Geometric Statistics
Univ. P. Sabatier, Toulouse
Aug. 30th - Sep. 5th, 2019

Towards a classification of metrics on Symmetric Positive Definite matrices

Based on:
- *Is affine-invariance well defined on SPD matrices? A principled continuum of metrics*
- *Exploration of Balanced Metrics on Symmetric Positive Definite Matrices*
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Outline

1. A zoo of Riemannian metrics on $SPD(n)$

2. $GL(n)$-invariant metrics

Paper 1: Is affine-invariance well defined on SPD matrices? A principled continuum of metrics

3. Balanced metrics

Paper 2: Exploration of Balanced Metrics on Symmetric Positive Definite Matrices

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A zoo of Riemannian metrics on $SPD(n)$

SPD matrices in applications

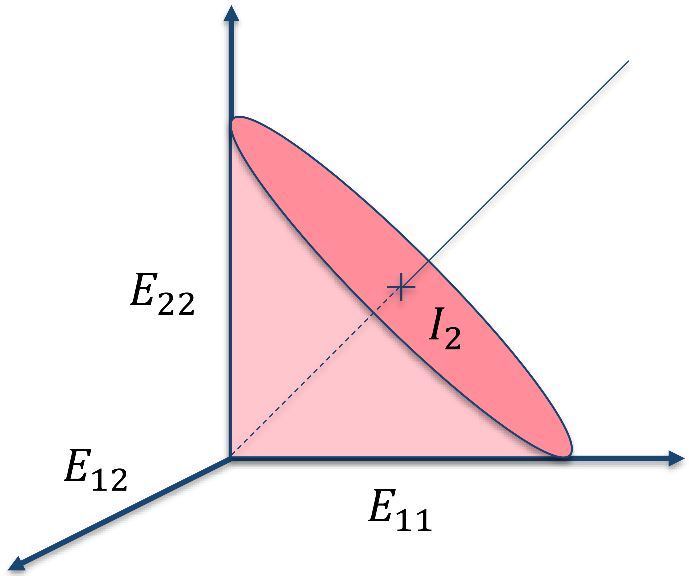
- Applications
  - Diffusion Tensor Imaging
  - Brain Computer Interfaces
  - Functional Magnetic Resonance Imaging
  - Computer Vision
  - RADAR
- SPD matrices
  - Diffusion tensors
  - Covariance matrices
  - Correlation matrices
  - Toeplitz matrices

Manifold of SPD matrices

Symmetric matrices $Sym(n) = \{M \in \mathbb{R}^{n \times n}, M = M^\top\}$

Spectral theorem $\Longrightarrow eig\big(Sym(n)\big) \subset \mathbb{R}$

$$SPD(n) := \{\Sigma \in Sym(n), eig(\Sigma) \subset \mathbb{R}_+^*\}$$



Manifold of SPD matrices

Symmetric matrices $Sym(n) = \{M \in \mathbb{R}^{n\times n}, M = M^\top\}$

Spectral theorem $\Longrightarrow eig\big(Sym(n)\big) \subset \mathbb{R}$

$$SPD(n) \coloneqq \{\Sigma \in Sym(n), eig(\Sigma) \subset \mathbb{R}_+^*\}$$

Matrix exponential $\exp M = \sum_{k=0}^{+\infty} \frac{M^k}{k!}$

Diffeomorphism $\exp: Sym(n) \longrightarrow SPD(n)$ of inverse $\log$

Power $\mathrm{pow}_p = \exp \circ\, p \log: SPD(n) \longrightarrow SPD(n)$

A zoo of Riemannian metrics on $SPD(n)$

Affine-invariant

Euclidean

Bogoliubov-Kubo-Mori

Inverse-Euclidean

Cholesky

Fisher

Bures-Wasserstein

Polar-affine

Power-Euclidean

Square-root

Log-Euclidean

Ref: [1] Dryden et al. 2009, [2] Michor et al. 2000, [3] Dryden et al. 2010

A zoo of Riemannian metrics on $SPD(n)$

	$O(n)$-invariant	Other
Positevely curved	Bures-Wasserstein	
Flat	Euclidean Inverse-Euclidean Log-Euclidean Power-Euclidean Square-root	Cholesky
Negatively curved	Affine-invariant Polar-affine Fisher	
Other	Bogoliubov-Kubo-Mori	

Ref: [1] Dryden et al. 2009, [2] Michor et al. 2000, [3] Dryden et al. 2010

A zoo of Riemannian metrics on $SPD(n)$

Flat metrics

$\Sigma \in SPD(n),\ X, Y \in T_\Sigma SPD(n)$

Name	Power	Riemannian Metric
Power-Euclidean	p	$g_\Sigma^{E,p}(X,Y) = \frac{1}{p^2}\mathrm{tr}\big(d\mathrm{pow}_p(\Sigma)[X]d\mathrm{pow}_p(\Sigma)[Y]\big)$
Euclidean	$p = 1$	$g_\Sigma^E(X,Y) = \mathrm{tr}(XY)$
Inverse-Euclidean	$p = -1$	$g_\Sigma^I(X,Y) = \mathrm{tr}(\Sigma^{-2}X\Sigma^{-2}Y)$
Square-root	$p = 1/2$	$g_\Sigma^{E,1/2}(X,Y) = 4\,\mathrm{tr}\big(d\mathrm{pow}_{1/2}(\Sigma)[X]d\mathrm{pow}_{1/2}(\Sigma)[Y]\big)$
Log-Euclidean	$p \longrightarrow 0$	$g_\Sigma^L(X,Y) = \mathrm{tr}(d\log(\Sigma)[X]d\log(\Sigma)[Y])$

Ref: [1] Dryden et al. 2009, [3] Dryden et al. 2010

A zoo of Riemannian metrics on $SPD(n)$
Negatively curved metrics with symmetric structure

- **Affine-invariant metrics**
  - Affine transformation of a random vector $X \longmapsto AX + B$
  - Transformation of its covariance matrix $\Sigma \longmapsto A\Sigma A^\top$
  - Group action $\begin{cases} GL(n) \times SPD(n) \longrightarrow SPD(n) \\ (A, \Sigma) \longmapsto A\Sigma A^\top \end{cases}$
  - One-parameter family of affine-invariant metrics, with $\alpha > 0$ and $\beta > -\alpha/n$

$$g_\Sigma^A(X, Y) = \alpha \operatorname{tr}(\Sigma^{-1}X\Sigma^{-1}Y) + \beta \operatorname{tr}(\Sigma^{-1}X) \operatorname{tr}(\Sigma^{-1}Y)$$

- **Fisher metric**
  - Multivariate centered Gaussian model $p_\Sigma(x) = \frac{1}{\sqrt{2\pi}^n} \frac{1}{\sqrt{\det \Sigma}} \exp\left(-\frac{1}{2} x^\top \Sigma^{-1} x\right)$
  - Fisher metric $g_\Sigma^F(X, Y) = \frac{1}{2} \operatorname{tr}(\Sigma^{-1}X\Sigma^{-1}Y)$

Ref: [4] Pennec et al. 2006, [5] Amari, Nagaoka 2000, [6] Skovgaard 1984

A zoo of Riemannian metrics on $SPD(n)$
Negatively curved metrics with symmetric structure

- **Polar-affine metric**
  - Polar decomposition $\begin{cases} GL(n) \longrightarrow SPD(n) \times O(n) \\ A \longmapsto \left(\sqrt{AA^\top}, \sqrt{AA^\top}^{-1} A\right) \end{cases}$
  - Quotient manifold and submersion $\begin{cases} GL(n) \longrightarrow GL(n)/O(n) \\ A \longmapsto A.O(n) \end{cases}$
  - 'Polar' diffeomorphism $\begin{cases} GL(n)/O(n) \longrightarrow SPD(n) \\ A.O(n) \longmapsto \sqrt{AA^\top} \end{cases}$
  - Frobenius inner product on $GL(n)$ is $O(n)$-invariant so it induces a metric on the quotient $GL(n)/O(n)$ and on $SPD(n)$, called the polar-affine metric

- **Questions**
  - **Do 'Affine-invariant' and 'Polar-affine' metrics belong to a wider family?**
  - **Does there exist a one-parameter family of polar-affine metrics?**

Ref: [7] Zhang, Su, Klassen, Le, Srivastava 2018

In the following sections

- **Section 2: $GL(n)$-invariant metrics**
  - Unification of Affine-invariant and Polar-affine metrics
  - Definition of Power-affine and Deformed-affine metrics
  - Relation with the Log-Euclidean metric
  - Relation with the Fisher metric

- **Section 3: Balanced metrics**
  - Relation between Affine-invariant, Euclidean and Inverse-Euclidean metrics
  - Relation between BKM, Euclidean and Log-Euclidean metrics
  - Principle of balanced metric
  - Definition of Mixed-power-Euclidean metrics

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$GL(n)$-invariant metrics

Is affine-invariance well defined on SPD matrices?
A principled continuum of metrics

Affine-invariant VS Polar-affine

'Quotient space' formalism

- Quotient manifold and submersion $\begin{cases} GL(n) \longrightarrow GL(n)/O(n) \\ A \longmapsto A.O(n) \end{cases}$
- $O(n)$-invariant inner product on $GL(n)$, with $\alpha > |\alpha'|$ and $\beta > -(\alpha + \alpha')/n$

$$\langle X|Y\rangle = \alpha \operatorname{tr}(XY^\top) + \alpha' \operatorname{tr}(XY) + \beta \operatorname{tr} X \operatorname{tr} Y$$

- Affine-invariant metric $\begin{cases} GL(n)/O(n) \longrightarrow SPD(n) \\ A.O(n) \longmapsto AA^\top \end{cases}$

$\uparrow \mathrm{pow}_2$

- Polar-affine metric $\begin{cases} GL(n)/O(n) \longrightarrow SPD(n) \\ A.O(n) \longmapsto \sqrt{AA^\top} \end{cases}$

Affine-invariant VS Polar-affine
'Group action' formalism

- Affine-invariant action $\eta^1: \begin{cases} GL(n) \times SPD(n) \longrightarrow SPD(n) \\ (A, \Sigma) \longmapsto A\Sigma A^\top \end{cases}$

$$\left(\eta^2(A,\Sigma)\right)^2 = \eta^1(A,\Sigma^2)$$

- Polar-affine action $\eta^2: \begin{cases} GL(n) \times SPD(n) \longrightarrow SPD(n) \\ (A, \Sigma) \longmapsto \sqrt{A\Sigma^2 A^\top} \end{cases}$

Affine-invariant VS Polar-affine

Unification and generalization

- Polar-affine metric $g^{A,2}$ $\mathrm{pow}_2 : (SPD(n), 4g^{A,2}) \longrightarrow (SPD(n), g^A)$
- Power-affine metric $g^{A,p}$ $\mathrm{pow}_p : (SPD(n), p^2 g^{A,p}) \longrightarrow (SPD(n), g^A)$
- Deformed-affine metric $g^{A,f}$ $f : \left(SPD(n), g^{A,f}\right) \longrightarrow (SPD(n), g^A)$
- These metrics are $GL(n)$-invariant under $\begin{cases} GL(n) \times SPD(n) \longrightarrow SPD(n) \\ (A, \Sigma) \longmapsto f^{-1}(Af(\Sigma)A^\top) \end{cases}$
- Relation with the log-Euclidean metric

$$\lim_{p \to 0} g^{A,p}(X, Y) = g^L(X, Y)$$

$GL(n)$-invariant metrics
Relation with the Fisher metric

- Centered Gaussian model

$$p_\Sigma(x) = \frac{1}{\sqrt{2\pi}^n} \frac{1}{\sqrt{\det \Sigma}} \exp\left(-\frac{1}{2} x^\top \Sigma^{-1} x\right)$$

- Deformed centered Gaussian model

$$p_\Sigma^f(x) = \frac{1}{\sqrt{2\pi}^n} \frac{1}{\sqrt{\det f(\Sigma)}} \exp\left(-\frac{1}{2} x^\top f(\Sigma)^{-1} x\right)$$

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Balanced metrics

Exploration of Balanced Metrics on Symmetric Positive Definite Matrices

α-connections of the centered Gaussian model

- The Fisher metric is the affine-invariant metric
- The m-connection ($\alpha = -1$) is the Euclidean Levi-Civita connection
- The e-connection ($\alpha = +1$) is the inverse-Euclidean Levi-Civita connection
- Note that:
  - $g_\Sigma^A(X,Y) = \mathrm{tr}\big((\Sigma^{-1}X\Sigma^{-1})Y\big) = \mathrm{tr}\big(X(\Sigma^{-1}Y\Sigma^{-1})\big)$
  - $g_\Sigma^E(X,Y) = \mathrm{tr}(XY)$
  - $g_\Sigma^I(X,Y) = \mathrm{tr}\big((\Sigma^{-1}X\Sigma^{-1})(\Sigma^{-1}Y\Sigma^{-1})\big)$
- And:
  - $g_\Sigma^{BKM}(X,Y) = \mathrm{tr}(d\log(\Sigma)[X]Y) = \mathrm{tr}(X d\log(\Sigma)[Y])$
  - $g_\Sigma^E(X,Y) = \mathrm{tr}(XY)$
  - $g_\Sigma^L(X,Y) = \mathrm{tr}(d\log(\Sigma)[X]d\log(\Sigma)[Y])$

Ref: [5] Amari, Nagaoka 2000

Principle of balanced metrics

- **Definition**:
  - Two flat metrics g et g^*
  - Their respective Levi-Civita connections ∇ and ∇^*
  - Their respective parallel transports Π and Π^*
  - The balanced bilinear form g^0 is defined by $g^0_\Sigma(X,Y) = \mathrm{tr}\left(\left(\Pi_{\Sigma\to I_n} X\right)\left(\Pi^*_{\Sigma\to I_n} Y\right)\right)$

- **Theorem**: If g^0 is a metric, then $(SPD(n), g^0, \nabla, \nabla^*)$ is a dually-flat manifold.

Mixed-power-Euclidean metrics

- **Definition**: Given two powers $p, q \neq 0$, we can define the balanced form

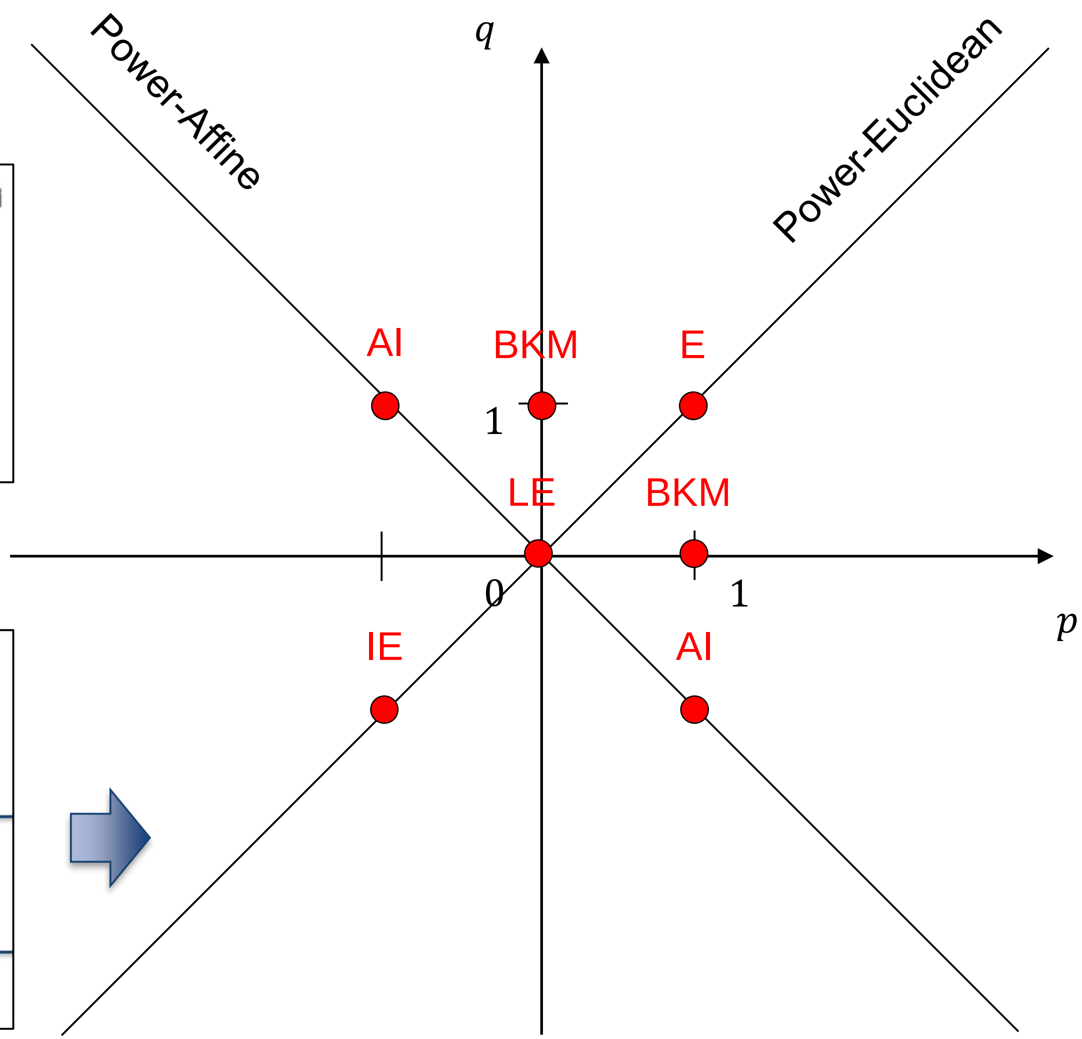
$$g_\Sigma^{E,p,q}(X,Y) = \mathrm{tr}\big(d\mathrm{pow}_p(\Sigma)[X]\, d\mathrm{pow}_q(\Sigma)[Y]\big)$$

- **Theorem**: It is symmetric and positive-definite, hence it is a metric.
- **Corollary**: The space $(SPD(n), g^{E,p,q}, \nabla^{E,p}, \nabla^{E,q})$ is dually-flat (where $\nabla^{E,p}$ and $\nabla^{E,q}$ are the Levi-Civita connections of the metrics $g^{E,p}$ and $g^{E,q}$)

Summary

Affine-invariant Euclidean Bogoliubov-Kubo-Mori
Inverse-Euclidean Fisher Cholesky
Bures-Wasserstein Polar-affine Power-Euclidean
Square-root Log-Euclidean

Flat	Euclidean, Inverse-Euclidean, Log-Euclidean, Power-Euclidean, Square-root
Negatively curved	Affine-invariant, Polar-affine, Fisher
Other	Bogoliubov-Kubo-Mori



Mixed-Power-Euclidean metrics $g^{E,p,q}$

Conclusion

- **Power-affine metrics**
  - Unified framework for affine-invariant, polar-affine and Fisher metrics
- **Mixed-power-Euclidean metrics**
  - Unified framework for power-Euclidean, power-affine and BKM metrics
- The **log-Euclidean metric** appears as a limit case in both frameworks, but also in the alpha-Procrustes framework [8, Ha Quang]

- **Future works**
  - Unified framework for power-Euclidean, power-affine and alpha-Procrustes metrics
  - Generalization to Positive Semi-Definite (PSD) matrices: boundary, strata…

References

[1] Dryden, Koloydenko, Zhou, Non-Euclidean Statistics for Covariance Matrices with Applications to Diffusion Tensor Imaging. *Annals of Applied Statistics*, 2009
[2] Michor, Petz, Andai, The Curvature of the Bogoliubov-Kubo-Mori Scalar Product on Matrices. *Infinite Dim. Analysis, Quantum Probability and Related Topics*, 2000
[3] Dryden, Pennec, Peyrat, Power-Euclidean metrics for covariance matrices with applications to diffusion tensor imaging. Arxiv, 2010
[4] Pennec, Fillard, Ayache, A Riemannian Framework for Tensor Computing. *International Journal of Computer Vision*, 2006
[5] Amari, Nagaoka, Methods of information geometry, 2000
[6] Skovgaard, A Riemannian geometry of the multivariate normal model. Scand. Journal of Statistics, 1984
[7] Zhang, Su, Klassen, Le, Srivastava, Rate-Invariant Analysis of Covariance Trajectories. Journal of Math. Imaging and Vision, 2018
[8] Ha Quang, Alpha Procrustes metrics between positive definite operators: a unifying formulation for the Bures-Wasserstein and Log-Euclidean/Log-Hilbert-Schmidt metrics, *Proceedings of GSI 2019*

Thank you for your attention

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