

# Riemannian Optimization with its Application to Averaging Positive Definite Matrices

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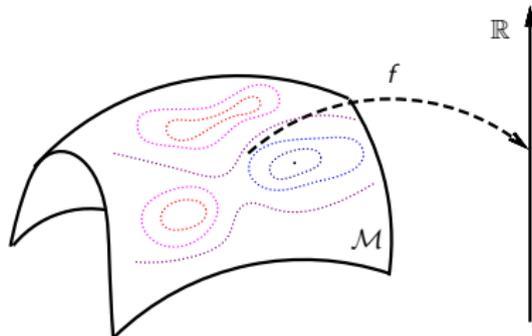
October 23, 2019

# Riemannian Optimization

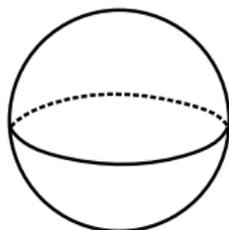
**Problem:** Given  $f(x) : \mathcal{M} \rightarrow \mathbb{R}$ , solve

$$\min_{x \in \mathcal{M}} f(x)$$

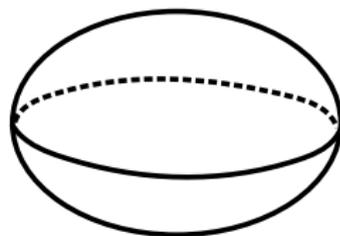
where  $\mathcal{M}$  is a Riemannian manifold.



# Examples of Manifolds



Sphere

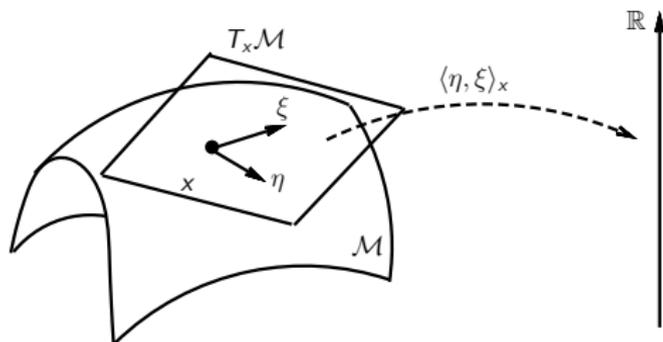


Ellipsoid

- Stiefel manifold:  $\text{St}(p, n) = \{X \in \mathbb{R}^{n \times p} \mid X^T X = I_p\}$
- Grassmann manifold: Set of all  $p$ -dimensional subspaces of  $\mathbb{R}^n$
- Set of fixed rank  $m$ -by- $n$  matrices
- And many more

# Riemannian Manifolds

Roughly, a Riemannian manifold  $\mathcal{M}$  is a smooth set with a smoothly-varying inner product on the tangent spaces.

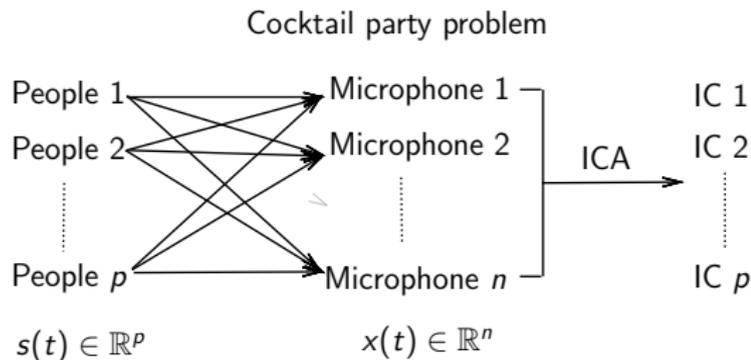


# Applications

Four applications are used to demonstrate the importances of the Riemannian optimization:

- Independent component analysis [CS93]
- Matrix completion problem [Van13]
- Geometric mean of symmetric positive definite matrices [ALM04, JVV12a, CS15]
- Elastic shape analysis of curves [SKJJ11, HGSA15]

# Application: Independent Component Analysis



- Observed signal is  $x(t) = As(t)$
- One approach:
  - Assumption:  $E\{s(t)s(t + \tau)\}$  is diagonal for all  $\tau$
  - $C_\tau(x) := E\{x(t)x(t + \tau)^T\} = AE\{s(t)s(t + \tau)^T\}A^T$

# Application: Independent Component Analysis

- Minimize joint diagonalization cost function on the Stiefel manifold [T106]:

$$f : \text{St}(p, n) \rightarrow \mathbb{R} : V \mapsto \sum_{i=1}^N \|V^T C_i V - \text{diag}(V^T C_i V)\|_F^2.$$

- $C_1, \dots, C_N$  are covariance matrices and  $\text{St}(p, n) = \{X \in \mathbb{R}^{n \times p} \mid X^T X = I_p\}$ .

# Application: Matrix Completion Problem

Matrix completion problem

	Movie 1	Movie 2		Movie $n$	
User 1		1		4	
User 2	3	5		4	
			5	1	
User $m$		2		5	3

Rate matrix  $M$

- The matrix  $M$  is sparse
- The goal: complete the matrix  $M$

# Application: Matrix Completion Problem

$$\begin{array}{ccc}
 & \text{movies} & & & \text{meta-user} & & \text{meta-movie} \\
 \left( \begin{array}{ccc}
 a_{11} & & a_{14} \\
 & & a_{24} \\
 & a_{33} & \\
 a_{41} & & \\
 & a_{52} & a_{53}
 \end{array} \right) & = & \left( \begin{array}{cc}
 b_{11} & b_{12} \\
 b_{21} & b_{22} \\
 b_{31} & b_{32} \\
 b_{41} & b_{42} \\
 b_{51} & b_{52}
 \end{array} \right) \left( \begin{array}{cccc}
 c_{11} & c_{12} & c_{13} & c_{14} \\
 c_{21} & c_{22} & c_{23} & c_{24}
 \end{array} \right)
 \end{array}$$

- Minimize the cost function

$$f : \mathbb{R}^{m \times n} \rightarrow \mathbb{R} : X \mapsto f(X) = \|P_{\Omega} M - P_{\Omega} X\|_F^2.$$

- $\mathbb{R}_r^{m \times n}$  is the set of  $m$ -by- $n$  matrices with rank  $r$ . It is known to be a Riemannian manifold.

# Application: Geometric Mean of Symmetric Positive Definite (SPD) Matrices

Computing the mean of a population of SPD matrices is important in medical imaging, image processing, radar signal processing, and elasticity. The desired properties are given in the ALM<sup>1</sup> list, some of which are

- if  $A_1, \dots, A_k$  commute, then  $G(A_1, \dots, A_k) = (A_1 \dots A_k)^{\frac{1}{k}}$ ;
- $G(A_{\pi(1)}, \dots, A_{\pi(k)}) = G(A_1, \dots, A_k)$ , with  $\pi$  a permutation of  $(1, \dots, k)$ ;
- $G(A_1, \dots, A_k) = G(A_1^{-1}, \dots, A_k^{-1})^{-1}$ ;
- $\det G(A_1, \dots, A_k) = (\det A_1 \dots \det A_k)^{\frac{1}{k}}$ ;

where  $A_1, \dots, A_k$  are SPD matrices, and  $G(\cdot, \dots, \cdot)$  denotes the geometric mean of arguments.

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<sup>1</sup>T. Ando, C.-K. Li, and R. Mathias, Geometric means, *Linear Algebra and Its Applications*, 385:305-334, 2004

# Application: Geometric Mean of Symmetric Positive Definite Matrices

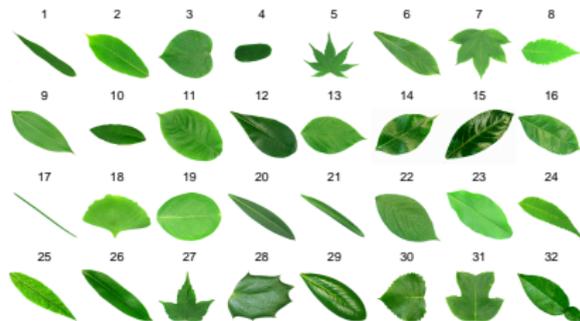
One geometric mean is the Karcher mean of the manifold of SPD matrices with the affine invariant metric, i.e.,

$$G(A_1, \dots, A_k) = \arg \min_{X \in \mathcal{S}_+^n} \frac{1}{2k} \sum_{i=1}^k \text{dist}^2(X, A_i),$$

where  $\text{dist}(X, Y) = \|\log(X^{-1/2} Y X^{-1/2})\|_F$  is the distance under the Riemannian metric

$$g(\eta_X, \xi_X) = \text{trace}(\eta_X X^{-1} \xi_X X^{-1}).$$

# Application: Elastic Shape Analysis of Curves



- Classification [LKS<sup>+</sup>12, HGSA15]
- Face recognition [DBS<sup>+</sup>13]



# Application: Elastic Shape Analysis of Curves

- Elastic shape analysis invariants:
  - Rescaling
  - Translation
  - Rotation
  - Reparametrization
- The shape space is a quotient space

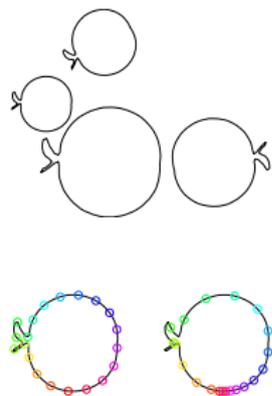
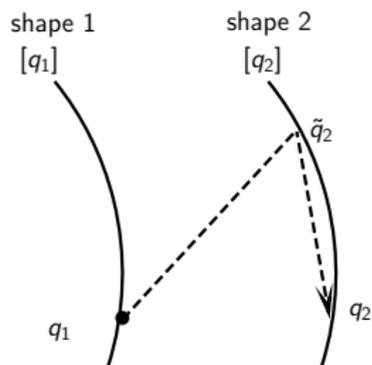


Figure: All are the same shape.

# Application: Elastic Shape Analysis of Curves



- Optimization problem  $\min_{q_2 \in [q_2]} \text{dist}(q_1, q_2)$  is defined on a Riemannian manifold
- Computation of a geodesic between two shapes
- Computation of Karcher mean of a population of shapes

# More Applications

- Role model extraction [MHB<sup>+</sup>16]
- Computations on SPD matrices [YHAG17]
- Phase retrieval problem [HGZ17]
- Blind deconvolution [HH17]
- Synchronization of rotations [Hua13]
- Computations on low-rank tensor
- Low-rank approximate solution for Lyapunov equation

# Iterations on the Manifold

Consider the following generic update for an iterative Euclidean optimization algorithm:

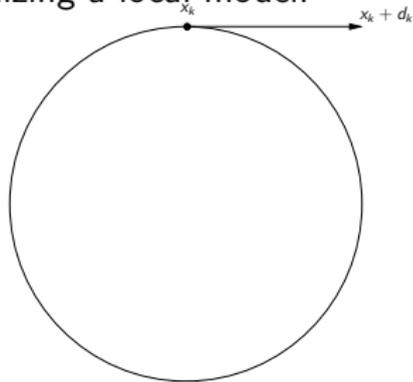
$$x_{k+1} = x_k + \Delta x_k = x_k + \alpha_k s_k .$$

This iteration is implemented in numerous ways, e.g.:

- Steepest descent:  $x_{k+1} = x_k - \alpha_k \nabla f(x_k)$
- Newton's method:  $x_{k+1} = x_k - [\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$
- Trust region method:  $\Delta x_k$  is set by optimizing a local model.

## Riemannian Manifolds Provide

- Riemannian concepts describing **directions** and **movement** on the manifold
- Riemannian analogues for **gradient** and **Hessian**



# Riemannian gradient and Riemannian Hessian

## Definition

The **Riemannian gradient** of  $f$  at  $x$  is the unique tangent vector in  $T_x M$  satisfying  $\forall \eta \in T_x M$ , the directional derivative

$$Df(x)[\eta] = \langle \text{grad } f(x), \eta \rangle$$

and  $\text{grad } f(x)$  is the direction of steepest ascent.

## Definition

The **Riemannian Hessian** of  $f$  at  $x$  is a symmetric linear operator from  $T_x M$  to  $T_x M$  defined as

$$\text{Hess } f(x) : T_x M \rightarrow T_x M : \eta \rightarrow \nabla_\eta \text{grad } f,$$

where  $\nabla$  is the affine connection.

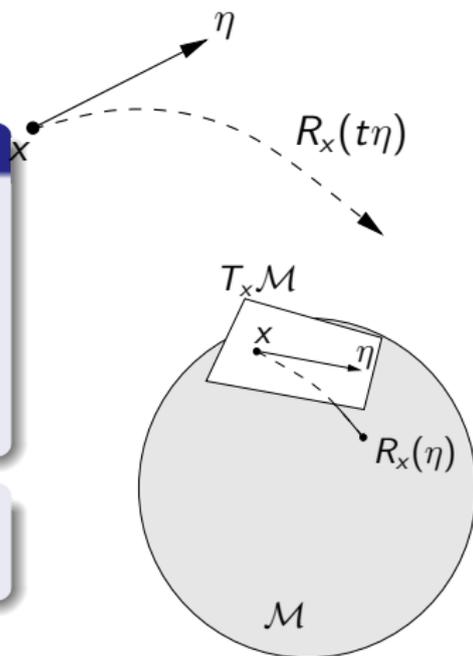
# Retractions

Euclidean	Riemannian
$x_{k+1} = x_k + \alpha_k d_k$	$x_{k+1} = R_{x_k}(\alpha_k \eta_k)$

## Definition

A **retraction** is a mapping  $R$  from  $TM$  to  $M$  satisfying the following:

- $R$  is continuously differentiable
  - $R_x(0) = x$
  - $D R_x(0)[\eta] = \eta$
- 
- maps tangent vectors back to the manifold
  - defines curves in a direction



# Categories of Riemannian optimization methods

Retraction-based: local information only

Line search-based: use local tangent vector and  $R_x(t\eta)$  to define line

- Steepest decent
- Newton

Local model-based: series of flat space problems

- Riemannian trust region Newton (RTR)
- Riemannian adaptive cubic overestimation (RACO)

# Categories of Riemannian optimization methods

## Retraction and transport-based: information from multiple tangent spaces

- Nonlinear conjugate gradient: multiple tangent vectors
- Quasi-Newton e.g. Riemannian BFGS: transport operators between tangent spaces

Additional element required for optimizing a cost function  $(M, g)$ :

- formulas for combining information from multiple tangent spaces.

# Vector Transports

## Vector Transport

- Vector transport: Transport a tangent vector from one tangent space to another
- $\mathcal{T}_{\eta_x} \xi_x$ , denotes transport of  $\xi_x$  to tangent space of  $R_x(\eta_x)$ .  $R$  is a retraction associated with  $\mathcal{T}$

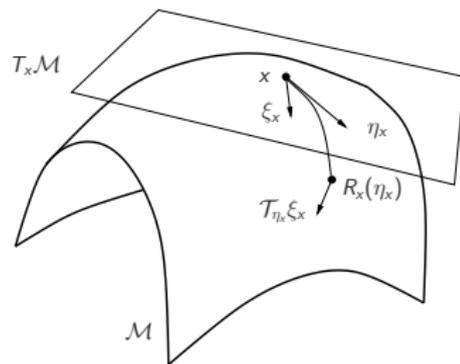


Figure: Vector transport.

# Retraction/Transport-based Riemannian Optimization

Given a retraction and a vector transport, we can generalize many Euclidean methods to the Riemannian setting. Do the Riemannian versions of the methods work well?

# Retraction/Transport-based Riemannian Optimization

Given a retraction and a vector transport, we can generalize many Euclidean methods to the Riemannian setting. Do the Riemannian versions of the methods work well?

No

- Lose many theoretical results and important properties;
- Impose restrictions on retraction/vector transport;

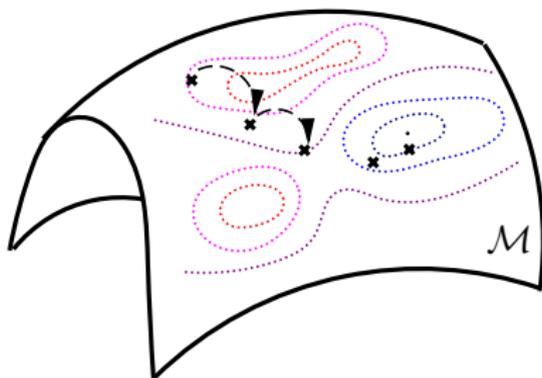
# Riemannian optimization methods

Elements required for optimizing a cost function  $(M, g)$ :

- an representation for points  $x$  on  $M$ , for tangent spaces  $T_x M$ , and for the inner products  $g_x(\cdot, \cdot)$  on  $T_x M$ ;
- choice of a retraction  $R_x : T_x M \rightarrow M$ ;
- formulas for  $f(x)$ ,  $\text{grad } f(x)$  and  $\text{Hess } f(x)$  (or its action);
- Computational and storage efficiency;

# Comparison with Constrained Optimization

- All iterates on the manifold
- Convergence properties of unconstrained optimization algorithms
- No need to consider Lagrange multipliers or penalty functions
- Exploit the structure of the constrained set



# Retraction/Transport-based Riemannian Optimization

## Benefits

- Increased generality does not compromise the **important theory**
- Less expensive than or similar to previous approaches
- May provide theory to explain behavior of algorithms specifically developed for a particular application – or closely related ones

## Possible Problems

- May be inefficient compared to algorithms that exploit application details

# Some History of Optimization On Manifolds (I)

[Luenberger \(1973\)](#), *Introduction to linear and nonlinear programming*. Luenberger mentions the idea of performing line search along geodesics, “which we would use if it were computationally feasible (which it definitely is not)”. Rosen (1961) essentially anticipated this but was not explicit in his Gradient Projection Algorithm.

[Gabay \(1982\)](#), *Minimizing a differentiable function over a differential manifold*. Steepest descent along geodesics; Newton’s method along geodesics; Quasi-Newton methods along geodesics. On Riemannian submanifolds of  $\mathbb{R}^n$ .

[Smith \(1993-94\)](#), *Optimization techniques on Riemannian manifolds*. Levi-Civita connection  $\nabla$ ; Riemannian exponential mapping; parallel translation.

# Some History of Optimization On Manifolds (II)

The “pragmatic era” begins:

[Manton \(2002\)](#), *Optimization algorithms exploiting unitary constraints*  
“The present paper breaks with tradition by not moving along geodesics”. The geodesic update  $\text{Exp}_x \eta$  is replaced by a projective update  $\pi(x + \eta)$ , the *projection* of the point  $x + \eta$  onto the manifold.

[Adler, Dedieu, Shub, et al. \(2002\)](#), *Newton's method on Riemannian manifolds and a geometric model for the human spine*. The exponential update is relaxed to the general notion of *retraction*. The geodesic can be replaced by any (smoothly prescribed) curve tangent to the search direction.

## Some History of Optimization On Manifolds (III)

Theory, efficiency, and library design improve dramatically:

[Absil, Baker, Gallivan \(2004-07\)](#), Theory and implementations of Riemannian Trust Region method. Retraction-based approach. Matrix manifold problems, software repository:

<http://www.math.fsu.edu/~cbaker/GenRTR>

Anasazi Eigenproblem package in Trilinos Library at Sandia National Laboratory

[Ring and With \(2012\)](#), combination of differentiated retraction and isometric vector transport for convergence analysis of RBFGS

[Absil, Gallivan, Huang \(2009-2017\)](#), Complete theory of Riemannian Quasi-Newton and related transport/retraction conditions, Riemannian SR1 with trust-region, RBFGS on partly smooth problems, A C++ library: <http://www.math.fsu.edu/~whuang2/ROPTLIB>

# Some History of Optimization On Manifolds (IV)

[Absil, Mahony, Sepulchre \(2007\)](#) Nonlinear conjugate gradient using retractions.

[Ring and With \(2012\)](#), Global convergence analysis for Fletcher-Reeves Riemannian nonlinear CG method with the strong wolfe conditions under a strong assumption.

[Sato, Iwai \(2013-2015\)](#), Global convergence analysis for Fletcher-Reeves type Riemannian nonlinear CG method with the strong wolfe conditions under a mild assumption; and global convergence for Dai-Yuan type Riemannian nonlinear CG method with the weak wolfe conditions under mild assumptions.

[Zhu \(2017\)](#), Global convergence for Riemannian version of Dai's nonmonotone nonlinear CG method.

# Some History of Optimization On Manifolds (V)

[Bonnabel \(2011\)](#), Riemannian stochastic gradient descent method.

[Sato, Kasai, Mishra\(2017\)](#), Riemannian stochastic gradient descent method using variance reduction or quasi-Newton.

[Becigneul, Ganea\(2018\)](#), Riemannian versions of ADAM, ADAGRAD, and AMSGRAD for geodesically convex functions.

[Zhang, Sra\(2016-2018\)](#), Riemannian first-order methods for geodesically convex optimization.

[Liu, Boumal\(2019\)](#), Riemannian optimization with constraints.

# Some History of Optimization On Manifolds (VI)

Hosseini, Grohs, Huang, Uschmajew, Boumal, (2015-2016),  
Lipschitz-continuous functions on Riemannian manifolds

Zhang, Sra(2016-2018), Riemannian first-order methods for geodesically  
convex optimization.

Bento, Ferreira, Melo(2017), Riemannian proximal point method for  
geodesically convex optimization.

Chen, Ma, So, Zhang(2018), Riemannian proximal gradient method.

Many people Application interests start to increase noticeably

# Riemannian Optimization Libraries

Riemannian optimization libraries for general problems:

- [Boumal, Mishra, Absil, Sepulchre\(2014\)](#)  
Manopt (Matlab library)
- [Townsend, Koep, Weichwald \(2016\)](#)  
Pymanopt (Python version of manopt)
- [Huang, Absil, Gallivan, Hand \(2018\)](#)  
ROPTLIB (C++ library, interfaces to Matlab and Julia)
- [Martin, Raim, Huang, Adraghi\(2018\)](#)  
ManifoldOptim (R wrapper of ROPTLIB)
- [Meghwanshi, Jawanpuria, Kunchukuttan, Kasai, Mishra \(2018\)](#)  
McTorch (Riemannian optimization for deep learning)

# Application: Averaging Symmetric Positive Definite matrices

Joint work with:

- Pierre-Antoine Absil, Professor of Mathematical Engineering, *Université catholique de Louvain*
- Kyle A. Gallivan, Professor of Mathematics, *Florida State University*
- Xinru Yuan, Data scientist, *Esurance*



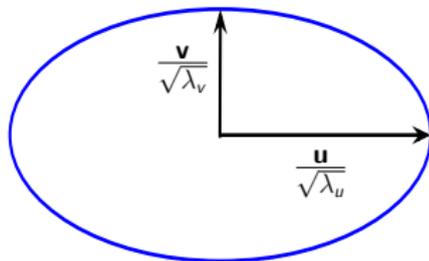
# Application: Averaging Symmetric Positive Definite matrices

## Definition

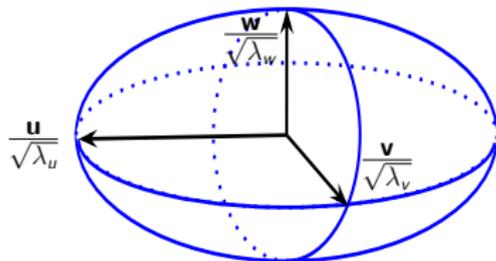
A symmetric matrix  $A$  is called **positive definite**  $A \succ 0$  iff all its eigenvalues are positive.

$$\mathcal{S}_{++}^n = \{A \in \mathbb{R}^{n \times n} : A = A^T, A \succ 0\}$$

2 × 2 SPD matrix



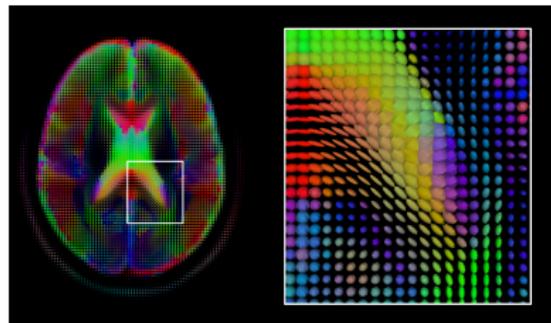
3 × 3 SPD matrix



# Motivation of Averaging SPD Matrices

- Possible applications of SPD matrices

- Diffusion tensors in medical imaging [CSV12, FJ07, RTM07]
- Describing images and video [LWM13, SFD02, ASF<sup>+</sup>05, TPM06, HWSC15]



- Motivation of averaging SPD matrices

- Aggregate several noisy measurements of the same object
- Subtask in interpolation methods, segmentation, and clustering

# Averaging Schemes: from Scalars to Matrices

Let  $A_1, \dots, A_K$  be SPD matrices.

- Generalized arithmetic mean:  $\frac{1}{K} \sum_{i=1}^K A_i$

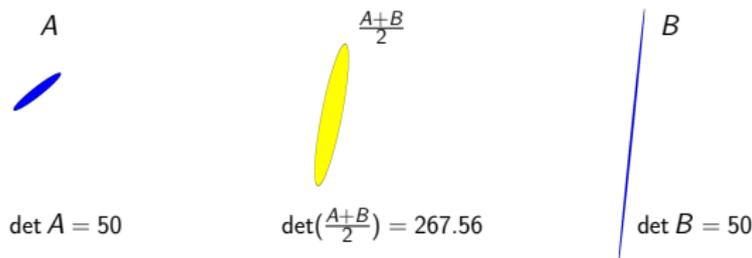
→ Not appropriate in many practical applications

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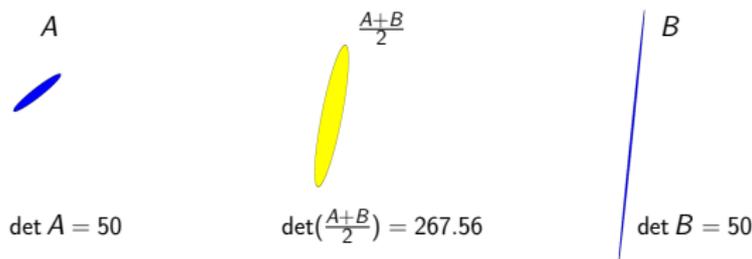


# Averaging Schemes: from Scalars to Matrices

Let  $A_1, \dots, A_K$  be SPD matrices.

- Generalized arithmetic mean:  $\frac{1}{K} \sum_{i=1}^K A_i$

→ Not appropriate in many practical applications



- Generalized geometric mean:  $(A_1 \cdots A_K)^{1/K}$

→ Not appropriate due to non-commutativity

→ How to define a matrix geometric mean?

# Desired Properties of a Matrix Geometric Mean

The desired properties are given in the ALM list<sup>2</sup>, some of which are:

- $G(A_{\pi(1)}, \dots, A_{\pi(K)}) = G(A_1, \dots, A_K)$  with  $\pi$  a permutation of  $(1, \dots, K)$
- if  $A_1, \dots, A_K$  commute, then  $G(A_1, \dots, A_K) = (A_1, \dots, A_K)^{1/K}$
- $G(A_1, \dots, A_K)^{-1} = G(A_1^{-1}, \dots, A_K^{-1})$
- $\det(G(A_1, \dots, A_K)) = (\det(A_1) \cdots \det(A_K))^{1/K}$

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<sup>2</sup>T. Ando, C.-K. Li, and R. Mathias, *Geometric means*, Linear Algebra and Its Applications, 385:305-334, 2004

# Geometric Mean of SPD Matrices

- A well-known mean on the manifold of SPD matrices is the **Karcher mean** [Kar77]:

$$G(A_1, \dots, A_K) = \arg \min_{X \in \mathcal{S}_{++}^n} \frac{1}{2K} \sum_{i=1}^K \delta^2(X, A_i), \quad (1)$$

where  $\delta(X, Y) = \|\log(X^{-1/2} Y X^{-1/2})\|_F$  is the geodesic distance under the affine-invariant metric

$$g(\eta_X, \xi_X) = \text{trace}(\eta_X X^{-1} \xi_X X^{-1})$$

- The Karcher mean defined in (1) satisfies all the geometric properties in the ALM list [LL11]

# Algorithms

$$G(A_1, \dots, A_k) = \operatorname{argmin}_{X \in \mathcal{S}_{++}^n} \frac{1}{2K} \sum_{i=1}^K \delta^2(X, A_i),$$

- Riemannian steepest descent [RA11, Ren13]
- Riemannian Barzilai-Borwein method [IP15]
- Riemannian Newton method [RA11]
- Richardson-like iteration [BI13]
- Riemannian steepest descent, conjugate gradient, BFGS, and trust region Newton methods [JVV12b]
- Limited-memory Riemannian BFGS method [YHAG16]

# Remarks

Previous work:

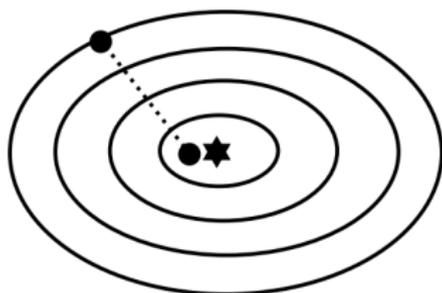
- Riemannian steepest descent and Riemannian CG methods are preferred in terms of computational time
- High rate of convergence of Riemannian Newton method does not make up for extra complexity

New results:

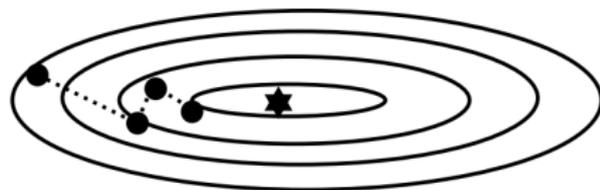
- Explain the preference for the first order methods
- More options of retractions and vector transports
- More efficient implementation
- Limited-memory Riemannian BFGS method

# Conditioning of the Objective Function

Hemstitching phenomenon  
for steepest descent



well-conditioned Hessian



ill-conditioned Hessian

- **Small** condition number  $\Rightarrow$  **fast** convergence
- **Large** condition number  $\Rightarrow$  **slow** convergence

# Conditioning of the Karcher Mean Objective Function

- **Riemannian metric:**

$$g_X(\xi, \eta) = \text{trace}(\xi X^{-1} \eta X^{-1})$$

- **Euclidean metric:**

$$g_X(\xi, \eta) = \text{trace}(\xi \eta)$$

## Condition number $\kappa$ of Hessian at the minimizer $\mu$ :

- Hessian of Riemannian metric:

- $\kappa(H^R) \leq 1 + \frac{\ln(\max \kappa_i)}{2}$ , where  $\kappa_i = \kappa(\mu^{-1/2} A_i \mu^{-1/2})$

- $\kappa(H^R) \leq 20$  if  $\max(\kappa_i) = 10^{16}$

- Hessian of Euclidean metric:

- $\frac{\kappa^2(\mu)}{\kappa(H^R)} \leq \kappa(H^E) \leq \kappa(H^R) \kappa^2(\mu)$

- $\kappa(H^E) \geq \kappa^2(\mu)/20$

# Implementations

- Retraction

- Exponential mapping:  $\text{Exp}_X(\xi) = X^{1/2} \exp(X^{-1/2} \xi X^{-1/2}) X^{1/2}$
- Second order approximation retraction [JVV12b]:

$$R_X(\xi) = X + \xi + \frac{1}{2} \xi X^{-1} \xi$$

- Vector transport

- Parallel translation:  $\mathcal{T}_{p_\eta}(\xi) = Q \xi Q^T$ , with  $Q = X^{\frac{1}{2}} \exp\left(\frac{X^{-\frac{1}{2}} \eta X^{-\frac{1}{2}}}{2}\right) X^{-\frac{1}{2}}$
- Vector transport by parallelization [HAG16]: essentially an identity
- Requires orthogonal basis for tangent spaces

# Implementations

- Cholesky  $X_k = L_k L_k^T$  assumed to be computed on each step
- $B_X$  of  $\mathbb{T}_X \mathcal{S}_{++}^n$ , the orthonormal basis of  $\mathbb{T}_X \mathcal{S}_{++}^n$

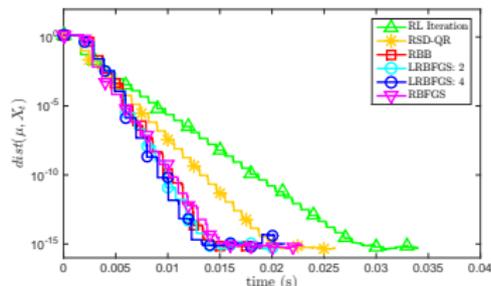
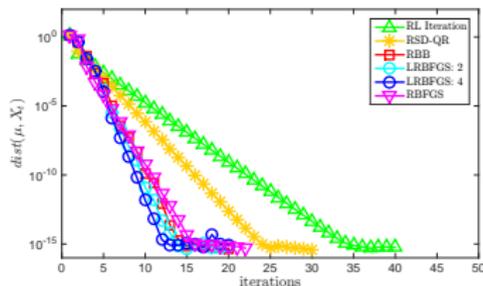
$$B_X = \{L e_i e_i^T L^T : i = 1, \dots, n\} \cup \left\{ \frac{1}{\sqrt{2}} L (e_i e_j^T + e_j e_i^T) L^T, \right. \\ \left. i < j, i = 1, \dots, n, j = 1, \dots, n \right\},$$

!where  $\{e_1, \dots, e_n\}$  is the standard basis of  $n$ -dimensional Euclidean space.

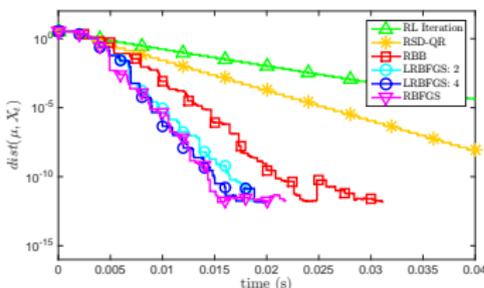
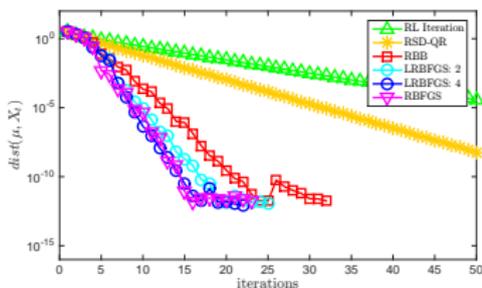
- orthonormal under  $g_X(\xi_X, \eta_X)$ .
- $\xi_X = B_X \hat{\xi}_X \leftrightarrow \xi_X = L S L^T$ , where  $S$  is symmetric and contains scale coefficients.
- intrinsic representation of tangent vectors is easily maintained.

Numerical Results:  $K = 100$ , size =  $3 \times 3$ ,  $d = 6$ 

- $1 \leq \kappa(A_i) \leq 200$

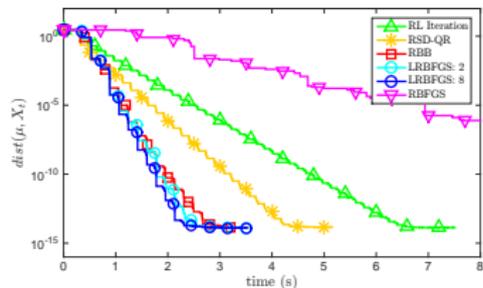
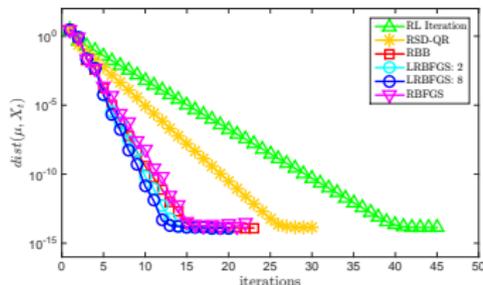


- $10^3 \leq \kappa(A_i) \leq 10^7$

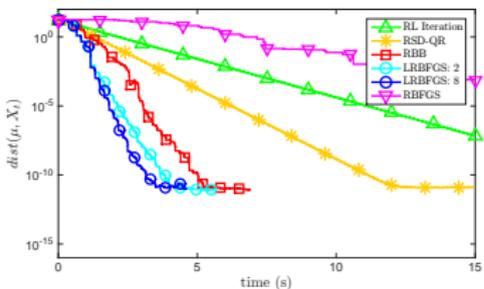
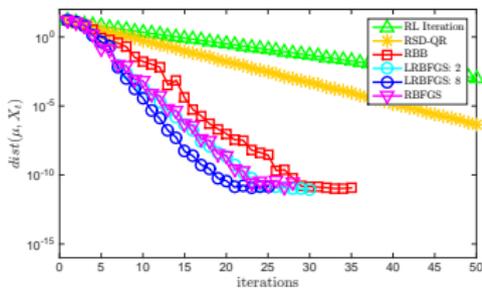


# Numerical Results: $K = 30$ , size = $100 \times 100$ , $d = 5050$

- $1 \leq \kappa(A_i) \leq 20$

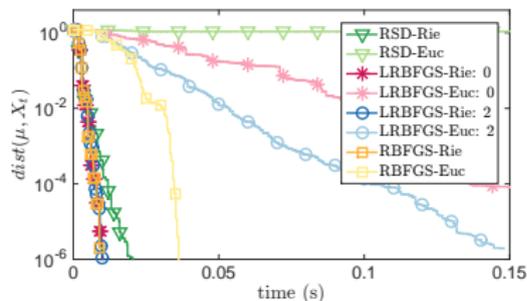
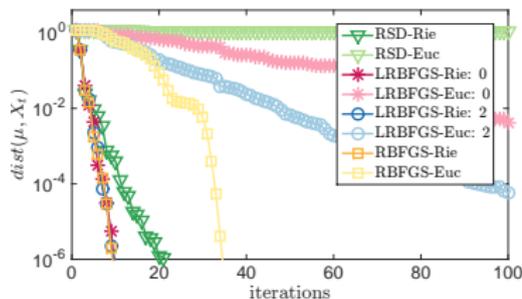


- $10^4 \leq \kappa(A_i) \leq 10^7$

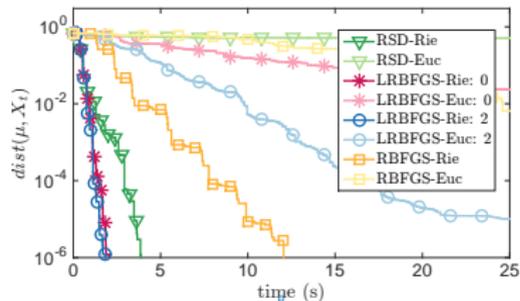
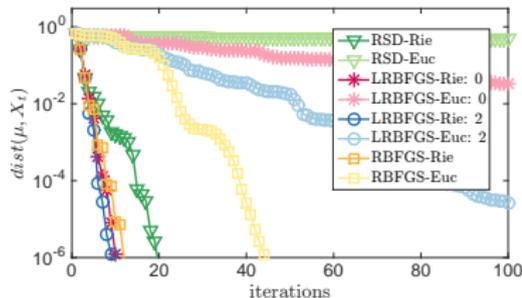


# Numerical Results: Riemannian vs. Euclidean Metrics

- $K = 100$ ,  $n = 3$ , and  $1 \leq \kappa(A_i) \leq 10^6$ .



- $K = 30$ ,  $n = 100$ , and  $1 \leq \kappa(A_i) \leq 10^5$ .



# Summary

- Introduced the framework of Riemannian optimization
- Used applications to show the importance of Riemannian optimization
- Briefly reviewed the history of Riemannian optimization
- Introduced the mean of SPD matrices
- Demonstrated the performance of the Riemannian methods

# Thank you

Thank you!

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