A Riemannian Limited-Memory BFGS Algorithm for Computing the Matrix Geometric Mean

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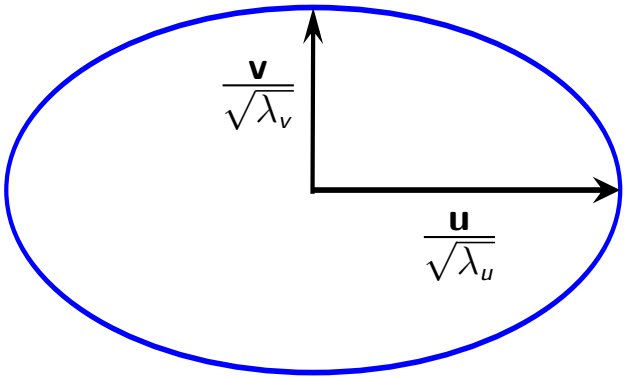
Symmetric Positive Definite (SPD) Matrix

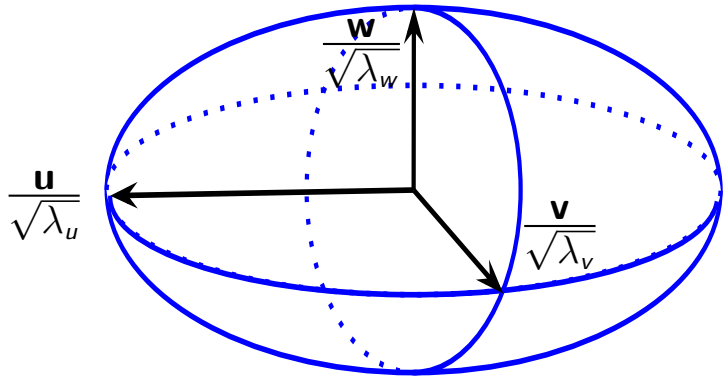
Definition

A symmetric matrix A is called positive definite if $x^T Ax > 0$ for all nonzero vector $x \in \mathbb{R}^n$.

2×2 SPD matrix

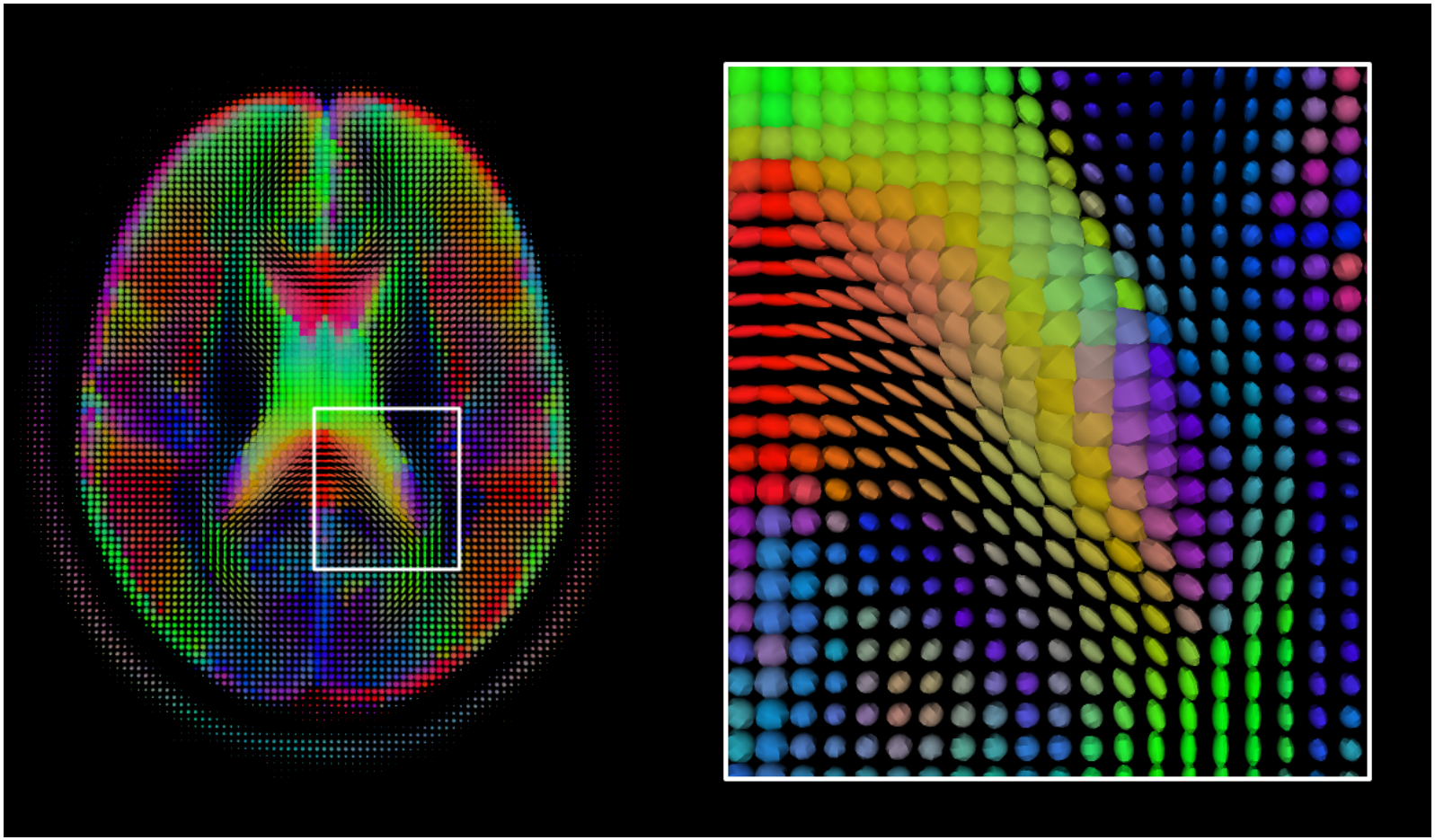


3×3 SPD matrix



Possible Applications of SPD Matrices

- Diffusion tensors in medical imaging



Motivation of Averaging SPD Matrices

- Subtask in interpolation schemes
  - Example: retrieve a tensor field between measured tensor values at sparse points [PFA06][1]

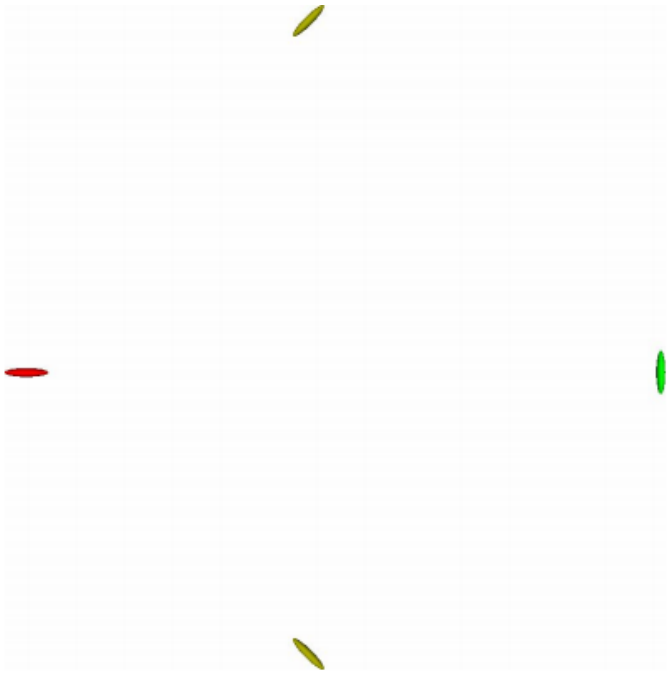


Figure : Initial tensor measurements

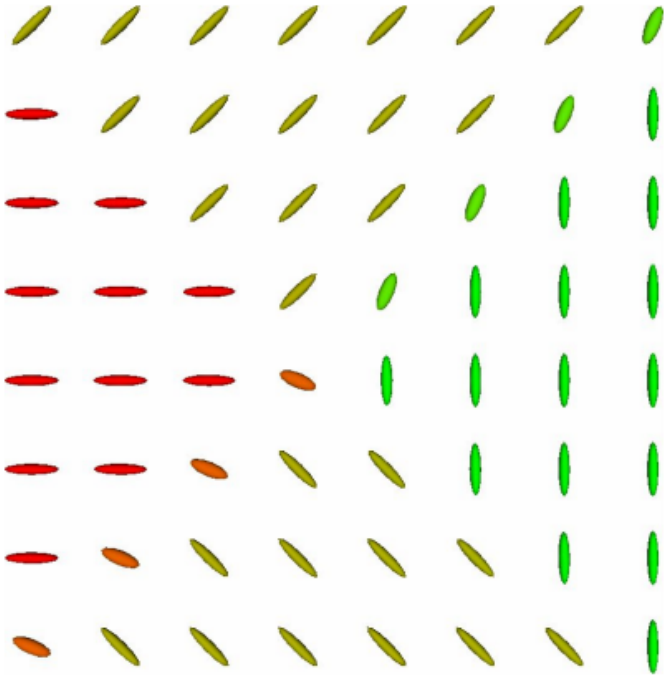


Figure : Retrieved tensor field after a certain interpolation scheme

[1] X. Pennec, P. Fillard and N. Ayache, *A Riemannian framework for tensor computing*, International Journal of Computer Vision, 2006

Averaging Schemes: from Scalars to Matrices

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

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

  $\rightarrow$ Not appropriate in many practical applications

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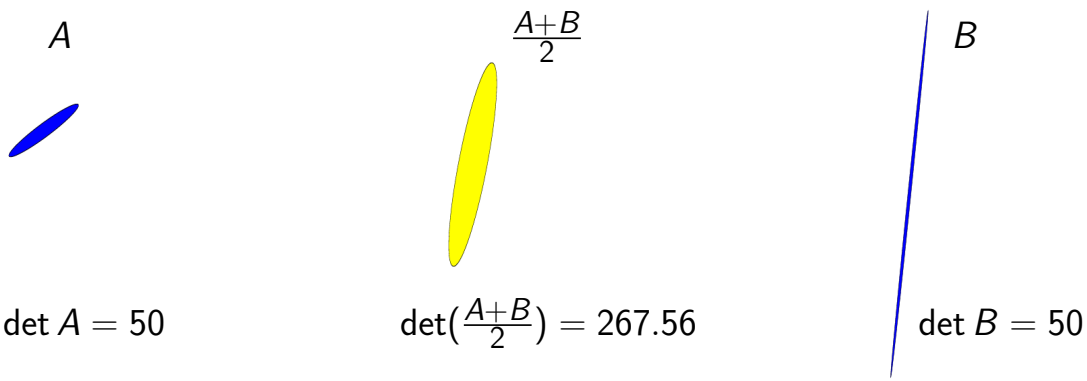

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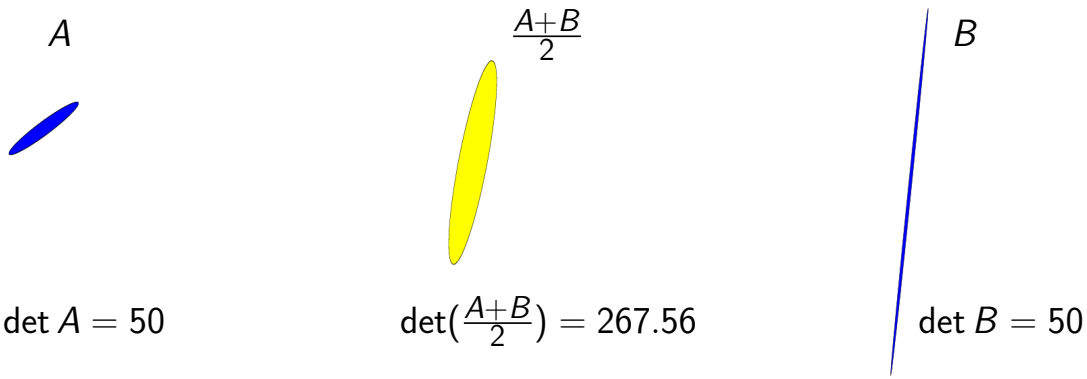

- Generalized geometric mean: $(A_1 \cdots A_K)^{1/K}$

  $\rightarrow$ Not appropriate due to non-commutativity

  $\rightarrow$ How to define a matrix geometric mean?

Desired Properties of a Matrix Geometric Mean

The desired properties are given in the ALM list[2], some of which are:

- Invariance under permutation:
  $G(A_{\pi(1)}, \ldots, A_{\pi(K)}) = G(A_1, \ldots, A_K)$ with π a permutation of $(1, \ldots, K)$

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

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- Invariance under inversion:
  $G(A_1, \ldots, A_K)^{-1} = G(A_1^{-1}, \ldots, A_K^{-1})$
- Determinant equality:
  $\det(G(A_1, \ldots, A_K)) = (\det(A_1) \cdots \det(A_K))^{1/K}$

[2] 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]:

$$G(A_1, \ldots, G_K) = \arg\min_{X \in \mathcal{S}^n_{++}} \frac{1}{2K} \sum_{i=1}^{K} \mathrm{dist}^2(X, A_i),$$

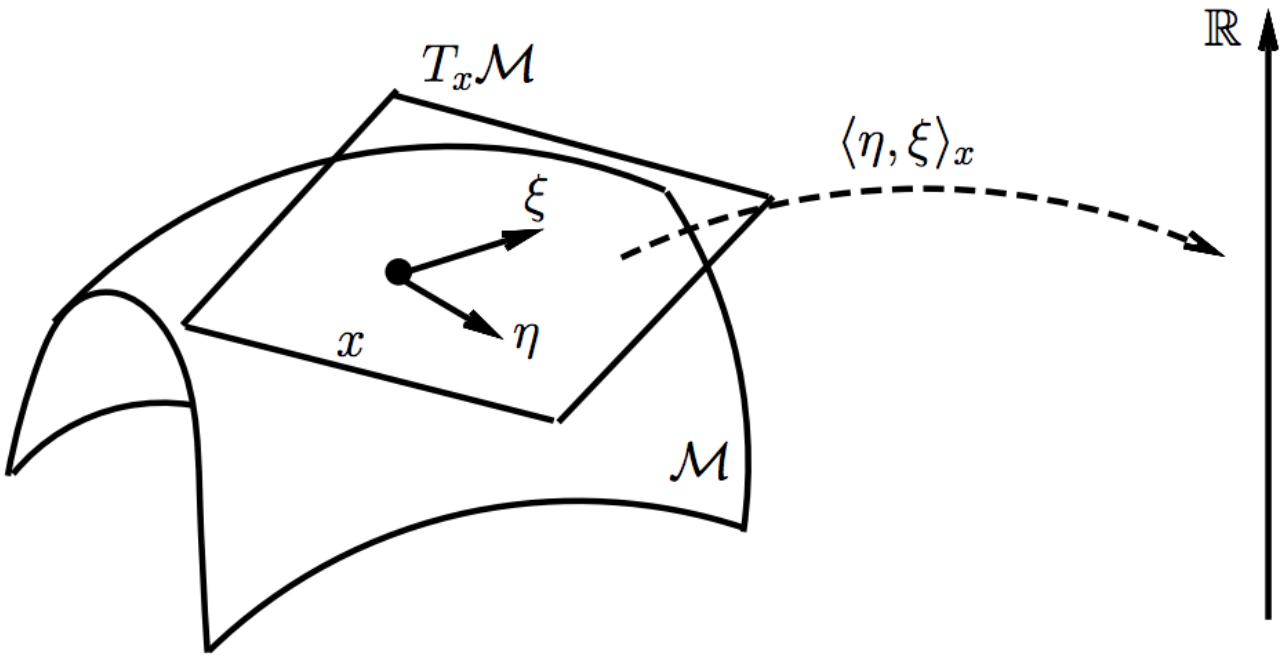
where $\mathrm{dist}(X, Y) = \| \log(X^{-1/2} Y X^{-1/2}) \|_F$ is the distance under the Riemannian metric

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

It has been shown recently [LL11] that the Karcher mean satisfies all the geometric properties in the ALM list.

Riemannian Manifolds

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



Manifold of SPD Matrices

- Let $\mathcal{S}_{++}^n$ be the manifold of SPD matrices
- Tangent space at $X \in \mathcal{S}_{++}^n$:

$$\mathrm{T}_X \mathcal{S}_{++}^n = \{S \in \mathbb{R}^{n \times n} : S = S^T\}$$

- Dimension: $d = n(n+1)/2$
- Riemannian metric:

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

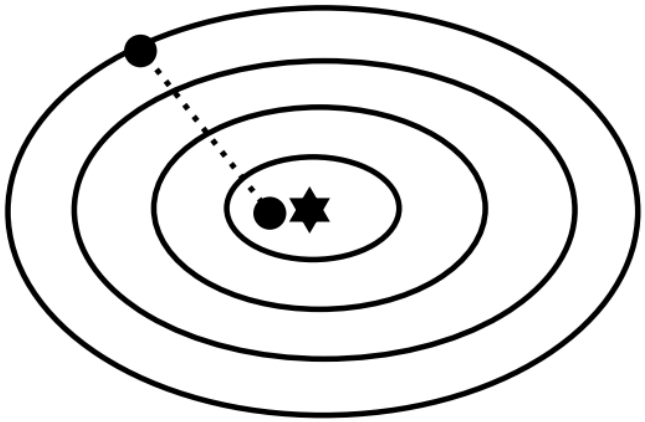
Algorithms

$$G(A_1, \ldots, G_K) = \arg\min_{X \in \mathcal{S}_{++}^n} \frac{1}{2K} \sum_{i=1}^{K} \mathrm{dist}^2(X, A_i),$$

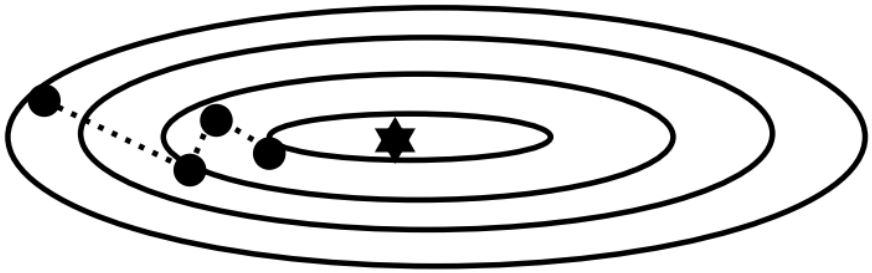
- Riemannian steepest descent [RA11]
- Riemannian steepest descent, conjugate gradient, BFGS, and trust region Newton methods [JVV12]
- Richardson-like iteration [BI13]
- Limited-memory Riemannian BFGS method [YHAG16]

Karcher Mean of SPD Matrices

Hemstitching phenomenon
for steepest descent



well-conditioned Hessian



ill-conditioned Hessian

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

Karcher Mean of SPD Matrices

Conditioning of the Riemannian Hessian of F at the minimizer:

- For the cost function $F(X) = \frac{1}{2K}\sum_{i=1}^{K} \mathrm{dist}^2(A_i, X)$, we have

$$1 \leq \frac{\mathrm{Hess}\, F(X)[\Delta X, \Delta X]}{\|\Delta X\|^2} \leq 1 + \frac{\ln(\max \kappa_i)}{2},$$

  where κ_i is the condition number of A_i.

- If $\max \kappa_i = 10^{10}$, then $1 + \frac{\ln(\max \kappa_i)}{2} \approx 12.51$.

Optimization Algorithm: from Euclidean to Riemannian

- Update formula:

$$x_{k+1} = x_k + \alpha_k \eta_k,$$

  where η_k is the search direction and α_k is the stepsize.

- Search direction:

$$\eta_k = -B_k^{-1} \operatorname{grad} f(x_k).$$

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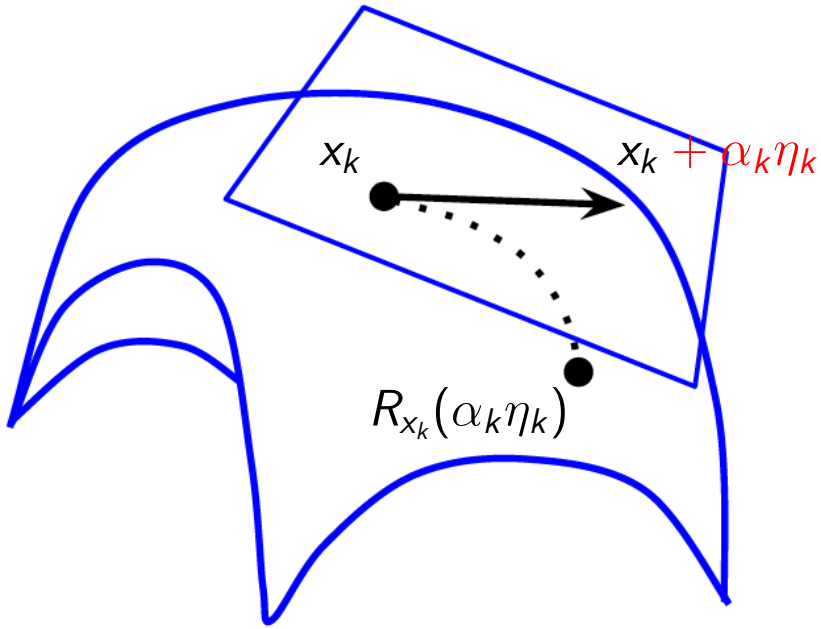


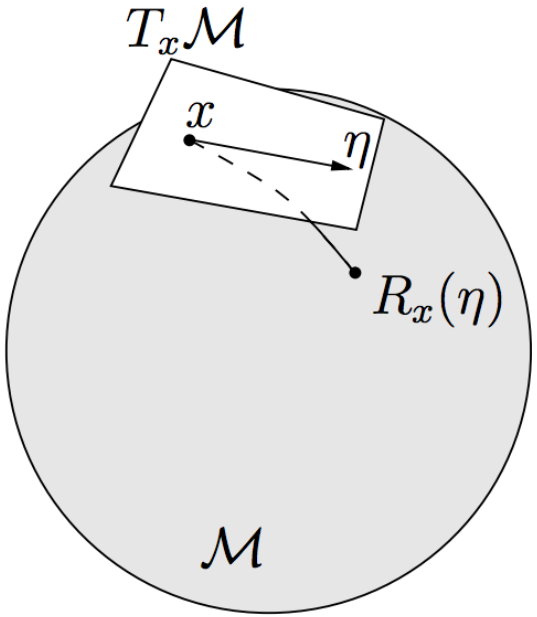
Optimization on a Manifold

Retraction

Definition

A retraction is a mapping R from $T\mathcal{M}$ to $\mathcal{M}$ satisfying the following:

- R is continuously differentiable
- $R_x(0) = x$
- $\mathrm{D}R_x(0)(\eta) = \eta$



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

Riemannian Optimization Algorithm

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

- Steepest Descent:

$$\eta_k = -\operatorname{grad} f(x_k)$$

- Newton's Method:

$$\eta_k = -\operatorname{Hess} f(x_k)^{-1} \operatorname{grad} f(x_k)$$

- Quasi-Newton Method:

$$\eta_k = -B_k^{-1} \operatorname{grad} f(x_k)$$

Riemannian Gradient and Hessian

- Riemannian gradient:

$$\operatorname{grad} F(X) = \frac{1}{K}\sum_{i=1}^{K} A_i^{1/2}\log(A_i^{-1/2}XA_i^{-1/2})A_i^{-1/2}X^{1/2}$$

- Riemannian Hessian:

$$\begin{aligned}\operatorname{Hess} F(X)[\xi_X] =& \frac{1}{2K}\sum_{i=1}^{K}\xi_X\log(A_i^{-1}X) - \frac{1}{2K}\sum_{i=1}^{K}\log(XA_i^{-1})\xi_X \\ &+ \frac{1}{K}\sum_{i=1}^{K} X\mathrm{D}(\log)(A_i^{-1}X)[A_i^{-1}\xi_X]\end{aligned}$$

Richardson-like Iteration [BI13]

- Update formula:

$$X_{k+1} = X_k - \alpha X_k^{1/2} \sum_{i=1}^{K} \log(X_k^{1/2} A_i^{-1} X_k^{1/2}) X_k^{1/2}$$

- Stepsize:

$$\alpha = 2/\sum_{i=1}^{K} \frac{\kappa_i + 1}{\kappa_i - 1} \log \kappa_i,$$

  where κ_i is the condition number of matrix $X_k^{1/2} A_i^{-1} X_k^{1/2}$

- Local linear convergence is proved

Richardson-like Iteration, Ctd

- The Richardson-like iteration can be considered from the view of Riemannian optimization algorithm

- $X_{k+1} = R_{X_k}(\alpha \eta_k)$
  - Search direction: $\eta_k = -\operatorname{grad} F(X_k)$
  - Choice of retraction: $R_X(\eta) = X + \eta$
  - Stepsize α satisfies the Wolfe condition

BFGS Quasi-Newton Algorithm: from Euclidean to Riemannian

- Search direction:

$$\eta_k = -B_k^{-1} \operatorname{grad} f(x_k)$$

- B_k update:

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k},$$

where $s_k = x_{k+1} - x_k$, and $y_k = \operatorname{grad} f(x_{k+1}) - \operatorname{grad} f(x_k)$.

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On a manifold:

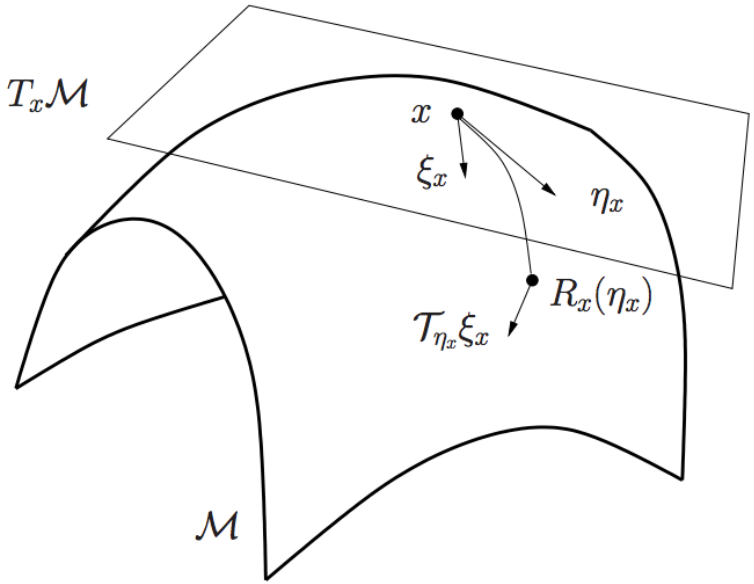
replaced by $R_{x_k}^{-1}(x_{k+1})$

on different tangent spaces

Vector Transport

Vector Transport

- Transport a tangent vector from one tangent space to another
- $\mathcal{T}_{\eta_x}\xi_x$, denotes transport of ξ_x to tangent space of $R_x(\eta_x)$



Riemannian BFGS (RBFGS) Algorithm

- Update formula:

$$x_{k+1} = R_{x_k}(\alpha_k \eta_k) \text{ with } \eta_k = -\mathcal{B}_k^{-1} \operatorname{grad} f(x_k)$$

- $\mathcal{B}_k$ update [HGA15]:

$$\mathcal{B}_{k+1} = \tilde{\mathcal{B}}_k - \frac{\tilde{\mathcal{B}}_k s_k (\tilde{\mathcal{B}}_k s_k)^\flat}{(\tilde{\mathcal{B}}_k s_k)^\flat s_k} + \frac{y_k y_k^\flat}{y_k^\flat s_k},$$

where $s_k = \mathcal{T}_{\alpha_k \eta_k} \alpha_k \eta_k$, $y_k = \beta_k^{-1} \operatorname{grad} f(x_{k+1}) - \mathcal{T}_{\alpha_k \eta_k} \operatorname{grad} f(x_k)$, and $\tilde{\mathcal{B}}_k = \mathcal{T}_{\alpha_k \eta_k} \circ \mathcal{B}_k \circ \mathcal{T}_{\alpha_k \eta_k}^{-1}$.

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- Stores and transports $\mathcal{B}_k^{-1}$ as a dense matrix

- Requires excessive computation time and storage space for large-scale problem

Limited-memory RBFGS (LRBFGS)

Riemannian BFGS:

- $\mathcal{B}_{k+1} = \tilde{\mathcal{B}}_k - \frac{\tilde{\mathcal{B}}_k s_k (\tilde{\mathcal{B}}_k s_k)^\flat}{(\tilde{\mathcal{B}}_k s_k)^\flat s_k} + \frac{y_k y_k^\flat}{y_k^\flat s_k}$,
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  and $\tilde{\mathcal{B}}_k = \mathcal{T}_{\alpha_k \eta_k} \circ \mathcal{B}_k \circ \mathcal{T}^{-1}_{\alpha_k \eta_k}$

Limited-memory Riemannian BFGS:

- Stores only the m most recent s_k and y_k
- Transports those vectors to the new tangent space rather than the entire matrix $\mathcal{B}_k^{-1}$
- Computational and storage complexity depends upon m

Limited-memory RBFGS (LRBFGS), Ctd

- $\mathcal{B}_k^{-1}$ update [HGA15]:

$$\begin{aligned}\mathcal{B}_k^{-1} &= \tilde{\mathcal{V}}_k^\flat \tilde{\mathcal{V}}_{k-1}^\flat \cdots \tilde{\mathcal{V}}_{k-m}^\flat \tilde{\mathcal{H}}_{k+1}^0 \tilde{\mathcal{V}}_{k-m} \cdots \tilde{\mathcal{V}}_{k-1} \tilde{\mathcal{V}}_k \\ &\quad + \rho_{k-m} \tilde{\mathcal{V}}_k^\flat \tilde{\mathcal{V}}_{k-1}^\flat \cdots \tilde{\mathcal{V}}_{k-m+1}^\flat s_{k-m}^{(k+1)} s_{k-m}^{(k+1)^\flat} \tilde{\mathcal{V}}_{k-m+1} \cdots \tilde{\mathcal{V}}_{k-1} \tilde{\mathcal{V}}_k \\ &\quad + \cdots + \rho_k s_k^{(k+1)} s_k^{(k+1)^\flat},\end{aligned}$$

  where $\tilde{\mathcal{V}}_i = \mathrm{id} - \rho_i y_i^{(k+1)} s_i^{(k+1)^\flat}$, $\rho_i = \frac{1}{g(y_i, s_i)}$, $\tilde{\mathcal{H}}_{k+1}^0 = \frac{g(s_k, y_k)}{g(y_k, y_k)}\,\mathrm{id}$, and $s_i^{(k+1)}$ represents a tangent vector in $\mathrm{T}_{x_{k+1}}\mathcal{M}$ given by transporting s_i, and likewise for $y_i^{(k+1)}$

- Avoids expensive matrix operations

- Requires less memory

Complexity Comparison

RBFGS		Limited-memory RBFGS	
Action	Complexity	Action	Complexity
get $\tilde{\mathcal{B}}_{k+1}^{-1}$ from $\mathcal{B}_k^{-1}$	$O(d^2)$	-	-
$\mathcal{B}^{-1}\eta$	$O(d^2)$	$\mathcal{B}^{-1}\eta$	$O(md)$

- d denotes the dimension of SPD manifold

Algorithm Comparison

Not sure where to put this table

Algorithm	Convergence
Riemannian steepest descent	global, linear
Riemannian BFGS	global(convex), superlinear
Riemannian limited-memory BFGS	global(convex), faster than linear
Riemannian Newton's method	global, quadratic

Outline

- Background of the SPD Karcher mean computation
- A brief description of the limited-memory RBFGS (LRBFGS) method
- Apply the LRBFGS to the SPD Karcher mean computation
  - Practical implementation
  - Experiments on various data sets

Implementations

- Cost function:

$$F(X) = \frac{1}{2K}\sum_{i=1}^{K} \mathrm{dist}^2(A_i, X)$$
$$= \frac{1}{2K}\sum_{i=1}^{K} \| \log(A_i^{-1/2} X A_i^{-1/2}) \|_F^2$$

- Riemannian gradient:

$$\mathrm{grad}\, F(X) = \frac{1}{K}\sum_{i=1}^{K} A_i^{1/2} \log(A_i^{-1/2} X A_i^{-1/2}) A_i^{-1/2} X^{1/2}$$

- The dominant computation time is on the function evaluation

Implementations

- Efficient representations of tangent vectors, see [YHAG16]
- Retraction
  - Exponential mapping: $\mathrm{Exp}_X(\xi_X) = X^{1/2}\exp(X^{-1/2}\xi_X X^{-1/2})X^{1/2}$
- Vector transport
  - Parallel translation: $\mathcal{T}_{p\eta_X}(\xi_X) = Q\xi_X Q^T$,

    where $Q = X^{1/2}\exp(\frac{X^{-1/2}\eta_X X^{-1/2}}{2})X^{-1/2}$

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  - Second order retraction [JVV12]: $R_X(\xi_X) = X + \xi_X + \frac{1}{2}\xi_X X^{-1}\xi_X$
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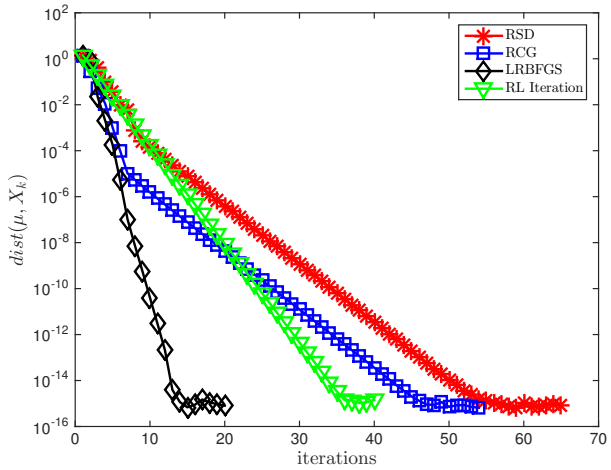
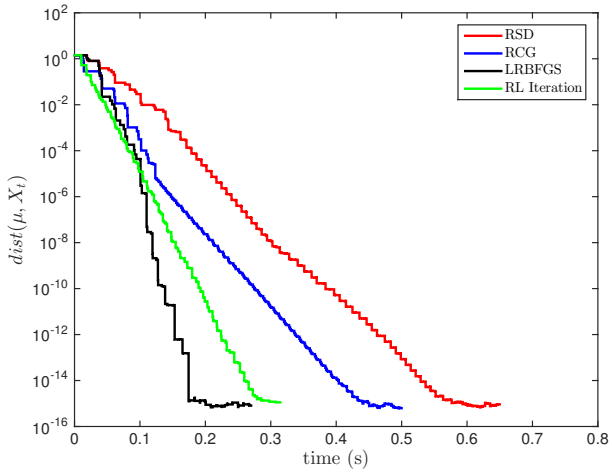
    where $Q = X^{1/2}\exp(\frac{X^{-1/2}\eta_X X^{-1/2}}{2})X^{-1/2}$
  - Vector transport by parallelization[3]: essentially an identity

[3] W. Huang, P.-A. Absil, and K. A. Gallivan, *A Riemannian symmetric rank-one trust-region method*, Mathematical Programming, 2014

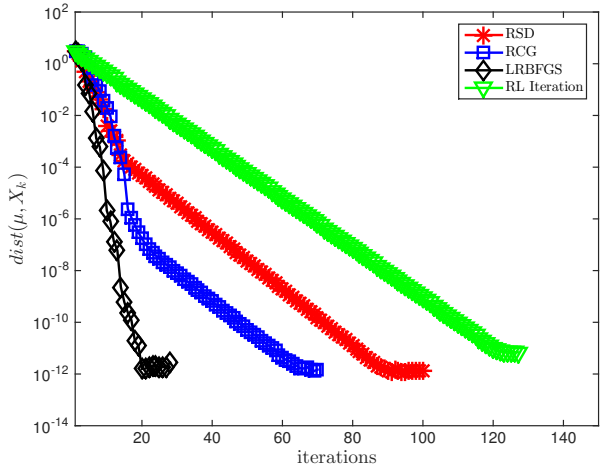
Numerical Results I: $K = 100$, 3×3, $d = 6$, $m = 2$

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





- $10^3 \leq \kappa(A_i) \leq 2 \cdot 10^6$



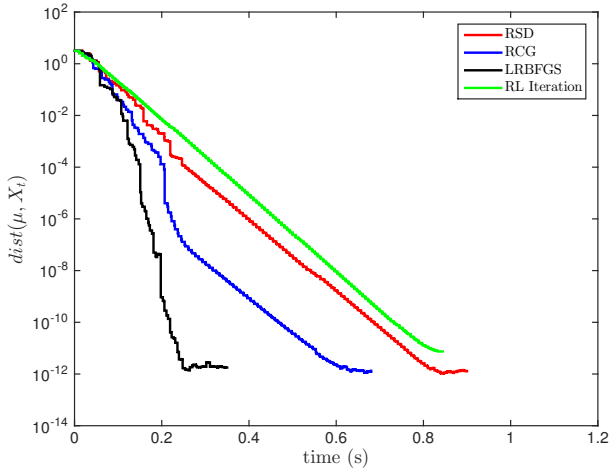
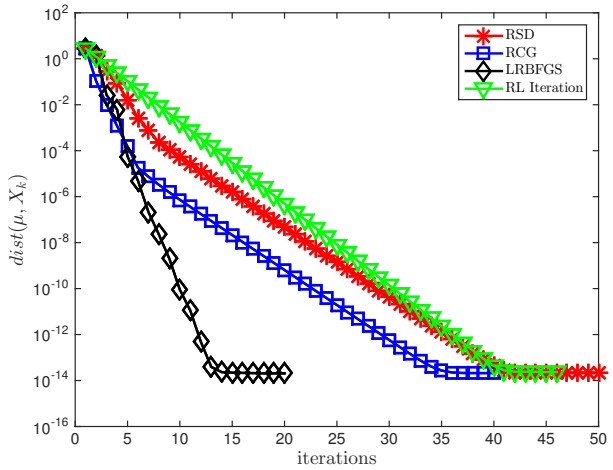
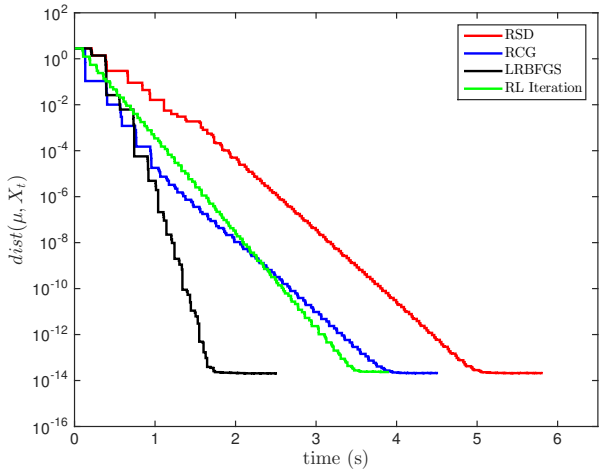


Figure : Evolution of averaged distance between current iterate and the exact Karcher mean with respect to time and iterations

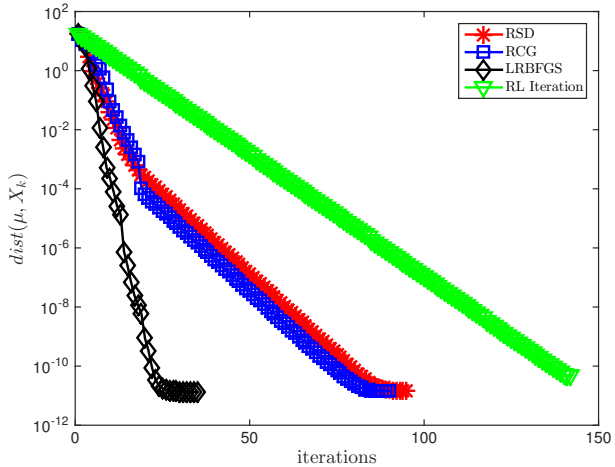
Numerical Results II: $K = 30$, 100×100, $d = 5050$, $m = 2$

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





- $10^4 \leq \kappa(A_i) \leq 2 \cdot 10^6$



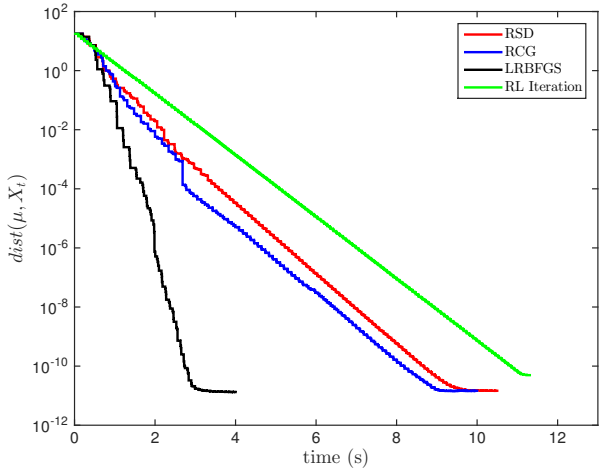


Figure : Evolution of averaged distance between current iterate and the exact Karcher mean with respect to time and iterations

Summary

- Analyze the conditioning of the Hessian of the Karcher cost function
- Apply a Riemannian version of limited-memory BFGS method to computing the SPD Karcher mean
- Present efficient implementations
- Compare with the state-of-the-art methods
- The proposed LRBFGS method is seen to be the method of choice for computing the SPD Karcher mean when the data matrices increase in size or number.

Implementation in Matlab

$$
\begin{aligned}
F(X) &= \frac{1}{2K}\sum_{i=1}^{K} \| \log(A_i^{-1/2} X A_i^{-1/2}) \|_F^2 \\
&= \frac{1}{2K}\sum_{i=1}^{K} \| \log(A_i^{-1/2} L L^T A_i^{-1/2}) \|_F^2 \\
&= \frac{1}{2K}\sum_{i=1}^{K} \| \log[(A_i^{-1/2} L)(A_i^{-1/2} L)^T] \|_F^2
\end{aligned}
$$

Let $S = A_i^{-1/2} L$, and $SS^T = QUQ^T$, where $QQ^T = I$, and U is an upper triangle matrix whose diagonal elements are the eigenvalues. Then

$$
\begin{aligned}
F(X) &= \frac{1}{2K}\sum_{i=1}^{K} \| \log(SS^T) \|_F^2 \\
&= \frac{1}{2K}\sum_{i=1}^{K} \| Q \log(\mathrm{diag}(U)) Q^T \|_F^2
\end{aligned}
$$

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