From Covariance Matrices to Covariance Operators Data Representation from Finite to Infinite-Dimensional Settings

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Covariance matrices & covariance operators

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Collaborators

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Symmetric Positive Definite (SPD) matrices

Sym⁺⁺(n) = set of $n \times n$ SPD matrices

- Have been studied extensively mathematically
- Numerous practical applications
 - Brain imaging (Arsigny et al 2005, Dryden et al 2009, Qiu et al 2015)
 - Computer vision: object detection (Tuzel et al 2008, Tosato et al 2013), image retrieval (Cherian et al 2013), visual recognition (Jayasumana et al 2015), many more
 - Radar signal processing: Barbaresco (2013), Formont et al 2013
 - Machine learning: kernel learning (Kulis et al 2009)

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- Overview of SPD, especially covariance matrices and their applications in computer vision
- Generalization to infinite-dimensional setting, namely covariance operators, via kernels
 - Nonlinear generalizations of covariance matrices
 - Can achieve substantial gains in practical performance compared to the finite-dimensional setting

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Part I: Finite-dimensional setting

Covariance Matrices and Applications

Part II: Infinite-dimensional setting

Covariance Operators and Applications

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Covariance Matrices and Applications

- Data Representation by Covariance Matrices
- ② Geometry of SPD matrices
- Machine Learning Methods on Covariance Matrices and Applications in Computer Vision

Covariance Operators and Applications

- Data Representation by Covariance Operators
- Geometry of Covariance Operators
- Machine Learning Methods on Covariance Operators and Applications in Computer Vision



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Covariance Matrices and Applications

- Data Representation by Covariance Matrices
- ② Geometry of SPD matrices
- Machine Learning Methods on Covariance Matrices and Applications in Computer Vision

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- Tuzel, Porikli, Meer (ECCV 2006, CVPR 2006): covariance matrices as region descriptors for images (covariance descriptors)
- Given an image *F* (or a patch in *F*), at each pixel, extract a feature vector (e.g. intensity, colors, filter responses etc)
- Each image corresponds to a data matrix X

 $\mathbf{X} = [x_1, \dots, x_m] = n \times m$ matrix

where

- *m* = number of pixels
- n = number of features at each pixel

.

Covariance matrix representation of images

 $\mathbf{X} = [x_1, \dots, x_m]$ = data matrix of size $n \times m$, with *m* observations

Empirical mean vector

$$\mu_{\mathbf{X}} = \frac{1}{m} \sum_{i=1}^{m} x_i = \frac{1}{m} \mathbf{X} \mathbf{1}_m, \quad \mathbf{1}_m = (1, \dots, 1)^T \in \mathbb{R}^m$$

Empirical covariance matrix

$$C_{\mathbf{X}} = \frac{1}{m} \sum_{i=1}^{m} (x_i - \mu_{\mathbf{X}}) (x_i - \mu_{\mathbf{X}})^T = \frac{1}{m} \mathbf{X} J_m \mathbf{X}^T$$
$$J_m = I_m - \frac{1}{m} \mathbf{1}_m \mathbf{1}_m^T = \text{ centering matrix}$$

Image $F \Rightarrow$ Data matrix $X \Rightarrow$ Covariance matrix C_X

- Each image is represented by a covariance matrix
- Example of image features

 $\mathbf{f}(x,y) = \left[I(x,y), R(x,y), G(x,y), B(x,y), \left| \frac{\partial R}{\partial x} \right|, \left| \frac{\partial R}{\partial y} \right|, \left| \frac{\partial G}{\partial x} \right|, \left| \frac{\partial B}{\partial x} \right|, \left| \frac{\partial B}{\partial y} \right| \right]$

at pixel location (x, y)

Example



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- Encode linear correlations (second order statistics) between image features
- Flexible, allowing the fusion of multiple and different features
 - Handcrafted features, e.g. colors and SIFT
 - Convolutional features
- Compact
- Robust to noise

- Covariance representation for video: e.g. Guo et al (AVSS 2010), Sanin et al (WACV 2013)
 - Employ features that capture temporal information, e.g. optical flow
- Covariance representation for 3D point clouds and 3D shapes: e.g. Fehr et al (ICRA 2012, ICRA 2014), Tabias et al (CVPR 2014), Hariri et al (Pattern Recognition Letters 2016)
 - Employ geometric features e.g. curvature, surface normal vectors

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Representing an image by a covariance matrix

is essentially equivalent to

Representing an image by a Gaussian probability density ρ in \mathbb{R}^n with mean zero Features extracted are random observations of a *n*-dimensional random vector with probability density ρ $X = (X_1, \dots, X_n)$ = random vector in \mathbb{R}^n with probability density function ρ

• Mean vector

$$\mu = \mathbb{E}(X)$$

• Covariance matrix

$$C = \mathbb{E}[(X - \mu)(X - \mu)^T]$$

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• Variance of the random variable X_i

$$C_{ii} = \mathbb{E}[(X_i - \mu_i)^2]$$

• Covariance between the random variables X_i and X_i

$$C_{ij} = \operatorname{cov}(X_i, X_j) = \mathbb{E}[(X_i - \mu_i)(X_j - \mu_j)]$$

• Correlation between X_i and X_j

$$\operatorname{corr}(X_i, X_j) = \begin{cases} \frac{C_{ij}}{\sqrt{C_{ii}C_{jj}}}, & i \neq j \\ 1, & i = j \end{cases}$$

Multivariate Gaussian probability density ρ = N(μ, C), with covariance matrix C ∈ Sym⁺⁺(n)

$$\rho(x) = \frac{1}{\sqrt{(2\pi)^n \det(C)}} \exp\left(-\frac{1}{2}(x-\mu)^T C^{-1}(x-\mu)\right)$$

• If $\mu = 0$, then ρ is completely determined by the covariance matrix C

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Empirical covariance matrix - MLE estimate

 $\mathbf{X} = [x_1, \dots, x_m], x_i$'s = IID samples drawn from $\mathcal{N}(\mu, C)$

Log-likelihood function

$$\log \mathcal{L}(\mu, C | \mathbf{X}) = -\frac{mn}{2} \log(2\pi) - \frac{m}{2} \log \det(C)$$

 $-\frac{1}{2} \sum_{i=1}^{m} (x_i - \mu)^T C^{-1} (x_i - \mu).$

• MLE estimates of μ and C

$$\mu_{\mathbf{X}} = \frac{1}{m} \sum_{i=1}^{m} x_i, \quad C_{\mathbf{X}} = \frac{1}{m} \sum_{i=1}^{m} (x_i - \mu_{\mathbf{X}}) (x_i - \mu_{\mathbf{X}})^T$$

Empirical covariance matrix - Unbiased estimate

• MLE estimate of μ is unbiased

 $\mathbb{E}(\mu_{\mathbf{X}}) = \mu$

• MLE estimate of *C* is biased

$$\mathbb{E}(C_{\mathbf{X}}) = \frac{m-1}{m}C \neq C$$

Unbiased estimate

$$\tilde{C}_{\mathbf{X}} = \frac{m}{m-1} C_{\mathbf{X}} = \frac{1}{m-1} \mathbf{X} J_m \mathbf{X}^{\mathsf{T}}$$

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 $C_{\mathbf{X}} = \frac{1}{m} \mathbf{X} J_m \mathbf{X}^T$ = MLE estimate, $\tilde{C}_{\mathbf{X}} = \frac{1}{m-1} \mathbf{X} J_m \mathbf{X}^T$ = unbiased estimate

• In the Gaussian case, in terms of MSE (mean square error)

 $MSE(C_{\mathbf{X}}) = \mathbb{E}||C_{\mathbf{X}} - C||_{F}^{2} < MSE(\tilde{C}_{\mathbf{X}}) = \mathbb{E}||\tilde{C}_{\mathbf{X}} - C||_{F}^{2}$

since C_X has smaller variance

- Both estimates are consistent: MSE \rightarrow 0 as $m \rightarrow \infty$
- The difference (by a factor $\frac{m-1}{m}$) diminishes as *m* becomes large
- Both estimates have been used in practice

- C_X is only guaranteed to be positive semi-definite
- C_X can be ill-conditioned
- For *C*_X to be positive definite/well-conditioned, need to use regularization in general
- Diagonal loading, widely used, readily generalizable to infinite-dimensional setting

 $C_{\mathbf{X}} + \gamma I \quad \gamma > 0$

 More generally, shrinkage estimators, Ledoit and Wolf (Journal of Multivariate Analysis, 2004)

$$\hat{C}_{\mathbf{X}} = (\mathbf{1} -
ho)C_{\mathbf{X}} +
ho
u I, \quad \mathbf{0} \le
ho \le \mathbf{1},
u > \mathbf{0}$$

- Some recent work also employ the mean μ in the representation, e.g. Wang et al (CVPR 2016), Li et al (PAMI 2017)
- Current presentation: assuming zero mean

Data Representation by Covariance Matrices

- Representation of images by covariance matrices and its generalizations
- Statistical interpretation

For practical applications, e.g. classification, clustering, regression etc

 We need notions of distances/similarities between covariance matrices

Covariance Matrices and Applications

- Data Representation by Covariance Matrices
- Geometry of SPD matrices
- Machine Learning Methods on Covariance Matrices and Applications in Computer Vision

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Geometry of SPD matrices - Outline

Three different views of the set of SPD matrices

- Subset of Euclidean space
 - Euclidean metric
 - Invariances and Interpretations
- Piemannian manifold
 - Affine-invariant Riemannian metric
 - Log-Euclidean metric
- Convex cone
 - Bregman divergences

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 $Mat(n) = set of real n \times n matrices$

 (Mat(n), +, ·) is a vector space, under standard matrix addition (+) and scalar multiplication (·)

 $\dim(\mathrm{Mat}(n)) = n^2$

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• Frobenius inner product between $A = (a_{ij})_{i,j=1}^n$, $B = (b_{ij})_{i,j=1}^n$

$$\langle A, B \rangle_F = \operatorname{tr}(A^T B) = \sum_{i,j=1^n} a_{ij} b_{ij}$$

• Frobenius norm of an $n \times n$ matrix $A = (a_{ij})_{i,j=1}^n$

$$||A||_{F}^{2} = \operatorname{tr}(A^{T}A) = \sum_{i,j=1}^{n} a_{ij}^{2}$$

• Euclidean (Frobenius) distance between two $n \times n$ matrices A, B

$$d_E(A,B) = ||A - B||_F$$

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In the Euclidean metric, each $n \times n$ matrix A is equivalent to its vectorized version $vec(A) \in \mathbb{R}^{n^2}$

 $\langle \boldsymbol{A}, \boldsymbol{B} \rangle_{\boldsymbol{F}} = \langle \operatorname{vec}(\boldsymbol{A}), \operatorname{vec}(\boldsymbol{B}) \rangle$

 $||A||_{F} = ||vec(A))||$

 $d_E(A,B) = ||A - B||_F = ||\operatorname{vec}(A) - \operatorname{vec}(B)||$

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Sym(n) = set of real, symmetric $n \times n$ matrices

• Sym(*n*) is a vector subspace of Mat(*n*)

$$\dim(\operatorname{Sym}(n)) = \frac{n(n+1)}{2}$$

Sym⁺⁺(*n*) = set of real SPD $n \times n$ matrices

Sym⁺⁺(n) is an open subset in Sym(n) ⊂ Mat(n)
Sym⁺⁺(n) automatically inherits the Euclidean metric on Mat(n)

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- Simple to implement and efficient to compute
- Essentially treats matrices as vectors, without taking into account their inherent structures
- Not intrinsic to Sym⁺⁺(*n*)
- May lead to swelling effect (mean of a set of SPD matrices might have larger determinant than the component matrices, Arsigny et al 2007)
- (Sym⁺⁺(n), d_E) is an incomplete metric space: Cauchy sequences, {A_n}, ||A_n − A_m||_F arbitrarily small, may not converge

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• Unitary (orthogonal) invariance: $CC^T = I \iff C^{-1} = C^T$

$$d_E(CAC^{-1}, CBC^{-1}) = d_E(A, B)$$

• Corresponds to e.g. rotation invariance of Euclidean distance in \mathbb{R}^n

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Geometry of SPD matrices - Outline

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- X = random vector in \mathbb{R}^n
 - Affine transformation

 $X \to \Gamma_{A,b}(X) = AX + b$, $A \in Mat(n)$ invertible $, b \in \mathbb{R}^n$

• Transformed mean vector

$$\mu_{\Gamma_{A,b}(X)} = A\mu_X + b$$

Transformed covariance matrix

 $C_{\Gamma_{A,b}(X)} = AC_X A^T$

.

d = distance or divergence on Sym⁺⁺(n) X, Y = random vectors in \mathbb{R}^n

$$X \rightarrow AX + b$$
, $Y \rightarrow AY + b$

Affine invariance

 $d(AC_XA^T, AC_YA^T) = d(C_X, C_Y)$

• Scale invariance: $A = \sqrt{sl}$, s > 0, b = 0

 $d(sC_X, sC_Y) = d(C_X, C_Y)$

d = distance or divergence on Sym⁺⁺(n) X, Y = random vectors in \mathbb{R}^n

 $X \rightarrow AX + b$, $Y \rightarrow AY + b$

• Unitary (orthogonal) invariance: $AA^T = I \iff A^T = A^{-1}, b = 0$ $d(AC_XA^{-1}, AC_YA^{-1}) = d(C_X, C_Y)$

e.g. A is a rotation matrix

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d = distance or divergence on Sym⁺⁺(n) X, Y = random vectors in \mathbb{R}^n

• Invariance under inversion

$$d(C_X^{-1}, C_Y^{-1}) = d(C_X, C_Y)$$

• For two Gaussian densities $\rho_1 = \mathcal{N}(0, C_X)$ and $\rho_2 = \mathcal{N}(0, C_Y)$

$$d(\rho_1, \rho_2) = d(C_X^{-1}, C_Y^{-1}) = d(C_X, C_Y)$$

 d(ρ₁, ρ₂) can be equally measured via either the distance/divergence between the corresponding covariance matrices or precision matrices.

- Affine invariance
- Scale invariance
- Unitary (orthogonal) invariance
- Invariance under inversion
- The corresponding data transformations

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$\mathcal{M} = n$ -dimensional manifold

- Locally Euclidean (ℝⁿ)
- Generalizations of two-dimensional regular surfaces in \mathbb{R}^3
- Examples
 - **R**^{*n*}
 - Open subsets of Rⁿ
 - n-dimensional unit sphere

$$\mathbb{S}^{n-1} = \{x \in \mathbb{R}^n : x_1^2 + \dots + x_n^2 = 1\}$$

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Smooth manifold - tangent vectors and tangent spaces

• Smooth curve $\gamma: (a, b) \to \mathbb{R}^3$, $\gamma'(t) \neq 0$

Tangent vector at t_0 : $V = \gamma'(t_0)$

- Regular surface $\mathcal{S} \subset \mathbb{R}^3$:
 - Tangent vector at a point $P \in S$

$$oldsymbol{V} = \gamma'(oldsymbol{0}), \hspace{1em} \gamma: (-\epsilon,\epsilon) o \mathcal{S}, \gamma(oldsymbol{0}) = oldsymbol{P}$$

• Tangent plane $T_P(S)$

 $T_P(S) = \{ \text{all tangent vectors at } P \}$ dim $(T_P(S)) = 2$ (2-dimensional plane)

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 $\mathcal{M} = n$ -dimensional smooth manifold

- Tangent vector: generalization of tangent vectors on regular surfaces (e.g. Do Carmo 1992, Jost 2008)
- Tangent space $T_P(\mathcal{M})$ at a point $P \in \mathcal{M}$

 $T_P(\mathcal{M}) = \{ \text{all tangent vectors at } P \}$ $\dim(T_P(\mathcal{M})) = n \text{ (}n\text{-dimensional vector space)}$

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Riemannian metric and Riemannian manifold

Riemannian manifold \mathcal{M} = smooth manifold \mathcal{M} + Riemannian metric

- Riemannian metric: a way to define distances on manifolds
- Riemannian metric: a family of inner products on the tangent spaces $T_P(\mathcal{M})$

$$\langle V, W \rangle_P, \quad V, W \in T_P(\mathcal{M})$$

that varies smoothly with P

• Length of a vector V in the tangent space $T_P(\mathcal{M})$

 $||V||_P = \sqrt{\langle V, V \rangle_P}$

Riemannian metric and Riemannian distance

A, *B* = two points on the manifold \mathcal{M} $\gamma : [a, b] \rightarrow \mathcal{M}$ = smooth curve joining *A*, *B*, $\gamma(a) = A$, $\gamma(b) = B$

- $\gamma'(t)$ is a tangent vector on the tangent space $T_{\gamma(t)}(\mathcal{M})$
- Length of the curve γ

$$L(\gamma) = \int_{a}^{b} ||\gamma'(t)||_{\gamma(t)} dt$$

• Riemannian distance between two points A and B on the manifold

$$d(A, B) = \inf\{L(\gamma) : \gamma(a) = A, \gamma(b) = B\}$$

• (*M*, *d*) is a metric space (satisfying positivity, symmetry, and triangle inequality)

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- Curves of zero acceleration (e.g. Do Carmo 1992)
- Generalization of straight lines in ℝⁿ
- Constant speed

$$\frac{d}{dt}||\gamma'(t)||_{\gamma(t)}=0$$

- Geodesically complete manifold:
 - (*M*, *d*) is a complete metric space
 - Geodesic of shortest length: ∃ a geodesic γ_{AB} joining any two points A, B, with

$$L(\gamma_{AB}) = d(A, B)$$

Geodesics - Example



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Riemannian exponential map

$$\begin{split} \mathrm{Exp}_{\mathcal{P}}: \ \mathcal{T}_{\mathcal{P}}(\mathcal{M}) \to \mathcal{M} \\ \text{Moving along the manifold, starting from point } \mathcal{P} \in \mathcal{M}, \text{ in the direction} \\ \mathcal{V} \in \mathcal{T}_{\mathcal{P}}(\mathcal{M}) \end{split}$$



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Covariance matrices & covariance operators

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Geodesics - Example

Geodesics may not be unique



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Sectional curvature: For a two-dimensional subspace
Σ_P ⊂ T_P(M) and a basis {X, Y} in Σ_P

$$\mathcal{K}(\Sigma_{\mathcal{P}}) = \mathcal{K}_{\mathcal{P}}(X, Y) = \frac{\langle \mathcal{R}(X, Y)X, Y \rangle_{\mathcal{P}}}{||X||_{\mathcal{P}}^{2}||Y||_{\mathcal{P}}^{2} - \langle X, Y \rangle_{\mathcal{P}}^{2}}$$

- R: Riemannian curvature tensor
- Measures how much a manifold deviates from Euclidean space
- Generalization of Gaussian curvature on regular surfaces in ℝ³
- Euclidean space \mathbb{R}^n : K = 0 (flat)
- Sphere \mathbb{S}^{n-1} : K = 1

- Cartan-Hadamard manifold: simply-connected, geodesically complete, nonpositive curvature
- Geodesics between any two points are unique
- Sym⁺⁺(n) under both the affine-invariant Riemannian metric and Log-Euclidean metric
- The exponential map Exp_P : T_P(M) → M is a diffeomorphism, i.e. it is a bijection, smooth, with smooth inverse

 $\mathrm{Log}_{P}:\mathcal{M}\to T_{P}(\mathcal{M})$

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Riemannian logarithm map

$\mathrm{Log}_{P}:\mathcal{M}\to T_{P}(\mathcal{M})$



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Riemannian manifold \mathcal{M} = smooth manifold \mathcal{M} + Riemannian metric

- $\bullet\,$ Every smooth manifold ${\cal M}$ admits a Riemannian metric
- Riemannian metrics are not unique
- $\bullet\,$ Each Riemannian metric defines a different distance on ${\cal M}$

Geometry of SPD matrices - Outline

Three different views of the set of SPD matrices

- Subset of Euclidean space
 - Euclidean metric
 - Invariances and Interpretations
- Piemannian manifold
 - Affine-invariant Riemannian metric
 - Log-Euclidean metric
- Convex cone
 - Bregman divergences

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Sym⁺⁺(*n*) = symmetric, positive definite $n \times n$ matrices

- Smooth manifold of dimension $\frac{n(n+1)}{2}$
- Tangent space T_P(Sym⁺⁺)(n) ≅ Sym(n) = vector space of symmetric matrices

- Has been studied extensively in mathematics
- Siegel (1943), Mostow (1955), Pennec et al (2006), Bhatia (2007), Moakher and Zéraï (2011), Bini and Iannazzo (2013)

Affine-invariant Riemannian metric

• Riemannian metric: On the tangent space $T_P(\text{Sym}^{++}(n)) \cong \text{Sym}(n)$, the inner product \langle , \rangle_P is

$$\langle V, W \rangle_{P} = \langle P^{-1/2} V P^{-1/2}, P^{-1/2} W P^{-1/2} \rangle_{F}$$

= tr(P^{-1} V P^{-1} W)
P \in Sym^{++}(n), V, W \in Sym(n)

Affine-invariance

$$\langle CAC^T, CBC^T \rangle_{CPC^T} = \langle A, B \rangle_P$$

for any invertible $n \times n$ matrix C

Affine-invariant Riemannian metric

- Geodesically complete Riemannian manifold, nonpositive curvature
- Unique geodesic joining $A, B \in \text{Sym}^{++}(n)$

$$\gamma_{AB}(t) = A^{1/2} (A^{-1/2} B A^{-1/2})^t A^{1/2}$$

 $\gamma_{AB}(0) = A, \quad \gamma_{AB}(1) = B$

• Riemannian (geodesic) distance

$$d_{\rm aiE}(A, B) = ||\log(A^{-1/2}BA^{-1/2})||_F$$

where log(A) is the principal logarithm of A

$$A = UDU^{T} = U \operatorname{diag}(\lambda_{1}, \dots, \lambda_{n})U^{T}$$
$$\log(A) = U \log(D)U^{T} = U \operatorname{diag}(\log \lambda_{1}, \dots, \log \lambda_{n})U^{T}$$

Affine-invariance

 $d_{aiE}(CAC^{T}, CBC^{T}) = d_{aiE}(A, B)$, any C invertible

• Scale invariance: $C = \sqrt{sI}$, s > 0,

 $d_{\mathrm{aiE}}(sA, sB) = d_{\mathrm{aiE}}(A, B)$

• Unitary (orthogonal) invariance: $CC^{T} = I \iff C^{-1} = C^{T}$

 $d_{\mathrm{aiE}}(CAC^{-1}, CBC^{-1}) = d_{\mathrm{aiE}}(A, B)$

• Invariance under inversion

$$d_{\mathrm{aiE}}(A^{-1},B^{-1})=d_{\mathrm{aiE}}(A,B)$$

• $(Sym^{++}(n), d_{aiE})$ is a complete metric space

- Close connection with Fisher-Rao metric in information geometry (e.g. Amari 1985, 2016)
- For two multivariate Gaussian probability densities $\rho_1 \sim \mathcal{N}(\mu, C_1)$, $\rho_2 \sim \mathcal{N}(\mu, C_2)$

 $d_{aiE}(C_1, C_2) = 2$ (Fisher-Rao distance between ρ_1 and ρ_2)

Affine-invariant Riemannian distance - Complexity

• For two matrices $A, B \in \text{Sym}^{++}(n)$

$$d_{\mathrm{aiE}}^2(A,B) = ||\log(A^{-1/2}BA^{-1/2})||_F^2 = \sum_{k=1}^{n} (\log \lambda_k)^2$$

where $\{\lambda_k\}_{k=1}^n$ are the eigenvalues of

 $A^{-1/2}BA^{-1/2}$ or equivalently $A^{-1}B$

- Matrix inversion, SVD, eigenvalue computation all have computational complexity O(n³)
- Therefore $d_{aiE}(A, B)$ has computational complexity $O(n^3)$

For a set $\{A_i\}_{i=1}^N$ of *N* SPD matrices, consider computing all the pairwise distances

 $d_{\mathrm{aiE}}(A_i, A_j) = ||\log(A_i^{-1/2}A_jA_i^{-1/2})||_F, \ 1 \le i, j \le N$

- The matrices A_i, A_i are all coupled together
- The computational complexity required is $O(N^2 n^3)$
- This is very large when N is large

Geometry of SPD matrices - Outline

Three different views of the set of SPD matrices

- Subset of Euclidean space
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- Log-Euclidean metric as a Riemannian metric
- Log-Euclidean distance as an approximation of the affine-invariant Riemannian distance
- Log-Euclidean vs. Euclidean

- N

- Arsigny, Fillard, Pennec, Ayache (SIAM Journal on Matrix Analysis and Applications 2007)
- Another Riemannian metric on Sym⁺⁺(n)
- Much faster to compute than the affine-invariant Riemannian distance on large sets of matrices
- Can be used to define many positive definite kernels on $Sym^{++}(n)$

Riemannian metric: On the tangent space $T_P(\text{Sym}^{++}(n))$

$$\langle V, W \rangle_P = \langle D \log(P)(V), D \log(P)(W) \rangle_F$$

 $P \in \text{Sym}^{++}(n), \quad V, W \in \text{Sym}(n)$

where

- D log is the Fréchet derivative of the function log : Sym⁺⁺(n) → Sym(n)
- $D\log(P)$: $Sym(n) \rightarrow Sym(n)$ is a linear map
- Explicit knowledge of (,)_P is not necessary for computing geodesics and Riemannian distances

.

• Unique geodesic joining $A, B \in Sym^{++}(n)$

 $\gamma_{AB}(t) = \exp[(1-t)\log(A) + t\log(B)]$

• Riemannian (geodesic) distance

 $d_{\mathrm{logE}}(A,B) = ||\log(A) - \log(B)||_{F}$

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• For two matrices $A, B \in \text{Sym}^{++}(n)$

$d_{\mathrm{logE}}(A,B) = ||\log(A) - \log(B)||_F$

- The computation of the log function, requiring an SVD, has computational complexity $O(n^3)$
- Therefore $d_{logE}(A, B)$ has computational complexity $O(n^3)$

.

For a set $\{A_i\}_{i=1}^N$ of *N* SPD matrices, consider computing all the pairwise distances

 $d_{\log E}(A_i, A_j) = ||\log(A_i) - \log(A_j)||_F, \quad 1 \leq i,j \leq N$

- The matrices A_i, A_j are all uncoupled
- The computational complexity required is O(Nn³)
- This is much faster than the affine-invariant Riemannian distance d_{aiE} when N is large

• Arsigny et al (2007): Log-Euclidean metric is a bi-invariant Riemannian metric associated with the Lie group operation

$$○: Sym^{++}(n) × Sym^{++}(n) → Sym^{++}(n) A ⊙ B = exp(log(A) + log(B)) = B ⊙ A$$

• Bi-invariance: for any $C \in \text{Sym}^{++}(n)$

 $d_{\text{logE}}[(A \odot C), (B \odot C)] = d_{\text{logE}}[(C \odot A), (C \odot B)] = d_{\text{logE}}(A, B)$

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Arsigny et al (2007): scalar multiplication operation

$$\circledast : \mathbb{R} \times \operatorname{Sym}^{++}(n) \to \operatorname{Sym}^{++}(n)$$
$$\lambda \circledast A = \exp(\lambda \log(A)) = A^{\lambda}$$

- (Sym⁺⁺(n), ⊙, ⊛) is a vector space, with ⊙ acting as vector addition and ⊛ acting as scalar multiplication
- Sym⁺⁺(n) under the Log-Euclidean metric is a Riemannian manifold with zero curvature

Vector space isomorphism

$$\log : (\operatorname{Sym}^{++}(n), \odot, \circledast) \to (\operatorname{Sym}(n), +, \cdot)$$
$$A \to \log(A)$$

The vector space (Sym⁺⁺(n), ⊙, ⊛) is not a subspace of the Euclidean vector space (Sym(n), +, ·)

Log-Euclidean inner product space

Log-Euclidean inner product (Li, Wang, Zuo, Zhang, ICCV 2013)

 $\langle A, B
angle_{\log E} = \langle \log(A), \log(B)
angle_F \ ||A||_{\log E} = ||\log(A)||_F$

• Log-Euclidean inner product space

 $(\text{Sym}^{++}(n), \odot, \circledast, \langle , \rangle_{\text{logE}})$

• Log-Euclidean distance

 $d_{\log E}(A, B) = ||\log(A) - \log(B)||_F = ||(A \odot B^{-1})||_{\log E}$

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Kernels with Log-Euclidean metric

- Positive definite kernels on Sym⁺⁺(n) defined with the Log-Euclidean inner product (,)_{logE} and norm || ||_{logE}
- Polynomial kernels

 $egin{aligned} \mathcal{K}(\mathcal{A},\mathcal{B}) &= (\langle \mathcal{A},\mathcal{B}
angle_{ ext{logE}} + oldsymbol{c}
angle)^d \ &= (\langle \log(\mathcal{A}),\log(\mathcal{B})
angle_{\mathcal{F}} + oldsymbol{c})^d, \quad oldsymbol{d} \in \mathbb{N}, oldsymbol{c} \geq 0 \end{aligned}$

Gaussian and Gaussian-like kernels

$$egin{aligned} \mathcal{K}(\mathcal{A},\mathcal{B}) &= \exp(-rac{1}{\sigma^2}||(\mathcal{A}\odot\mathcal{B}^{-1})||_{\mathrm{logE}}^p), & 0$$

- Log-Euclidean metric as a Riemannian metric
- Log-Euclidean distance as an approximation of the affine-invariant Riemannian distance
- Log-Euclidean vs. Euclidean

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Log-Euclidean distance as an approximation of the affine-invariant Riemannian distance

Affine-invariant Riemannian metric

- Riemannian exponential map: $\operatorname{Exp}_{P} : T_{P}(\operatorname{Sym}^{++}(n)) \to \operatorname{Sym}^{++}(n)$ $\operatorname{Exp}_{P}(V) = P^{1/2} \exp(P^{-1/2}VP^{-1/2})P^{1/2}$
- Riemannian logarithm map: $\text{Log}_P : \text{Sym}^{++}(n) \to T_P(\text{Sym}^{++}(n))$

$$Log_P(A) = P^{1/2} log(P^{-1/2}AP^{-1/2})P^{1/2} A \in Sym^{++}(n)$$

• At the identity matrix /

$$\operatorname{Exp}_{I}(V) = \exp(V), \quad \operatorname{Log}_{I}(A) = \log(A)$$

Log-Euclidean distance as an approximation of the affine-invariant Riemannian distance

• Affine-invariant Riemannian metric on the tangent space $T_P(\text{Sym}^{++}(n))$

$$\langle V, W \rangle_P = \langle P^{-1/2} V P^{-1/2}, P^{-1/2} W P^{-1/2} \rangle_F$$

 $V, W \in \text{Sym}(n)$

• On the tangent space $T_l(\text{Sym}^{++}(n))$

 $\langle V, W \rangle_I = \langle V, W \rangle_F, \quad ||V - W||_I = ||V - W||_F$

.

Log-Euclidean distance as an approximation of the affine-invariant Riemannian distance

• At the identity matrix /

 $||\log(A) - \log(B)||_F = ||\mathrm{Log}_I(A) - \mathrm{Log}_I(B)||_I$

- Log-Euclidean distance is obtained by projecting A, B onto the tangent space at the identity T_l(Sym⁺⁺(n))
- This viewpoint does not capture the intrinsic nature of the Log-Euclidean metric

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- Log-Euclidean metric as a Riemannian metric
- Log-Euclidean distance as an approximation of the affine-invariant Riemannian distance
- Log-Euclidean vs. Euclidean

- Euclidean: Sym⁺⁺(n) is an open subset in the Euclidean vector space (Sym(n), +, ·)
- Log-Euclidean: $(Sym^{++}(n), \odot, \circledast)$ is a vector space
- The two vector space structures are fundamentally different
- The differences between the metrics can be seen via the invariance properties

Unitary (orthogonal) invariance $CC^T = I \iff C^T = C^{-1}$

• Euclidean distance

$$d_E(CAC^{-1}, CBC^{-1}) = ||CAC^{-1} - CBC^{-1}||_F$$

= $||A - B||_F = d_E(A, B)$

• Log-Euclidean distance

$$d_{\log E}(CAC^{-1}, CBC^{-1}) = ||\log(CAC^{-1}) - \log(CBC^{-1})||_F$$

= $||\log(A) - \log(B)||_F = d_{\log E}(A, B)$

Log-Euclidean distance is scale-invariant

 $\begin{aligned} d_{\text{logE}}(sA, sB) &= ||\log(sA) - \log(sB)||_F \\ &= ||\log(A) - \log(B)||_F = d_{\text{logE}}(A, B) \end{aligned}$

• Euclidean distance is not scale-invariant

 $d_E(sA, sB) = s||A - B||_F = sd_E(A, B)$

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• Log-Euclidean distance is inversion-invariant

$$d_{\log E}(A^{-1}, B^{-1}) = ||\log(A^{-1}) - \log(B^{-1})||$$

= || - log(A) + log(B)||_F = d_{\log E}(A, B)

• Euclidean distance is not inversion-invariant

$$d_E(A^{-1}, B^{-1}) = ||A^{-1} - B^{-1}||_F$$

 $\neq ||A - B||_F = d_E(A, B)$

As metric spaces

- $(Sym^{++}(n), d_E)$ is incomplete
- $(Sym^{++}(n), d_{logE})$ is complete

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Summary of comparison

- The two metrics are fundamentally different
- Euclidean metric is extrinsic to Sym⁺⁺(*n*)
- Log-Euclidean metric is intrinsic to $Sym^{++}(n)$
- The vector space structures are fundamentally different
- They have different invariance properties

Geometry of SPD matrices - Outline

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 - Bregman divergences

Bregman divergences

- $\Omega = \text{convex subset in } \mathbb{R}^n$
- $\phi: \Omega \to \mathbb{R}$ = differentiable, strictly convex function
- Bregman divergence on Ω (Bregman, 1967)

$$B_{\phi}(x, y) = \phi(x) - \phi(y) - \langle \nabla \phi(y), x - y \rangle$$

Divergence properties

 $egin{aligned} & B_{\phi}(x,y) \geq 0, \ & B_{\phi}(x,y) = 0 \Longleftrightarrow x = y \end{aligned}$

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Bregman divergences

More generally, ϕ induces a parametrized family of divergences $\{d_{\phi}^{\alpha}\}$ (Zhang, Neural Computation, 2004)

$$d^{\alpha}_{\phi}(x,y) = \frac{4}{1-\alpha^2} \left[\frac{1-\alpha}{2} \phi(x) + \frac{1+\alpha}{2} \phi(y) - \phi\left(\frac{1-\alpha}{2}x + \frac{1+\alpha}{2}y\right) \right]$$
$$-1 < \alpha < 1$$

Limiting cases

$$d_{\phi}^{1}(x,y) = \lim_{\alpha \to 1} d_{\phi}^{\alpha}(x,y) = B_{\phi}(x,y)$$
$$d_{\phi}^{-1}(x,y) = \lim_{\alpha \to -1} d_{\phi}^{\alpha}(x,y) = B_{\phi}(y,x)$$

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Alpha Log-Determinant divergences

Chebbi and Moakher (Linear Algebra and Its Applications 2012) $\Omega = \text{Sym}^{++}(n), \phi(X) = -\log \det(X)$

$$d_{\text{logdet}}^{\alpha}(A, B) = \frac{4}{1 - \alpha^2} \log \frac{\det(\frac{1 - \alpha}{2}A + \frac{1 + \alpha}{2}B)}{\det(A)^{\frac{1 - \alpha}{2}} \det(B)^{\frac{1 + \alpha}{2}}}$$
$$-1 < \alpha < 1$$

Limiting cases

 $d_{\text{logdet}}^{1}(A, B) = \lim_{\alpha \to 1} d_{\text{logdet}}^{\alpha}(A, B) = \text{tr}(B^{-1}A - I) - \log \det(B^{-1}A)$ (Burg divergence) $d_{\text{logdet}}^{-1}(A, B) = \lim_{\alpha \to -1} d_{\text{logdet}}^{\alpha}(A, B) = \text{tr}(A^{-1}B - I) - \log \det(A^{-1}B)$

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Alpha Log-Determinant divergences

• $\alpha = 0$: Symmetric Stein divergence (also called *S*-divergence)

$$d_{\text{logdet}}^{0}(A,B) = 4\left[\log \det\left(\frac{A+B}{2}\right) - \frac{1}{2}\log \det(AB)\right] = 4d_{\text{stein}}^{2}(A,B)$$

• Sra (NIPS 2012):

$$d_{\text{stein}}(A,B) = \sqrt{\log \det \left(rac{A+B}{2}
ight) - rac{1}{2}\log \det(AB)}$$

is a metric (satisfying positivity, symmetry, and triangle inequality)

Alpha Log-Determinant divergences - Properties

Positivity

 $egin{aligned} & d^lpha_{ ext{logdet}}(A,B) \geq 0 \ & d^lpha_{ ext{logdet}}(A,B) = 0 \Longleftrightarrow A = B \end{aligned}$

• In general, they are not symmetric and are not metrics.

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Alpha Log-Determinant divergences - Properties

Affine-invariance

 $d_{\text{logdet}}^{\alpha}(CAC^{T}, CBC^{T}) = d_{\text{logdet}}^{\alpha}(A, B), \text{ any } C \text{ invertible}$

• Scale invariance: $C = \sqrt{sI}$, s > 0,

$$\textit{d}^{lpha}_{
m logdet}(\textit{sA},\textit{sB}) = \textit{d}^{lpha}_{
m logdet}(\textit{A},\textit{B})$$

• Unitary (orthogonal) invariance: $CC^{T} = I \iff C^{-1} = C^{T}$

$$d_{\text{logdet}}^{\alpha}(CAC^{-1}, CBC^{-1}) = d_{\text{logdet}}^{\alpha}(A, B)$$

Alpha Log-Determinant divergences - Properties

Dual-symmetry

 $\textit{d}^{lpha}_{
m logdet}(\textit{A},\textit{B}) = \textit{d}^{-lpha}_{
m logdet}(\textit{B},\textit{A})$

 $\alpha = 0$: symmetry

$$d^0_{\mathrm{logdet}}(A,B) = d^0_{\mathrm{logdet}}(B,A)$$

• Dual-invariance under inversion

$$d_{\text{logdet}}^{\alpha}(A^{-1}, B^{-1}) = d_{\text{logdet}}^{-\alpha}(A, B)$$

 $\alpha = 0$: invariance under inversion

$$d_{\text{logdet}}^0(A^{-1}, B^{-1}) = d_{\text{logdet}}^0(A, B)$$

Connection with the Rényi divergences

- P_1, P_2 = Borel probability density functions on \mathbb{R}^n
 - For 0 < r < 1, the Rényi divergence (Rényi, 1961) of order r between P₁ and P₂ is

$$d_R^r(P_1, P_2) = -\frac{1}{1-r} \log \int_{\mathbb{R}^n} P_1(x)^r P_2(x)^{1-r} dx$$

 As r → 1, the Rényi divergence becomes the Kullback-Leibler divergence (Kullback, 1951)

$$d_{KL}(P_1, P_2) = \int_{\mathbb{R}^n} P_1(x) \log \frac{P_1(x)}{P_2(x)} dx$$

Connection with the Rényi divergences

For two multivariate Gaussian density functions $P_1 \sim \mathcal{N}(\mu, C_1)$ and $P_2 \sim \mathcal{N}(\mu, C_2)$ (same mean)

$$d_{R}^{r}(P_{1}, P_{2}) = \frac{1}{2(1-r)} \log \left[\frac{\det[(1-r)C_{1} + rC_{2}]}{\det(C_{1})^{1-r}\det(C_{2})^{r}} \right]$$
$$= \frac{r}{2} d_{\text{logdet}}^{(2r-1)}(C_{1}, C_{2})$$

$$d_{KL}(P_1, P_2) = \frac{1}{2} [tr(C_2^{-1}C_1 - I) - \log \det(C_2^{-1}C_1)]$$
$$= \frac{1}{2} d_{logdet}^1(C_1, C_2)$$

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- Can compute the log det function using the Cholesky decomposition. The computational complexity $O(n^3)$.
- For a set of *N* SPD matrices, the computational complexity required for computing all pairwise divergences $d_{logdet}^{\alpha}(A_i, A_j)$ is $O(N^2 n^3)$.
- No need to carry out matrix inversion and multiplication
- Much faster than affine-invariant Riemannian metric

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Cichocki, Cruces, Amari (Entropy 2015)

$$D^{(\alpha,\beta)}(A,B) = \frac{1}{\alpha\beta} \log \det \left[\frac{\alpha (AB^{-1})^{\beta} + \beta (AB^{-1})^{-\alpha}}{\alpha + \beta} \right],$$
$$\alpha > 0, \beta > 0$$

- A highly general family of divergences, encompassing many divergences and distances on Sym⁺⁺(n)
- Affine-invariant divergences

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Alpha-Beta Log-Determinant divergences

• Alpha Log-Determinant divergences

$$d_{\text{logdet}}^{\alpha}(A,B) = D^{(\frac{1-\alpha}{2},\frac{1+\alpha}{2})}(A,B)$$

• $\sqrt{D^{(\alpha,\alpha)}(A,B)}$ is a metric on Sym⁺⁺(*n*)

$$D^{(1/2,1/2)}(A,B) = 4d_{stein}^2(A,B)$$

• Squared affine-invariant Riemannian distance

$$\lim_{\alpha \to 0} D^{(\alpha,\alpha)}(A,B) = \frac{1}{2} ||\log(A^{-1/2}BA^{-1/2})||_F^2$$

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 $\{\lambda_k\}_{k=1}^n$ = eigenvalues of AB^{-1}

$$D^{(\alpha,\beta)}(A,B) = \frac{1}{\alpha\beta} \log\left(\frac{\alpha\lambda_k^{\beta} + \beta\lambda_k^{-\alpha}}{\alpha + \beta}\right)$$

- Require the computation of the eigenvalues of AB⁻¹
- Generally have the same computational complexity as the affine-invariant Riemannian distance

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Dryden, Koloydenko, Zhou (Annals of Applied Statistics 2009)

$$d_{E,\alpha}(A,B) = \frac{1}{\alpha} ||A^{\alpha} - B^{\alpha}||_{F}, \quad \alpha > 0$$

- Euclidean distance $d_{E,1}(A, B) = d_E(A, B)$
- Log-Euclidean distance as a limiting case

 $\lim_{\alpha \to 0} \textit{d}_{\textit{E},\alpha}(\textit{A},\textit{B}) = ||\log(\textit{A}) - \log(\textit{B})||_{\textit{F}}$

$$d_{E,\alpha}(A,B) = \frac{1}{lpha} ||A^{lpha} - B^{lpha}||_{F}, \quad lpha > 0$$

- Do not share the same invariance properties as the Log-Euclidean distance (neither scale-invariant nor inversion-invariant)
- For α ∉ N, these divergences have the same computational complexity as the Log-Euclidean distance

- Euclidean (Frobenius) distance and inner product
- Affine-invariant Riemannian distance
- Log-Euclidean distance and inner product
- Alpha Log-Determinant divergences, including symmetric Stein divergence
- Alpha-Beta Log-Determinant divergences
- Power-Euclidean distances

Properties of common distances and divergences

	Euclidean	Log-E	Affine-invariant	Stein
geodesic distance	Yes	Yes	Yes	No
affine invariance	No	No	Yes	Yes
scale invariance	No	Yes	Yes	Yes
unitary invariance	Yes	Yes	Yes	Yes
inversion invariance	No	Yes	Yes	Yes
inner product distance	Yes	Yes	No	No

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- Data representation by covariance matrices
- Geometry of SPD matrices
- Machine learning methods on covariance matrices

- Sparse coding and dictionary learning: Cherian and Sra (Trans. Neural Net. Learning Systems 2016), Harandi et al (Trans. Neural Net. Learning Systems 2016), Li et al (ICCV 2013), Sivalingam et al (PAMI 2016), Wu et al (Trans. Image Processing 2015)
- Metric learning: Huang et al (ICML 2015), Matsuzawa et al (ECCV 2016)
- Dimensionality reduction: Harandi et al (PAMI 2017)
- Kernel methods on covariance matrices

- Positive definite kernels defined with the Frobenius inner product $\langle\;,\;\rangle_{\it F}$ and norm $||\;||_{\it F}$
- Polynomial kernels

 $K(A,B) = (\langle A,B \rangle_F + c \rangle)^d = [\operatorname{tr}(A^TB) + c]^d, \quad d \in \mathbb{N}, c \ge 0$

• Gaussian and Gaussian-like kernels

$$K(A,B) = \exp(-\frac{1}{\sigma^2}||A-B||_F^p), \quad 0$$

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Kernels on SPD matrices with Log-Euclidean metric

- Positive definite kernels on Sym⁺⁺(n) defined with the Log-Euclidean inner product (,)_{logE} and norm || ||_{logE}
- Polynomial kernels

 $egin{aligned} \mathcal{K}(\mathcal{A},\mathcal{B}) &= (\langle \mathcal{A},\mathcal{B}
angle_{ ext{logE}} + oldsymbol{c}
angle)^d \ &= (\langle \log(\mathcal{A}),\log(\mathcal{B})
angle_{\mathcal{F}} + oldsymbol{c})^d, \quad oldsymbol{d} \in \mathbb{N}, oldsymbol{c} \geq 0 \end{aligned}$

Gaussian and Gaussian-like kernels

$$egin{aligned} \mathcal{K}(\mathcal{A},\mathcal{B}) &= \exp(-rac{1}{\sigma^2}||(\mathcal{A}\odot\mathcal{B}^{-1})||_{\mathrm{logE}}^p), & 0$$

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• Sra (NIPS 2012)

$$K(A, B) = \exp[-\sigma d_{\text{stein}}^2(A, B)]$$

is positive definite if and only if

$$\sigma \in \left\{\frac{1}{2}, 1 \dots, \frac{n-1}{2}\right\} \cup \left\{\sigma \in \mathbb{R} : \sigma > \frac{n-1}{2}\right\}$$

• One needs to be careful when fine-tuning σ to ensure the kernel remains positive definite.

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Kernels on SPD matrices with Affine-invariant Riemannian distance?

$K(A, B) = \exp[-\sigma d_{aiE}^2(A, B)]$

- *K* cannot be positive definite for all $\sigma > 0$, since the Riemannian manifold has nonpositive curvature (Feragen et al, CVPR 2015)
- Open question: Can K be positive definite for some specific choices of *σ*?

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- P. Li, Q. Wang, W. Zuo, and L. Zhang. Log-Euclidean kernels for sparse representation and dictionary learning, ICCV 2013
- D. Tosato, M. Spera, M. Cristani, and V. Murino. Characterizing humans on Riemannian manifolds, PAMI 2013

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Kernel methods with Log-Euclidean metric for image classification



H.Q. Minh (IIT)

Covariance matrices & covariance operators

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Example: KTH-TIPS2b data set



 $\mathbf{f}(x, y) = \left[R(x, y), G(x, y), B(x, y), \left| G^{0,0}(x, y) \right|, \dots \left| G^{3,4}(x, y) \right| \right]$

Example: ETH-80 data set



$\mathbf{f}(x,y) = [x,y,l(x,y),|l_x|,|l_y|]$

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Covariance matrices & covariance operators

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Better results with covariance operators (Part II)!

Method	KTH-TIPS2b	ETH-80
E	55.3%	64.4%
	(±7.6%)	(±0.9%)
Stein	73.1%	67.5%
	(±8.0%)	(±0.4%)
Log-E	74.1 %	71.1%
	(±7.4%)	(±1.0%)

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(4) (5) (4) (5)

Results from Cherian et al (PAMI 2013) using Nearest Neighbor

Method	Texture	Activity
Affine-invariant	85.5%	99.5%
Stein	85.5%	99.5%
Log-E	82.0%	96.5%

Texture: images from Brodatz and CURET datasets Activity: videos from Weizmann, KTH, and UT Tower datasets **Covariance Matrices and Applications**

- Data Representation by Covariance Matrices
- Geometry of SPD matrices
- Machine Learning Methods on Covariance Matrices and Applications in Computer Vision

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Thank you for listening! Questions, comments, suggestions?

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