

RMLR: Extending Multinomial Logistic Regression into General Geometries

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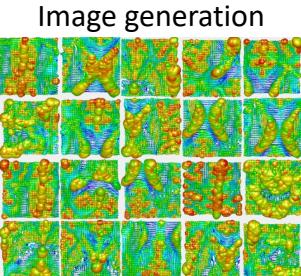


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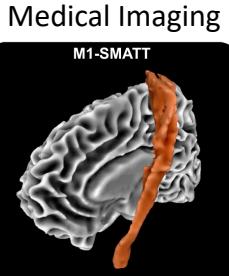


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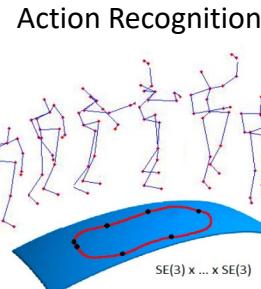
Applications of Riemannian Manifolds



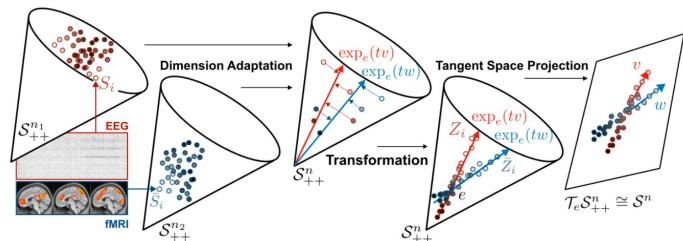
Huang et al., 2019



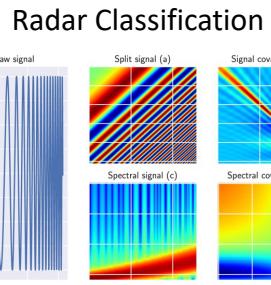
Chakraborty et al., 2020



Vemulapalli, Raviteja 2014



Ju et al., 2024



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Motivation



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



$$p(y = k | x) \propto \exp(\text{sign}(\langle a_k, x - p_k \rangle) \|a_k\| d(x, H_{a_k, p_k})),$$

$$H_{a_k, p_k} = \{x \in \mathbb{R}^n : \langle a_k, x - p_k \rangle = 0\},$$

General geometries



Eqs. (2) and (3) can be naturally extended into manifolds \mathcal{M} by Riemannian operators:

$$p(y = k | S) \propto \exp\left(\text{sign}(\langle \tilde{A}_k, \text{Log}_{P_k}(S) \rangle_{P_k}) \|\tilde{A}_k\|_{P_k} \tilde{d}(S, \tilde{H}_{\tilde{A}_k, P_k})\right), \quad (4)$$

$$\tilde{H}_{\tilde{A}_k, P_k} = \{S \in \mathcal{M} : g_{P_k}(\text{Log}_{P_k} S, \tilde{A}_k) = 0\}, \quad (5)$$

where $P_k \in \mathcal{M}$, $\tilde{A}_k \in T_{P_k} \mathcal{M} \setminus \{\mathbf{0}\}$, g_{P_k} is the Riemannian metric at P_k , and Log_{P_k} is the Riemannian logarithm at P_k . The margin distance is defined as an infimum:

$$\tilde{d}(S, \tilde{H}_{\tilde{A}_k, P_k}) = \inf_{Q \in \tilde{H}_{\tilde{A}_k, P_k}} d(S, Q). \quad (6)$$

- The key is to solve the margin distance, which could be non-convex on general geometries

Reformulation by Riemannian Trigonometry



$$p(y = k \mid x) \propto \exp(\text{sign}(\langle a_k, x - p_k \rangle) \|a_k\| d(x, H_{a_k, p_k})),$$

$$H_{a_k, p_k} = \{x \in \mathbb{R}^n : \langle a_k, x - p_k \rangle = 0\},$$

Reformulation

$$d(x, H_{a,p})) = \sin(\angle xpy^*)d(x, p), \quad \text{with } y^* = \arg \max_{y \in H_{a,p} \setminus \{p\}} (\cos \angle xpy). \quad (7)$$

Riemannian trigonometry

Definition 3.1 (Riemannian Margin Distance). Let $\tilde{H}_{\tilde{A}, P}$ be a Riemannian hyperplane defined in Eq. (5), and $S \in \mathcal{M}$. The Riemannian margin distance from S to $\tilde{H}_{\tilde{A}, P}$ is defined as

$$d(S, \tilde{H}_{\tilde{A}, P}) = \sin(\angle SPY^*)d(S, P), \quad (8)$$

where $d(S, P)$ is the geodesic distance, and $Y^* = \operatorname{argmax}(cos \angle SPY)$ with $Y \in \tilde{H}_{\tilde{A}, P} \setminus \{P\}$. The initial velocities of geodesics define $\cos \angle SPY$:

$$\cos \angle SPY = \frac{\langle \text{Log}_P Y, \text{Log}_P S \rangle_P}{\|\text{Log}_P Y\|_P, \|\text{Log}_P S\|_P}, \quad (9)$$

where $\langle \cdot, \cdot \rangle_P$ is the Riemannian metric at P , and $\|\cdot\|_P$ is the associated norm.

General Results

Riemannian Margin distance

Riemannian MLR

Optimization

Generality

Theorem 3.2. [↓] The Riemannian margin distance defined in Def. 3.1 is given as

$$d(S, \tilde{H}_{\tilde{A}, P}) = \frac{|\langle \text{Log}_P S, \tilde{A} \rangle_P|}{\|\tilde{A}\|_P}. \quad (10)$$

Putting the Eq. (10) into Eq. (4), we can a closed-form expression for Riemannian MLR.

Theorem 3.3 (RMLR). [↓] Given a Riemannian manifold $\{\mathcal{M}, g\}$, the Riemannian MLR induced by g is

$$p(y = k \mid S \in \mathcal{M}) \propto \exp \left(\langle \text{Log}_{P_k} S, \tilde{A}_k \rangle_{P_k} \right), \quad (11)$$

where $P_k \in \mathcal{M}$, $\tilde{A}_k \in T_{P_k} \mathcal{M} \setminus \{\mathbf{0}\}$, and Log is the Riemannian logarithm.

$$\tilde{A}_k = \Gamma_{Q \rightarrow P_k} A_k, \quad (12)$$

$$\tilde{A}_k = L_{P_k \odot Q_\odot^{-1} *, Q} A_k, \quad (13)$$

where $Q \in \mathcal{M}$ is a fixed point, $A_k \in T_Q \mathcal{M} \setminus \{\mathbf{0}\}$, Γ is the parallel transportation along geodesic connecting Q and P_k , and $L_{P_k \odot Q_\odot^{-1} *, Q}$ denotes the differential map at Q of left translation $L_{P_k \odot Q_\odot^{-1}}$

Table 1: Several MLRs on different geometries are special cases of our MLR.

MLR	Geometries	Requirements	Incorporated by Our MLR
Euclidean MLR (Eq. (1))	Euclidean geometry	N/A	✓(App. C)
Gyro SPD MLRs [50]	AIM, LEM & LCM on \mathcal{S}_{++}^n	Gyro structures	✓(Rem. 4.3)
Gyro SPSD MLRs [51]	SPSD product gyro spaces	Gyro structures	✓(App. D)
Flat SPD MLRs [16]	(α, β) -LEM & (θ) -LCM on \mathcal{S}_{++}^n	Pullback metrics from the Euclidean space	✓(Rem. 4.3)
Ours	General Geometries	Riemannian logarithm	N/A

Deformed SPD Geometries

Table 12: The associated Riemannian operators and properties of five basic metrics on SPD manifolds.

Metrics	$g_P(V, W)$	$\text{Log}_P Q$	$\Gamma_{P \rightarrow Q}(V)$	Properties
(α, β) -LEM	$\langle \log_{*, P}(V), \log_{*, P}(W) \rangle^{(\alpha, \beta)}$	$(\log_{*, P})^{-1} [\log(Q) - \log(P)]$	$(\log_{*, Q})^{-1} \circ \log_{*, P}(V)$	$O(n)$ -Invariance, Geodesically Completeness
(α, β) -AIM	$\langle P^{-1}V, WP^{-1} \rangle^{(\alpha, \beta)}$	$P^{1/2} \log (P^{-1/2} Q P^{-1/2}) P^{1/2}$	$(QP^{-1})^{1/2} V (P^{-1}Q)^{1/2}$	Lie Group Left-Invariance, $O(n)$ -Invariance, Geodesically Completeness
(α, β) -EM	$\langle V, W \rangle^{(\alpha, \beta)}$	$Q - P$	V	$O(n)$ -Invariance
LCM	$\sum_{i>j} \tilde{V}_{ij} \tilde{W}_{ij} + \sum_{j=1}^n \tilde{V}_{jj} \tilde{W}_{jj} L_{jj}^{-2}$	$(\text{Chol}^{-1})_{*, L} [\lfloor K \rfloor - \lfloor L \rfloor + \mathbb{D}(L) \text{Dlog}(\mathbb{D}(L)^{-1} \mathbb{D}(K))]$	$(\text{Chol}^{-1})_{*, K} [\lfloor \tilde{V} \rfloor + \mathbb{D}(K) \mathbb{D}(L)^{-1} \mathbb{D}(\tilde{V})]$	Lie Group Bi-Invariance, Geodesically Completeness
BWM	$\frac{1}{2} \langle \mathcal{L}_P[V], W \rangle$	$(PQ)^{1/2} + (QP)^{1/2} - 2P$	$U \left[\sqrt{\frac{\delta_i + \delta_j}{\sigma_i + \sigma_j}} [U^\top VU]_{ij} \right] U^\top$	$O(n)$ -Invariance

$$\tilde{g}_P(V, W) = \frac{1}{\theta^2} g_{P^\theta}((\phi_\theta)_{*, P}(V), (\phi_\theta)_{*, P}(W)), \forall P \in \mathcal{S}_{++}^n, V, W \in T_P \mathcal{S}_{++}^n, \quad (14)$$

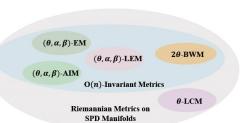
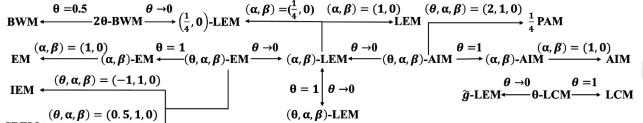


Figure 1: Illustration on the deformation (left) and Venn diagram (right) of metrics on SPD manifolds, where IEM, SREM, and $\frac{1}{4}$ PAM denotes Inverse Euclidean Metric, Square Root Euclidean Metric, and Polar Affine Metric scaled by $1/4$.

Table 2: Properties of deformed metrics on SPD manifolds ($\theta \neq 0$ and $\min(\alpha, \alpha + n\beta) > 0$).

Name	Properties
(θ, α, β) -LEM	Bi-Invariance, $O(n)$ -Invariance, Geodesically Completeness
(θ, α, β) -AIM	Lie Group Left-Invariance, $O(n)$ -Invariance, Geodesically Completeness
(θ, α, β) -EM	$O(n)$ -Invariance
θ -LCM	Lie Group Bi-Invariance, Geodesically Completeness
2θ-BWM	$O(n)$ -Invariance

Manifestation



SPD MLR

Theorem 4.2 (SPD MLRs). [↓] By abuse of notation, we omit the subscripts k of A_k and P_k . Given SPD feature S , the SPD MLRs, $p(y = k \mid S \in \mathcal{S}_{++}^n)$, are proportional to

$$(\alpha, \beta)\text{-LEM} : \exp \left[\langle \log(S) - \log(P), A \rangle^{(\alpha, \beta)} \right], \quad (16)$$

$$(\theta, \alpha, \beta)\text{-AIM} : \exp \left[\frac{1}{\theta} \langle \log(P^{-\frac{\theta}{2}} S^\theta P^{-\frac{\theta}{2}}), A \rangle^{(\alpha, \beta)} \right], \quad (17)$$

$$(\theta, \alpha, \beta)\text{-EM} : \exp \left[\frac{1}{\theta} \langle S^\theta - P^\theta, A \rangle^{(\alpha, \beta)} \right], \quad (18)$$

$$\theta\text{-LCM} : \exp \left[\frac{1}{\theta} \langle [\tilde{K}] - [\tilde{L}] + [\text{Dlog}(\mathbb{D}(\tilde{K})) - \text{Dlog}(\mathbb{D}(\tilde{L}))], [A] + \frac{1}{2}\mathbb{D}(A) \rangle \right], \quad (19)$$

$$2\theta\text{-BWM} : \exp \left[\frac{1}{4\theta} \langle (P^{2\theta} S^{2\theta})^{\frac{1}{2}} + (S^{2\theta} P^{2\theta})^{\frac{1}{2}} - 2P^{2\theta}, \mathcal{L}_{P^{2\theta}}(\bar{L} A \bar{L}^\top) \rangle \right], \quad (20)$$

where $A \in T_I \mathcal{S}_{++}^n \setminus \{0\}$ is a symmetric matrix, $\log(\cdot)$ is the matrix logarithm, $\mathcal{L}_P(V)$ is the solution to the matrix linear system $\mathcal{L}_P[V]P + P\mathcal{L}_P[V] = V$, known as the Lyapunov operator, $\text{Dlog}(\cdot)$ is the diagonal element-wise logarithm, $[\cdot]$ is the strictly lower part of a square matrix, and $\mathbb{D}(\cdot)$ is a diagonal matrix with diagonal elements of a square matrix. Besides, $\log_{*, P}$ is the differential maps at P , $\tilde{K} = \text{Chol}(S^\theta)$, $\tilde{L} = \text{Chol}(P^\theta)$, and $\bar{L} = \text{Chol}(P^{2\theta})$.

Lie MLR

Theorem 5.2. [↓] The Lie MLR on $\text{SO}(n)$ is given as

$$p(y = k \mid R \in \text{SO}(n)) \propto \langle \log(P_k^\top S), A_k \rangle, \quad (22)$$

where $P_k \in \text{SO}(n)$ and $A_k \in \mathfrak{so}(n)$.

Visualization

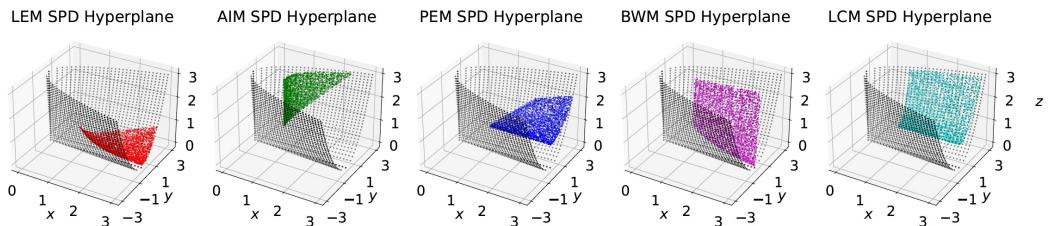


Figure 2: Conceptual illustration of SPD hyperplanes induced by five families of Riemannian metrics. The black dots denote the boundary of S^2_{++} .

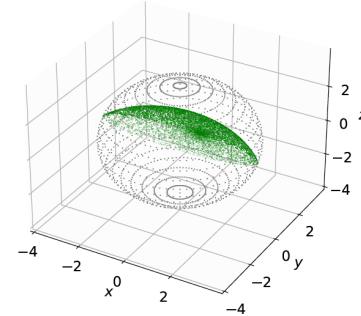


Figure 3: Conceptual illustration of a Lie hyperplane. Each pair of antipodal black dots corresponds to a rotation matrix with an Euler angle of π , while the green dots denote a Lie hyperplane.

Results

Table 3: Comparison of SPDNet with LogEig against SPD MLRs on the Radar dataset.

Architectures	LogEig MLR	(θ, α, β)-AIM		(θ, α, β)-EM		(α, β)-LEM		2 θ -BWM		θ -LCM	
		(1,1,0)	(1,1,0)	(1,1,1/8)	(1,1,0)	(1,1,1)	(0.5)	(0.25)	(1)	(0.5)	
2-Block	92.88±1.05	94.53±0.95	94.24±0.55	94.93±0.60	93.55±1.21	95.64±0.83	92.22±0.83	94.99±0.47	93.49±1.25	94.59±0.82	
5-Block	93.47±0.45	94.32±0.94	95.11±0.82	95.01±0.84	94.60±0.70	95.87±0.58	93.69±0.66	94.84±0.68	93.93±0.98	95.16±0.67	

Table 4: Comparison of SPDNet with LogEig against SPD MLRs on the HDM05 dataset.

Architectures	LogEig MLR	(θ, α, β)-AIM		(θ, α, β)-EM		(α, β)-LEM		2 θ -BWM		θ -LCM	
		(1,1,0)	(1,1,0)	(0.5,1.0,1/30)	(1,1,0)	(0.5)	(1)	(0.5)	(1)	(0.5)	
1-Block	57.42±1.31	58.07±0.64	66.32±0.63	71.65±0.88	56.97±0.61	70.24±0.92	63.84±1.31	65.66±0.73			
2-Block	60.69±0.66	60.72±0.62	66.40±0.87	70.56±0.39	60.69±1.02	70.46±0.71	62.61±1.46	65.79±0.63			
3-Block	60.76±0.80	61.14±0.94	66.70±1.26	70.22±0.81	60.28±0.91	70.20±0.91	62.33±2.15	65.71±0.75			

Table 5: Inter-session experiments of TSMNet with different MLRs on the Hinss2021 dataset.

Classifiers	LogEig MLR	(θ, α, β)-AIM		(θ, α, β)-EM		(α, β)-LEM		2 θ -BWM		θ -LCM	
		(1,1,0)	(0.5,1.0,0.05)	(1,1,0)	(1,1,0)	(0.5)	(1)	(1.5)			
Balanced Acc.	53.83±9.77	53.36±9.92	55.27±8.68	54.48±9.21	53.51±10.02	55.54±7.45	55.71±8.57	56.43±8.79			

Table 6: Inter-subject experiments of TSMNet with different MLRs on the Hinss2021 dataset.

Classifiers	LogEig MLR	(θ, α, β)-AIM		(θ, α, β)-EM		(α, β)-LEM		2 θ -BWM		θ -LCM	
		(1,1,0)	(1.5,1,0)	(1,1,0)	(1.5,1,1/20)	(1,1,0)	(0.5)	(0.75)	(1)	(0.5)	
Balanced Acc.	49.68±7.88	50.65±8.13	51.15±7.83	50.02±5.81	51.38±5.77	51.41±7.98	50.26±7.23	51.67±8.73	52.93±7.76	54.14±8.36	

Results

Riemannian GCN

Table 8: Comparison of LogEig against SPD MLRs under the SPDGCN architecture.

Classifiers	Disease		Cora		Pubmed	
	Mean±STD	Max	Mean±STD	Max	Mean±STD	Max
LogEig MLR	90.55 ± 4.83	96.85	78.04 ± 1.27	79.6	70.99 ± 5.12	77.6
(θ, α, β)-AIM	94.84 ± 2.27	98.43	79.79 ± 1.44	81.6	77.83 ± 1.08	80
(θ, α, β)-EM	90.87 ± 5.14	98.03	79.05 ± 1.23	81	78.16 ± 2.41	79.5
(α, β)-LEM	96.33 ± 2.19	98.82	79.89 ± 0.99	81.8	78.16 ± 2.41	79.5
2 θ -BWM	91.93 ± 3.64	96.85	73.46 ± 2.18	77.7	73.22 ± 4.06	78.1
θ -LCM	93.01 ± 2.14	98.43	77.59 ± 1.20	80.1	74.46 ± 5.81	78.9

RResNet

Table 7: Comparison of LogEig against SPD MLRs under the RResNet architecture.

Datasets	LogEigMLR	(θ, α, β)-AIM	(θ, α, β)-EM	(α, β)-LEM	2 θ -BWM	θ -LCM
HDM05	58.17 ± 2.07	60.23 ± 1.26	71.89 ± 0.60 ($\uparrow 13.72$)	59.44 ± 0.87	69.85 ± 0.23	65.76 ± 0.96
NTU60	45.22 ± 1.23	48.94 ± 0.68	52.24 ± 1.25	46.99 ± 0.41	50.56 ± 0.59	53.63 ± 0.95 ($\uparrow 8.41$)

Table 9: Comparison of LogEig against SPD MLRs for direct classification.

Riemannian VS. Tangent MLR

Classifiers	Radar	HDM05	Hinss2021	
			Inster-session	Inster-subject
LogEig MLR	91.93 ± 1.30	48.43 ± 1.25	39.76 ± 7.60	44.66 ± 7.17
(θ, α, β)-AIM	95.21 ± 0.81	49.17 ± 1.08	41.14 ± 7.26	45.89 ± 6.52
(θ, α, β)-EM	92.25 ± 1.20	61.60 ± 0.69	45.78 ± 8.51 ($\uparrow 6.02$)	45.84 ± 4.75
(α, β)-LEM	95.09 ± 0.57	49.05 ± 0.91	40.88 ± 7.46	46.02 ± 5.96 ($\uparrow 1.36$)
2 θ -BWM	94.89 ± 0.41	66.77 ± 1.34 ($\uparrow 18.34$)	44.84 ± 8.00	45.21 ± 7.44
θ -LCM	95.67 ± 0.61 ($\uparrow 3.74$)	58.66 ± 0.51	43.17 ± 6.21	45.10 ± 6.20

Results



Efficiency

Table 16: Training efficiency (s/epoch).

Methods	Radar	HDM05	Hinss2021	
			Inter-session	Inter-subject
Baseline	1.36	1.95	0.18	8.31
AIM-MLR	1.75	31.64	0.38	13.3
EM-MLR	1.34	3.91	0.19	8.23
LEM-MLR	1.5	4.7	0.24	10.13
BWM-MLR	1.75	33.14	0.38	13.84
LCM-MLR	1.35	3.29	0.18	8.35

Table 10: Results of LogEig MLR against Lie MLR under the LieNet architecture.

LieNet

Classifiers	G3D		HDM05	
	Mean±STD	Max	Mean±STD	Max
LogEig MLR	87.91±0.90	89.73	76.92±1.27	79.11
Lie MLR	89.13±1.7	92.12	78.24±1.03	80.25

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