A Riemannian Proximal Newton-CG Method

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Joint work with Wutao Si in University Grenoble Alpes

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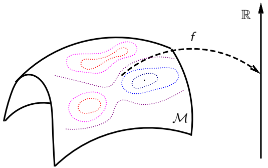
Problem Statement

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
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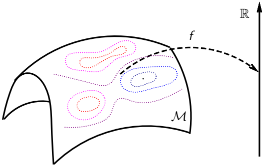

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Applications: sparse PCA [ZHT06], compressed modes [OLCO13], sparse partial least squares regression [CSG+18], sparse inverse covariance estimation [BESS19], sparse blind deconvolution [ZLK+17], and clustering [HWGVD22].

Outline

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

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

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- Proximal Gradient
- Accelerated versions
- Proximal inexact Newton
- Proximal quasi-Newton

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Given x_0[1],

$$\begin{cases} d_k = \arg\min_p \langle \nabla f(x_k), p \rangle + \frac{L}{2} \|p\|_{\mathrm{F}}^2 + h(x_k + p) \\ x_{k+1} = x_k + d_k. \end{cases}$$

1. The update rule: $x_{k+1} = \arg\min_x \langle \nabla f(x_k), x - x_k \rangle + \frac{L}{2} \|x - x_k\|^2 + h(x)$.

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- $h = 0$: reduce to steepest descent method;
- Any limit point is a critical point;
- $O\left(\frac{1}{k}\right)$ sublinear convergence rate for convex f and h;
- Linear convergence rate for strongly convex f and convex h;
- Local convergence rate by KL property;

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Given x_0, let $y_0 = x_0, t_0 = 1$;

$$\begin{cases} d_{y_k} = \operatorname{argmin}_p \langle \nabla f(y_k), p \rangle + \frac{L}{2} \|p\|_{\mathrm{F}}^2 + h(y_k + p) \\ x_{k+1} = y_k + d_{y_k} \\ t_{k+1} = \frac{\sqrt{4t_k^2+1}+1}{2} \\ y_{k+1} = x_{k+1} + \frac{t_k - 1}{t_{k+1}} (x_{k+1} - x_k). \end{cases}$$

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- A representative one: FISTA [BT09];
- Based on the Nesterov momentum technique;
- $O\left(\frac{1}{k^2}\right)$ sublinear convergence rate for convex f and h;

[BT09] A. Beck and M. Teboulle. A fast iterative shrinkage-thresholding algorithm for linear inverse problems. SIAM Journal on Imaging Sciences, 2(1):183-202, January 2009.

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Given x_0;

$$\begin{cases} d_k = \mathrm{argmin}_p \langle \nabla f(x_k), p \rangle + \frac{1}{2} \langle p, H_k p \rangle + h(x_k + p) \\ x_{k+1} = x_k + t_k d_k, \text{ for a step size } t_k \end{cases}$$

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- H_k is Hessian or a positive definite approximation to Hessian [LSS14];
- t_k is one for sufficiently large k;
- Quadratic/Superlinear convergence rate for strongly convex f and convex h;
- Josephy-Newton algorithm[Jos79];

[LLS14] Jason D Lee, Yuekai Sun, and Michael A Saunders. Proximal newton-type methods for minimizing composite functions. SIAM Journal on Optimization, 24(3):1420-1443, 2014.

[Jos79] N. Josephy, Newton's method for generalized equations. Technical Summary Report 1965, Mathematics Research Center, University of Wisconsin, Madison, Wisconsin (1979)

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[ST16] K. Scheinberg and X. Tang. Practical inexact proximal quasi-Newton method with global complexity analysis. Mathematical Programming, (160):495-529, 2016.

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- Dennis-Moré condition $\Longrightarrow$ superlinear convergence rate for strongly convex f and convex h [LSS14];
- Sublinear without the accuracy assumption on H_k [ST16];

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Proximal Gradient Method and its variants

Euclidean to Riemannian

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Riemannian versions

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[CMSZ20], ManPG: Given x_0,

$$\begin{cases} \eta_k = \arg\min_{\eta \in \mathrm{T}_{x_k}\mathcal{M}} \langle \nabla f(x_k), \eta \rangle + \frac{L}{2}\|\eta\|_F^2 + h(x_k + \eta) \\ x_{k+1} = R_{x_k}(\alpha_k \eta_k) \text{ with an appropriate step size } \alpha_k; \end{cases}$$

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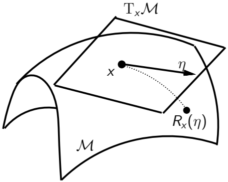

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[HW21a], RPG: Given x_0,

$$\begin{cases} \text{Let } \ell_{x_k}(\eta) = \langle \mathrm{grad} f(x_k), \eta \rangle_{x_k} + \frac{L}{2} \|\eta\|_{x_k}^2 + h(R_{x_k}(\eta)); \\ \eta_k \text{ is a stationary point of } \ell_{x_k} \text{ and } \ell_{x_k}(0) \geq \ell_k(\eta_k); \\ x_{k+1} = R_{x_k}(\eta_k); \end{cases}$$

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- [CMSZ20]: numerical aspect;
- [HW21a]: theoretical aspect;

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[HW21b] W. Huang and K. Wei. An extension of fast iterative shrinkage-thresholding algorithm to Riemannian optimization for sparse principal component analysis. Numerical Linear Algebra with Applications, p.e2409, 2021.

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- A representative on in [HW21b], also see [HW21a];
- Observe acceleration empirically;
- No theoretical guarantee for acceleration;

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[WY23, WY24], ManRQN, ARPQN, ARPN: Given x_0

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[WY23] Q. Wang and W. Yang. Proximal Quasi-Newton Method for Composite Optimization over the Stiefel Manifold, 95:39, 2023.
[WY24] Q. Wang and W. Yang. An adaptive regularized proximal Newton-type methods for composite optimization over the Stiefel manifold, Computational Optimization and Applications, 2024

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- $\mathcal{H}_k$: an approximation of quasi-Newton update or Riemannian Hessian;
- Local superlinear convergence results: $h(R_{x_k}(\eta))$;
- Only use diagonal $\mathcal{H}_k$ and $h(x_k+\eta)$ numerically.

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Good theoretical results

but not practical algorithms with a local superlinear convergence rate

Outline

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

A practical algorithm with a local superlinear convergence rate

W. Si, P.-A. Absil, W. Huang, R. Jiang, and S. Vary. A Riemannian Proximal Newton Method, SIAM Journal on Optimization, 34:1, p.654-681, 2024.

Outline

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Note that this method focuses on:

- $\mathcal{M}$ is an Riemannian embedded submanifold of a Euclidean space;
- $h(x) = \mu \|x\|_1$;

A Riemannian proximal Newton method

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

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

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

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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

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A Riemannian proximal Newton method (RPN)

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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 $\hat{x} + \hat{v} = 0$.

A Riemannian proximal Newton method

Local superlinear convergence rate

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]

A Riemannian proximal Newton method

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

A Riemannian proximal Newton 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];

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

for $k = 0, 1, \ldots$ **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 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];

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

1: **for** $k = 0, 1, \ldots$ **do**
2: Compute a ManPG direction v_k;
3: If $\|v_k\| \leq \epsilon$, then $K = k$ and break;
4: $x_{k+1} = R_{x_k}(\alpha v_k)$ with an appropriate step size;
5: **end for**
6: **for** k = K+1, K+2, ... **do**
7: Compute u_k by solving $J(x_k) u_k = -v_k$ with v_k being the ManPG direction;
8: $x_{k+1} = R_{x_k}(u_k)$;
9: **end for**

The switching parameter ϵ is crucial for the performance.

Outline

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

A practical and robust algorithm with
global convergence and local superlinear convergence guarantee

W. Huang, and W. Si. A Riemannian Proximal Newton-CG Method, arxiv:2405.08365, 2024.

Outline

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

Also focus on:

- $\mathcal{M}$ is an Riemannian embedded submanifold of a Euclidean space;
- $h(x) = \mu \|x\|_1$;

A Riemannian proximal Newton-CG method

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

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 $\underbrace{J(x_k)[u(x_k)] = -v(x_k)}_{tCG?}$

A Riemannian proximal Newton-CG method

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!

A Riemannian proximal Newton-CG method

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.

A Riemannian proximal Newton-CG method

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

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

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

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

A Riemannian proximal Newton-CG method

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

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-CG method

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_*?

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 $\mathfrak{L}_{x_*} = \{w \mid \bar{B}_{x_*}^T w = 0\}$.

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

A Riemannian proximal Newton-CG method

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:

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

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

- 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)

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

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)

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

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)

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

```
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;

A Riemannian proximal Newton-CG method

Early termination conditions in tCG

Algorithm: Truncated conjugate gradient (tCG)

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

...... (See the previous slide)
$w_0 = 0$, $r_0 = P_x(\ell_x)$, $o_0 = -r_0$, $\delta_0 = \langle r_0, r_0 \rangle$, $t_0 = z$;
for $i = 0, 1, \ldots$ **do**
    $p_i = \mathcal{B} o_i$ and $q_i = P_x(p_i)$;
    if $\langle o_i, q_i \rangle \leq \vartheta \delta_i$ **then**
        return $w(x) = w_i$ and $\mathrm{status} =' neg'$;
    end if
    ...... (Remaining CG iterations)
end for

An existing early termination condition

Early termination conditions in tCG

Algorithm: Truncated conjugate gradient (tCG)

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

...... (See previous slides)
for $i = 0, 1, \ldots$ **do**
    ...... (See previous slides)
    $\alpha_i = \frac{\langle r_i, r_i \rangle}{\langle o_i, q_i \rangle}$; $w_{i+1} = w_i + \alpha_i o_i$; $r_{i+1} = r_i + \alpha_i q_i$;
    $d_{i+1} = \begin{pmatrix} \bar{v}(x) + w_{i+1} \\ \hat{v}(x) \end{pmatrix}$, $t_{i+1} = t_i + \alpha_i \begin{pmatrix} p_i \\ \mathfrak{B}_{21} o_i \end{pmatrix}$;
    if $\langle d_{i+1}, t_{i+1} \rangle + \tau \|\hat{v}(x)\|_F^2 < \gamma \|d_{i+1}\|_F^2$ or $G_x(d_{i+1}) > G_x(0)$ **then**
        return $w(x) = w_i$ and $\mathrm{status} = ' early3'$;
    end if
    ...... (Remaining CG iterations)
end for

Use to guarantee global convergence

Early termination conditions in tCG

Algorithm: Truncated conjugate gradient (tCG)

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

...... (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 $\mathrm{status} = '\mathit{lin}'$ if $\|r_0\|_F^\theta > \kappa$ and $\mathrm{status} = '\mathit{sup}'$ otherwise;
  end if
end for

An existing early termination condition

A Riemannian proximal Newton-CG method

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

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

A Riemannian proximal Newton-CG method

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

A Riemannian proximal Newton-CG method

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 $\hat{x} + \hat{v} = 0$;
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$$F(y) \geq F(x_*) + \frac{\varsigma}{2} \| \mathrm{Exp}_{x_*}^{-1}(y) \|_F^2$$
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* $C_{\mathrm{up}} > 0$.

A Riemannian proximal Newton-CG method

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.

A Riemannian proximal Newton-CG method

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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.

- 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 $F : \mathbb{R}^2 \to \mathbb{R} : (x_1, x_2)^T \mapsto \underbrace{x_1^2 - 3x_1 + 1 + x_2^2}_{f(x)} + \underbrace{|x_1| + |x_2|}_{g(x)};$
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- $F(R_x(u(x))) - F(x) = 4\epsilon^4 + \epsilon^2 > 0$;
- 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.

A Riemannian proximal Newton-CG method

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 $x_{++} = R_{x_+}(d(x_+))$.

A Riemannian proximal Newton-CG method

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

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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 $\mathcal{M}_{sub}$;

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No counterpart in the Euclidean space.

Outline

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

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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- Stop criterion: iter≥ 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.

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

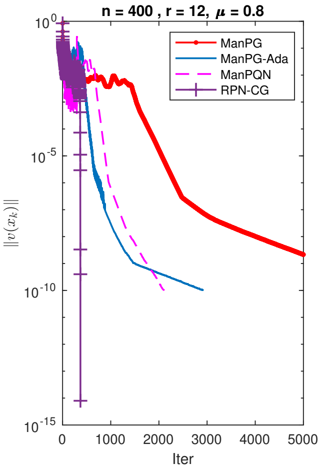

Figure: Sparse PCA: plots of $\|v(x_k)\|$ versus iterations and CPU times respectively.

The compressed modes (CM) problem aims to seek sparse solution of the independent-particle Schrödinger equation. It can be formulated as

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

where $H \in \mathbb{R}^{n \times n}$ denotes the discretized Schrödinger operator.

Table: An average result of 50 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
(256, 4, 0.1)	ManPG	3000.00	2.49	4.03_{-5}	0.75	0.85
(256, 4, 0.1)	ManPG-Ada	3000.00	2.49	9.49_{-5}	0.88	0.85
(256, 4, 0.1)	ManPQN	3000.00	2.49	9.06_{-6}	1.22	0.84
(256, 4, 0.1)	RPN-CG	92.54	2.49	2.66_{-9}	0.20	0.86
(512, 4, 0.1)	ManPG	3000.00	3.29	3.83_{-5}	0.76	0.86
(512, 4, 0.1)	ManPG-Ada	3000.00	3.29	1.16_{-4}	0.88	0.86
(512, 4, 0.1)	ManPQN	3000.00	3.30	1.44_{-6}	2.98	0.86
(512, 4, 0.1)	RPN-CG	147.40	3.29	2.29_{-9}	0.48	0.88

- Stop criterion: iter$\geq$ 3000 or $\|v(x)\|_F \leq 10^{-8}$;
- Different runs may converge to different points;

Table: An average result of 50 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
(256, 4, 0.1)	ManPG	3000.00	2.49	4.03_{-5}	0.75	0.85
(256, 4, 0.1)	ManPG-Ada	3000.00	2.49	9.49_{-5}	0.88	0.85
(256, 4, 0.1)	ManPQN	3000.00	2.49	9.06_{-6}	1.22	0.84
(256, 4, 0.1)	RPN-CG	92.54	2.49	2.66_{-9}	0.20	0.86
(512, 4, 0.1)	ManPG	3000.00	3.29	3.83_{-5}	0.76	0.86
(512, 4, 0.1)	ManPG-Ada	3000.00	3.29	1.16_{-4}	0.88	0.86
(512, 4, 0.1)	ManPQN	3000.00	3.30	1.44_{-6}	2.98	0.86
(512, 4, 0.1)	RPN-CG	147.40	3.29	2.29_{-9}	0.48	0.88

RPN-CG always stops due to $\|v\|_F \leq 10^{-8}$ and is the most efficient one.

None of other methods find a solution with $\|v\|_F \leq 10^{-8}$.

Numerical Experiments

Compressed modes

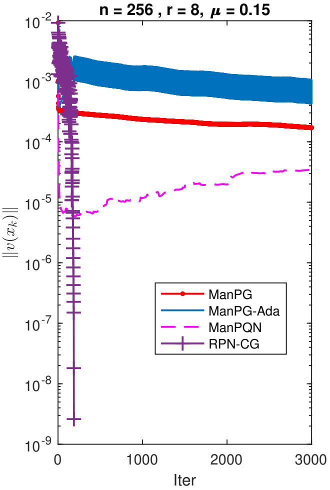

Figure: CM: plots of $\|v(x_k)\|$ versus iterations and CPU times respectively.

Summary

- Briefly review Euclidean and Riemannian proximal gradient method and its variants;
- Review the existing Riemannian proximal Newton method;
- Propose a Riemannian proximal Newton-CG method with global and local superlinear convergence gauranteed;
- Numerical experiments show its performance;

Future work

- Other types of $h(x)$;
- General manifold;
- Riemannian proximal quasi-Newton methods;
- Accelerated Riemannian proximal gradient method with theoretical guaranteed;

Thank you

Thank you!

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