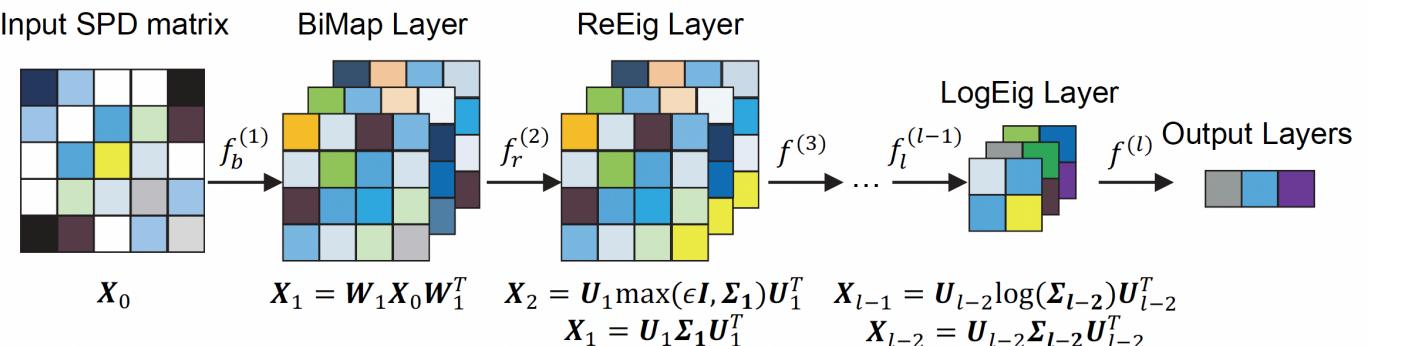


Riemannian Multinomial Logistics Regression for SPD Neural Networks

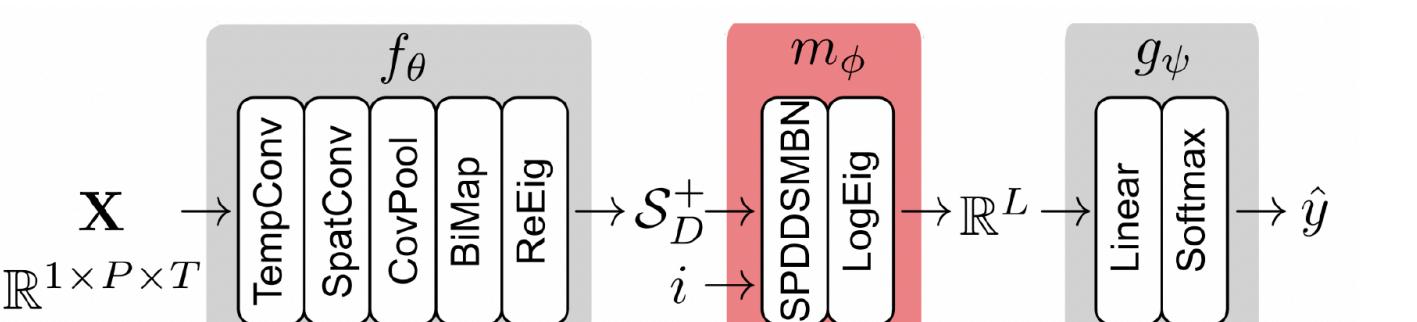
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Motivation

Classification layers in typical SPD neural networks are non-intrinsic



Tangent Space [1-2]



Parameterization [3]

$$\begin{aligned} Y_t &= \text{FM}\left(\left\{M_{t-1}^{(\alpha)}\right\}, \left\{w^{(y, \alpha)}\right\}\right), & R_t &= \mathbb{T}(Y_t, g^{(r)}) \\ T_t &= \text{FM}\left(\{R_t, X_t\}, w^{(t)}\right), & \Phi_t &= \mathbb{T}(T_t, g^{(p)}) \\ \forall \alpha \in J, \quad M_t^{(\alpha)} &= \text{FM}\left(\left\{M_{t-1}^{(\alpha)}\right\}, \Phi_t\right), & O_t &= \text{Chol}\left(\text{ReLU}\left(\text{Chol}\left(\mathbb{T}(S_t, g^{(y)})\right)\right)\right) \end{aligned}$$

Theoretical Contributions

- a general framework for building SPD MLRs under PEMs
- specific SPD MLRs under parameterized LCM and LEM
- An intrinsic theoretical explanation of the most popular LogEig classifier

Preliminaries

Pullback Euclidean Metrics (PEMs) [4]

Definition 2.1 (Pullback Metrics). Suppose \mathcal{M}, \mathcal{N} are smooth manifolds, g is a Riemannian metric on \mathcal{N} , and $f : \mathcal{M} \rightarrow \mathcal{N}$ is a diffeomorphism. Then f can induce a Riemannian metric on \mathcal{M} defined as

$$(f^*g)_p(V_1, V_2) = g_{f(p)}(f_{*,p}(V_1), f_{*,p}(V_2)), \quad (1)$$

where $p \in \mathcal{M}$, $f_{*,p}(\cdot)$ is the differential map of f at p , $V_i \in T_p \mathcal{M}$, and f^*g is the pullback metric by f from \mathcal{N} .

Theorem 2.2 (Pullback Euclidean Metrics (PEMs)). Let $S, S_1, S_2 \in \mathcal{S}_{++}^n$ and $V_1, V_2 \in T_S \mathcal{S}_{++}^n$, $\phi : \mathcal{S}_{++}^n \rightarrow \mathcal{S}^n$ is a diffeomorphism. We define the following operations.

$$S_1 \odot_\phi S_2 = \phi^{-1}(\phi(S_1) + \phi(S_2)), \quad (3)$$

$$g_S^\phi(V_1, V_2) = \langle \phi_{*,S}(V_1), \phi_{*,S}(V_2) \rangle, \quad (4)$$

where $\phi_{*,S} : T_S \mathcal{S}_{++}^n \rightarrow T_{\phi(S)} \mathcal{S}^n$ is the differential map of ϕ at S , and $\langle \cdot, \cdot \rangle$ is the standard Frobenius inner product. Then, we have the following conclusions: $\{\mathcal{S}_{++}^n, \odot_\phi\}$ is an Abelian Lie group, $\{\mathcal{S}_{++}^n, g^\phi\}$ is a Riemannian manifold, and g^ϕ is a bi-invariant metric, called Pullback Euclidean Metric (PEM). The associated geodesic distance is

$$d^\phi(S_1, S_2) = \|\phi(S_1) - \phi(S_2)\|_F, \quad (5)$$

where $\|\cdot\|_F$ is the norm induced by $\langle \cdot, \cdot \rangle$. The Riemannian operators are as follows

$$\text{Exp}_{S_1} V = \phi^{-1}(\phi(S_1) + \phi_{*,S_1} V), \quad (6)$$

$$\text{Log}_{S_1} S_2 = \phi_{*,\phi(S_1)}^{-1}(\phi(S_2) - \phi(S_1)), \quad (7)$$

$$\Gamma_{S_1 \rightarrow S_2}(V) = \phi_{*,\phi(S_2)}^{-1} \circ \phi_{*,S_1}(V), \quad (8)$$

where $V \in T_{S_1} \mathcal{S}_{++}^n$ is a tangent vector, Exp_{S_1} is the Riemannian exponential at S_1 , and ϕ_*^{-1} are the differential maps ϕ^{-1} .

SPD Geometries

Name	$g_P(V, W)$	$\text{Log}_P Q$	$\Gamma_{P \rightarrow Q}(V)$
(α, β) -LEM	$\langle \text{mlog}_{*,P}(V), \text{mlog}_{*,P}(W) \rangle^{(\alpha, \beta)}$	$(\text{mlog}_{*,P})^{-1}[\text{mlog}(Q) - \text{mlog}(P)]$	$(\text{mlog}_{*,Q})^{-1} \circ \text{mlog}_{*,P}(V)$
LCM	$\sum_{i>j} V_{ij} \tilde{W}_{ij} + \sum_{j=1}^n \tilde{V}_{jj} \tilde{W}_{jj} L_{jj}^{-2}$	$(\text{Chol}^{-1})_{*,L} [[K] - [L] + \mathbb{D}(L) \text{Diag}(\mathbb{D}(L)^{-1} \mathbb{D}(K))]$	$(\text{Chol}^{-1})_{*,K} [[\tilde{V}] + \mathbb{D}(K) \mathbb{D}(L)^{-1} \mathbb{D}(\tilde{V})]$

Table 2. Riemannian operators of (α, β) -LEM and LCM on SPD manifolds.

Methods

Exsiting Multinomial Logistics Regression (MLR)

$$\forall k \in \{1, \dots, C\}, p(y = k | x) \propto \exp((\langle a_k, x \rangle - b_k))$$

Euclidean MLR:

$$\begin{aligned} \text{Reformulation} \\ p(y = k | x) &\propto \exp(\text{sign}(\langle a_k, x - p_k \rangle) \|a_k\| d(x, H_{a_k, p_k})) \\ H_{a_k, p_k} &= \{x \in \mathbb{R}^n : \langle a_k, x - p_k \rangle = 0\} \end{aligned}$$

Euclidean MLR has been generalized into hyperbolic [6] and SPD manifolds [5]. However, existing gyro SPD MLRs require:

- Gyro vector structures
- Solving formulation case by case

SPD MLR under PEMs

General Formulation

Theorem 3.8 (SPD MLR under a PEM). Under any PEM, SPD MLR and SPD hyperplane is

$$p(y = k | S) \propto \exp(\langle \phi(S) - \phi(P_k), \phi_{*,I}(\tilde{A}_k) \rangle), \quad (19)$$

$$\tilde{H}_{\tilde{A}_k, P_k} = \{S \in \mathcal{S}_{++}^n : \langle \phi(S) - \phi(P_k), \phi_{*,I}(\tilde{A}_k) \rangle = 0\}, \quad (20)$$

where $\tilde{A}_k \in T_I \mathcal{S}_{++}^n / \{0\} \cong \mathcal{S}^n / \{0\}$ is a symmetric matrix, and $P_k \in \mathcal{S}_{++}^n$ is an SPD matrix.

Definition 3.1 (SPD hyperplanes). Given $P \in \mathcal{S}_{++}^n$, $A \in T_P \mathcal{S}_{++}^n \setminus \{0\}$, we define the SPD hyperplane as

$$\tilde{H}_{A, P} = \{S \in \mathcal{S}_{++}^n : g_P(\text{Log}_P S, A) = \langle \text{Log}_P S, A \rangle_P = 0\}, \quad (12)$$

where P and A are referred to as shift and normal matrices, respectively.

Definition 3.2 (SPD MLR). SPD MLR is defined as

$$p(y = k | S) \propto \exp(\text{sign}(\langle A_k, \text{Log}_{P_k}(S) \rangle_{P_k}) \|A_k\|_{P_k} d(S, \tilde{H}_{A_k, P_k})), \quad (13)$$

where $P_k \in \mathcal{S}_{++}^n$, $A_k \in T_{P_k} \mathcal{S}_{++}^n \setminus \{0\}$, $\langle \cdot, \cdot \rangle_{P_k} = g_{P_k}$, and $\|\cdot\|_{P_k}$ is the norm on $T_{P_k} \mathcal{S}_{++}^n$ induced by g at P_k , and \tilde{H}_{A_k, P_k} is a margin hyperplane in \mathcal{S}_{++}^n as defined in Eq. (12). $d(S, \tilde{H}_{A_k, P_k})$ denotes the margin distance between S and SPD hyperplane \tilde{H}_{A_k, P_k} , which is formulated as:

$$d(S, \tilde{H}_{A_k, P_k}) = \inf_{Q \in \tilde{H}_{A_k, P_k}} d(S, Q), \quad (14)$$

where $d(S, Q)$ is the geodesic distance induced by g .

SPD hyperplanes are submanifolds, which generalize hyperplane in Euclidean spaces.

Proposition 3.3 (Submanifolds). The SPD hyperplane (as defined in Eq. (12)) under any geometrically complete Riemannian metric g is a regular submanifold of SPD manifolds.

Lemma 3.5. Given a PEM g , the margin distance defined in Eq. (14) has a closed-form solution:

$$d(S, \tilde{H}_{A_k, P_k}) = d(\phi(S), H_{\phi_{*,P_k}(A_k), \phi(P_k)}), \quad (15)$$

$$= \frac{|\langle \phi(S) - \phi(P_k), \phi_{*,P_k}(A_k) \rangle|}{\|A_k\|_{P_k}}, \quad (16)$$

where $|\cdot|$ is the absolute value.

SPD MLR: $p(y = k | S) \propto \exp(\langle A_k, \text{Log}_{P_k}(S) \rangle_{P_k}) = \exp(\langle \phi(S) - \phi(P_k), \phi_{*,P_k}(A_k) \rangle)$

Optmizing $A_k \in T_{P_k} \mathcal{S}_{++}^n \setminus \{0\}$

Lemma 3.6. Given a PEM, any parallel transportation is equivalent to the differential map of a left translation and vice versa.

Lemma 3.7. Given two fixed SPD matrices $Q_1, Q_2 \in \mathcal{S}_{++}^n$, we have the following equivalence for parallel transportations under a PEM,

$$\begin{aligned} \forall \tilde{A}_{1,k} \in T_{Q_1} \mathcal{S}_{++}^n, \exists! \tilde{A}_{2,k} \in T_{Q_2} \mathcal{S}_{++}^n, \\ s.t. \Gamma_{Q_1 \rightarrow P_k}(\tilde{A}_{1,k}) = \Gamma_{Q_2 \rightarrow P_k}(\tilde{A}_{2,k}). \end{aligned} \quad (18)$$

Lems 3.6-3.7 indicates that we can either use parallel transportation or left translation.

SPD MLR under deformed LEM and LCM

Power deformation can interpolates between different metrics [7, 8]

$$\text{Power deformation: } \tilde{g} = \frac{1}{\theta^2} \text{Pow}_\theta^* g,$$

Corollary 4.1 (SPD MLRs under the deformed LEM and LCM). The SPD MLRs under (α, β) -LEM is

$$p(y = k | S) \propto \exp\left[\langle \text{mlog}(S) - \text{mlog}(P_k), \tilde{A}_k \rangle^{(\alpha, \beta)}\right],$$

where $\tilde{A}_k \in T_I \mathcal{S}_{++}^n \cong \mathcal{S}^n$ and $P_k \in \mathcal{S}_{++}^n$. The SPD MLRs under (θ) -LCM is

$$p(y = k | S) \propto \exp\left[\frac{1}{\theta} [\tilde{K}] - [\tilde{L}_k] + [\text{Dlog}(\mathbb{D}(\tilde{K})) - \text{Dlog}(\mathbb{D}(\tilde{L}_k))] + [\tilde{A}_k] + \frac{1}{2} \mathbb{D}(\tilde{A}_k)\right], \quad (22)$$

where $\tilde{K} = \text{Chol}(S^0)$, $\tilde{L}_k = \text{Chol}(P_k^0)$, and $\mathbb{D}(\tilde{A}_k)$ denotes a diagonal matrix with diagonal elements of \tilde{A}_k .

SPD Hyperplanes

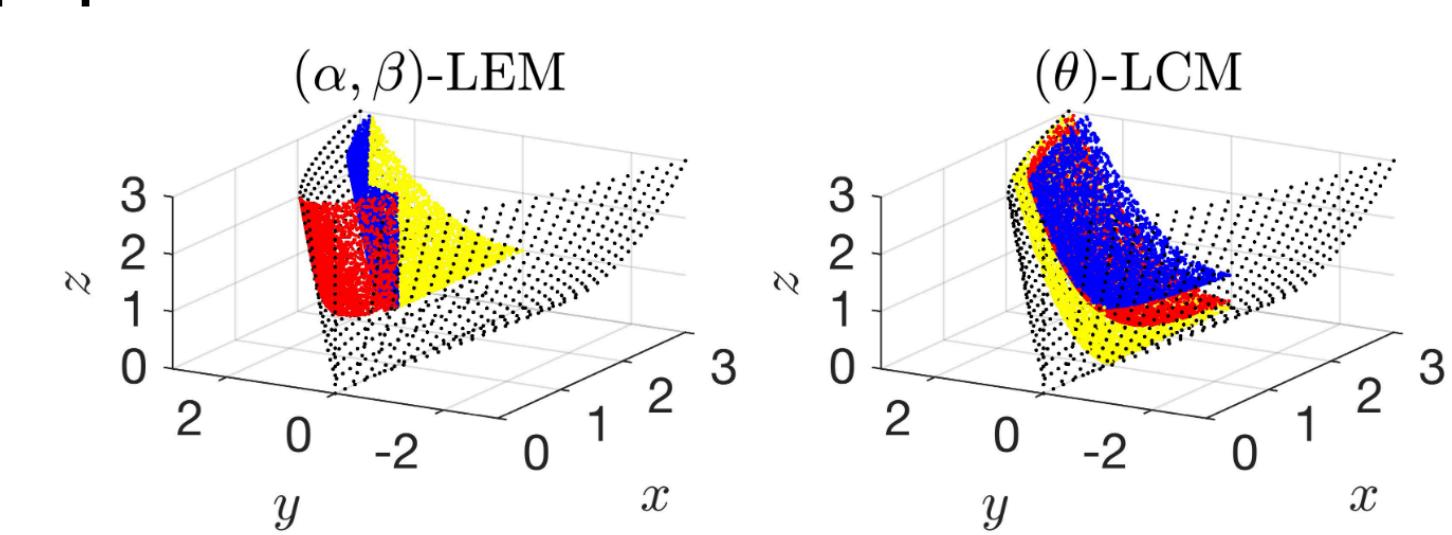


Figure 1. Conceptual illustration of SPD hyperplanes induced by (α, β) -LEM and (θ) -LCM. In each subfigure, the black dots are symmetric positive semi-definite (SPSD) matrices, denoting the boundary of \mathcal{S}_{++}^2 , while the blue, red, and yellow dots denote three SPD hyperplanes.

An Intrinsic theoretical explanation for LogEig MLR

Proposition 5.1. Endowing SPD manifolds with the standard LEM, optimizing SPD parameter P_k in Eq. (21) by LEM-based RSGD and Euclidean parameter A_k by Euclidean SGD, the LEM-based SPD MLR is equivalent to a LogEig MLR with parameters in FC layer optimized by Euclidean SGD.

Experiments

SPDNet

Backbone	Classifier	[20,16,8]	[20,16,14,12,10,8]
SPDNet			