Riemannian Optimization and a Riemannian Proximal Newton-CG Method

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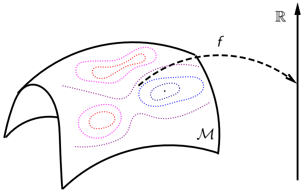
Outline

- Riemannian optimization;
  - Problem statement;
  - Applications;
  - Smooth optimization framework;
  - Research foci of Riemannian optimization;
- A Riemannian proximal Newton-CG method;
  - Optimization with a structure;
  - Proximal gradient-type methods;
  - A Riemannian proximal Newton method;
  - Globalization by truncated CG;
  - Numerical experiments;
- 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.



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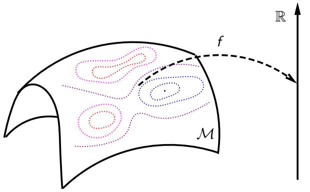
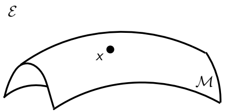
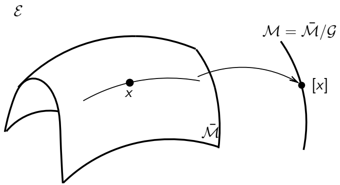


Two kinds of commonly-encountered manifolds

Embedded submanifold of a Euclidean space



Quotient manifold from an embedded submanifold



Riemannian Optimization

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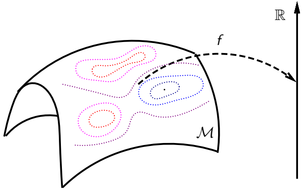
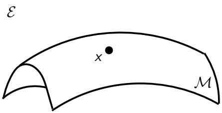


Examples:

- 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



Riemannian Optimization

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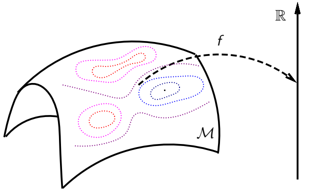
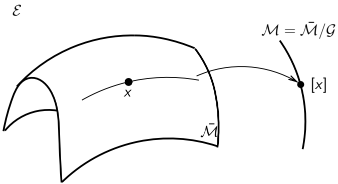


Examples:

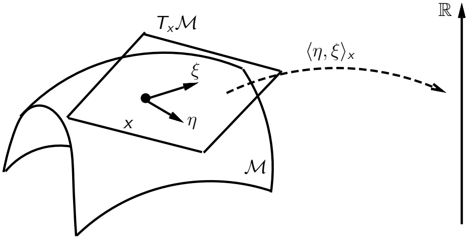
- Grassmann manifold: the set of p dimensional linear spaces in $\mathbb{R}^n$ $\mathrm{Gr}(p, n) = \mathrm{St}(p, n)/\mathcal{O}_p$;
- Shape space;
- etc;

Quotient manifold from an embedded submanifold



Riemannian Optimization

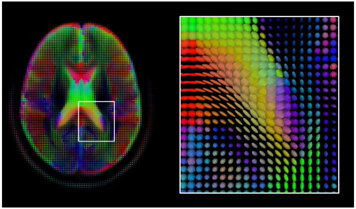
Roughly, a Riemannian manifold $\mathcal{M}$ is a smooth set with a smoothly-varying inner product on the tangent spaces.



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

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Why shall we use Riemannian optimization approach?

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

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

Condition number of the Riemannian Hessian [YHAG2020]

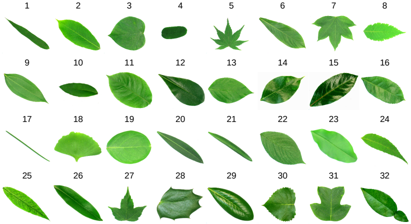
- $\kappa(H^R) \leq 1 + \frac{\ln(\max \kappa_i)}{2}$, where $\kappa_i = \kappa(\mu^{-1/2} A_i \mu^{-1/2})$
- $\kappa(H^R) \leq 20$ if $\max(\kappa_i) = 10^{16}$

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

[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

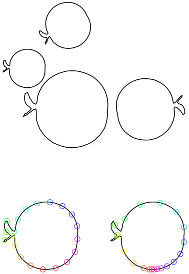
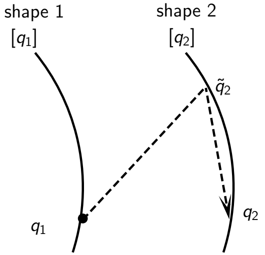
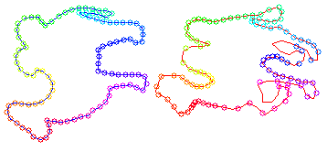


Figure: All are the same shape.

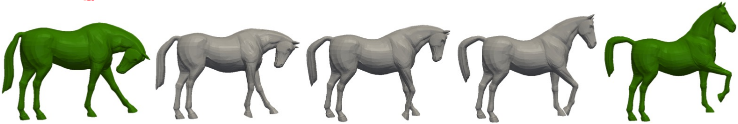
Quotient manifold: Computation on shape space
Registration





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

Quotient manifold: Computation on shape space
Geodesic / Interpolation

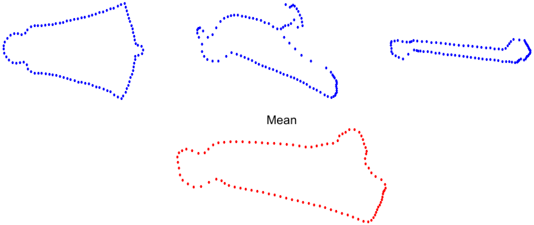


$$\min_{\alpha \in \mathcal{H}_{x,y}} \frac{1}{2} \int_0^1 \langle \dot{\alpha}(\tau), \dot{\alpha}(\tau) \rangle_{\alpha(\tau)} \mathrm{d}\tau$$

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

Quotient manifold: Computation on shape space

Karcher mean

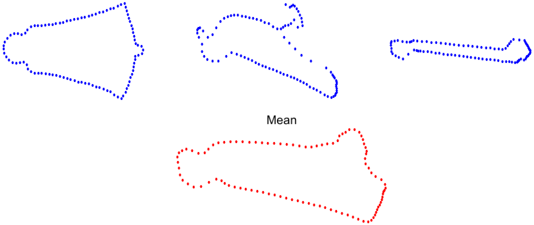


$$\min_{X \text{ is a shape}} \frac{1}{2k} \sum_{i=1}^{k} \mathrm{dist}^2(X, S_i),$$

- 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:

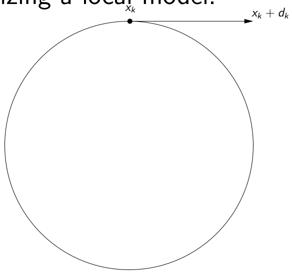
$$x_{k+1} = x_k + \Delta x_k = x_k + \alpha_k s_k \ .$$

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

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

and $\operatorname{grad} f(x)$ 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

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

where ∇ is the affine connection.

Smooth Optimization Framework

Retractions

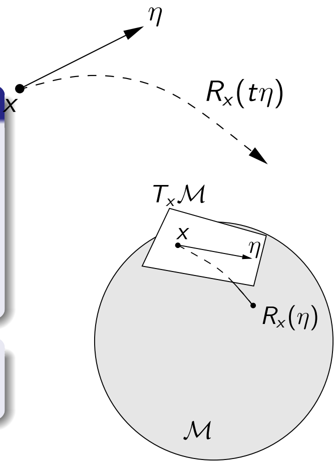
Euclidean	Riemannian
$x_{k+1} = x_k + \alpha_k d_k$	$x_{k+1} = R_{x_k}(\alpha_k \eta_k)$

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.

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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 $\mathcal{T}$;

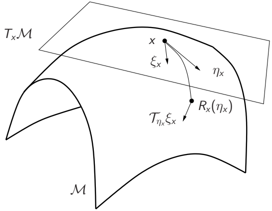

Figure: Vector transport.

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

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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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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

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

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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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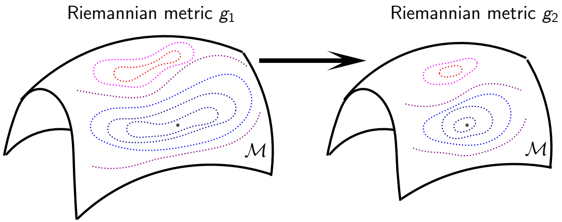

Figure: Changing Riemannian metric may influence the difficulty of a problem.

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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)]

1. Manifold recognition, geometry structure analyses and computations;
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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;

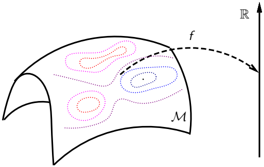
[MBDG2023] P. Mlinaric, C. Beattie, Z. Drmac, and S. Gugercin. IRKA is a Riemannian Gradient Descent Method. arxiv:2311.02031, 2023

[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

Optimization on Manifolds with Structure:

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



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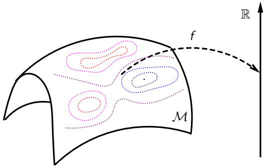

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Applications: sparse PCA [ZHT06], compressed modes [OLCO13], sparse partial least squares regression [CSG+18], sparse inverse covariance estimation [BESS19], sparse blind deconvolution [ZLK+17], and clustering [HWGVD22].

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

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

Given x_0,

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

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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;

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How to generalize to the Riemannian setting?

Euclidean Proximal gradient:

Given x_0,

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Riemannian generalization 1: (for embedded submanifold)

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

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

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)

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

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

Euclidean proximal Newton:

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

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:

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

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Does it converge superlinearly locally?

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

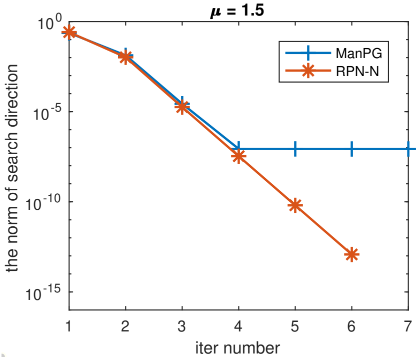

Figure: Comparisons of native generalization (RPN-N) and the proximal gradient method (ManPG) in [CMSZ20].

Euclidean version:

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

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

Euclidean version:

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

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

$\min_{x \in \mathcal{M}} F(x) = f(x) + h(x), h(x) = \mu \|x\|_1$

A Riemannian proximal Newton method (RPN)

1. Compute the ManPG direction
   $v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$
2. Find $u(x_k) \in \mathrm{T}_{x_k} \mathcal{M}$ by solving
   $$J(x_k)[u(x_k)] = -v(x_k),$$
   where $J(x_k) = -\left[I_n - \Lambda_{x_k} + t\Lambda_{x_k} (\nabla^2 f(x_k) - \mathcal{L}_{x_k}) \right]$, 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-CG method

$\min_{x \in \mathcal{M}} F(x) = f(x) + h(x), h(x) = \mu\|x\|_1$

A Riemannian proximal Newton method (RPN)

1. Compute the ManPG direction
   $v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t}\|v\|_F^2 + h(x_k + v);$
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3. $x_{k+1} = R_{x_k}(u(x_k));$

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

$$\min_{x \in \mathcal{M}} F(x) = f(x) + h(x), h(x) = \mu \|x\|_1$$

A Riemannian proximal Newton method (RPN)

1. Compute the ManPG direction
   $$v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$$
2. Find $u(x_k) \in \mathrm{T}_{x_k} \mathcal{M}$ by solving
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   where $J(x_k) = -\left[I_n - \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) - \mathcal{L}_{x_k})\right]$, 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 $v(x_k)$;

$$\min_{x \in \mathcal{M}} F(x) = f(x) + h(x), h(x) = \mu \|x\|_1$$

A Riemannian proximal Newton method (RPN)

1. Compute the ManPG direction
$$v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$$
2. Find $u(x_k) \in \mathrm{T}_{x_k} \mathcal{M}$ by solving
$$J(x_k)[u(x_k)] = -v(x_k),$$
where $J(x_k) = -\left[I_n - \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) - \mathcal{L}_{x_k})\right]$, 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;

Without loss of generality, we assume that the nonzero entries of x_* are in the first part, i.e., $x_* = [\bar{x}_*^T, 0^T]^T$. B_x denotes an orthonormal basis of $\mathrm{T}_x^\perp \mathcal{M}$ at 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 $x = [\bar{x}^T, \hat{x}^T]^T \in \mathcal{U}$, it holds that $\bar{x} + \bar{v} \neq 0$ and $\hat{x} + \hat{v} = 0$.

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_*.

The convergence rate is improved to quadratically convergence in [SAH$^+$24a]

- Similar to the Riemannian Newton method, this Riemannian proximal Newton method does not guarantee global convergence;

A Riemannian proximal Newton-CG method

A Riemannian proximal Newton method: a hybrid version

- Similar to the Riemannian Newton method, this Riemannian proximal Newton method does not guarantee global convergence;
- A hybrid method that merges ManPG with RPN is proposed in [SAH+24b];

Require: $x_0 \in \mathcal{M}$, $t > 0$, $\epsilon > 0$;

for $k = 0, 1, \dots$ **do**

  Compute a ManPG direction v_k;

  If $\|v_k\| \leq \epsilon$, then $K = k$ and break;

  $x_{k+1} = R_{x_k}(\alpha v_k)$ with an appropriate step size;

end for

for k = K+1, K+2, ... **do**

  Compute u_k by solving $J(x_k) u_k = -v_k$ with v_k being the ManPG direction;

  $x_{k+1} = R_{x_k}(u_k)$;

end for

A Riemannian proximal Newton-CG method

- Similar to the Riemannian Newton method, this Riemannian proximal Newton method does not guarantee global convergence;
- A hybrid method that merges ManPG with RPN is proposed in [SAH+24b];

Require: $x_0 \in \mathcal{M}$, $t > 0$, $\epsilon > 0$;

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  If $\|v_k\| \leq \epsilon$, then $K = k$ and break;

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end for

for k = K+1, K+2, ... **do**

  Compute u_k by solving $J(x_k) u_k = -v_k$ with v_k being the ManPG direction;

  $x_{k+1} = R_{x_k}(u_k)$;

end for

The switching parameter ϵ is crucial for the performance.

A Riemannian proximal Newton method (RPN)

1. Compute the ManPG direction
$$v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k}\mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t}\|v\|_F^2 + h(x_k + v);$$
2. Find $u(x_k) \in \mathrm{T}_{x_k}\mathcal{M}$ by solving
$$J(x_k)[u(x_k)] = -v(x_k);$$
3. $x_{k+1} = R_{x_k}(u(x_k));$

Smooth case:

- $v(x_k) = -t \, \mathrm{grad} \, f(x_k);$
- $J(x_k) = -t \, \mathrm{Hess} \, f(x_k);$
- $J(x_k)[u(x_k)] = -v(x_k) \Longrightarrow \underbrace{\mathrm{Hess} \, f(x_k)[u(x_k)] = -\,\mathrm{grad} \, f(x_k)}_{\text{truncated conjugate gradient (tCG)}}.$

A Riemannian proximal Newton-CG method

Truncated conjugate gradient

A Riemannian proximal Newton method (RPN)

1. Compute the ManPG direction
   $v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v)$;
2. Find $u(x_k) \in \mathrm{T}_{x_k} \mathcal{M}$ by solving
   $$J(x_k)[u(x_k)] = -v(x_k);$$
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Smooth case:

- $v(x_k) = -t \, \mathrm{grad} \, f(x_k)$;
- $J(x_k) = -t \, \mathrm{Hess} \, f(x_k)$;
- $J(x_k)[u(x_k)] = -v(x_k) \Longrightarrow$ $\underbrace{\mathrm{Hess} \, f(x_k)[u(x_k)] = -\mathrm{grad} \, f(x_k)}_{\text{truncated conjugate gradient (tCG)}}$.

Nonsmooth case:

- $v(x_k)$: ManPG direction;
- $J(x_k)$: Generalized Jacobi of v;
- $u(x_k)$: solving a linear system by $\underbrace{J(x_k)[u(x_k)] = -v(x_k)}_{tCG?}$

A Riemannian proximal Newton method (RPN)

1. Compute the ManPG direction
$$v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$$
2. Find $u(x_k) \in \mathrm{T}_{x_k} \mathcal{M}$ by solving
$$J(x_k)[u(x_k)] = -v(x_k);$$
3. $x_{k+1} = R_{x_k}(u(x_k))$;

Smooth case:

- $v(x_k) = -t \,\mathrm{grad}\, f(x_k)$;
- $J(x_k) = -t \,\mathrm{Hess}\, f(x_k)$;
- $J(x_k)[u(x_k)] = -v(x_k) \Longrightarrow \underbrace{\mathrm{Hess}\, f(x_k)[u(x_k)] = -\,\mathrm{grad}\, f(x_k)}_{\text{truncated conjugate gradient (tCG)}}$.

Nonsmooth case:

- $v(x_k)$: ManPG direction;
- $J(x_k)$: Generalized Jacobi of v;
- $u(x_k)$: solving a linear system by $\underbrace{J(x_k)[u(x_k)] = -v(x_k)}_{tCG?}$

Problem: $J(x_k)$ is not symmetric!

Notation:

$$\mathfrak{B}_{x_k} = \nabla^2 f(x_k) - \mathcal{L}_{x_k} = \begin{pmatrix} \mathfrak{B}_{x_k}^{(11)} & \mathfrak{B}_{x_k}^{(12)} \\ \mathfrak{B}_{x_k}^{(21)} & \mathfrak{B}_{x_k}^{(22)} \end{pmatrix}, \mathcal{B}_{x_k} = \mathfrak{B}_{x_k}^{(11)}.$$

$$J(x_k) = -\begin{pmatrix} \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger} + t(I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger})\mathcal{B}_{x_k} & t(I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger})\mathfrak{B}_{x_k}^{(12)} \\ 0_{(n-j_k)\times j_k} & I_{n-j_k} \end{pmatrix}$$

$$\begin{cases} [\bar{B}_{x_k}\bar{B}_{x_k}^{\dagger} + t(I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger})\mathcal{B}_{x_k}]\bar{u}(x_k) = \bar{v}(x_k) - t(I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger})\mathfrak{B}_{x_k}^{(12)}\hat{u}(x_k) \\ \hat{u}(x_k) = \hat{v}(x_k) \end{cases}.$$

$$\Longrightarrow \bar{u}(x_k) = \bar{v}(x_k) - \{I_{j_k} + (I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger})N_{x_k}\}^{-1}(I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger})\ell_{x_k}$$

where $\ell_{x_k} = \frac{1}{t_k}(-I_{j_k} + t_k\mathcal{B}_{x_k})\bar{v}(x_k) + \mathfrak{B}_{x_k}^{(12)}\hat{v}(x_k)$ and $N_{x_k} = -I_{j_k} + t\mathcal{B}_{x_k}$ is symmetric.

$$\bar{u}(x_k) = \bar{v}(x_k) - \{I_{j_k} + (I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger}) \underbrace{N_{x_k}}_{symmetric} \}^{-1}(I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger})\ell_{x_k}$$

Lemma

Let $N \in \mathbb{R}^{j\times j}$ and $B \in \mathbb{R}^{j\times m}$ with $m \leq j$. Suppose that $I_j + N$ is symmetric positive definite on $\{w \mid B^T w = 0\}$ and that B is full column rank. Then it holds that the unique solution of the problem

$$\min_{B^T w = 0} \ell^T w + \frac{1}{2} w^T (I_j + N) w$$

is given by

$$w_* = -\left[I_j + (I_j - BB^{\dagger})N\right]^{-1}\left[I_j - BB^{\dagger}\right]\ell.$$

A Riemannian proximal Newton-CG method

Truncated conjugate gradient

$$\bar{u}(x_k) = \bar{v}(x_k) - \{I_{j_k} + (I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger}) \underbrace{N_{x_k}}_{symmetric} \}^{-1}(I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger})\ell_{x_k}$$

Corollary

Suppose $\bar{B}_{x_k}$ has full column rank, $\mathcal{B}_{x_k}$ is symmetric positive definite on $\{w \mid B^T w = 0\}$. Then the proximal Newton equation $J(x_k)[u(x_k)] = -v(x_k)$ can be computed by

$$u(x_k) = \begin{pmatrix} \bar{v}(x_k) + w(x_k) \\ \hat{v}(x_k) \end{pmatrix},$$

where $w(x_k) = \mathrm{argmin}_{\bar{B}_{x_k}^T w = 0}\, \ell_{x_k}^T w + \frac{1}{2} w^T \mathcal{B}_{x_k} w$.

$$\bar{u}(x_k) = \bar{v}(x_k) - \{I_{j_k} + (I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger}) \underbrace{N_{x_k}}_{symmetric} \}^{-1}(I_{j_k} - \bar{B}_{x_k}\bar{B}_{x_k}^{\dagger})\ell_{x_k}$$

Corollary

Suppose $\bar{B}_{x_k}$ has full column rank, $\mathcal{B}_{x_k}$ is symmetric positive definite on $\{w \mid B^T w = 0\}$. Then the proximal Newton equation $J(x_k)[u(x_k)] = -v(x_k)$ can be computed by

$$u(x_k) = \begin{pmatrix} \bar{v}(x_k) + w(x_k) \\ \hat{v}(x_k) \end{pmatrix},$$

where $w(x_k) = \mathrm{argmin}_{\bar{B}_{x_k}^T w = 0}\, \ell_{x_k}^T w + \frac{1}{2} w^T \mathcal{B}_{x_k} w$.

tCG can be used for the computation of $w(x_k)$.

A Riemannian proximal Newton method (RPN)

1. $v(x_k) = \mathrm{argmin}_{v \in \mathrm{T}_{x_k} \mathcal{M}} \; f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$
2. $d(x_k) = \begin{pmatrix} \bar{d}(x_k) \\ \hat{d}(x_k) \end{pmatrix} = \begin{pmatrix} \bar{v}(x_k) + w(x_k) \\ \hat{v}(x_k) \end{pmatrix}$, where $w(x_k)$ is an output of tCG for solving $\min_{\bar{B}_{x_k}^T w = 0} \langle \ell_{x_k}, w \rangle + \frac{1}{2} \langle w, \mathcal{B}_{x_k} w \rangle$.
3. $x_{k+1} = R_{x_k}(\alpha_k d(x_k))$ with an appropriate step size α_k;

Question:

- Is $\mathcal{B}_{x_k}$ symmetric positive definite near a local minimizer x_*?
- What is the early termination conditions for tCG?
  - Guarantee global convergence;
  - Guarantee local superlinear convergence;

Is $\mathcal{B}_{x_k}$ symmetric positive definite near x_*?

Is $\mathcal{B}_{x_k}$ symmetric positive definite near x_*?

Assumption:

1. The function f is twice continuously differentiable with a Lipschitz continuous Euclidean Hessian;
2. 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;
3. 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 $\hat{x} + \hat{v} = 0$;
4. The linear operator $\mathcal{B}_{x_*}$ is positive definite on the subspace $\mathfrak{L}_{x_*} = \{w \mid \bar{B}_{x_*}^T w = 0\}$.

Is $\mathcal{B}_{x_k}$ symmetric positive definite near x_*?

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4. The linear operator $\mathcal{B}_{x_*}$ is positive definite on the subspace $\mathfrak{L}_{x_*} = \{w \mid \bar{B}_{x_*}^T w = 0\}$.

- Under the second assumption, the intersection of the manifold and the sparsity constraints forms an embedded submanifold around x_*;
- $\mathcal{B}_{x_*}$ is the Riemannian Hessian of F at x_* for the submanifold;
- $\mathcal{B}_{x_*}$ is symmetric positive semidefinite on $\mathfrak{L}_{x_*}$;

Is $\mathcal{B}_{x_k}$ symmetric positive definite near x_*?

Assumption:

1. The function f is twice continuously differentiable with a Lipschitz continuous Euclidean Hessian;
2. 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;
3. 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 $\hat{x} + \hat{v} = 0$;
4. The linear operator $\mathcal{B}_{x_*}$ is positive definite on the subspace $\mathfrak{L}_{x_*} = \{w \mid \bar{B}_{x_*}^T w = 0\}$.

Lemma

Suppose the above Assumption holds. Then there exists a neighborhood of x_*, denoted by $\mathcal{V}_2$, and a positive constant χ_ϵ such that the smallest eigenvalue of $\mathcal{B}_x$ on $\mathfrak{L}_x$ is greater than χ_ϵ for all $x \in \mathcal{V}_2$. This implies $\mathcal{B}_x$ is positive definite on $\mathfrak{L}_x$ for all $x \in \mathcal{V}_2$.

Early termination conditions in tCG

tCG step

2. $d(x_k) = \begin{pmatrix} \bar{d}(x_k) \\ \hat{d}(x_k) \end{pmatrix} = \begin{pmatrix} \bar{v}(x_k) + w(x_k) \\ \hat{v}(x_k) \end{pmatrix}$, where $w(x_k)$ is an output of tCG for solving $\min_{\bar{B}_{x_k}^T w = 0} \langle \ell_{x_k}, w \rangle + \frac{1}{2} \langle w, \mathcal{B}_{x_k} w \rangle$.

Early termination conditions in tCG

tCG step

2. $d(x_k) = \begin{pmatrix} \bar{d}(x_k) \\ \hat{d}(x_k) \end{pmatrix} = \begin{pmatrix} \bar{v}(x_k) + w(x_k) \\ \hat{v}(x_k) \end{pmatrix}$, where $w(x_k)$ is an output of tCG for solving $\min_{\bar{B}_{x_k}^T w = 0} \langle \ell_{x_k}, w \rangle + \frac{1}{2} \langle w, \mathcal{B}_{x_k} w \rangle$.

Difficulty

- Smooth:

$$\text{approximately} \quad \min_{d \in \mathrm{T}_{x_k} \mathcal{M}} \langle \mathrm{grad}\, f(x_k), d \rangle + \frac{1}{2} \langle \mathrm{Hess}\, f(x_k)[d], d \rangle,$$

find $d(x_k)$ such that $\langle d(x_k), \mathrm{grad}\, f(x_k) \rangle < 0$;

- Nonsmooth:

$$\text{approximately} \quad \min_{\bar{B}_{x_k}^T w = 0} \langle \ell_{x_k}, w \rangle + \frac{1}{2} \langle w, \mathcal{B}_{x_k} w \rangle,$$

find $w(x_k)$ such that $d(x_k)$ is a descent direction;

Early termination conditions in tCG

tCG step

2. $d(x_k) = \begin{pmatrix} \bar{d}(x_k) \\ \hat{d}(x_k) \end{pmatrix} = \begin{pmatrix} \bar{v}(x_k) + w(x_k) \\ \hat{v}(x_k) \end{pmatrix}$, where $w(x_k)$ is an output of tCG for solving $\min_{\bar{B}_{x_k}^T w = 0} \langle \ell_{x_k}, w \rangle + \frac{1}{2} \langle w, \mathcal{B}_{x_k} w \rangle$.

Difficulty

- Smooth:

  $$\text{approximately} \quad \min_{d \in \mathrm{T}_{x_k} \mathcal{M}} \langle \mathrm{grad}\, f(x_k), d \rangle + \frac{1}{2} \langle \mathrm{Hess}\, f(x_k)[d], d \rangle,$$

  find $d(x_k)$ such that $\langle d(x_k), \mathrm{grad}\, f(x_k) \rangle < 0$;
- Nonsmooth:

  $$\text{approximately} \quad \min_{\bar{B}_{x_k}^T w = 0} \langle \ell_{x_k}, w \rangle + \frac{1}{2} \langle w, \mathcal{B}_{x_k} w \rangle,$$

  find $w(x_k)$ such that $d(x_k)$ is a descent direction;

The early termination conditions for the smooth case are not sufficient.

Early termination conditions in tCG

Algorithm: Truncated conjugate gradient (tCG)

Require: $\vartheta > 0$, $\gamma > 0$, $\tau > 0$, $\theta > 0$, and $\kappa \in (0, 1)$;
Ensure: $(w(x), \mathrm{status})$;
if $G_x(v(x)) > G_x(0)$ **then**
    return $w(x) = 0$ and $\mathrm{status} =' early1'$;
end if
$z = \mathfrak{B} v(x)$;
if $\langle v(x), z \rangle + \tau \|\hat{v}(x)\|_F^2 < \gamma \|v(x)\|_F^2$ **then**
    return $w(x) = 0$ and $\mathrm{status} =' early2'$;
end if
$w_0 = 0$, $r_0 = P_x(\ell_x)$, $o_0 = -r_0$, $\delta_0 = \langle r_0, r_0 \rangle$, $t_0 = z$;
...... (CG iterations)

Omit subscript k for simplicity

Early termination conditions in tCG

Algorithm: Truncated conjugate gradient (tCG)

Require: $\vartheta > 0$, $\gamma > 0$, $\tau > 0$, $\theta > 0$, and $\kappa \in (0, 1)$;
Ensure: $(w(x), \mathrm{status})$;
1: **if** $G_x(v(x)) > G_x(0)$ **then**
2: return $w(x) = 0$ and $\mathrm{status} =' early1'$;
3: **end if**
4: $z = \mathfrak{B} v(x)$;
5: **if** $\langle v(x), z \rangle + \tau \|\hat{v}(x)\|_F^2 < \gamma \|v(x)\|_F^2$ **then**
6: return $w(x) = 0$ and $\mathrm{status} =' early2'$;
7: **end if**
8: $w_0 = 0$, $r_0 = P_x(\ell_x)$, $o_0 = -r_0$, $\delta_0 = \langle r_0, r_0 \rangle$, $t_0 = z$;
9: ...... (CG iterations)

- $G_x(u) = f(x) + \langle \nabla f(x), u \rangle + \frac{1}{2}\langle u, \mathfrak{B}_x u \rangle + \frac{\tau}{2}\|\hat{u}(x)\|_F^2 + h(x+u)$;
- Use to guarantee global convergence;
- $\frac{\tau}{2}\|\hat{u}(x)\|_F^2$ is added for the condition in Step 5;

Early termination conditions in tCG

Algorithm: Truncated conjugate gradient (tCG)

Require: $\vartheta > 0$, $\gamma > 0$, $\tau > 0$, $\theta > 0$, and $\kappa \in (0, 1)$;
Ensure: $(w(x), \mathrm{status})$;

```
if  G_x(v(x)) > G_x(0)  then
    return w(x) = 0 and status = 'early1';
end if
z = 𝔅 v(x);
if  ⟨v(x), z⟩ + τ‖v̂(x)‖_F^2 < γ‖v(x)‖_F^2  then
    return w(x) = 0 and status = 'early2';
end if
w_0 = 0, r_0 = P_x(ℓ_x), o_0 = −r_0, δ_0 = ⟨r_0, r_0⟩, t_0 = z;
...... (CG iterations)
```

- Use to guarantee global convergence;
- $\tau\|\hat{v}(x)\|_F^2$ is used since $\mathfrak{B}_x \succ 0$ may not hold;

Early termination conditions in tCG

Algorithm: Truncated conjugate gradient (tCG)

Require: $\vartheta > 0$, $\gamma > 0$, $\tau > 0$, $\theta > 0$, and $\kappa \in (0, 1)$;
Ensure: $(w(x), \mathrm{status})$;
1: ...... (See the previous slide)
2: $w_0 = 0$, $r_0 = P_x(\ell_x)$, $o_0 = -r_0$, $\delta_0 = \langle r_0, r_0 \rangle$, $t_0 = z$;
3: **for** $i = 0, 1, \dots$ **do**
4: $p_i = \mathcal{B} o_i$ and $q_i = P_x(p_i)$;
5: **if** $\langle o_i, q_i \rangle \le \vartheta \delta_i$ **then**
6: return $w(x) = w_i$ and $\mathrm{status} =' neg'$;
7: **end if**
8: ...... (Remaining CG iterations)
9: **end for**

An existing early termination condition

Early termination conditions in tCG

Algorithm: Truncated conjugate gradient (tCG)

Require: $\vartheta > 0$, $\gamma > 0$, $\tau > 0$, $\theta > 0$, and $\kappa \in (0, 1)$;
Ensure: $(w(x), \mathrm{status})$;

```
...... (See previous slides)
for i = 0, 1, ... do
    ...... (See previous slides)
    α_i = ⟨r_i, r_i⟩ / ⟨o_i, q_i⟩; w_{i+1} = w_i + α_i o_i; r_{i+1} = r_i + α_i q_i;
    d_{i+1} = ( v̄(x) + w_{i+1} ; v̂(x) ), t_{i+1} = t_i + α_i ( p_i ; 𝔅_21 o_i );
    if ⟨d_{i+1}, t_{i+1}⟩ + τ‖v̂(x)‖_F^2 < γ‖d_{i+1}‖_F^2 or G_x(d_{i+1}) > G_x(0) then
        return w(x) = w_i and status = 'early3';
    end if
    ...... (Remaining CG iterations)
end for
```

$$\alpha_i = \frac{\langle r_i, r_i\rangle}{\langle o_i, q_i\rangle};\ w_{i+1} = w_i + \alpha_i o_i;\ r_{i+1} = r_i + \alpha_i q_i;$$

$$d_{i+1} = \begin{pmatrix} \bar{v}(x) + w_{i+1} \\ \hat{v}(x) \end{pmatrix},\ t_{i+1} = t_i + \alpha_i \begin{pmatrix} p_i \\ \mathfrak{B}_{21} o_i \end{pmatrix};$$

$$\text{if } \langle d_{i+1}, t_{i+1}\rangle + \tau \|\hat{v}(x)\|_F^2 < \gamma \|d_{i+1}\|_F^2 \text{ or } G_x(d_{i+1}) > G_x(0) \text{ then return } w(x) = w_i \text{ and } \mathrm{status} = \text{'}early3\text{'};$$

Use to guarantee global convergence

Early termination conditions in tCG

Algorithm: Truncated conjugate gradient (tCG)

Require: $\vartheta > 0$, $\gamma > 0$, $\tau > 0$, $\theta > 0$, and $\kappa \in (0, 1)$;
Ensure: $(w(x), \mathrm{status})$;

...... (See previous slides)
for $i = 0, 1, \dots$ **do**
    ...... (See previous slides)
    $\beta_{i+1} = \frac{\langle r_{i+1}, r_{i+1} \rangle}{\langle r_i, r_i \rangle}$; $o_{i+1} = -r_{i+1} + \beta_{i+1} o_i$;
    $\delta_{i+1} = \langle r_{i+1}, r_{i+1} \rangle + \beta_{i+1}^2 \delta_i$; (Note that $\delta_{i+1} = \langle o_{i+1}, o_{i+1} \rangle$)
    $i = i + 1$;
    if $\|r_i\|_F \leq \|r_0\|_F \min(\|r_0\|_F^\theta, \kappa)$ **then**
        return $w(x) = w_i$, and $\mathrm{status} =' lin'$ if $\|r_0\|_F^\theta > \kappa$ and $\mathrm{status} =' sup'$ otherwise;
    end if
end for

An existing early termination condition

Assumption:

1. The function f is twice continuously differentiable with a Lipschitz continuous gradient;

Theorem

Suppose the above Assumption holds and the parameters are appropriately chosen. Then it holds that

$$\lim_{k \to \infty} \|v(x_k)\|_F = 0.$$

Assumption:

1. The function f is twice continuously differentiable with a Lipschitz continuous Euclidean Hessian;
2. 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;
3. 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 $\hat{x} + \hat{v} = 0$;
4. The function F is ς-geodesically strongly convex at x_*, i.e., there exists a neighborhood $\tilde{\mathcal{U}}_{x_*}$ of x_* in $\mathcal{M}$ such that
$$F(y) \geq F(x_*) + \frac{\varsigma}{2} \| \mathrm{Exp}_{x_*}^{-1}(y) \|_F^2$$
holds for any $y \in \tilde{\mathcal{U}}_{x_*}$.

Assumption:

1. The function f is twice continuously differentiable with a Lipschitz continuous Euclidean Hessian;
2. 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;
3. 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 $\hat{x} + \hat{v} = 0$;
4. The function F is ς-geodesically strongly convex at x_*, i.e., there exists a neighborhood $\tilde{\mathcal{U}}_{x_*}$ of x_* in $\mathcal{M}$ such that

$$F(y) \geq F(x_*) + \frac{\varsigma}{2} \| \mathrm{Exp}_{x_*}^{-1}(y) \|_F^2$$

holds for any $y \in \tilde{\mathcal{U}}_{x_*}$.

Lemma

Suppose the last Assumption holds, that is, the function $F = f + h$ is ς-geodesically strongly convex at x_*. Then the linear operator $\mathcal{B}_{x_*}$ is positive definite on $\mathfrak{L}_{x_*}$.

Assumption:

1. The function f is twice continuously differentiable with a Lipschitz continuous Euclidean Hessian;
2. 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;
3. 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 $\hat{x} + \hat{v} = 0$;
4. The function F is ς-geodesically strongly convex at x_*, i.e., there exists a neighborhood $\tilde{\mathcal{U}}_{x_*}$ of x_* in $\mathcal{M}$ such that

$$F(y) \geq F(x_*) + \frac{\varsigma}{2} \| \mathrm{Exp}_{x_*}^{-1}(y) \|_F^2$$

holds for any $y \in \tilde{\mathcal{U}}_{x_*}$.

Theorem

Suppose the previous assumptions hold. If x is sufficiently close x_* and the parameters are appropriately chosen, then tCG terminates only due to the accurate condition, i.e., $\|r_i\|_F \leq \|r_0\|_F \min(\|r_0\|_F^{\theta}, \kappa)$.

Theorem

Suppose the previous Assumptions hold and the parameters are appropriately chosen. Then there exists a neighborhood of x_*, *denoted by* $\mathcal{V}_8$, *such that if the step size one is used, then the convergence rate is* $\min(1+\theta, 2)$, *i.e.,* $\|R_x(d(x)) - x_*\|_F \leq C_{\mathrm{up}} \|x - x_*\|_F^{\min(1+\theta,2)}$ *holds for any* $x \in \mathcal{V}_8$ *and a constant* $C_{\mathrm{up}} > 0$.

Theorem

Suppose the previous Assumptions hold and the parameters are appropriately chosen. Then there exists a neighborhood of x_*, denoted by $\mathcal{V}_8$, such that if the step size one is used, then the convergence rate is $\min(1+\theta, 2)$, *i.e.,* $\|R_x(d(x)) - x_*\|_F \leq C_{\mathrm{up}} \|x - x_*\|_F^{\min(1+\theta,2)}$ *holds for any* $x \in \mathcal{V}_8$ *and a constant* $C_{\mathrm{up}} > 0$.

Is step size one acceptable for x sufficiently close to x_*?
That is to make objective function sufficiently descent.

Theorem

Suppose the previous Assumptions hold and the parameters are appropriately chosen. Then there exists a neighborhood of x_*, denoted by $\mathcal{V}_8$, such that if the step size one is used, then the convergence rate is $\min(1+\theta, 2)$, i.e., $\|R_x(d(x)) - x_*\|_F \leq C_{\rm up}\|x - x_*\|_F^{\min(1+\theta,2)}$ holds for any $x \in \mathcal{V}_8$ and a constant $C_{\rm up} > 0$.

Is step size one acceptable for x sufficiently close to x_*?
That is to make objective function sufficiently descent.

- For smooth Riemannian optimization problem, step size one is acceptable eventually for Riemannian Newton method;
- For Euclidean nonsmooth optimization problem $F = f + g$, step size one is also acceptable eventually for proximal Newton method [LSS14];

Example

- Consider $F : \mathbb{R}^2 \to \mathbb{R} : (x_1, x_2)^T \mapsto \underbrace{x_1^2 - 3x_1 + 1 + x_2^2}_{f(x)} + \underbrace{|x_1| + |x_2|}_{g(x)}$;
- The unique minimizer: $x_* = (1, 0)^T$;
- $x = (1 + \epsilon, 0)^T$ with $|\epsilon|$ being arbitrarily small;
- Proximal Newton direction: $u(x) = -(\epsilon, 0)^T$;
- Retraction: $R : \mathrm{T}\,\mathcal{M} \to \mathcal{M} : \eta_x \mapsto x + \eta_x + \begin{pmatrix} 0 \\ 2\eta_x^T \eta_x \end{pmatrix}$;
- $R(u(x)) = (1, 2\epsilon^2)^T$;
- $F(R_x(u(x))) - F(x) = 4\epsilon^4 + \epsilon^2 > 0$;
- Step size one is not acceptable for any $\epsilon > 0$;

Example

- Consider $F : \mathbb{R}^2 \to \mathbb{R} : (x_1, x_2)^T \mapsto \underbrace{x_1^2 - 3x_1 + 1 + x_2^2}_{f(x)} + \underbrace{|x_1| + |x_2|}_{g(x)}$;
- The unique minimizer: $x_* = (1, 0)^T$;
- $x = (1 + \epsilon, 0)^T$ with $|\epsilon|$ being arbitrarily small;
- Proximal Newton direction: $u(x) = -(\epsilon, 0)^T$;
- Retraction: $R : \mathrm{T}\,\mathcal{M} \to \mathcal{M} : \eta_x \mapsto x + \eta_x + \begin{pmatrix} 0 \\ 2\eta_x^T \eta_x \end{pmatrix}$;
- $R(u(x)) = (1, 2\epsilon^2)^T$;
- $F(R_x(u(x))) - F(x) = 4\epsilon^4 + \epsilon^2 > 0$;
- Step size one is not acceptable for any $\epsilon > 0$;

The answer is negative for nonsmooth Riemannian problems.

Difficulty comes from the nonsmoothness and the curvature.

Two consecutive iterations near x_* guarantee sufficient descent.

Theorem

Suppose that the previous Assumptions hold and that there exists a neighborhood of x_*, denoted by $\mathcal{V}_9$, such that for any $x \in \mathcal{V}_9$, it holds that $\|R_x(d(x)) - x_*\|_F \leq C_{\mathrm{up}}\|x - x_*\|_F^{\varkappa}$ for a $\varkappa > \sqrt{2}$ and $R_x(d(x)) \in \mathcal{V}_9$. Then there exists a neighborhood of x_*, denoted by $\mathcal{V}_{10}$, and a constant $\rho_1 > 0$ such that for any $x \in \mathcal{V}_{10}$, it holds that

$$F(x_{++}) \leq F(x) - \rho_1\|v(x)\|_F^2,$$

where $x_+ = R_x(d(x))$ and $x_{++} = R_{x_+}(d(x_+))$.

Two consecutive iterations near x_* guarantee sufficient descent.

Theorem

Suppose that the previous Assumptions hold and that there exists a neighborhood of x_*, denoted by $\mathcal{V}_9$, such that for any $x \in \mathcal{V}_9$, it holds that $\|R_x(d(x)) - x_*\|_F \leq C_{\mathrm{up}} \|x - x_*\|_F^{\varkappa}$ for a $\varkappa > \sqrt{2}$ and $R_x(d(x)) \in \mathcal{V}_9$. Then there exists a neighborhood of x_*, denoted by $\mathcal{V}_{10}$, and a constant $\rho_1 > 0$ such that for any $x \in \mathcal{V}_{10}$, it holds that

$$F(x_{++}) \leq F(x) - \rho_1 \|v(x)\|_F^2,$$

where $x_+ = R_x(d(x))$ and $x_{++} = R_{x_+}(d(x_+))$.

The global convergence result becomes: $\liminf_{k\to\infty} \|v(x_k)\|_F = 0$.

A new interpretation of RPN

Lemma

Suppose the previous Assumptions hold. Then there exists a neighborhood of x_*, denoted by $\mathcal{V}_5$, such that

$$u(x) = \operatorname*{argmin}_{u \in \mathrm{T}_x \mathcal{M}, \hat{u} = \hat{v}(x)} G_x(u) = \frac{1}{2}\langle u, \mathfrak{B}_x u \rangle + \nabla f(x)^T u + \mu \|x + u\|_1 \quad (1)$$

holds for any $x \in \mathcal{V}_5$.

- First, find the ManPG search direction $v(x)$;
- Fixed the entries that corresponds to the zero of $x + v$;
- Solve (1) for $u(x)$;

A new interpretation of RPN

Lemma

Suppose the previous Assumptions hold. Then there exists a neighborhood of x_*, denoted by $\mathcal{V}_5$, such that

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holds for any $x \in \mathcal{V}_5$.

- $\mathcal{M}_{sub}$: submanifold of the intersection of $\mathcal{M}$ and the sparse constraints;
- $\mathfrak{B}_x^{(11)}$ is the Riemannian Hessian at x with respect to $\mathcal{M}_{sub}$;
- $u(x)$ is the Riemannian Newton direction on $\mathcal{M}_{sub}$;

A new interpretation of RPN

Lemma

Suppose the previous Assumptions hold. Then there exists a neighborhood of x_*, denoted by $\mathcal{V}_5$, such that

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- $u(x)$ is the Riemannian Newton direction on $\mathcal{M}_{sub}$;

No counterpart in the Euclidean space.

Sparse PCA problem

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

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

Table: An average result of 20 random runs for random data. Multiple values of n, p, and μ are used. The subscript k indicates a scale of 10^k.

(n, p, μ)	Algo	iter	Fval	$\|v(x_k)\|_F$	time	sparsity
(400, 8, 0.8)	ManPG	3416.15	-2.16_1	3.66_{-9}	2.69	0.63
(400, 8, 0.8)	ManPG-Ada	1281.55	-2.16_1	1.06_{-10}	1.21	0.63
(400, 8, 0.8)	ManPQN	1260.40	-2.16_1	9.83_{-11}	0.72	0.63
(400, 8, 0.8)	RPN-CG	204.85	-2.16_1	1.16_{-11}	0.37	0.63
(800, 8, 0.8)	ManPG	4232.80	-5.92_1	1.84_{-7}	3.56	0.48
(800, 8, 0.8)	ManPG-Ada	1867.05	-5.92_1	2.57_{-10}	1.80	0.48
(800, 8, 0.8)	ManPQN	1883.80	-5.92_1	1.22_{-10}	1.43	0.48
(800, 8, 0.8)	RPN-CG	215.05	-5.92_1	1.07_{-11}	0.60	0.48

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- Proximal gradient on Stiefel manifold: ManPG, ManPG-Ada [CMSZ20];
- Proximal quasi-Newton on Stiefel manifold: ManPQN [WY23];
- The proposed method: RPN-CG;

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(400, 8, 0.8)	ManPG	3416.15	-2.16_1	3.66_{-9}	2.69	0.63
(400, 8, 0.8)	ManPG-Ada	1281.55	-2.16_1	1.06_{-10}	1.21	0.63
(400, 8, 0.8)	ManPQN	1260.40	-2.16_1	9.83_{-11}	0.72	0.63
(400, 8, 0.8)	RPN-CG	204.85	-2.16_1	1.16_{-11}	0.37	0.63
(800, 8, 0.8)	ManPG	4232.80	-5.92_1	1.84_{-7}	3.56	0.48
(800, 8, 0.8)	ManPG-Ada	1867.05	-5.92_1	2.57_{-10}	1.80	0.48
(800, 8, 0.8)	ManPQN	1883.80	-5.92_1	1.22_{-10}	1.43	0.48
(800, 8, 0.8)	RPN-CG	215.05	-5.92_1	1.07_{-11}	0.60	0.48

- Stop criterion: iter$\geq$ 5000 or $\|v(x)\|_F \leq 10^{-10}$;
- The entries of A are drawn from the standard normal distribution;
- Runs that converges to the same minimizer are reported;
- Support estimation: $(x + v(x))_i$ nonzero and $|(x)_i| \geq \|v(x)\|_F$;

Table: An average result of 20 random runs for random data. Multiple values of n, p, and μ are used. The subscript k indicates a scale of 10^k.

(n, p, μ)	Algo	iter	Fval	$\|v(x_k)\|_F$	time	sparsity
(400, 8, 0.8)	ManPG	3416.15	-2.16_1	3.66_{-9}	2.69	0.63
(400, 8, 0.8)	ManPG-Ada	1281.55	-2.16_1	1.06_{-10}	1.21	0.63
(400, 8, 0.8)	ManPQN	1260.40	-2.16_1	9.83_{-11}	0.72	0.63
(400, 8, 0.8)	RPN-CG	204.85	-2.16_1	1.16_{-11}	0.37	0.63
(800, 8, 0.8)	ManPG	4232.80	-5.92_1	1.84_{-7}	3.56	0.48
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(800, 8, 0.8)	ManPQN	1883.80	-5.92_1	1.22_{-10}	1.43	0.48
(800, 8, 0.8)	RPN-CG	215.05	-5.92_1	1.07_{-11}	0.60	0.48

RPN-CG always stops due to $\|v\|_F \leq 10^{-10}$
and is the most efficient one.

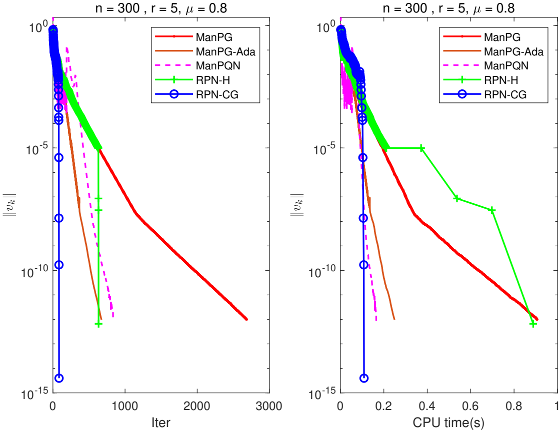

Figure: Sparse PCA: plots of $\|v(x_k)\|$ versus iterations and CPU times respectively.

[HS2025]: W. Huang*, W. Si. "A Riemannian Proximal Newton-CG Method", arxiv:2405.08365, 2025.

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-CG method;
  - A Riemannian proximal Newton method;
  - Truncated conjugate gradient;
  - Superlinear convergence approach;
  - Numerical experiments;
- Summary;

Thank you

Thank you!

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