Riemannian Proximal Gradient Methods

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This is joint work with Ke Wei at Fudan University.

Problem Statement

Optimization on Manifolds with Structure:

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



- \mathcal{M} is a Riemannian manifold;
- f is Lipschitz continuously differentiable and may be nonconvex; and
- g is continuous and convex, but may be not differentiable.

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Applications: sparse PCA, sparse blind deconvolution, sparse low rank image representation, etc [JTU03, GHT15, SQ16, ZLK $^+$ 17]

Existing Nonsmooth Optimization on Manifolds

 $F:\mathcal{M}\rightarrow\mathbb{R}$ is Lipschitz continuous

- Huang (2013), Gradient sampling method without convergence analysis.
- Grohs and Hosseini (2015), Two ε-subgradient-based optimization methods using line search strategy and trust region strategy, respectively. Any limit point is a critical point.
- Hosseini and Uschmajew (2017), Gradient sampling method and any limit point is a critical point.
- Hosseini and Huang and Yousefpour (2018), Merge ε-subgradient-based and quasi-Newton ideas and show any limit point is a critical point.

Existing Nonsmooth Optimization on Manifolds

$F:\mathcal{M} \to \mathbb{R}$ is convex

- Zhang and Sra (2016), subgradient-based method and function value converges to the optimal $O(1/\sqrt{k})$.
- Ferreira and Oliveira (2002) and Bento, Ferreira and Melo (2017), proximal point method and function value converges to the optimal O(1/k) on Hadamard manifold.
- Liu, Shang, Cheng, Cheng, and Jiao (2017), F is Lipschitz-continuously differentiable, function value converges to the optimal O(1/k²)

Existing Nonsmooth Optimization on Manifolds

F = f + g, where f is L-con, and g is non-smooth

- Chen, Ma, So, and Zhang (2018), A proximal gradient method with global convergence
- Huang and Wei (2019), A FISTA on manifolds with global convergence
- Huang and Wei (2019), A Riemannian proximal gradient method and its invariant with acceleration. Convergence rate analyses are given

A Euclidean Proximal Gradient Method

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

$$\min_{x \in \mathbb{R}^{n \times m}} F(x) = f(x) + g(x), \tag{1}$$

Proximal gradient method and its invariants are excellent methods for solving (1).

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A proximal gradient method¹:

initial iterate: x₀,

$$\begin{cases} d_k = \arg\min_{p \in \mathbb{R}^{n \times m}} \langle \nabla f(x_k), p \rangle + \frac{L}{2} \|p\|_F^2 + g(x_k + p), & (\text{Proximal mapping}) \\ x_{k+1} = x_k + d_k. & (\text{Update iterates}) \end{cases}$$

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

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Convergence Rates

Assumption

$$\min_{x \in \mathbb{R}^{n \times m}} F(x) = f(x) + g(x)$$
, with convex f ;

• O(1/k) sublinear convergence rate:

 $F(x_k) - F(x_*) \le C/k$, for a constant C;

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- Here, we consider FISTA [BT09]

initial iterate: x_0 and let $y_0 = x_0$, $t_0 = 1$, $\begin{cases}
d_k = \arg \min_{p \in \mathbb{R}^{n \times m}} \langle \nabla f(y_k), p \rangle + \frac{L}{2} \|p\|_F^2 + g(y_k + p), \\
x_{k+1} = y_k + d_k, \\
t_{k+1} = \frac{1 + \sqrt{4t_k^2 + 1}}{2}, \\
y_{k+1} = x_{k+1} + \frac{t_k - 1}{t_{k+1}} (x_{k+1} - x_k).
\end{cases}$

Difficulties in the Riemannian Setting

Euclidean proximal mapping

$$d_k = \arg\min_{p \in \mathbb{R}^{n \times m}} \langle \nabla f(x_k), p \rangle + \frac{L}{2} \|p\|_F^2 + g(x_k + p)$$

In the Riemannian setting:

- How to define the proximal mapping?
- Can be solved cheaply?
- Share the same convergence rate?

A Riemannian Proximal Gradient Method in [CMSZ18]

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A Riemannian proximal mapping [CMSZ18]

• Only works for embedded submanifold;

 $^1[\mathsf{CMSZ18}]$: S. Chen, S. Ma, M. C. So, and T. Zhang, Proximal gradient method for nonsmooth optimization over the Stiefel manifold. arXiv:1811.00980v2

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- Proximal mapping is defined in tangent space;
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- Solved efficiently for the Stiefel manifold by a semi-Newton algorithm [XLWZ18];

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• Convergence to a stationary point [HW19];

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2 $x_{k+1} = R_{x_k}(\alpha_k \eta_k)$ with an appropriate step size α_k ;

- Convergence to a stationary point [HW19];
- No convergence rate analysis (expect rate O(1/k) if f is convex);

New Riemannian Proximal Gradient Methods

GOAL:

Numerical aspect:

An accelerated Riemannian proximal gradient method with good numerical performance

Output: Control of the section of

An accelerated Riemannian proximal gradient method with convergence rate analysis and good numerical performance for some instances

Numerical aspect: A New Riemannian Proximal Gradient

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A Riemannian FISTA with a safeguard

initial iterate: x_0 and let $y_0 = x_0$, $t_0 = 1$;

Invoke a safeguard every N iterations;

3
$$x_{k+1} = R_{y_k}(\eta_k);$$

$$t_{k+1} = \frac{1 + \sqrt{4t_k^2 + 1}}{2};$$

• Compute
$$y_{k+1} = R_{x_{k+1}} \left(\frac{1-t_k}{t_{k+1}} R_{x_{k+1}}^{-1}(x_k) \right);$$

Numerical aspect: A New Riemannian Proximal Gradient

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9 Compute
$$y_{k+1} = R_{x_{k+1}} \left(\frac{1-t_k}{t_{k+1}} R_{x_{k+1}}^{-1}(x_k) \right);$$

- Run proximal gradient method every N iterations
- If the iterate by FISTA has larger function value than that by proximal gradient, then the safeguard takes effect.

Numerical aspect: A New Riemannian Proximal Gradient

A Riemannian FISTA with a safeguard

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initial iterate: x_0 and let $y_0 = x_0$, $t_0 = 1$;

- Invoke a safeguard every N iterations;
- $x_{k+1} = R_{y_k}(\eta_k);$
- Solution $y_{k+1} = R_{x_{k+1}} \left(\frac{1-t_k}{t_{k+1}} R_{x_{k+1}}^{-1}(x_k) \right);$

FISTA initial iterate: x_0 and let $y_0 = x_0$, $t_0 = 1$,

$$\begin{cases} d_{k} = \arg\min_{p \in \mathbb{R}^{n \times m}} \langle \nabla f(y_{k}), p \rangle + \frac{L}{2} \|p\|_{F}^{2} + g(y_{k} + p), \\ x_{k+1} = y_{k} + d_{k}, \\ t_{k+1} = \frac{1 + \sqrt{4t_{k}^{2} + 1}}{2}, \\ y_{k+1} = x_{k+1} + \frac{t_{k} - 1}{t_{k+1}} (x_{k+1} - x_{k}). \end{cases}$$

Riemannian Proximal Gradient Methods

Numerical aspect: A New Riemannian Proximal Gradient

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- Invoke a safeguard every N iterations;
- $x_{k+1} = R_{y_k}(\eta_k);$ • $t_{k+1} = \frac{1 + \sqrt{4t_k^2 + 1}}{1 + \sqrt{4t_k^2 + 1}};$
 - **3** Compute $y_{k+1} = R_{x_{k+1}} \left(\frac{1-t_k}{t_{k+1}} R_{x_{k+1}}^{-1}(x_k) \right);$

A Riemannian generalization: $R_x(\eta) = x + \eta$, $R_x^{-1}(y) = y - x$: $y_{k+1} = x_{k+1} + \frac{1 - t_k}{t_{k+1}}$ $(x_k - x_{k+1})$, replaced by $R_{x_{k+1}}^{-1}(x_k)$ replaced by $R_{x_{k+1}}(\frac{1 - t_k}{t_{k-1}}, R_{x_{k-1}}^{-1}(x_k))$

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3 Compute
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- Works well in practice
- Convergence globally
- No convergence rate analysis

Theoretical aspect: A New Riemannian Proximal Gradient

GOAL: Develop an accelerated Riemannian proximal gradient method with convergence rate analysis and good numerical performance for some instances

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• General framework for Riemannian optimization;

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- The tangent space may be too rough to approximate manifold for convergence analysis;

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- General framework for Riemannian optimization;
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- Step size can be fixed to be 1;

Assumptions and Convergence Result

Assumption:

 f is Lipschitz continuously differentiable in a Riemannian sense (L-retraction-smooth);

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Definition

A function $h: \mathcal{M} \to \mathbb{R}$ is called *L*-retraction-smooth with respect to a retraction R in $\mathcal{N} \subset \mathcal{M}$ if for any $x \in \mathcal{N}$ and any $\mathcal{S}_x \subset T_x \mathcal{M}$ such that $R_x(\mathcal{S}_x) \subset \mathcal{N}$, we have that $q_x = h \circ R_x$ satisfies

$$q_x(\eta) \leq q_x(\xi) + \langle ext{grad} \ q_x(\xi), \eta - \xi
angle_x + rac{L}{2} \| \eta - \xi \|_x^2 \ \ orall \eta, \xi \in \mathcal{S}_x.$$
Assumptions and Convergence Result

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 f is Lipschitz continuously differentiable in a Riemannian sense (L-retraction-smooth);

Theoretical results:

• For any accumulation point x_* of $\{x_k\}$, x_* is a stationary point, i.e., $0 \in \partial F(x_*)$.

Assumptions and Convergence Rate

Additional Assumptions:

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$$q_{x}(\eta) \geq q_{x}(\xi) + \langle \zeta, \eta - \xi \rangle_{x} \quad \forall \eta, \xi \in \mathcal{S}_{x}.$$
(2)

Note that $\zeta = \operatorname{grad} q_x(\xi)$ if *h* is differentiable; otherwise, ζ is any subgradient of q_x at ξ .

Assumptions and Convergence Rate

Additional Assumptions:

- f is convex in a Riemannian sense (retraction-convex);
- Retraction approximately satisfies the triangle relation:

 $\left| \|\xi_x - \eta_x\|_x^2 - \|\zeta_y\|_y^2 \right| \le \kappa \|\eta_x\|_x^2$, for a constant κ

where $\eta_x = R_x^{-1}(y)$, $\xi_x = R_x^{-1}(z)$, $\zeta_y = R_y^{-1}(z)$.

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Table: Exponential mapping on the Stifel manifold with the Euclidean metric $\langle \eta_x, \xi_x \rangle_x = \operatorname{trace}(\eta_x^T \xi_x)$. Left $= \left| \|\xi_x - \eta_x\|_x^2 - \|\zeta_y\|_y^2 \right|$

(n, p) =	: (10, 1)	(n, p) =	= (10, 4)	(n,p) = (10,10)		
$\ \eta_x\ $	Left	$\ \eta_{\mathbf{x}}\ $	Left	$\ \eta_{\mathbf{x}}\ $	Left	
5.00_{-2}	7.83 ₋₅	5.00_{-2}	1.83_{-5}	5.00_{-2}	2.14_{-6}	
2.50_{-2}	1.80_{-5}	2.50_{-2}	4.27_{-6}	2.50_{-2}	4.72_{-7}	
1.25_{-2}	4.25_{-6}	1.25_{-2}	1.01_{-6}	1.25_{-2}	1.11_{-7}	
6.25 ₋₃	1.03_{-6}	6.25 ₋₃	2.46_{-7}	6.25 ₋₃	2.68_8	
3.12_{-3}	2.54_{-7}	3.12_3	6.05_{-8}	3.13_3	6.61_{-9}	

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Table: Exponential mapping on the Stifel manifold with the canonical metric $\langle \eta_x, \xi_x \rangle_x = \operatorname{trace}(\eta_x^T (I - XX^T/2)\xi_x)$. Left $= \left| \|\xi_x - \eta_x\|_x^2 - \|\zeta_y\|_y^2 \right|$

(n, p) =	= (10, 2)	(n, p) =	= (10, 4)	(n,p) = (10,9)		
$\ \eta_{\mathbf{x}}\ $	Left	$\ \eta_{\mathbf{x}}\ $	Left	$\ \eta_{\mathbf{x}}\ $	Left	
5.00_{-2}	3.55_{-5}	5.00_{-2}	1.15_{-5}	5.00_2	8.39_6	
2.50_{-2}	8.06_{-6}	2.50_{-2}	2.58_{-6}	2.50_{-2}	1.89_{-6}	
1.25_{-2}	1.90_{-6}	1.25_{-2}	6.08_7	1.25_{-2}	4.45_{-7}	
6.25_{-3}	4.61_{-7}	6.25 ₋₃	1.47_{-7}	6.25 ₋₃	1.08_{-7}	
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where
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, $\xi_x = R_x^{-1}(z)$, $\zeta_y = R_y^{-1}(z)$.

Theoretical results:

• Convergence rate O(1/k):

$$F(x_k) - F(x_*) \leq \frac{1}{k} \left(\frac{L}{2} \| R_{x_0}^{-1}(x_*) \|_{x_0}^2 + \frac{L\kappa C}{2} (F(x_0) - F(x_*)) \right).$$

A Riemannian FISTA

A Riemannian FISTA

initial iterate: x_0 and let $y_0 = x_0$, $t_0 = 1$; $\eta_k = \arg \min_{\eta \in \mathbf{T}_{y_k}} \mathcal{M} \langle \operatorname{grad} f(y_k), \eta \rangle_{y_k} + \frac{L}{2} \|\eta\|_{y_k}^2 + g(R_{y_k}(\eta));$ $x_{k+1} = R_{y_k}(\eta_k);$ $t_{k+1} = \frac{1 + \sqrt{4t_k^2 + 1}}{2};$ Compute $y_{k+1} = R_{y_k} \left(\frac{t_{k+1} + t_k - 1}{t_{k+1}} \eta_{y_k} - \frac{t_k - 1}{t_{k+1}} R_{y_k}^{-1}(x_k) \right);$ FISTA initial iterate: x_0 and let $y_0 = x_0$, $t_0 = 1$

$$\begin{cases} d_k = \arg\min_{p \in \mathbb{R}^{n \times m}} \langle \nabla f(y_k), p \rangle + \frac{l}{2} \|p\|_F^2 + g(y_k + p), \\ x_{k+1} = y_k + d_k, \\ t_{k+1} = \frac{1 + \sqrt{4t_k^2 + 1}}{2}, \\ y_{k+1} = x_{k+1} + \frac{t_k - 1}{t_{k+1}} (x_{k+1} - x_k). \end{cases}$$

A Riemannian FISTA

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initial iterate: x_0 and let $y_0 = x_0$, $t_0 = 1$; **a** $\eta_k = \arg \min_{\eta \in T_{y_k}} \mathcal{M} \langle \operatorname{grad} f(y_k), \eta \rangle_{y_k} + \frac{L}{2} \|\eta\|_{y_k}^2 + g(R_{y_k}(\eta))$; **a** $x_{k+1} = R_{y_k}(\eta_k)$; **b** $t_{k+1} = \frac{1 + \sqrt{4t_k^2 + 1}}{2}$; **c** Compute $y_{k+1} = R_{y_k} \left(\frac{t_{k+1} + t_k - 1}{t_{k+1}} \eta_{y_k} - \frac{t_k - 1}{t_{k+1}} R_{y_k}^{-1}(x_k) \right)$;

A Riemannian generalization:

$$y_{k+1} = y_k + \frac{t_{k+1} + t_k - 1}{t_{k+1}} (x_{k+1} - y_k) - \frac{t_k - 1}{t_{k+1}} (x_k - y_k)$$
$$= x_{k+1} + \frac{t_k - 1}{t_{k+1}} (x_{k+1} - x_k),$$

Assumptions and Convergence Rate

Additional Assumptions:

 $\bullet\,$ There exists a constant $\tilde{\kappa}$ such that

$$\begin{split} \|(t_{k+1}-1)(R_{y_k}^{-1}(x_{k+1})-R_{y_k}^{-1}(y_{k+1}))+R_{y_k}^{-1}(x_*)-R_{y_k}^{-1}(y_{k+1})\|_{y_k}^2\\ &-\|(t_{k+1}-1)R_{y_{k+1}}^{-1}(x_{k+1})+R_{y_{k+1}}^{-1}(x_*)\|_{y_{k+1}}^2\Big|\leq \tilde{\kappa}\|R_{y_k}^{-1}(y_{k+1})\|_{y_k}^2. \end{split}$$

• $\phi(k) := \sum_{i=0}^{k} \|R_{y_k}^{-1}(y_{k+1})\|_{y_k}^2$ increases on the order of $O((k+1)^{\theta})$ for $\theta \in [0, 1]$, i.e., $\frac{\phi(k)}{(k+1)^{\theta}} < C_{\phi}$ for all k.

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Assumptions and Convergence Rate

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•
$$\phi(k) := \sum_{i=0}^{k} \|R_{y_k}^{-1}(y_{k+1})\|_{y_k}^2$$
 increases on the order of $O((k+1)^{\theta})$ for $\theta \in [0, 1]$, i.e., $\frac{\phi(k)}{(k+1)^{\theta}} < C_{\phi}$ for all k .

Theoretical results:

• Convergence rate $O(1/k^2)$ if $\theta = 0$:

$$F(x_k) - F(x_*) \leq \frac{2L}{k^2} \|R_{x_0}^{-1}(x_*)\|_{x_0}^2 + \frac{2L\tilde{\kappa}C_{\phi}}{k^{2-\theta}}(F(x_0) - F(x_*)).$$

The Proposed Algorithm

A Riemannian FISTA with a safeguard

initial iterate: x_0 and let $y_0 = x_0$, $t_0 = 1$;

• Invoke a safeguard every N iterations;

•
$$x_{k+1} = R_{y_k}(\eta_k);$$

$$t_{k+1} = \frac{1+\sqrt{4t_k^2+1}}{2};$$

3 Compute
$$y_{k+1} = R_{y_k} \left(\frac{t_{k+1} + t_k - 1}{t_{k+1}} \eta_{y_k} - \frac{t_k - 1}{t_{k+1}} R_{y_k}^{-1}(x_k) \right);$$

• Convergence globally;

 Convergence rate ¹/_{k^{2-θ}} if previous assumptions hold and safeguard takes effect for finite iterations;

Riemannian subproblem

$$\eta_u = \arg\min_{\eta \in \mathbb{T}_u \mathcal{M}} \ell_u(\eta) := \langle \nabla f(u), \eta \rangle_u + \frac{L}{2} \|\eta\|_u^2 + g(R_u(\eta))$$

Riemannian subproblem

$$\eta_u = \arg\min_{\eta \in \mathrm{T}_u \,\mathcal{M}} \ell_u(\eta) := \langle \nabla f(u), \eta \rangle_u + \frac{L}{2} \|\eta\|_u^2 + g(R_u(\eta))$$

In some cases, the subproblem can be solved by exploiting the structure of the manifold;

Riemannian subproblem

$$\eta_u = \arg\min_{\eta \in \mathbb{T}_u \mathcal{M}} \ell_u(\eta) := \langle \nabla f(u), \eta \rangle_u + \frac{L}{2} \|\eta\|_u^2 + g(R_u(\eta))$$

.

Solving the Riemannian Proximal Mapping

initial iterate: $\eta_0 \in T_u \mathcal{M}$, $\sigma \in (0, 1)$, k = 0;

$$v_k = R_u(\eta_k);$$

Compute

$$\xi_k^* = \arg \min_{\xi \in \mathrm{T}_{\nu_k} \mathcal{M}} \langle \mathcal{T}_{R_{\eta_k}}^{-\sharp}(\operatorname{grad} f(u) + \tilde{L}\eta_k), \xi \rangle_u + \frac{L}{4} \|\xi\|_F^2 + g(\nu_k + \xi);$$

• Find $\alpha > 0$ such that $\ell_u(\eta_k + \alpha \mathcal{T}_{R_{\eta_k}}^{-1} \xi_k^*) < \ell_u(\eta_k) - \sigma \alpha \|\xi_k^*\|_u^2$;

•
$$\eta_{k+1} = \eta_k + lpha \mathcal{T}_{R_{\eta_k}}^{-1} \xi_k^*$$
, $k \leftarrow k+1$ and goto Step 1;

Above algorithm is used if the ambient space is \mathbb{R}^n

Riemannian subproblem

$$\eta_u = \arg\min_{\eta \in \mathbb{T}_u \mathcal{M}} \ell_u(\eta) := \langle \nabla f(u), \eta \rangle_u + \frac{L}{2} \|\eta\|_u^2 + g(R_u(\eta))$$

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Solving the Riemannian Proximal Mapping

initial iterate: $\eta_0 \in T_u \mathcal{M}$, $\sigma \in (0, 1)$, k = 0;

$$v_k = R_u(\eta_k);$$

Compute

$$\xi_k^* = \arg \min_{\xi \in \operatorname{T}_{\nu_k} \mathcal{M}} \langle \mathcal{T}_{R_{\eta_k}}^{-\sharp} (\operatorname{grad} f(u) + \tilde{L}\eta_k), \xi \rangle_u + \frac{L}{4} \|\xi\|_F^2 + g(\nu_k + \xi);$$

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$$\eta_u = \arg\min_{\eta \in \mathbb{T}_u \mathcal{M}} \ell_u(\eta) := \langle \nabla f(u), \eta \rangle_u + \frac{L}{2} \|\eta\|_u^2 + g(R_u(\eta))$$

.

Solving the Riemannian Proximal Mapping

initial iterate: $\eta_0 \in T_u \mathcal{M}$, $\sigma \in (0, 1)$, k = 0;

$$v_k = R_u(\eta_k);$$

Compute

$$\xi_k^{\pm} = \arg \min_{\xi \in \mathrm{T}_{v_k} \mathcal{M}} \langle \mathcal{T}_{R_{\eta_k}}^{\pm} (\operatorname{grad} f(u) + \tilde{L}\eta_k), \xi \rangle_u + \frac{L}{4} \|\xi\|_F^2 + g(v_k + \xi);$$

• Find $\alpha > 0$ such that $\ell_u(\eta_k + \alpha \mathcal{T}_{R_{\eta_k}}^{-1} \xi_k^*) < \ell_u(\eta_k) - \sigma \alpha \|\xi_k^*\|_u^2$;

•
$$\eta_{k+1} = \eta_k + lpha \mathcal{T}_{R_{\eta_k}}^{-1} \xi_k^*$$
, $k \leftarrow k+1$ and goto Step 1;

An application of [CMSZ18] if $R_u^{-1}(\eta)$ exists.

Numerical Experiments

Sparse PCA problem [GHT15]

$$\min_{X \in OB(p,n)} \|X^{\mathsf{T}}A^{\mathsf{T}}AX - D^2\|_F^2 + \lambda \|X\|_1,$$

where $A \in \mathbb{R}^{m \times n}$, D is the diagonal matrix with dominant singular values of A, $OB(p, n) = \{X \in \mathbb{R}^{n \times p} \mid \text{diag}(X^T X) = I_p\}$, $p \le m$;

Numerical Experiments

Solve the proximal mapping:

$$\eta_k = \arg\min_{\eta \in \mathrm{T}_x \mathcal{M}} \langle \nabla f(x_k), \eta \rangle_{x_k} + \frac{L}{2} \|\eta\|_{x_k}^2 + g(R_{x_k}(\eta));$$

• Exponential mapping (each column): $R_x(\eta_x) = x \cos(||\eta_x||) + \frac{\eta_x}{||\eta_x||} \sin(||\eta_x||);$

Numerical Experiments

Solve the proximal mapping:

$$\eta_k = \arg\min_{\eta \in \mathrm{T}_x \mathcal{M}} \langle
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- Exponential mapping (each column): $R_x(\eta_x) = x \cos(||\eta_x||) + \frac{\eta_x}{||\eta_x||} \sin(||\eta_x||);$
- Explore the fact that the following problem has a closed solution:

$$\min_{x \in OB(p,n)} \|x - y\|_F^2 + \frac{1}{2\lambda} \|x\|_1 \text{ for any } y \in \mathbb{R}^{n \times p}.$$

Numerical Experiments

Solve the proximal mapping:

$$\eta_k = \arg\min_{\eta \in \mathrm{T}_x \,\mathcal{M}} \langle \nabla f(x_k), \eta \rangle_{x_k} + \frac{L}{2} \|\eta\|_{x_k}^2 + g(R_{x_k}(\eta));$$

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A conditional gradient (Frank-Wolfe) method is used;

Numerical Experiments

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- A conditional gradient (Frank-Wolfe) method is used;
- Numerically, using approximate 2 iterations is enough for high accuracy;

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- A conditional gradient (Frank-Wolfe) method is used;
- Numerically, using approximate 2 iterations is enough for high accuracy;

Numerical Experiments

Table: An average result of 10 random tests. n = 128, m = 20, r = 4. $\delta = (L ||x_{k+1} - x_k||)^2$. The subscript k indicates a scale of 10^k .

λ	Algo	iter	time	f	δ	spar.	navar
	ManPG	11791	1.40	8.33 ₁	5.11_{-6}	0.54	0.86
2	RPG	11679	0.94	8.33 ₁	5.11_{-6}	0.54	0.86
5	ManPG-Ada	1398	0.30	8.33 ₁	1.67_{-3}	0.54	0.86
	A-ManPG	273	0.09	8.33 ₁	9.19_{-4}	0.54	0.86
	A-RPG	263	0.06	8.33 ₁	1.12_{-3}	0.54	0.86

- ManPG: the method in [CMSZ18];
- RPG: the new Riemannian proximal gradient without acceleration;
- A-ManPG: Use similar technique to accelerate ManPG;
- A-RPG: the new Riemannian proximal gradient with acceleration;

Numerical Experiments

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ManPG-Ada:

•
$$\eta_k = \arg \min_{\eta \in T_{x_k} \mathcal{M}} \langle \nabla f(x_k), \eta \rangle + \frac{\tilde{L}}{2} \|\eta\|_F^2 + g(x_k + \eta);$$

2
$$x_{k+1} = R_{x_k}(lpha_k \eta_k)$$
 with an appropriate step size $lpha_k$

• Update \tilde{L} ;

Numerical Experiments

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- ManPG and RPG: Stop when $\delta < 10^{-8} nr$;
- A-ManPG and A-RPG: Stop when F is smaller than the minimum of ManPG and RPG;

Numerical Experiments

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- spar.: sparsity of the solution;
- navar: the adjusted variance normalized by the variance from the standard PCA;

Numerical Experiments

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• PG without acceleration is slower than PG with acceleration;

• RPG is slightly faster ManPG in term of computational time;

Numerical Experiments

Table: An average result of 10 random tests. n = 128, m = 20, r = 4. $\delta = (L ||x_{k+1} - x_k||)^2$. The subscript k indicates a scale of 10^k .

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	A-RPG	263	0.06	8.33 ₁	1.12_{-3}	0.54	0.86

 ManPG and RPG: similarly; and A-ManPG and A-RPG: similarly; in term of:

- number of iterations;
- function values;
- sparsity;
- adjusted variance;

Numerical Experiments



Figure: Two typical runs of ManPG, RPG, A-ManPG, and A-RPG for the Sparse PCA problem. n = 1024, p = 4, $\lambda = 2$, m = 20.

Numerical Experiments

Sparse PCA problem (Another model) [CMSZ18, HW19]

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

where $A \in \mathbb{R}^{m \times n}$ is a data matrix.

Numerical Experiments

Solve the proximal mapping:

$$\eta_k = \arg\min_{\eta \in \mathrm{T}_x \mathcal{M}} \langle \nabla f(x_k), \eta \rangle_{x_k} + \frac{L}{2} \|\eta\|_{x_k}^2 + g(R_{x_k}(\eta));$$

.

• Exponential mapping:

$$\operatorname{Exp}_{X}(\eta_{X}) = \begin{bmatrix} X & Q \end{bmatrix} \exp\left(\begin{bmatrix} \Omega & -R^{T} \\ R & 0 \end{bmatrix} \right) \begin{bmatrix} I_{p} \\ 0 \end{bmatrix},$$

where $\Omega = X^T \eta_X$, Q and R are from the compact QR factorization of $(I - XX^T)\eta_X$.

Numerical Experiments

Solve the proximal mapping:

$$\eta_k = \arg \min_{\eta \in \mathrm{T}_{\mathsf{x}} \,\mathcal{M}} \langle \nabla f(\mathbf{x}_k), \eta \rangle_{\mathsf{x}_k} + \frac{L}{2} \|\eta\|_{\mathsf{x}_k}^2 + g(R_{\mathsf{x}_k}(\eta));$$

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- Ingredients for the algorithm on Page 17:
 - R^{-1} by iterative methods [Zim17]
 - $\mathcal{T}_{R}^{-\sharp}$ by iterative methods
Numerical Experiments

Lemma

The adjoint operator of the inverse differentiated retraction is

$$\begin{aligned} \mathcal{T}_{\eta_{X}}^{-\sharp}\xi_{X} &= \begin{bmatrix} X & Q_{1} \end{bmatrix} \exp\left(\begin{bmatrix} \Omega_{\eta_{X}} & -R_{1}^{T} \\ R_{1} & 0_{\rho \times \rho} \end{bmatrix} \right) \begin{bmatrix} X & Q_{1} \end{bmatrix}^{T} \omega_{x} \\ &+ \begin{pmatrix} I - \begin{bmatrix} X & Q_{1} \end{bmatrix} \begin{bmatrix} X & Q_{1} \end{bmatrix}^{T} \end{pmatrix} \omega_{x}, \end{aligned}$$

where $\omega_{X} = X\Omega_{\zeta_{Y}} + QR_{2}$, $Y = \operatorname{Exp}_{X}(\eta_{X})$, $Q_{1}R_{1} = (I - XX^{T})\eta_{X}$ and $Q_{2}\tilde{R}_{2} = (I - [XQ_{1}][XQ_{1}]^{T})\xi_{X}$ are qr decompositions, $Q = [Q_{1} \quad Q_{2}]$, $\tilde{M}_{1} = \begin{bmatrix} \Omega_{\eta_{X}} & -R_{1}^{T} & 0_{p \times p} \\ R_{1} & 0_{p \times p} & 0_{p \times p} \end{bmatrix}$, $\tilde{Z}\tilde{\Lambda}\tilde{Z}^{H} = \tilde{M}_{1}$, and $\Omega_{\zeta_{Y}}$ and R_{2} are $g_{0p \times p} \quad 0_{p \times p} \quad 0_{p \times p} \end{bmatrix}$, $\tilde{Z}\tilde{\Lambda}Z^{H} = \tilde{M}_{1}$, \tilde{L}^{T} ,

Numerical Experiments

Table: An average result of 10 random tests. n = 1024, m = 20, r = 4. $\delta = (L||x_{k+1} - x_k||)^2$. The subscript k indicates a scale of 10^k .

λ	Algo	iter	time	f	δ	spar.	navar
3	ManPG	1572	0.92	-7.28	4.76_{-5}	0.64	0.74
	RPG	1464	5.46	-7.28	4.06_{-5}	0.64	0.74
	ManPG-Ada	376	0.22	-7.28	3.99_{-4}	0.64	0.74
	A-ManPG	110	0.20	-7.28	1.06_{-3}	0.64	0.74
	A-RPG	88	1.61	-7.28	2.05_{-4}	0.64	0.74

- Same notation, same stopping criterion, same parameter setting;
- New approaches take more time due to excessive cost on R^{-1} and $\mathcal{T}^{-\sharp}$;
- New approaches take less iterations;

Numerical Experiments

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	RPG	1464	5.46	-7.28	4.06_{-5}	0.64	0.74
	ManPG-Ada	376	0.22	-7.28	3.99_{-4}	0.64	0.74
	A-ManPG	110	0.20	-7.28	1.06_{-3}	0.64	0.74
	A-RPG	88	1.61	-7.28	2.05_{-4}	0.64	0.74

- Same notation, same stopping criterion, same parameter setting;
- New approaches take more time due to excessive cost on R^{-1} and $\mathcal{T}^{-\sharp}$;
- New approaches take less iterations;

Numerical Experiments



Figure: Two typical runs of ManPG, RPG, A-ManPG, and A-RPG for the Sparse PCA problem. n = 1024, p = 4, $\lambda = 2$, m = 20.

Acceleration for SPCA on the Stiefel manifold

Scaled proximal mapping:

$$\eta_{k} = \arg \min_{\eta \in \mathrm{T}_{x_{k}} \mathcal{M}} \langle \nabla f(x_{k}), \eta \rangle + \frac{L}{2} \|\eta\|_{F}^{2} + g(x_{k} + \eta)$$
$$\implies \eta_{k} = \arg \min_{\eta \in \mathrm{T}_{x_{k}} \mathcal{M}} \langle \nabla f(x_{k}), \eta \rangle + \frac{L}{2} \|\eta\|_{W}^{2} + g(x_{k} + \eta)$$

where $\|\eta\|_W^2 = \operatorname{vec}(\eta)^T W \operatorname{vec}(\eta)$ and W is symmetric positive definite.

Acceleration for SPCA on the Stiefel manifold

Scaled proximal mapping:

$$\eta_{k} = \arg \min_{\eta \in \mathrm{T}_{x_{k}} \mathcal{M}} \langle \nabla f(x_{k}), \eta \rangle + \frac{L}{2} \|\eta\|_{F}^{2} + g(x_{k} + \eta)$$
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where $\|\eta\|_{W}^{2} = \operatorname{vec}(\eta)^{T} W \operatorname{vec}(\eta)$ and W is symmetric positive definite.

• Difficult to solve in general

Acceleration for SPCA on the Stiefel manifold

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$$\eta_{k} = \arg\min_{\eta \in \mathcal{T}_{x_{k}} \mathcal{M}} \langle \nabla f(x_{k}), \eta \rangle + \frac{L}{2} \|\eta\|_{F}^{2} + g(x_{k} + \eta)$$
$$\implies \eta_{k} = \arg\min_{\eta \in \mathcal{T}_{x_{k}} \mathcal{M}} \langle \nabla f(x_{k}), \eta \rangle + \frac{L}{2} \|\eta\|_{W}^{2} + g(x_{k} + \eta)$$

where $\|\eta\|_{W}^{2} = \operatorname{vec}(\eta)^{T} W \operatorname{vec}(\eta)$ and W is symmetric positive definite.

- Difficult to solve in general
- Diagonal matrix *W* inspired by the Riemannian Hessian of the smooth term.

Acceleration for SPCA on the Stiefel manifold

The diagonal weight W

• Riemannian Hessian of $f : \operatorname{St}(p, n) \to \mathbb{R} : X \mapsto -\operatorname{trace}(X^T A^T A X)$:

$$Hess f(X)[\eta_X] = P_{T_X \operatorname{St}(p,n)}(-2A^T A \eta_X + 2\eta_X (X^T A^T A X)), \\ \forall \eta_X \in T_X \operatorname{St}(p,n)$$

• An *np*-by-*np* matrix representation of $\operatorname{Hess} f(X)$:

$$\langle \eta_{X}, \operatorname{Hess} f(X)[\eta_{X}] \rangle = \langle \eta_{X}, -2A^{T}A\eta_{X} + 2\eta_{X}(X^{T}A^{T}AX) \rangle \\ = \langle \operatorname{vec}(\eta_{X}), J\operatorname{vec}(\eta_{X}) \rangle,$$

where $J = -2I_{\rho} \otimes (A^{T}A) + 2(X^{T}A^{T}AX) \otimes I_{n}$.

• The diagonal matrix $W = \max(\operatorname{diag}(J), \tau I_{np})$.

Acceleration for SPCA on the Stiefel manifold

Numerical experiments

Table: An average result of 20 random runs for the random data: r = 4, n = 3000 and m = 40. The subscript k indicates a scale of 10^k .

λ	Algo	iter	time	f	$\ \eta_{z_k}\ $	sparsity	variance
2.5	ManPG-D	1538	1.67	-1.48_{1}	1.09_{-3}	0.65	0.72
2.5	ManPG	2155	2.20	-1.48_{1}	1.09_{-3}	0.65	0.72
2.5	ManPG-Ada-D	469	0.60	-1.48_{1}	1.03_{-3}	0.65	0.72
2.5	ManPG-Ada	508	0.60	-1.48_{1}	1.04_{-3}	0.65	0.72
2.5	AManPG-D	201	0.39	-1.48_{1}	1.02_{-3}	0.65	0.72
2.5	AManPG	237	0.43	-1.49_{1}	1.05_{-3}	0.65	0.72

Acceleration for SPCA on the Stiefel manifold

Numerical experiments

Table: The result for the DNA methylation data: r = 4, n = 24589 and m = 113. The subscript k indicates a scale of 10^k .

λ	Algo	iter	time	f	$\ \eta_{z_k}\ $	sparsity	variance
6.0	ManPG-D	706	7.37	-7.74 ₃	3.11_{-3}	0.29	0.96
6.0	ManPG	2206	20.10	-7.74_{3}	3.14_{-3}	0.29	0.96
6.0	ManPG-Ada-D	369	4.58	-7.74_{3}	3.03_{-3}	0.29	0.96
6.0	ManPG-Ada	957	10.18	-7.74_{3}	3.11_{-3}	0.29	0.96
6.0	AManPG-D	93	2.33	-7.74_{3}	2.91_{-3}	0.29	0.96
6.0	AManPG	183	3.46	-7.74_{3}	2.96_{-3}	0.29	0.96



- Propose first Riemannian proximal gradient methods with convergence rate analyses;
- Propose Riemannian proximal gradient methods with acceleration;
- Apply the methods to sparse PCA problems on the oblique manifold and the Stiefel manifold;
- Compare the new proximal gradient method with the existing proximal gradient method;

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