Beyond Euclidean Space: Geometric Deep Learning for Brain Connectomics

Surpassing NeuroGraph SOTA using SPDNet

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Introduction & Benchmark

- **Domain:**
  - Functional MRI (fMRI) data represented as **Connectomes**.
  - Nodes: brain ROIs, Edges: correlation matrices.
- **Benchmark:**
  - **NeuroGraph**: standardized datasets like HCP-Gender, HCP-Age, HCP-Task.
- **Objective:**
  - Predict demographics (Gender, Age, Task) using brain connectivity.
  - Beat the NeuroGraph SOTA.

Problem Statement

> ### Euclidean Error
>
> Standard GNNs treat correlation matrices as flat Euclidean vectors. However, these matrices are SPD and lie on a curved Riemannian manifold.
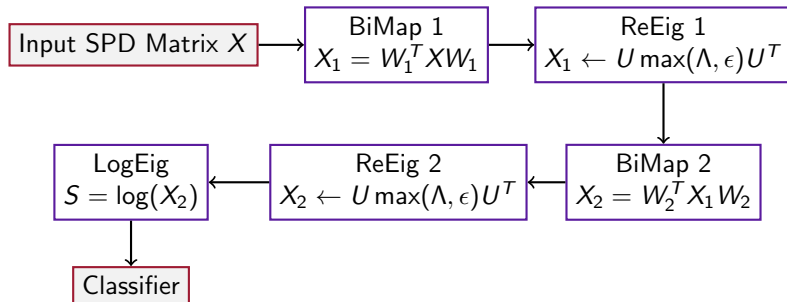
- Treating curved data as flat causes **"swelling effect"**.
- Distances between subjects are distorted.
- Analogy: measuring globe distances with a flat map $\rightarrow$ errors near poles.

Solution: SPDNet (Full Flow)

- **Manifold-Aware Network:**
  - Processes data directly on the **curved SPD manifold** before flattening.
- **Pipeline:**

Input SPD Matrix X → BiMap 1 $X_1 = W_1^T X W_1$ → ReEig 1 $X_1 \leftarrow U \max(\Lambda, \epsilon) U^T$

BiMap 2 $X_2 = W_2^T X_1 W_2$ → ReEig 2 $X_2 \leftarrow U \max(\Lambda, \epsilon) U^T$ → LogEig $S = \log(X_2)$

LogEig → Classifier

BiMap Layer

- Weight matrix $W \in \mathbb{R}^{d_{in} \times d_{out}}$.
- Forward pass:

$$X_{new} = W^T X W$$

- Preserves SPD: $X_{new} = X_{new}^T$, $\lambda_i > 0$.
- Geometric intuition: rotates and reduces dimensionality of the manifold.
- Example: $X \in \mathbb{R}^{4 \times 4}$, $W \in \mathbb{R}^{4 \times 2} \Rightarrow X_{new} \in \mathbb{R}^{2 \times 2}$.

ReEig Layer

- Eigen-decomposition: $X = U \Lambda U^T$
- Rectify eigenvalues: $\Lambda \leftarrow \max(\Lambda, \epsilon)$
- Reconstruct: $X_{\text{rect}} = U \Lambda_{\text{rect}} U^T$
- Removes small noisy eigenvalues, preserves SPD

LogEig: Tangent Projection

- Matrix logarithm:

$$S = \log(X) = U \log(\Lambda) U^T$$

- Maps SPD manifold $\rightarrow$ flat tangent space
- Allows standard linear classifier
- Flatten vector: $v = \text{vec}(\text{upper-triangular}(S))$

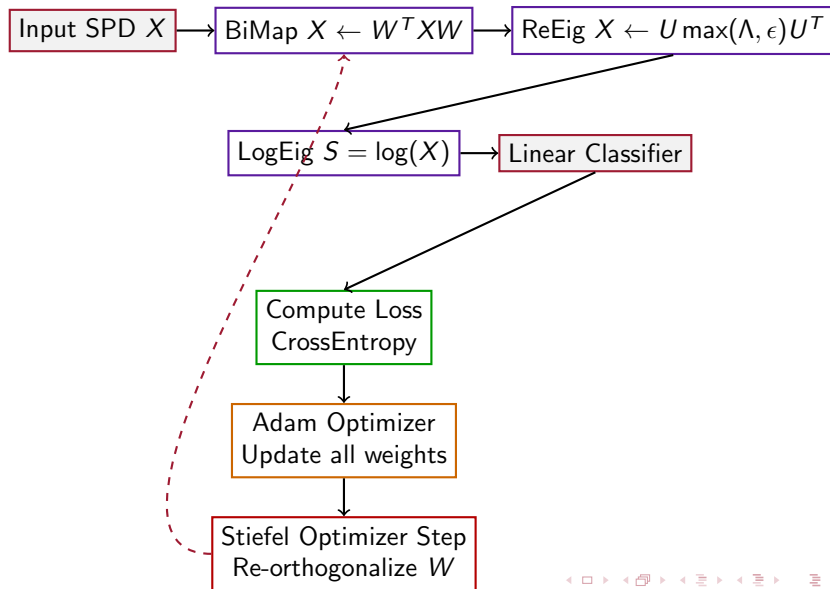## Updating W: Adam + Stiefel Step

- Standard update with Adam:

$$W \leftarrow W - \alpha \cdot \mathsf{AdamGrad}(W)$$

- Problem: breaks orthonormality
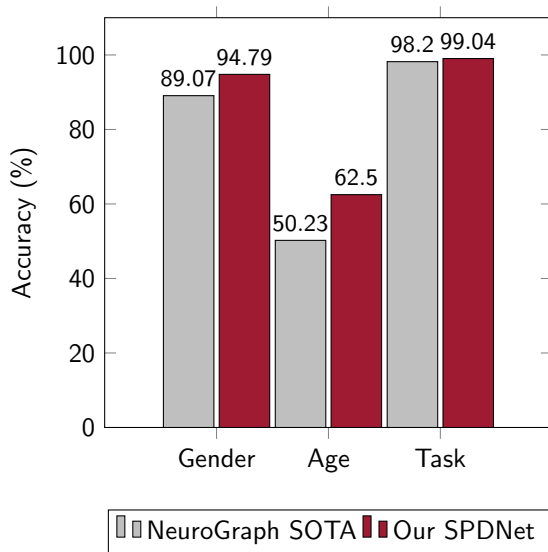- Fix: Stiefel Projection (QR decomposition)

$$Q, R = \mathsf{qr}(W), \quad W \leftarrow Q$$

- Ensures $W^T W = I$.
- Flow:
  1. Forward: $X_{new} = W^T X W$
  2. Backprop: $\nabla_W \mathcal{L}$
  3. Adam step: $W' = W - \alpha \nabla_W$
  4. Stiefel step: $W \leftarrow QR(W')$

SPDNet Training Flow

Input SPD X → BiMap $X \leftarrow W^T X W$ → ReEig $X \leftarrow U \max(\Lambda, \epsilon) U^T$

LogEig $S = \log(X)$ → Linear Classifier

Compute Loss
CrossEntropy

Adam Optimizer
Update all weights

Stiefel Optimizer Step
Re-orthogonalize W

Results: Smashing the Benchmark

Gains:

- Gender: $+5.7\%$
- Age: $+12.27\%$
- Task: $+0.84\%$

Conclusion

- SPDNet processes data **on the manifold**, not flattening first.
- BiMap + ReEig + LogEig pipeline preserves geometry and reduces noise.
- Adam + Stiefel ensures W stays orthonormal.
- Results: Significant gains in Gender and Age prediction over NeuroGraph SOTA.