Riemannian Optimization: A Proximal Newton Method

Speaker: Wen Huang

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January 12, 2024

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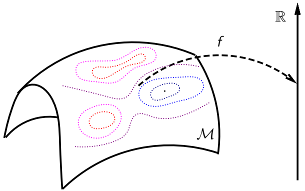
Outline

- Riemannian optimization;
- Applications;
- Smooth optimization framework;
- Research foci of Riemannian optimization;
- A Riemannian proximal Newton method;
- Summary;

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

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

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



Riemannian Optimization

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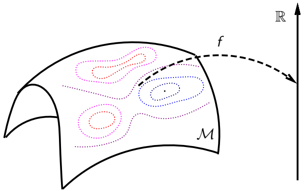
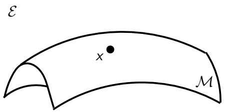
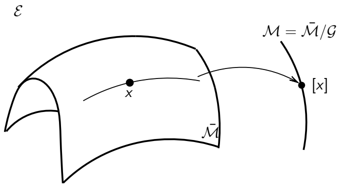


Two kinds of commonly-encountered manifolds

Embedded submanifold of a Euclidean space



Quotient manifold from an embedded submanifold



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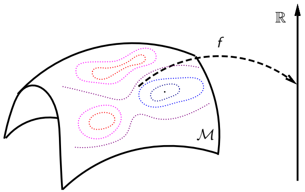
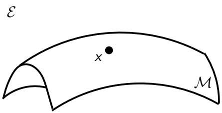


Examples:

- Sphere: $\{x \in \mathbb{R}^n \mid \|x\| = 1\}$;
- Stiefel manifold: $\mathrm{St}(p, n) = \{X \in \mathbb{R}^{n \times p} \mid X^T X = I_p\}$;
- Fixed rank: $\mathbb{R}_r^{m \times n} = \{X \in \mathbb{R}^{m \times n} : \mathrm{rank}(X) = r\}$;
- etc;

Embedded submanifold of a Euclidean space



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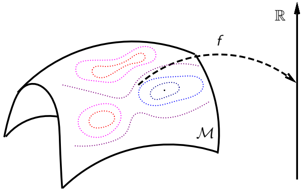
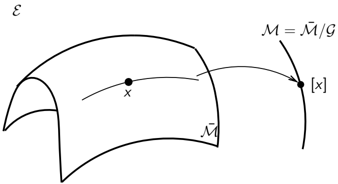


Examples:

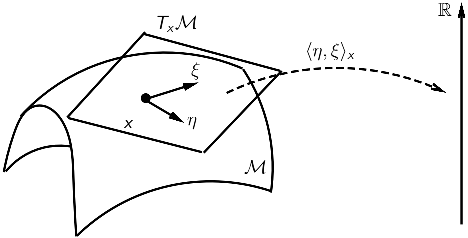
- Grassmann manifold: the set of p dimensional linear spaces in $\mathbb{R}^n$ $\mathrm{Gr}(p, n) = \mathrm{St}(p, n)/\mathcal{O}_p$;
- Shape space;
- etc;

Quotient manifold from an embedded submanifold



Riemannian Optimization

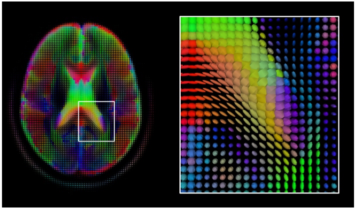
Roughly, a Riemannian manifold $\mathcal{M}$ is a smooth set with a smoothly-varying inner product on the tangent spaces.



Riemannian manifold = Manifold + Riemannian metric (inner products)

Embedded submanifold: Computation on SPD manifold

- SPD manifold:
  $\mathcal{S}_{++}^n = \{X \in \mathbb{R}^{n \times n} : X = X^T, X \succ 0\}$;
- Applications of SPD matrices
  - Diffusion tensors in medical imaging [CSV12, FJ07, RTM07]
  - Describing images and video [LWM13, SFD02, ASF$^+$05, TPM06, HWSC15]
- Motivation of averaging SPD matrices
  - denoising / interpolation
  - clustering / classification



Embedded submanifold: Computation on SPD manifold

One averaging SPD matrices method:

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

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

Applications

Embedded submanifold: Computation on SPD manifold

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Why shall we use Riemannian optimization approach?

Metric: $\langle \eta_X, \xi_X \rangle_X = \mathrm{trace}(\eta_X X^{-1} \xi_X X^{-1})$

- $\kappa(H^R) \leq 1 + \frac{\ln(\max \kappa_i)}{2}$, where $\kappa_i = \kappa(\mu^{-1/2} A_i \mu^{-1/2})$
- $\kappa(H^R) \leq 20$ if $\max(\kappa_i) = 10^{16}$

Metric: $\langle \eta, \xi \rangle_X = \mathrm{trace}(\eta^T \xi)$

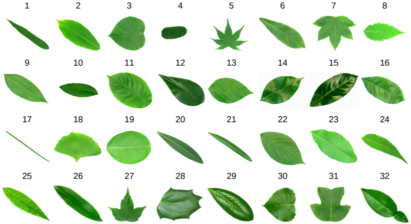
- $\frac{\kappa^2(\mu)}{\kappa(H^{\mathrm{R}})} \leq \kappa(H^{\mathrm{E}}) \leq \kappa(H^{\mathrm{R}}) \kappa^2(\mu)$
- $\kappa(H^E) \geq \kappa^2(\mu)/20$

Condition number of the Riemannian Hessian [YHAG2020]

[YHAG2020]: X. Yuan, W. Huang*, P.-A. Absil, K. A. Gallivan. "Computing the matrix geometric mean: Riemannian vs Euclidean conditioning, implementation techniques, and a Riemannian BFGS method", *Numerical Linear Algebra with Applications*, 27:5, 1-23, 2020.

Applications

Quotient manifold: Computation on shape space



- Classification [LKS+12, HGSA15]
- Face recognition [DBS+13]

Quotient manifold: Computation on shape space

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

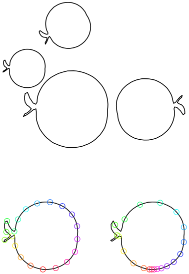
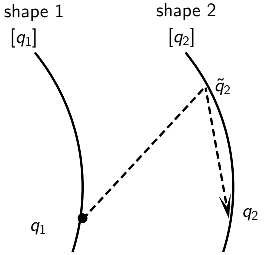
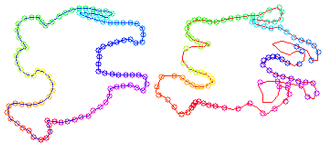


Figure: All are the same shape.

Quotient manifold: Computation on shape space
Registration

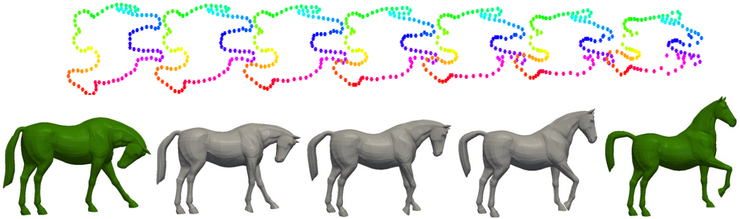




- Optimization problem $\min_{q_2 \in [q_2]} \mathrm{dist}(q_1, q_2)$ is defined on a Riemannian manifold

Applications

Quotient manifold: Computation on shape space
Geodesic / Interpolation

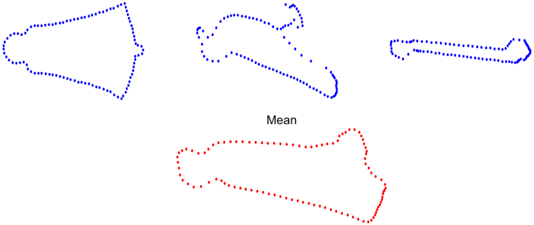


$$\min_{\alpha \in \mathcal{H}_{x,y}} \frac{1}{2} \int_0^1 \langle \dot{\alpha}(\tau), \dot{\alpha}(\tau) \rangle_{\alpha(\tau)} \mathrm{d}\tau$$

- Computation of a geodesic between two shapes
- Interpolation in shape space

Quotient manifold: Computation on shape space

Karcher mean

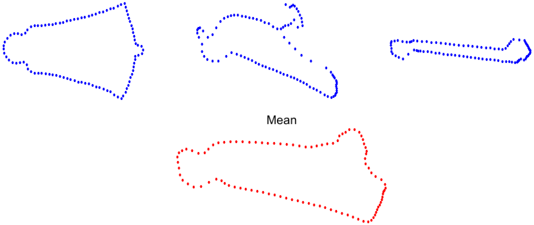


$$\min_{X \text{ is a shape}} \frac{1}{2k} \sum_{i=1}^{k} \mathrm{dist}^2(X, S_i),$$

- Computation of Karcher mean of a population of shapes

Quotient manifold: Computation on shape space

Karcher mean



$$\min_{X \text{ is a shape}} \frac{1}{2k} \sum_{i=1}^{k} \mathrm{dist}^2(X, S_i),$$

- Computation of Karcher mean of a population of shapes

Riemannian optimization is used since these problems naturally involve a Riemannian manifold

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

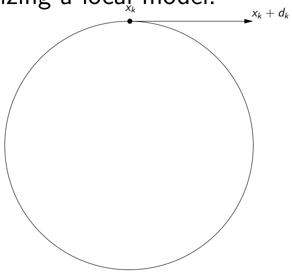
$$x_{k+1} = x_k + \Delta x_k = x_k + \alpha_k s_k \ .$$

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: $x_{k+1} = x_k - \left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k)$
- Trust region method: Δx_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



Definition

The Riemannian gradient of f at x is the unique tangent vector in $\mathrm{T}_x \mathcal{M}$ satisfying $\forall \eta \in \mathrm{T}_x \mathcal{M}$, the directional derivative

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

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

Definition

The Riemannian Hessian of f at x is a symmetric linear operator from $\mathrm{T}_x \mathcal{M}$ to $\mathrm{T}_x \mathcal{M}$ defined as

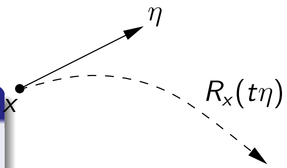
$$\mathrm{Hess}\, f(x) : \mathrm{T}_x \mathcal{M} \to \mathrm{T}_x \mathcal{M} : \eta \to \nabla_\eta \,\mathrm{grad}\, f,$$

where ∇ is the affine connection.

Smooth Optimization Framework

Retractions

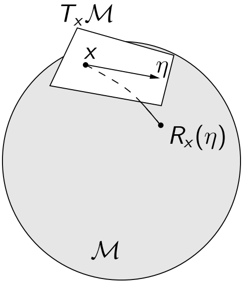
Euclidean	Riemannian
$x_{k+1} = x_k + \alpha_k d_k$	$x_{k+1} = R_{x_k}(\alpha_k \eta_k)$



Definition

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

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



- maps tangent vectors back to the manifold
- defines curves in a direction

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)

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;

- formulas for combining information from multiple tangent spaces.

Retraction and transport-based: information from multiple tangent spaces

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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 $R_x(\eta_x)$. R is a retraction associated with $\mathcal{T}$;

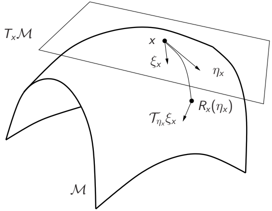

Figure: Vector transport.

Given a retraction and a vector transport, we can generalize classical unconstrained smooth optimization methods from Euclidean space to the Riemannian manifold.

Smooth Optimization Framework

Retraction/Transport-based Riemannian Optimization

Given a retraction and a vector transport, we can generalize classical unconstrained smooth optimization methods from Euclidean space to the Riemannian manifold.

Do the Riemannian versions of those methods work well?

Given a retraction and a vector transport, we can generalize classical unconstrained smooth optimization methods from Euclidean space to the Riemannian manifold.

Do the Riemannian versions of those methods work well?

No, generally

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

Research Foci of Riemannian Optimization

1. Manifold recognition, geometry structure analyses and computations;
2. Generalization Euclidean algorithms to the Riemannian setting;
3. Algorithms specialization for applications;
4. Library developments;

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2. Generalization Euclidean algorithms to the Riemannian setting;
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4. Library developments;

- Manifold recognition
- Riemannian metric
- Retraction / Geodesic
- Vector transport / Parallel translation

[EAS1998] A. Edelman, T. A. Arias, and S. T. Smith. The geometry of algorithms with orthogonality constraints. *SIAM Journal on Matrix Analysis and Applications*, 20(2):303–353, 1998

[CMV2017] T Carson, D. G. Mixon, and S. Villar. Manifold optimization for k-means clustering. In *2017 International Conference on Sampling Theory and Applications (SampTA)*, 73–77. IEEE, 2017

[SDN2021] G. Song, W. Ding, and M. K. Ng, Low rank pure quaternion approximation for pure quaternion matrices, *SIAM Journal on Matrix Analysis and Applications*, 42, pp. 58–82, 2021

[VAV2013] B. Vandereycken, P.-A. Absil, and S. Vandewalle. A Riemannian geometry with complete geodesics for the set of positive semidefinite matrices of fixed rank, *IMA Journal of Numerical Analysis*, 33.2, 481–514, 2013.

[Zim2017] R. Zimmermann. A matrix-algebraic algorithm for the Riemannian logarithm on the Stiefel manifold under the canonical metric. *SIAM Journal on Matrix Analysis and Applications*, 38.2, 322–342, 2017.

Research Foci of Riemannian Optimization

1. Manifold recognition, geometry structure analyses and computations;
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- Smooth unconstrained optimization algorithms
- Nonsmooth unconstrained optimization algorithms
- Constrained optimization algorithms

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Riemannian optimization mainly focuses on this topic.
Discuss later.

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4. Library developments;

- Computations on the SPD manifold;
- Computations on the shape space;
- Clustering and graph partitions;
- Beamforming in wireless communication;
- Blind source separation;
- etc

Research Foci of Riemannian Optimization

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- Representation of a manifold and tangent spaces;
- Choose a Riemannian metric;
- Choose a retraction;
- Choose a vector transport;

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Above factors may influence algorithms significantly.

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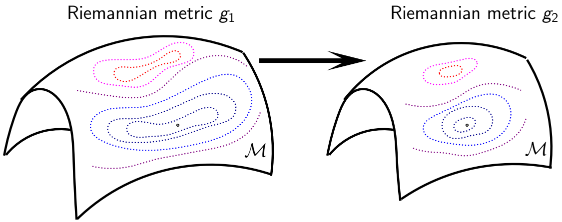

Figure: Changing Riemannian metric may influence the difficulty of a problem.

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- Manopt (Matlab library) [Boumal, Mishra, Absil, Sepulchre(2014)]
- Pymanopt (Python version of Manopt) [Townsend, Koep, Weichwald (2016)]
- Manoptjl (Julia, nonsmooth methods) [Bergmann (2019)]
- ROPTLIB (C++ library, interfaces to Matlab and Julia) [Huang, Absil, Gallivan, Hand (2018)]
- ManifoldOptim (R wrapper of ROPTLIB) [Martin, Raim, Huang, Adragni (2018)]
- McTorch (Python, GPU acceleration) [Meghawanshi, Jawanpuria, Kunchukuttan, Kasai, Mishra (2018)]
- CDOpt (Python, embedded submanifold in the form of $c(x) = 0$) [Xiao, Hu, Liu, Toh (2022)]

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Provide theories to explain behaviors of existing algorithms for particular applications

- [MBDG2023]: IRKA is a Riemannian gradient descent method;
- [YHAG2020]: Richardson-like iteration for matrix geometric mean is a Riemannian gradient descent method;
- [BM2006]: The improved BFGS method is a Riemannian BFGS method using vector transport by parallelization;

[MBDG2023] P. Mlinaric, C. Beattie, Z. Drmac, and S. Gugercin. IRKA is a Riemannian Gradient Descent Method. arxiv:2311.02031, 2023

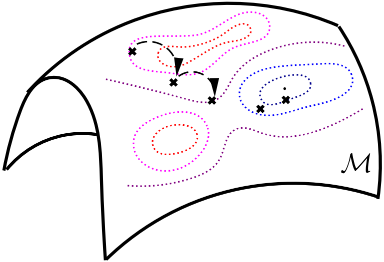
[YHAG2020] X. Yuan, W. Huang, P.-A. Absil, K. A. Gallivan. Computing the matrix geometric mean: Riemannian vs Euclidean conditioning, implementation techniques, and a Riemannian BFGS method, *Numerical Linear Algebra with Applications*, 27:5, 1-23, 2020

[BM2006] I. Brace and J. H. Manton. An improved BFGS-on-manifold algorithm for computing weighted low rank approximations. *Proceedings of 17th international Symposium on Mathematical Theory of Networks and Systems*, P.1735–1738, 2006

Comparison with Constrained Optimization

Not all Riemannian optimization problem can be formulated as constrained optimization problems, and vice versa.

- 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



A Non-exhaustive Review

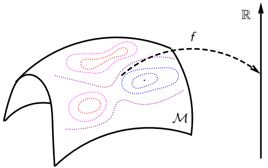
- Smooth unconstrained problems
  - Steepest descent: Smith 1994; Helmke-Moore 1994; Iannazzo-Porcelli 2019;
  - Conjugate gradient: Smith 1994; Gallivan-Absil 2010; Ring-Wirth 2012; Sato-Iwai 2015;
  - Quasi-Newton: Ring-Wirth 2012; Huang-Absil-Gallivan 2018; Huang-Gallivan 2022
  - Newton-CG: Absil-Baker-Gallivan 2007; Huang-Huang 2023
- Nonsmooth unconstrained problems
  - Proximal point method: Ferreira-Oliveira 2002;
  - Optimality conditions: Yang-Zhang-Song 2014;
  - Gradient sampling: Huang 2013; Hosseini and Uschmajew 2017;
  - ϵ-subgradient-based methods: Grohs-Hosseini 2015;
  - Proximal gradient methods: Huang-Wei 2022;
  - Proximal Newton method: Si-Absil-Huang-Jiang-Vary 2023;
- Constrained problems:
  - Augmented Lagrangian methods: Boumal-Liu 2019;
  - Sequential quadratic programming: Obara-Okuno-Takeda 2022;
  - Frank-Wolfe Methods: Weber-Sra 2023;

A Non-exhaustive Review

- Smooth unconstrained problems:
  - Stiefel manifold: Wen-Yin 2012; Jiang-Dai 2014; Xiao-Liu-Yuan 2020; Dai-Wang-Zhou 2020
  - Symplectic Stiefel manifold: Gao-Son-Absil-Stykel 2021
  - Symmetric positive definite manifold: Bini-Iannazzo 2013; Zhang 2017; Yuan-Huang-Absil-Gallivan 2020;
  - Fixed rank manifold: Wen-Yin-Zhang 2012; Mishra 2014; Sutti-Vandereycken 2021; Levin-Kileel-Boumal 2022
- Nonsmooth unconstrained problems:
  - Stiefel Manifold: Huang-Wei 2019; Chen-Ma-So-Zhang 2020; Xiao-Liu-Yuan 2020;
  - Fixed rank manifold: Cambier-Absil 2016;
  - Matrix manifolds: Zhou-Bao-Ding-Zhu 2022
  - Smooth equation constraints: Xiao-Liu-Toh 2023
- Constrained problems:
  - Stiefel + non-negativity: Jiang-Meng-Wen-Chen 2019;
  - Symmetric positive definite + zeros: Phan-Menickelly 2020;

Optimization on Manifolds with Structure:

$$\min_{x \in \mathcal{M}} F(x) = f(x) + h(x),$$

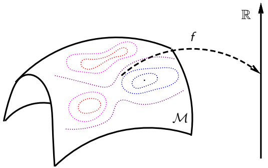


- $\mathcal{M}$ is a finite-dimensional Riemannian manifold;
- f is smooth and may be nonconvex; and
- $h(x)$ is continuous and convex but may be nonsmooth;

A Riemannian Proximal Newton Method

Optimization on Manifolds with Structure:

$$\min_{x \in \mathcal{M}} F(x) = f(x) + h(x),$$



- $\mathcal{M}$ is a finite-dimensional Riemannian manifold;
- f is smooth and may be nonconvex; and
- $h(x)$ is continuous and convex but may be nonsmooth;

Applications: sparse PCA [ZHT06], compressed model [OLCO13], sparse partial least squares regression [CSG$^+$18], sparse inverse covariance estimation [BESS19], sparse blind deconvolution [ZLK$^+$17], and clustering [HWGVD22].

Euclidean Proximal Gradient/Newton Method

Optimization with Structure: $\mathcal{M} = \mathbb{R}^n$

$$\min_{x \in \mathbb{R}^n} F(x) = f(x) + h(x),$$

Given x_0,

$$\begin{cases} d_k = \arg\min_{p \in \mathbb{R}^n} f(x_k) + \langle \nabla f(x_k), p \rangle + \frac{1}{2} \langle p, H_k p \rangle + h(x_k + p) \\ x_{k+1} = x_k + d_k. \end{cases}$$

Euclidean Proximal Gradient/Newton Method

Optimization with Structure: $\mathcal{M} = \mathbb{R}^n$

$$\min_{x \in \mathbb{R}^n} F(x) = f(x) + h(x),$$

Given x_0,

$$\begin{cases} d_k = \arg\min_{p \in \mathbb{R}^n} f(x_k) + \langle \nabla f(x_k), p \rangle + \frac{1}{2} \langle p, H_k p \rangle + h(x_k + p) \\ x_{k+1} = x_k + d_k. \end{cases}$$

proximal gradient: $H_k = L I_n$

- $h \equiv 0 \Rightarrow$ Steepest descent;
- Linear convergence;

proximal Newton: $H_k = \nabla^2 f(x_k)$

- $h \equiv 0 \Rightarrow$ Newton;
- Superlinear convergence;

Euclidean Proximal Gradient/Newton Method

Optimization with Structure: $\mathcal{M} = \mathbb{R}^n$

$$\min_{x \in \mathbb{R}^n} F(x) = f(x) + h(x),$$

Given x_0,

$$\begin{cases} d_k = \arg\min_{p \in \mathbb{R}^n} f(x_k) + \langle \nabla f(x_k), p \rangle + \frac{1}{2}\langle p, H_k p \rangle + h(x_k + p) \\ x_{k+1} = x_k + d_k. \end{cases}$$

proximal gradient: $H_k = L I_n$

- $h \equiv 0 \Rightarrow$ Steepest descent;
- Linear convergence;

proximal Newton: $H_k = \nabla^2 f(x_k)$

- $h \equiv 0 \Rightarrow$ Newton;
- Superlinear convergence;

How to generalize to the Riemannian setting?

Generalizations of Proximal Gradient Method

Euclidean Proximal gradient:

Given x_0,

$$\begin{cases} d_k = \arg\min_{p \in \mathbb{R}^n} f(x_k) + \langle \nabla f(x_k), p \rangle + \frac{L}{2}\langle p, p \rangle + h(x_k + p) \\ x_{k+1} = x_k + d_k. \end{cases}$$

Riemannian generalization 1: (for embedded submanifold)

$$\left.\begin{array}{c} \nabla f(x_k) \Longrightarrow \mathrm{grad}\, f(x_k) \\ x_{k+1} = x_k + d_k \Longrightarrow x_{k+1} = R_{x_k}(d_k) \\ p \in \mathbb{R}^n \Longrightarrow p \in \mathrm{T}_{x_k}\mathcal{M} \end{array}\right\} \Longrightarrow \text{Converge globally}$$

$$\begin{cases} d_k = \arg\min_{p \in \mathrm{T}_{x_k}\mathcal{M}} f(x_k) + \langle \mathrm{grad}\, f(x_k), p \rangle + \frac{L}{2}\langle p, p \rangle + h(x_k + p) \\ x_{k+1} = R_{x_k}(d_k). \end{cases}$$

Generalizations of Proximal Gradient Method

Euclidean Proximal gradient:

Given x_0,

$$\begin{cases} d_k = \arg\min_{p \in \mathbb{R}^n} f(x_k) + \langle \nabla f(x_k), p \rangle + \frac{L}{2}\langle p, p \rangle + h(x_k + p) \\ x_{k+1} = x_k + d_k. \end{cases}$$

Riemannian generalization 2: (for general manifold)

$$\left.\begin{array}{c} \nabla f(x_k) \Longrightarrow \mathrm{grad}\, f(x_k) \\ x_{k+1} = x_k + d_k \Longrightarrow x_{k+1} = R_{x_k}(d_k) \\ p \in \mathbb{R}^n \Longrightarrow p \in \mathrm{T}_{x_k}\mathcal{M} \\ h(x_k + p) \Longrightarrow h(R_{x_k}(p)) \end{array}\right\} \Longrightarrow \begin{array}{l} \text{Converge globally} \\ \text{Convergence rate analyses} \end{array}$$

$$\begin{cases} d_k = \arg\min_{p \in \mathrm{T}_{x_k}\mathcal{M}} f(x_k) + \langle \mathrm{grad}\, f(x_k), p \rangle + \frac{L}{2}\langle p, p \rangle + h(R_{x_k}(p)) \\ x_{k+1} = R_{x_k}(d_k). \end{cases}$$

Euclidean proximal Newton:

$$\begin{cases} d_k = \mathrm{argmin}_{p \in \mathbb{R}^n} f(x_k) + \langle \nabla f(x_k), p \rangle + \frac{1}{2} \langle p, \nabla^2 f(x_k) p \rangle + h(x_k + p) \\ x_{k+1} = x_k + d_k \end{cases}$$

A native generalization by replacing the Euclidean gradient and Hessian by the Riemannian gradient and Hessian:

$$\begin{cases} \eta_k = \arg\min_{\eta \in \mathrm{T}_{x_k} \mathcal{M}} f(x_k) + \langle \mathrm{grad}\, f(x_k), \eta \rangle + \frac{1}{2} \langle \eta, \mathrm{Hess}\, f(x_k) \eta \rangle + h(x_k + \eta) \\ x_{k+1} = R_{x_k}(\eta_k) \end{cases}$$

Euclidean proximal Newton:

$$\begin{cases} d_k = \operatorname{argmin}_{p \in \mathbb{R}^n} f(x_k) + \langle \nabla f(x_k), p \rangle + \frac{1}{2} \langle p, \nabla^2 f(x_k) p \rangle + h(x_k + p) \\ x_{k+1} = x_k + d_k \end{cases}$$

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Does it converge superlinearly locally?

Euclidean proximal Newton:

$$\begin{cases} d_k = \mathrm{argmin}_{p \in \mathbb{R}^n} f(x_k) + \langle \nabla f(x_k), p \rangle + \frac{1}{2} \langle p, \nabla^2 f(x_k) p \rangle + h(x_k + p) \\ x_{k+1} = x_k + d_k \end{cases}$$

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Does it converge superlinearly locally?

Not necessarily!

Consider the Sparse PCA over sphere:

$$\min_{x \in \mathbb{S}^{n-1}} -x^{\mathrm{T}} A^{\mathrm{T}} A x + \mu \|x\|_1,$$

where $f(x) = -x^{\mathrm{T}} A^{\mathrm{T}} A x$, $h(x) = \mu \|x\|_1$.

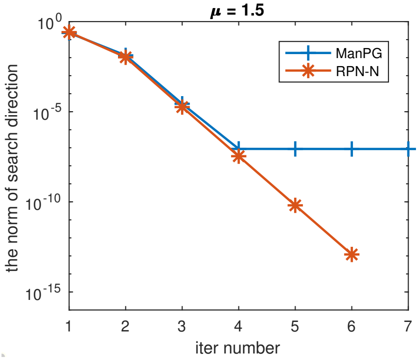

Figure: Comparisons of native generalization (RPN-N) and the proximal gradient method (ManPG) in [CMSZ20].

Euclidean version:

$$\begin{cases} d_k = \mathrm{argmin}_p \langle \nabla f(x_k), p \rangle + \frac{1}{2} \langle p, \nabla^2 f(x_k) p \rangle + h(x_k + p) \\ x_{k+1} = x_k + d_k \end{cases}$$

A native generalization by replacing the Euclidean gradient and Hessian by the Riemannian gradient and Hessian:

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- $x_k + \eta$ in h is only a first order approximation;

Euclidean version:

$$\begin{cases} d_k = \mathrm{argmin}_p \langle \nabla f(x_k), p \rangle + \frac{1}{2}\langle p, \nabla^2 f(x_k) p \rangle + h(x_k + p) \\ x_{k+1} = x_k + d_k \end{cases}$$

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$$\begin{cases} \eta_k = \arg\min_{\eta \in \mathrm{T}_{x_k}\mathcal{M}} f(x_k) + \langle \mathrm{grad}\, f(x_k), \eta \rangle + \frac{1}{2}\langle \eta, \mathrm{Hess}\, f(x_k)\eta \rangle + h(x_k + \eta + \frac{1}{2}\Pi(\eta, \eta)) \\ x_{k+1} = R_{x_k}(\eta_k) \end{cases}$$

- $x_k + \eta$ in h is only a first order approximation;
- If an second order approximation is used, then the subproblem is difficult to solve;

A Riemannian proximal Newton method (RPN)

1. Compute
   $v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$
2. Find $u(x_k) \in \mathrm{T}_{x_k} \mathcal{M}$ by solving
   $$J(x_k)[u(x_k)] = -v(x_k),$$
   where $J(x_k) = -\left[\mathrm{I}_n - \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) - \mathcal{L}_{x_k})\right]$, Λ_{x_k} and $\mathcal{L}_{x_k}$ are defined later ;
3. $x_{k+1} = R_{x_k}(u(x_k));$

A Riemannian proximal Newton method (RPN)

1. Compute
$v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v)$;
2. Find $u(x_k) \in \mathrm{T}_{x_k} \mathcal{M}$ by solving
$$J(x_k)[u(x_k)] = -v(x_k),$$
where $J(x_k) = -\left[\mathrm{I}_n - \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) - \mathcal{L}_{x_k})\right]$, Λ_{x_k} and $\mathcal{L}_{x_k}$ are defined later ;
3. $x_{k+1} = R_{x_k}(u(x_k))$;

1. Step 1: compute a Riemannian proximal gradient direction (ManPG)

A Riemannian proximal Newton method (RPN)

1. Compute
   $v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$
2. Find $u(x_k) \in \mathrm{T}_{x_k} \mathcal{M}$ by solving
   $$J(x_k)[u(x_k)] = -v(x_k),$$
   where $J(x_k) = -\left[\mathrm{I}_n - \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) - \mathcal{L}_{x_k})\right]$, Λ_{x_k} and $\mathcal{L}_{x_k}$ are defined later ;
3. $x_{k+1} = R_{x_k}(u(x_k));$

1. Step 1: compute a Riemannian proximal gradient direction (ManPG)
2. Step 2: compute the Riemannian proximal Newton direction, where $J(x_k)$ is from a generalized Jacobi of $v(x_k)$;

A Riemannian Proximal Newton Method

The proposed approach

A Riemannian proximal Newton method (RPN)

1. Compute
   $v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$
2. Find $u(x_k) \in \mathrm{T}_{x_k} \mathcal{M}$ by solving
   $$J(x_k)[u(x_k)] = -v(x_k),$$
   where $J(x_k) = -\left[\mathrm{I}_n - \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) - \mathcal{L}_{x_k})\right]$, Λ_{x_k} and $\mathcal{L}_{x_k}$ are defined later ;
3. $x_{k+1} = R_{x_k}(u(x_k));$

1. Step 1: compute a Riemannian proximal gradient direction (ManPG)
2. Step 2: compute the Riemannian proximal Newton direction, where $J(x_k)$ is from a generalized Jacobi of $v(x_k)$;
3. Step 3: Update iterate by a retraction;

A Riemannian proximal Newton method (RPN)

1. Compute
   $v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$
2. Find $u(x_k) \in \mathrm{T}_{x_k} \mathcal{M}$ by solving
   $$J(x_k)[u(x_k)] = -v(x_k),$$
   where $J(x_k) = -\left[\mathrm{I}_n - \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) - \mathcal{L}_{x_k})\right]$, Λ_{x_k} and $\mathcal{L}_{x_k}$ are defined later ;
3. $x_{k+1} = R_{x_k}(u(x_k));$

Next, we will show:

1. G-semismoothness of $v(x_k)$ and its generalized Jacobi;
2. Superlinear convergence rate;

Definition (G-Semismoothness [Gow04])

Let $F : \mathcal{D} \to \mathbb{R}^m$ where $\mathcal{D} \subset \mathbb{R}^n$ be an open set, $\mathcal{K} : \mathcal{D} \rightrightarrows \mathbb{R}^{m \times n}$ be a nonempty set-valued mapping. We say that F is G-semismooth at $x \in \mathcal{D}$ with respect to $\mathcal{K}$ if for any $J \in \mathcal{K}(x + d)$,

$$F(x + d) - F(x) - Jd = o(\|d\|) \text{ as } d \to 0.$$

If F is G-semismooth at any $x \in \mathcal{D}$ with respect to $\mathcal{K}$, then F is called a G-semismooth function with respect to $\mathcal{K}$.

The standard definition of semismoothness additional requires:

- $\mathcal{K}$ is compact valued, upper semicontinuous set-valued mapping;
- F is a locally Lipschitz continuous function;
- F is directionally differentiable at x;

[Gow04] M Seetharama Gowda. Inverse and implicit function theorems for h-differentiable and semismooth functions. Optimization Methods and Software, 19(5):443-461, 2004.

$v(x)$ (dropping the subscript for simplicity)

$$v(x) = \operatorname*{argmin}_{v \in \mathrm{T}_x \mathcal{M}} f(x) + \langle \nabla f(x), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x + v);$$

$v(x)$ (dropping the subscript for simplicity)

$$v(x) = \operatorname*{argmin}_{v \in \mathrm{T}_x \mathcal{M}} f(x) + \langle \nabla f(x), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x + v);$$

Above problem can be rewritten as

$$\arg \min_{B_x^T v = 0} \langle \xi_x, v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x + v)$$

where $B_x^T v = (\langle b_1, v \rangle, \langle b_2, v \rangle, \dots, \langle b_m, v \rangle)^T$, and $\{b_1, \dots, b_m\}$ forms an orthonormal basis of $\mathrm{T}_x^{\perp} \mathcal{M}$.

The Lagrangian function:

$$\mathcal{L}(v, \lambda) = \langle \xi_x, v \rangle + \frac{1}{2t} \langle v, v \rangle + h(X + v) - \langle \lambda, B_x^T v \rangle.$$

Therefore

$$\text{KKT: } \left\{ \begin{array}{c} \partial_v \mathcal{L}(v, \lambda) = 0 \\ B_x^T v = 0 \end{array} \right. \Longrightarrow \left\{ \begin{array}{c} v = \mathrm{Prox}_{th} \left(x - t(\xi_x - B_x \lambda) \right) - x \\ B_x^T v = 0 \end{array} \right.$$

where $\mathrm{Prox}_{tg}(z) = \mathrm{argmin}_{v \in \mathbb{R}^{n \times p}} \frac{1}{2} \|v - z\|_F^2 + th(v)$.

Define

$$\mathcal{F} : \mathbb{R}^n \times \mathbb{R}^{n+d} \mapsto \mathbb{R}^{n+d} : (x; v, \lambda) \mapsto \begin{pmatrix} v + x - \mathrm{Prox}_{th}(x - t[\nabla f(x) + B_x \lambda]) \\ B_x^T v \end{pmatrix}.$$

$v(x)$ is the solution of the system $\mathcal{F}(x, v(x), \lambda(x)) = 0$;

Define

$$\mathcal{F} : \mathbb{R}^n \times \mathbb{R}^{n+d} \mapsto \mathbb{R}^{n+d} : (x; v, \lambda) \mapsto \begin{pmatrix} v + x - \mathrm{Prox}_{th}(x - t[\nabla f(x) + B_x \lambda]) \\ B_x^T v \end{pmatrix}.$$

- $\mathcal{F}$ is semismooth;
- $v(x)$ is G-semismooth by the G-semismooth Implicit Function Theorem in [Gow04, PSS03];

[Gow04] M Seetharama Gowda. Inverse and implicit function theorems for h-differentiable and semismooth functions. Optimization Methods and Software, 19(5):443-461, 2004.
[PSS03] Jong-Shi Pang, Defeng Sun, and Jie Sun. Semismo oth homeomorphisms and strong stability of semidefinite and Lorentz complementarity problems. Mathematics of Operations Research, 28(1):39-63, 2003.

Lemma (Semismooth Implicit Function Theorem)

Suppose that $F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^m$ is a semismooth function with respect to $\partial_{\mathrm{B}} F$ in an open neighborhood of (x^0, y^0) with $F(x^0, y^0) = 0$. Let $H(y) = F(x^0, y)$, if every matrix in $\partial_C H(y^0)$ is nonsingular, then there exists an open set $\mathcal{V} \subset \mathbb{R}^n$ containing x^0, a set-valued fucntion $\mathcal{K} : \mathcal{V} \to \mathbb{R}^{m \times n}$, and a G-semismooth function $f : \mathcal{V} \to \mathbb{R}^m$ with respect to $\mathcal{K}$ satisfying $f(x^0) = y^0$, for every $x \in \mathcal{V}$,

$$F(x, f(x)) = 0,$$

and the set-valued function $\mathcal{K}$ is

$$\mathcal{K} : x \mapsto \{-(A_y)^{-1} A_x : [A_x \; A_y] \in \partial_{\mathrm{B}} F\big(x, f(x)\big)\},$$

where the map $x \mapsto \mathcal{K}(x)$ is compact valued and upper semicontinuous.

A Riemannian Proximal Newton Method

G-semismoothness of $v(x)$

Without loss of generality, we assume that the nonzero entries of x_* are in the first part, i.e., $x_* = [\bar{x}_*^T, 0^T]^T$

Assumption

Let $B_{x_*}^{\mathrm{T}} = [\bar{B}_{x_*}^{\mathrm{T}}, \hat{B}_{x_*}^{\mathrm{T}}]$, where $\bar{B}_{x_*} \in \mathbb{R}^{j \times d}$ and $\hat{B}_{x_*} \in \mathbb{R}^{(n-j) \times d}$. It is assumed that $j \geq d$ and $\bar{B}_{x_*}$ is full column rank.

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$v(x)$ is a G-semismooth function of x in a neighborhood of x_*

Under the above Assumption, there exists a neighborhood $\mathcal{U}$ of x_* such that $v : \mathcal{U} \to \mathbb{R}^n : x \mapsto v(x)$ is a G-semismooth function with respect to $\mathcal{K}_v$, where

$$\mathcal{K}_v : x \mapsto \left\{ -[\mathrm{I}_n,\ 0] B^{-1} A : [A\ B] \in \partial_{\mathrm{B}} \mathcal{F}\big(x, v(x), \lambda(x)\big) \right\}.$$

For $x \in \mathcal{U}$, any element of $\mathcal{K}_v(x)$ is called a generalized Jacobi of v at x.

Here, the semismooth implicit function theorem is used

The generalized Jacobi of v at x is

$$\Big\{ \mathcal{J}_x \,|\, \mathcal{J}_x[\omega] = -\left[\mathrm{I}_n - \Lambda_x + t\Lambda_x(\nabla^2 f(x) - \mathcal{L}_x)\right]\omega - M_x B_x H_x(\mathrm{D}B_x^{\mathrm{T}}[\omega])v, \forall \omega \\ M_x \in \partial_C \mathrm{prox}_{th}(x) \Big\},$$

where $\Lambda_x = M_x - M_x B_x H_x B_x^T M_k$, $H_x = \left(B_x^T M_x B_x\right)^{-1}$, $\mathcal{L}_x(\cdot) = \mathcal{W}_x(\cdot, B_x \lambda(x))$, and $\mathcal{W}_x$ denotes the Weingarten map;

- $v(x_*) = 0$;
- Set $J(x) = \mathrm{I}_n - \Lambda_x + t\Lambda_x(\nabla^2 f(x) - \mathcal{L}_x)$;
- The Riemannian proximal Newton direction: $J(x)u(x) = -v(x)$;
- Let $u(x) = (\bar{u}(x); \hat{u}(x))$, then

$$\hat{u}(x) = \hat{v} \text{ and } \bar{J}(x)\bar{u}(x) = -\bar{v}(x)$$

Assumption:

1. Let $B_{x_*}^T = [\bar{B}_{x_*}^T, \hat{B}_{x_*}^T]$, where $\bar{B}_{x_*} \in \mathbb{R}^{j \times d}$ and and $\hat{B}_{x_*} \in \mathbb{R}^{(n-j)\times d}$. It is assumed that $j \geq d$ and $\bar{B}_{x_*}$ is full column rank;

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2. There exists a neighborhood $\mathcal{U}$ of $x_* = [\bar{x}_*^T, 0^T]^T$ on $\mathcal{M}$ such that for any $x = [\bar{x}^T, \tilde{x}^T]^T \in \mathcal{U}$, it holds that $\bar{x} + \bar{v} \neq 0$ and $\hat{x} + \hat{v} = 0$.

$$v(x) = \operatorname*{argmin}_{v \in \mathrm{T}_x \mathcal{M}} f(x) + \langle \nabla f(x), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x + v)$$

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Theorem

Suppose that x_* be a local optimal minimizer. Under the above Assumptions, assume that $J(x_*)$ is nonsingular. Then there exists a neighborhood $\mathcal{U}$ of x_* on $\mathcal{M}$ such that for any $x_0 \in \mathcal{U}$, RPN Algorithm generates the sequence $\{x_k\}$ converging superlinearly to x_*.

Assumption:

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Theorem

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If the intersection of manifold and sparsity constraints forms an embedded manifold around x_*, then $\nabla^2 \bar{f}(x_*) - \bar{\mathcal{L}} \succeq 0$. If $\nabla^2 \bar{f}(x_*) - \bar{\mathcal{L}} \succ 0$, then $J(x_*)$ is nonsingular.

$$\text{Smooth case: } \min_{x \in \mathcal{M}} f(x)$$

- KKT conditions:

$$\nabla f(x) + \frac{1}{t} v + B_x \lambda = 0, \text{ and } B_x^T v = 0;$$

- Closed form solutions:

$$\lambda(x) = -B_x^{\mathrm{T}} \nabla f(x), \qquad v = -t \operatorname{grad} f(x);$$

- Action of $J(x)$: for $\omega \in \mathrm{T}_x \mathcal{M}$

$$J(x)[\omega] = -\, t P_{\mathrm{T}_x \mathcal{M}} (\nabla^2 f(x) - \mathcal{L}_x) P_{\mathrm{T}_x \mathcal{M}} \omega = -t \operatorname{Hess} f(x)[\omega]$$

- $J(x) u(x) = -v(x) \Longrightarrow \operatorname{Hess} f(x)[u(x)] = -\operatorname{grad} f(x);$
- It is the Riemannian Newton method;

- Euclidean proximal gradient method and its variants;
- Riemannian proximal gradient method and its variants;
- A Riemannian proximal Newton method;
- Numerical experiments;

Numerical Experiments

Sparse PCA problem

$$\min_{X \in \mathrm{St}(r,n)} -\mathrm{trace}(X^T A^T A X) + \mu \|X\|_1,$$

where $A \in \mathbb{R}^{m \times n}$ is a data matrix and
$\mathrm{St}(r,n) = \{X \in \mathbb{R}^{n \times r} \mid X^T X = I_r\}$ is the compact Stiefel manifold.

- $R_x(\eta_x) = (x + \eta_x)(I + \eta_x^T \eta_x)^{-1/2}$;
- $t = 1/(2\|A\|_2^2)$;
- Run ManPG until $\|v\|$ reaches 10^{-4}, i.e., it reduces by a factor of 10^3. The resulting x as the input of RPN;

Numerical Experiments

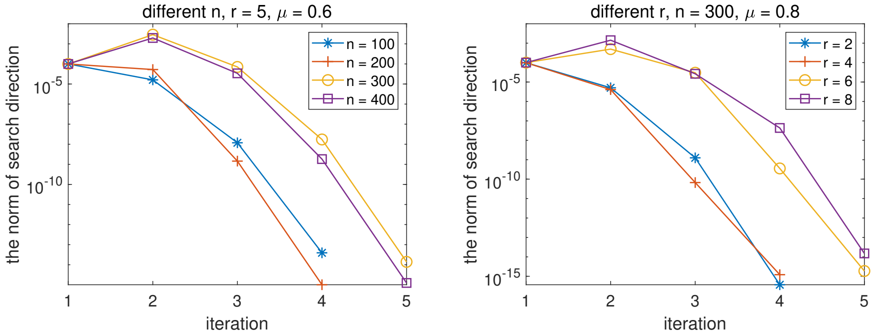

Figure: Random data. Left: different $n = \{100, 200, 300, 400\}$ with $r = 5$ and $\mu = 0.6$; Right: different $r = \{2, 4, 6, 8\}$ with $n = 300$ and $\mu = 0.8$

Collaborators

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W. Si, P.-A. Absil, W. Huang*, R. Jiang, and S. Vary,
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Summary

- Riemannian optimization;
- Applications;
  - An example on an embedded submanifold;
  - An example on a quotient manifold;
- Smooth optimization framework;
  - Search direction/Riemannian metric;
  - Riemannian gradient/Hessian;
  - Retraction/vector transport;
- Research foci of Riemannian optimization;
  - Manifold recognition/structures;
  - Algorithm generalizations;
  - Applications/Libraries;
- A Riemannian proximal Newton method;
  - Naive generalization;
  - Superlinear convergence approach;
- Summary;

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Thank you

Thank you!