Data Analysis with the Riemannian Geometry of SPD Matrices

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- **P:** Datasets often comprise multiple domains:
 - Sessions
 - Subjects
 - Batches
- **Q:** How to adapt a given model that is well performing on a particular domain to a different yet related domain?
- Q: How to train a classifier based on data from one domain and apply it to data from another domain?

- Highly researched subject
- Many previous studies, e.g.:
 - [Ben-David et al, 07]
 - [Raina et al, 07]
 - [Dai et al, 09]
 - [Pan et al, 10]
 - ...

Data Analysis in High Dimension

- P: The data do not live in a Euclidean space
 - Multiple modalities
 - Dependence between coordinates
- **Q:** What is the proper non-Euclidean metric?
- **Q:** How to find an embedding into a Euclidean space?

• P: Unsupervised



- Brain Computer Interface (BCI) [Barachant et al, 13]
- Data: [recent BCI competition]
 - EEG from 9 subjects
 - 22 electrodes
 - 2 days of experiments
 - 288 trials per subject
- In each trial, imagine performing 1 of 4 motor tasks:
 - Left hand
 - Right hand
 - Both feet
 - Tongue



Consider two datasets from two subjects:



- Each set contains N_k matrices of observations • d - dimension (# of EEG electrodes) d • $T_i^{(k)}$ - observation length • $u_i^{(k)}$ - bidder

 - $y_i^{(k)}$ hidden label (imagined motor task)



• Let $P_i^{(k)} \in \mathbb{R}^{d \times d}$ be the (sample) covariance of $X_i^{(k)}$



Low dimensional representation of the covariance matrices from two subjects



Identify the imagined motor activity per trial *from multiple subjects*

- → Training a classifier from one subject and testing on another subject
- → Unsupervised



Our Solution

Riemannian Geometry of SPD matrices

Benefits

- *Known* non-Euclidean space facilitating comparisons, additions, subtractions
- Joint representation from multiple domains
- Following recent work:
 - Theory [Pennec et al, 06], [Sra & Hosseini, 15]
 - Applications in BCI [Barachant et al, 13]
 - Applications in computer vision [Tuzel el al, 08], [Freifeld et al, 14], [Bergman et al, 17]

Preliminaries on Riemannian Geometry

- Let $x, y \in \mathcal{M}$ be two points on a Riemannian manifold
- Let $\mathcal{T}_x \mathcal{M}$ be the tangent plane at the point x
- Define the following operations:

	Vector Space	Riemannian Manifold
Subtraction	$\overrightarrow{xy} = y - x$	$\overrightarrow{xy} = \text{Log}_{x}(y)$
Addition	$egin{array}{c} egin{array}{c} egin{array}$	$oldsymbol{y} = \operatorname{Exp}_{oldsymbol{x}}\left(\overrightarrow{oldsymbol{x}oldsymbol{y}} ight)$
Mean	$ig rgmin_{oldsymbol{x}} \sum_i ig\ oldsymbol{x} - oldsymbol{x}_i ig\ _i^2$	$lpha \mathrm{rgmin}_{oldsymbol{x}}\sum_{i}d_{R}^{2}\left(oldsymbol{x},oldsymbol{x}_{i} ight)$



The SPD Cone

- The SPD matrices constitute a convex half-cone in the space of real symmetric matrices
- This cone forms a differentiable Riemannian manifold ${\mathcal M}$ equipped with the inner product

$$\langle S_1, S_2 \rangle_{\mathcal{T}_P \mathcal{M}} = \langle P^{-\frac{1}{2}} S_1 P^{-\frac{1}{2}}, P^{-\frac{1}{2}} S_2 P^{-\frac{1}{2}} \rangle$$

- $\mathcal{T}_P\mathcal{M}$ is the tangent plane at $P \in \mathcal{M}$
- $S_1, S_2 \in \mathcal{T}_P\mathcal{M}$
- $\langle \cdot, \cdot \rangle$ is the standard Euclidean inner product
- The symmetric matrices $S \in \mathcal{T}_P \mathcal{M}$ live in a linear space
 - We can view them as vectors



The SPD Cone – Properties

 There exists a unique geodesic curve between any two SPD matrices P₁, P₂ ∈ M:

$$\varphi(t) = P_1^{\frac{1}{2}} \left(P_1^{-\frac{1}{2}} P_2 P_1^{-\frac{1}{2}} \right)^t P_1^{\frac{1}{2}}, \qquad 0 \le t \le 1$$

• Define a **Riemannian distance** on the manifold as the arc-length of the geodesic curve:

$$d_R^2(P_1, P_2) = \left\| \log \left(P_2^{-\frac{1}{2}} P_1 P_2^{-\frac{1}{2}} \right) \right\|_F^2$$
$$= \sum_{i=1}^n \log^2 \left(\lambda_i \left(P_2^{-\frac{1}{2}} P_1 P_2^{-\frac{1}{2}} \right) \right)$$

- $\lambda_i(P)$ is the i-th eigenvalue of P
- Scale-invariant

The SPD Cone – Properties

$$M = \begin{bmatrix} x & y \\ y & z \end{bmatrix}$$

$$\Rightarrow \begin{cases} \operatorname{Tr}(M) = x + z > 0 \\ |(M)| = xz - y^2 > 0 \end{cases} \Rightarrow \begin{cases} x > 0 \\ z > 0 \end{cases} \Rightarrow \boxed{|y| < \sqrt{xz}}$$

The SPD Cone – Properties

• Logarithm map:

$$S_1 = \text{Log}_P(P_1) = P^{\frac{1}{2}} \log \left(P^{-\frac{1}{2}} P_1 P^{-\frac{1}{2}} \right) P^{\frac{1}{2}} \in \mathcal{T}_P \mathcal{M}$$

- Exponential map: $P_1 = \operatorname{Exp}_P(S_1) = P^{\frac{1}{2}} \exp\left(P^{-\frac{1}{2}}S_1P^{-\frac{1}{2}}\right)P^{\frac{1}{2}} \in \mathcal{M}$
- Relation to the (unique) geodesic curve $\varphi(t)$ from P_1 to P_2 is given by the initial velocity

$$\varphi'(0) = \operatorname{Log}_{P_1}(P_2) \in \mathcal{T}_{P_1}\mathcal{M}$$



Formulation

- Consider two subsets $\mathcal{P}^{(1)}$ (target) and $\mathcal{P}^{(2)}$ (source) of SPD matrices from two different domains
 - $\overline{P}^{(1)}$ and $\overline{P}^{(2)}$ Riemannian means
 - $\varphi(t)$ the unique geodesic from $\overline{P}^{(2)}$ to $\overline{P}^{(1)}$
 - $S_i^{(k)}$ the symmetric matrix (or vector) in $\mathcal{T}_{\overline{P}^{(k)}}\mathcal{M}$

$$S_i^{(k)} = \operatorname{Log}_{\overline{P}^{(k)}}\left(P_i^{(k)}\right)$$

Formulation

- **Goal:** Derive a new representation $\Gamma(S_i^{(2)})$: $\Gamma: \mathcal{T}_{\overline{P}^{(2)}}\mathcal{M} \to \mathcal{T}_{\overline{P}^{(1)}}\mathcal{M}$ so that $\{S_i^{(1)}\}$ and $\{\Gamma(S_i^{(2)})\}$ live in the same linear space
- Benefit: Relate samples from the two subsets
 - Compute quantities such as $\langle S_i^{(1)}, \Gamma(S_j^{(2)}) \rangle_{\overline{P}^{(1)}}$

Formulation

- Constraints:
 - Zero mean:

$$\frac{1}{N_2} \sum_{i=1}^{N_2} \Gamma(S_i^{(2)}) = \frac{1}{N_1} \sum_{i=1}^{N_1} S_i^{(1)} = 0$$

• Inner product preservation:

$$\big\langle \Gamma\big(S_i^{(2)}\big), \Gamma\big(S_j^{(2)}\big)\big\rangle_{\overline{P}^{(1)}} = \big\langle S_i^{(2)}, S_j^{(2)}\big\rangle_{\overline{P}^{(2)}}$$

• Geodesic velocity preservation:

$$\Gamma\left(\varphi'\left(0\right)\right) = \varphi'\left(1\right)$$

Formulation

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Imply that the map preserves inter-sample relations

Formulation

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Not unique: If Γ admits to these properties, then also $R \circ \Gamma$ where R is an arbitrary rotation

Formulation

- Constraints:
 - Zero mean:

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Simple implementation by mean subtraction

Formulation

- Constraints:
 - Geodesic velocity preservation:

$$\Gamma\left(\varphi'\left(0\right)\right) = \varphi'\left(1\right)$$

Use the *unique* geodesic to resolve the arbitrary degree of freedom

The two intrinsic symmetric matrices (vectors) $\varphi'(0) \in \mathcal{T}_{\overline{P}^{(2)}}\mathcal{M}$ and $\varphi'(1) \in \mathcal{T}_{\overline{P}^{(1)}}\mathcal{M}$ are used to fix the rotation

Formulation

- Constraints:
 - Geodesic velocity preservation:

$$\Gamma\left(\varphi'\left(0\right)\right) = \varphi'\left(1\right)$$

Unsupervised – no labels are used

Present a closed-form expression (no optimization)

Parallel Transport

Lemma (Parallel Transport)
Let
$$A, B \in \mathcal{M}$$
.
The PT from B to A of any $S \in \mathcal{T}_B \mathcal{M}$ is:
 $\Gamma_{B \to A} (S) \triangleq ESE^T$
where $E = (AB^{-1})^{\frac{1}{2}}$.

Theorem. The representation $\Gamma_{\overline{P}^{(2)}} \rightarrow \overline{P}^{(1)}(S_i^{(2)}),$

i.e., the unique PT of $S_i^{(2)}$ from $\overline{P}^{(2)}$ to $\overline{P}^{(1)}$, is well defined and satisfies properties (1) - (3).

Parallel Transport



Domain Adaptation with PT

Algorithm:

- 1. Project the SPD matrix $\boldsymbol{P}_{i}^{(2)}$ to the tangent plane $\mathcal{T}_{\overline{\boldsymbol{P}}^{(2)}}\mathcal{M}$ $\boldsymbol{S}_{i}^{(2)} = \operatorname{Log}_{\overline{\boldsymbol{P}}^{(2)}}(\boldsymbol{P}_{i}^{(2)})$
- 2. Parallel transport $S_i^{(2)}$ from $\overline{P}^{(2)}$ to $\overline{P}^{(1)}$ by computing

$$\boldsymbol{S}_{i}^{(2) \to (1)} = \Gamma_{\overline{\boldsymbol{P}}^{(2)} \to \overline{\boldsymbol{P}}^{(1)}} \left(\boldsymbol{S}_{i}^{(2)} \right)$$

3. Project the symmetric matrix $S_i^{(2)\to(1)} \in \mathcal{T}_{\overline{P}^{(1)}}\mathcal{M}$ back to the manifold using $\operatorname{Exp}_{\overline{P}^{(1)}}(S_i^{(2)\to(1)})$.

Domain Adaptation with PT

Define the map $\Psi:\mathcal{M}\to\mathcal{M}$ that adapts the domain of $\mathcal{P}^{(2)}$ to the domain of $\mathcal{P}^{(1)}$

$$\begin{split} \Psi\big(P_i^{(2)}\big) = \mathrm{Exp}_{\overline{P}^{(1)}} \left(\Gamma_{\overline{P}^{(2)} \to \overline{P}^{(1)}} \left(\mathrm{Log}_{\overline{P}^{(2)}} \left(P_i^{(2)}\right)\right)\right) \\ \text{for any } P_i^{(2)} \in \mathcal{P}^{(2)} \end{split}$$

Implementation

Theorem. Let $A, B, P \in \mathcal{M}$ and let $S = \text{Log}_B(P) \in \mathcal{T}_B \mathcal{M}$. Then, $\text{Exp}_A(\Gamma_{B \to A}(S)) = EPE^T$, where $E = (AB^{-1})^{\frac{1}{2}}$.

• Ψ can be efficiently implemented

$$\Psi\left(P_i^{(2)}\right) = \Gamma_{\overline{P}^{(2)} \to \overline{P}^{(1)}}\left(P_i^{(2)}\right) = EP_i^{(2)}E^T$$
$$E \triangleq \left(\overline{P}^{(1)}\left(\overline{P}^{(2)}\right)^{-1}\right)^{\frac{1}{2}}$$

Implementation

- Important consequence:
 - The covariance adaptation:

$$EP_i^{(2)}E^T$$

where

$$E \triangleq \left(\overline{P}^{(1)} \left(\overline{P}^{(2)}\right)^{-1}\right)^{\frac{1}{2}}$$

• Can be applied directly to data by:

 $EX_i^{(2)}$

Toy Problem

- Consider the set of hidden multi-dimensional times series $\{s_i[n]\}_{i=1}^{100}$:

$$\boldsymbol{s}_{i}\left[n\right] = \begin{bmatrix} \sin\left(2\pi f_{0}n/T\right) \\ \cos\left(2\pi f_{0}n/T + \phi_{i}\right) \end{bmatrix}, n = 0, \dots, T-1$$

where $f_0\!=\!10$, $T\!=\!500$, and $\phi_i\sim U\left[-\pi/2,0\right]$

- Short segments of two oscillatory signals
- Governed by a 1-dimensional hidden variable ϕ_i (the initial phase of the oscillations)



• The population covariance of $s_i[n]$ is

$$\frac{1}{2} \begin{bmatrix} 1 & -\sin(\phi_i) \\ -\sin(\phi_i) & 1 \end{bmatrix}$$

which depends only on ϕ_i

• <u>Note</u>:

when presenting the population covariances as vectors in \mathbb{R}^3 , two coordinates are fixed and only one varies

Toy Problem

• We generate two observable subsets

$$\mathcal{X}^{(1)} \!=\! \big\{ \boldsymbol{x}_{i}^{(1)}[n] \big\}_{i=1}^{100}, \mathcal{X}^{(2)} \!=\! \big\{ \boldsymbol{x}_{i}^{(2)}[n] \big\}_{i=1}^{100}$$

such that:

$$x_{i}^{(k)}[n] = M^{(k)}s_{i}[n]$$

where

- $M^{(1)}$ is randomly chosen
- $M^{(2)} = 1.5 \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} M^{(1)}$

Toy Problem





* PT of the source and target sets to the mid-point

- Data: [BCI competition]
 - 22 EEG electrodes
 - 9 subjects
 - 2 days of experiments
 - 288 trials per subject
 - In each trial the subject is asked to imagine performing 1 out of 4 motor tasks: left hand, right hand, both feet, tongue

tSNE [v. d. Maaen & Hinton, 08] representation of Covariance matrices







After PT

Two subjects





After PT



Mean subtraction [Barachant et al, 13]

• Using *affine transformation* [Zanini et al, 18]:

$$\left(\overline{P}^{(k)}\right)^{-\frac{1}{2}} P_i^{(k)} \left((\overline{P}^{(k)})^{-\frac{1}{2}} \right)^T$$

• Equivalent to parallel transport to the identity:

$$\Psi\left(P_{i}^{(k)}\right) = \Gamma_{\overline{P}^{(k)} \to I}\left(P_{i}^{(k)}\right) = EP_{i}^{(k)}E^{T}$$
$$E \triangleq \left(I\left(\overline{P}^{(k)}\right)^{-1}\right)^{\frac{1}{2}}$$

• When there are two sets, it is equivalent to

$$\Gamma_{I \to \overline{P}^{(1)}} \circ \Gamma_{\overline{P}^{(2)} \to I}$$

(PC)

Coincides with our work when

$$\begin{split} \Gamma_{\overline{P}^{(2)}\to\overline{P}^{(1)}} &= \Gamma_{I\to\overline{P}^{(1)}} \circ \Gamma_{\overline{P}^{(2)}\to I} \\ \bullet \quad \overline{P}^{(1)} \text{ and } \overline{P}^{(2)} \text{ commute and have the same eigenvectors} \end{split}$$

• **Q:** what is special about the proposed transport?

Definition (Equivalent Pairs) Two pairs (A_1, B_1) and (A_2, B_2) , such that $A_1, B_1, A_2, B_2 \in \mathcal{M}$, are *equivalent* if there exists an invertible matrix E such that

$$A_2 = \Gamma(A_1) = EA_1E^T$$

 $B_2 = \Gamma(B_1) = EB_1E^T$

We denote this relation by

$$(oldsymbol{A}_1,oldsymbol{B}_1)\sim(oldsymbol{A}_2,oldsymbol{B}_2)$$



Definition (Equivalent Pairs) Two pairs (A_1, B_1) and (A_2, B_2) , such that $A_1, B_1, A_2, B_2 \in \mathcal{M}$, are *equivalent* if there exists an invertible matrix E such that

$$A_2 = \Gamma(A_1) = EA_1E^T$$

 $B_2 = \Gamma(B_1) = EB_1E^T$

We denote this relation by

$$(\boldsymbol{A}_1, \boldsymbol{B}_1) \sim (\boldsymbol{A}_2, \boldsymbol{B}_2)$$

Lemma.

The relation \sim is an equivalence relation, satisfying reflexivity, symmetry, and transitivity.

- Interpretation:
 - Equivalent pairs are matrices with equivalent intrarelations
 - E.g. if $(A_1, B_1) \sim (A_2, B_2)$ then

 $d_R(A_1, B_1) = d_R(A_2, B_2)$

but with a different global position on the manifold



Proposition.

Let (A_1, B_1) be a pair of SPD matrices $A_1, B_1 \in \mathcal{M}$, and let $[(A_1, B_1)]$ denote the equivalence class

$$[(A_1, B_1)] = \{(A_2, B_2) \in \mathcal{M} \times \mathcal{M} | (A_2, B_2) \sim (A_1, B_1) \},\$$

of all matrix pairs that are equivalent to (A_1, B_1) . Then, for any $(A_2, B_2) \in [(A_1, B_1)]$:

$$\Gamma \circ \Gamma_{B_1 \to A_1} = \Gamma_{B_2 \to A_2} \circ \Gamma \,,$$

where $\Gamma(P) = EPE^T$ and E satisfies the equivalence relation.



- Direct consequence:
 - Domain adaptation via $\Psi\,$ is invariant to the relative position of $\overline{P}^{(1)}$ and $\overline{P}^{(2)}$ on the manifold
 - It is constructed equivalently for every pair in the equivalence class

$$\left[(\overline{P}^{(1)},\overline{P}^{(2)})
ight]$$

- Guarantees consistence
 - For example, two subjects in two sessions in the BCI problem

Extension to Multiple Subsets

Algorithm. Input: $\{P_i^{(1)}\}_{i=1}^{N_1}, \{P_i^{(2)}\}_{i=1}^{N_2}, \dots, \{P_i^{(K)}\}_{i=1}^{N_K}$ Output: $\{\tilde{S}_i^{(1)}\}_{i=1}^{N_1}, \{\tilde{S}_i^{(2)}\}_{i=1}^{N_2}, \dots, \{\tilde{S}_i^{(K)}\}_{i=1}^{N_K}$

- 1. For each $k \in \{1, 2, ..., K\}$, compute $\overline{\mathbf{P}}^{(k)}$ the Riemannian mean of the subset $\{\mathbf{P}_i^{(k)}\}$.
- 2. Compute $\hat{\boldsymbol{P}}$, the Riemannian mean of $\{\overline{\boldsymbol{P}}^{(k)}\}_{k=1}^{K}$.
- 3. For all k and all i, apply Parallel Transport using:

$$\boldsymbol{\Gamma}_{i}^{(k)} = \Gamma_{\overline{\boldsymbol{P}}^{(k)} \to \hat{\boldsymbol{P}}} \big(\boldsymbol{P}_{i}^{(k)} \big).$$

4. For all k and all i, project the transported matrix to the tangent space via:

$$ilde{oldsymbol{S}}_i^{(k)} = \logig(\hat{oldsymbol{P}}^{-rac{1}{2}} oldsymbol{\Gamma}_i^{(k)} \hat{oldsymbol{P}}^{-rac{1}{2}}ig).$$



- Objective evaluation via classification
 - Leave-one-subject-out
 - Linear SVM



Sleep Stage Identification

- Six different sleep stages: awake, REM, and sleep stages 1-4
- Recordings [PhysioNet.org]:
 - Two EEG channels
 - One electrooculography (EOG) channel
- Data from three subjects

Sleep Stage Identification

0

Subject #

Subject #2

-1

-2

* REM

0.5

0

-0.5

0.5

REM

Sleep Stage

2

3

0.5

Sleep Stage

0

Sleep Stage 3

REM

0

-1

-2

-1

0

-2

Subject #1

Subject #2

Subject #3

0.5

0

-0.5

0.5

0

0.5

-0

Subject #'

Subject #2

Subject #

3

2

PCA of the covariance matrices¹







-1

0

Sleep Stage Identification

Baseline

Mean Subtraction

Parallel Transport



Mental Arithmetic Identification

- Recordings [Shin et al, 17]:
 - EEG from 29 subjects
 - 30 electrodes at 1000Hz
 - 3 sessions per subject
 - 20 repetitions/trials per session
- Two mental states:
 - Performing repeated simple arithmetic calculations
 - Baseline resting state

Mental Arithmetic Identification







Baseline

Parallel Transport

Mental Arithmetic Identification

- Average classification results over all 29 subjects
 - Leave-one-session-out cross-validation
 - Linear SVM

Baseline	Mean Subtraction	Parallel Transport
74%	73%	78%

Extensions and Outlook

- To facilitate the internal structure of each subset:
 - Rotation following the PT
 - Unsupervised moments alignment



Baseline





Parallel Transport



Mean Subtraction

Parallel Transport & Moments Alignment

Extensions and Outlook

- Take home message
 - High-dimensional data live in a non-Euclidean space
 - Covariance matrices are informative features
 - They live in a non-Euclidean space with operations given in closed-form
- Covariance matrices might be insufficient features
- Instead, we could use:
 - Correlation and Partial Correlation matrices
 - Positive Kernels
 - Graph Laplacians
 - Transition probability matrices of random walks on graphs

Thank you

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