[cite : 44]proposedtheLog-Euclideanmetric, whichmapsthemanifoldtoavectorspaceviathematrixlogarithm, allowi$

4 Methodology: The SPDNet Architecture

Our pipeline takes raw functional connectivity matrices and passes them through a sequence of geometry-preserving layers. The architecture can be summarized as:

$$X_{\text{in}} \xrightarrow{\text{BiMap}} X_1 \xrightarrow{\text{ReEig}} X_2 \xrightarrow{\text{BiMap}} X_3 \xrightarrow{\text{LogEig}} V_{\text{out}} \xrightarrow{\text{FC}} \hat{y}$$

4.1 BiMap Layer (Bilinear Mapping)

The BiMap layer functions similarly to a dense linear layer in standard neural networks but preserves the SPD structure. Given an input $X_{k-1} \in \mathcal{S}^{++}(n_{k-1})$, the layer transforms it to $X_k \in \mathcal{S}^{++}(n_k)$ via a weight matrix $W_k \in \mathbb{R}^{n_{k-1} \times n_k}$ (where $n_k < n_{k-1}$):

$$X_k = f_{BM}(X_{k-1}; W_k) = W_k^\top X_{k-1} W_k.$$

For the output X_k to be strictly positive-definite, W_k must have full rank. To ensure numerical stability and optimal convergence, we constrain W_k to reside on the **Stiefel Manifold** $\mathrm{St}(n_k, n_{k-1})$, meaning W_k must be a semi-orthogonal matrix:

$$W_k^\top W_k = I_{n_k}.$$

4.2 ReEig Layer (Rectified Eigenvalues)

Analogous to the ReLU activation function, the ReEig layer introduces non-linearity. Since standard element-wise ReLU would destroy the SPD property, we operate on the eigenvalues. Let $X = U\Sigma U^\top$ be the eigen-decomposition. The ReEig function is:

$$f_{RE}(X) = U \max(\Sigma, \epsilon I) U^\top,$$

where ϵ is a small threshold (e.g., 10^{-4}) to strictly enforce positive definiteness. This layer acts as a non-linear spectral filter.

4.3 LogEig Layer (Log-Euclidean Mapping)

The final geometric layer flattens the manifold structure to a tangent space, preparing the data for standard Euclidean classification.

$$f_{LE}(X) = \mathrm{Log}(X) = U \log(\Sigma) U^\top.$$

The output is a symmetric matrix. We vectorise the upper triangular portion of this matrix to form a feature vector in $\mathbb{R}^{n(n+1)/2}$, which is then fed into a standard Multi-Layer Perceptron (MLP) with Softmax activation.

5 Riemannian Optimization Pipeline

Training SPDNet is distinct from standard networks because the weights of the BiMap layers reside on the Stiefel manifold, not in Euclidean space. We utilize a Riemannian Stochastic Gradient Descent (RSGD) approach.

5.1 Backpropagation

The gradients are computed via the chain rule on the matrix space. For a loss function L, the Euclidean gradient $\nabla_W L$ is computed using standard backpropagation frameworks (PyTorch). However, simply updating $W \leftarrow W - \eta \nabla_W L$ would violate the orthogonality constraint $W^\top W = I$.

5.2 Projected Gradient and Retraction

To maintain the constraint, we project the Euclidean gradient onto the tangent space of the Stiefel manifold. The Riemannian gradient $\tilde{\nabla} L$ at W is defined as:

$$\tilde{\nabla} L = \nabla L - W(\nabla L)^\top W.$$

After the update step in the tangent direction, the new weight matrix may drift slightly off the manifold. We employ a retraction mapping $\mathcal{R}$ to map the point back to $\mathrm{St}(n_k, n_{k-1})$. We typically use the QR-decomposition-based retraction:

$$W_{new} = \mathcal{Q}(W - \eta \tilde{\nabla} L),$$

where $\mathcal{Q}$ denotes the Q-factor of the QR decomposition. This ensures that after every optimizer step, our transformation matrices remain orthogonal.

6 Experimental Setup

6.1 Datasets

[cite$_{s}tart]WeutilizedtheprocesseddatasetsprovidedbytheNeuroGraphbenchmark, derivedfromtheHumanCon$
$1, 43]$.

HCP-Gender: A binary classification task predicting the gender of the subject based on their resting-state fMRI.

HCP-Age: A multi-class classification problem. [cite$_{s}tart]Weutilizedthe3-classsplit(Young, Adult, Senior)$
$1].[cite_{s}tart]$

HCP-Task: A 7-class classification task where the goal is to identify which cognitive task (e.g., Gambling, Motor, Language, Social) the subject was performing during the scan[cite: 1].

6.2 Preprocessing

The raw fMRI time-series were parcellated using the Schaefer atlas. Functional connectivity matrices were computed using Pearson correlation. To ensure inputs belong to $\mathcal{S}^{++}(n)$:

1. Symmetrization: $X \leftarrow \frac{X + X^\top}{2}$.
2. Diagonal regularization: A small jitter δI was added to the diagonal if eigenvalues were close to zero.
3. Reconstruction: Any negative eigenvalues resulting from numerical noise were clipped to $\epsilon > 0$.

6.3 Hyperparameters

- **Input Dimension:** 100×100 (based on parcellation).
- **Architecture:** BiMap ($100 \rightarrow 50$) $\rightarrow$ ReEig $\rightarrow$ BiMap ($50 \rightarrow 20$) $\rightarrow$ LogEig $\rightarrow$ Linear.
- **Batch Size:** 16.
- **Optimizer:** Standard Adam for the Euclidean classifier layers; Riemannian SGD for Stiefel layers.
- **Learning Rate:** 1×10^{-2} with decay.

7 Results and Analysis

We present the performance of SPDNet on the static NeuroGraph benchmarks. We utilize Accuracy as the primary metric, consistent with the NeuroGraph leaderboard.

7.1 Quantitative Results

Table 1: SPDNet test accuracies on NeuroGraph tasks compared to baseline expectations.

Dataset	Classes	SPDNet Accuracy
HCP-Gender	2	**94.79%**
HCP-Age	3	**62.50%**
HCP-Task	7	**99.04%**

7.2 Performance Analysis

HCP-Gender: The model achieved near 95% accuracy. Gender differences in brain connectivity are diffuse and involve subtle shifts in inter-hemispheric connection strengths. The BiMap layer's ability to learn a reduced-rank projection that maximizes class separability while maintaining covariance structure proved superior to node-aggregation methods used in GNNs.

HCP-Task: The 99.04% accuracy on the Task dataset is particularly notable. Cognitive tasks induce strong, global changes in functional connectivity (e.g., the visual cortex coupling with the motor cortex). These global changes are essentially large deformations of the SPD covariance ellipsoid. SPDNet, designed to measure geodesic distances between these ellipsoids, can separate these states with almost perfect precision.

HCP-Age: The performance on Age (62.50%) was lower than the other tasks. Aging is a continuous, heterogeneous process that affects individual connections differently. The lower performance suggests that while global geometric structure is informative, local topological features (which GNNs excel at) might also be necessary for this specific trait. This points towards a future hybrid approach.

7.3 Convergence and Stability

We observed that the Stiefel manifold correction was critical. Without the QR-retraction step, the weight matrices W rapidly lost orthogonality, leading to the collapse of the SPD property in deeper layers and resulting in 'NaN' loss values due to the logarithm of negative eigenvalues.

8 Discussion

8.1 Geometry vs. Topology

Traditional GNNs rely on the graph topology (the adjacency matrix). In fMRI functional connectivity, the graph is often dense (all-to-all). Thresholding this matrix to create a sparse graph for GCNs results in information loss. SPDNet treats the dense matrix as a single geometric object (a point on the manifold $\mathcal{S}^{++}(n)$). Our results confirm that for dense functional connectomes, the geometric perspective is more robust than the topological approximation.

8.2 Computational Complexity

The primary bottleneck of SPDNet is the Eigen-decomposition (SVD) required in the ReEig and LogEig layers, which scales cubically $O(n^3)$. However, given the typical ROI count in fMRI (ranging from 100 to 400), this computational cost is manageable on modern GPUs compared to the massive adjacency multiplications required by dense Graph Transformers.

9 Implementation Availability

To foster reproducibility and further research in geometric deep learning for neuroscience, we have released our complete codebase. The repository includes:

- Custom PyTorch 'Function' implementations for BiMap and ReEig backward passes.
- Integration scripts for the NeuroGraph data loader.
- Pre-trained weights for the best performing models:
  - `spdnet_best_HCPGender_0.9479.pkl`
  - `spdnet_best_HCPAge_0.6250.pkl`
  - `spdnet_best_HCPTask_0.9904.pkl`

Repository URL: `https://github.com/MIbrahim-86/Neurograph_SNA.git`

10 Conclusion and Future Work

In this work, we demonstrated that treating functional brain connectomes as points on a Riemannian manifold yields superior classification performance compared to Euclidean baselines. By employing SPDNet, we achieved state-of-the-art results on the NeuroGraph benchmarks, particularly in Task decoding and Gender classification.

Future work will focus on two directions:

1. **Temporal Dynamics:** Extending the SPDNet architecture to handle dynamic functional connectivity (dFC) by implementing Recurrent Neural Networks on the SPD manifold (SPD-LSTM).
2. **Hybrid Models:** Combining the local feature aggregation of GCNs with the global geometric pooling of SPDNet to improve performance on complex tasks like Age prediction.

References

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