# Riemannian Optimization and a Riemannian Proximal Newton-CG Method

Speaker: Wen Huang

Xiamen University

October 31, 2024

东莞理工学院

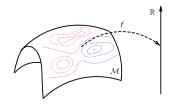
#### Outline

- 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

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

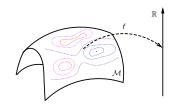
where  ${\mathcal M}$  is a Riemannian manifold.



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

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

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

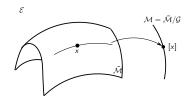


#### Two kinds of commonly-encountered manifolds

Embedded submanifold of a Euclidean space



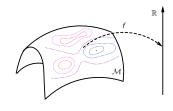
Quotient manifold from an embedded submanifold



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

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

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



#### Examples:

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

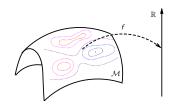
Embedded submanifold of a Euclidean space



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

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

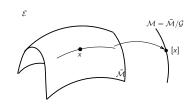
where  $\mathcal{M}$  is a Riemannian manifold.



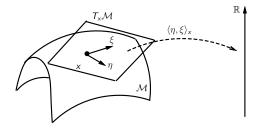
#### **Examples**:

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

Quotient manifold from an embedded submanifold



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



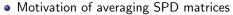
 $Riemannian\ manifold = Manifold + Riemannian\ metric\ (inner\ products)$ 

#### Embedded submanifold: Computation on SPD manifold

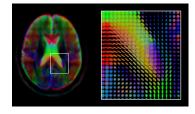
SPD manifold:

$$\mathcal{S}^n_{++} = \{X \in \mathbb{R}^{n \times n} : X = X^T, X \succ 0\};$$

- Applications of SPD matrices
  - Diffusion tensors in medical imaging [CSV12, FJ07, RTM07]
  - Describing images and video [LWM13, SFD02, ASF+05, TPM06, HWSC15]



- denoising / interpolation
- clustering / classification



#### Embedded submanifold: Computation on SPD manifold

One averaging SPD matrices method:

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

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

#### Embedded submanifold: Computation on SPD manifold

One averaging SPD matrices method:

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

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

#### Why shall we use Riemannian optimization approach?

Metric: 
$$\langle \eta_X, \xi_X \rangle_X = \operatorname{trace}(\eta_X X^{-1} \xi_X X^{-1})$$
 Metric:  $\langle \eta, \xi \rangle_X = \operatorname{trace}(\eta^T \xi)$ 

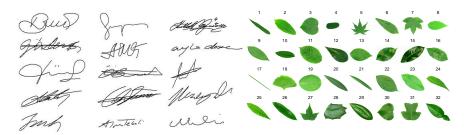
#### Condition number of the Riemannian Hessian [YHAG2020]

$$\begin{array}{ll} -\kappa(H^R) \leq 1 + \frac{\ln(\max \kappa_i)}{2}, \text{ where} \\ \kappa_i = \kappa(\mu^{-1/2}A_i\mu^{-1/2}) \\ -\kappa(H^R) \leq 20 \text{ if } \max(\kappa_i) = 10^{16} \end{array} \qquad \begin{array}{ll} -\frac{\kappa^2(\mu)}{\kappa(H^R)} \leq \kappa(H^R) \kappa^2(\mu) \\ -\kappa(H^E) \geq \kappa^2(\mu)/20 \end{array}$$

Riemannian Optimization: A Proximal Newton-CG Method

Speaker: Wen Huang

#### Quotient manifold: Computation on shape space



- Classification [LKS<sup>+</sup>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

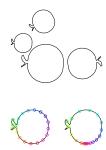
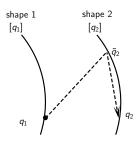


Figure: All are the same shape.

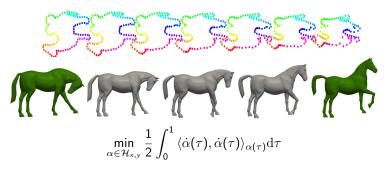
## Quotient manifold: Computation on shape space Registration





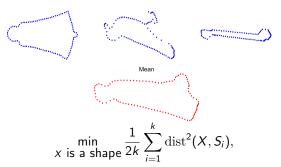
• Optimization problem  $\min_{q_2 \in [q_2]} \operatorname{dist}(q_1, q_2)$  is defined on a Riemannian manifold

#### Quotient manifold: Computation on shape space Geodesic / Interpolation



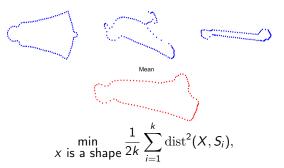
- Computation of a geodesic between two shapes
- Interpolation in shape space

#### Quotient manifold: Computation on shape space Karcher mean



• Computation of Karcher mean of a population of shapes

#### Quotient manifold: Computation on shape space Karcher mean



• Computation of Karcher mean of a population of shapes

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

Iterations on the Manifold

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

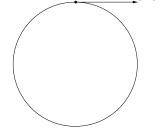
$$x_{k+1} = x_k + \Delta x_k = x_k + \alpha_k s_k.$$

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:  $\Delta x_k$  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



Riemannian gradient and Riemannian Hessian

#### Definition

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

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

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  $T_x \mathcal{M}$  to  $T_x \mathcal{M}$  defined as

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

where  $\nabla$  is the affine connection.

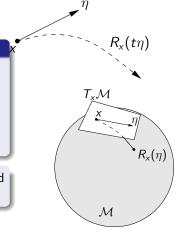
Retractions

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  $T\mathcal{M}$  to  $\mathcal{M}$  satisfying the following:

- *R* is continuously differentiable
- $R_x(0) = x$
- $D R_x(0)[\eta] = \eta$
- maps tangent vectors back to the manifold
- defines curves in a direction



Categories of Riemannian smooth optimization methods

#### 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)

Categories of Riemannian smooth optimization methods

#### 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.

Categories of Riemannian smooth optimization methods

#### 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.

#### **Vector Transport:**

- Vector transport: Transport a tangent vector from one tangent space to another;
- $\mathcal{T}_{\eta_x}\xi_x$ , denotes transport of  $\xi_x$  to tangent space of  $R_x(\eta_x)$ . R is a retraction associated with  $\mathcal{T}$ :

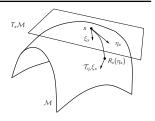


Figure: Vector transport.

Retraction/Transport-based Riemannian optimization

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

Retraction/Transport-based Riemannian optimization

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

Do the Riemannian versions of those methods work well?

Retraction/Transport-based Riemannian optimization

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

Do the Riemannian versions of those methods work well?

No, generally

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

- Manifold recognition, geometry structure analyses and computations;
- @ Generalization Euclidean algorithms to the Riemannian setting;
- Algorithms specialization for applications;
- Library developments;

- Manifold recognition, geometry structure analyses and computations;
- @ Generalization Euclidean algorithms to the Riemannian setting;
- Algorithms specialization for applications;
- Library developments;
- Manifold recognition
- Riemannian metric
- Retraction / Geodesic
- Vector transport / Parallel translation

<sup>[</sup>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

<sup>[</sup>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

<sup>[</sup>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

<sup>[</sup>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.

<sup>[</sup>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.

- Manifold recognition, geometry structure analyses and computations;
- Generalization Euclidean algorithms to the Riemannian setting;
- Algorithms specialization for applications;
- Library developments;
  - Smooth unconstrained optimization algorithms
  - Nonsmooth unconstrained optimization algorithms
- Constrained optimization algorithms

- Manifold recognition, geometry structure analyses and computations;
- @ Generalization Euclidean algorithms to the Riemannian setting;
- Algorithms specialization for applications;
- Library developments;
  - Smooth unconstrained optimization algorithms
  - Nonsmooth unconstrained optimization algorithms
  - Constrained optimization algorithms

Riemannian optimization mainly focuses on this topic.

Discuss later.

- Manifold recognition, geometry structure analyses and computations;
- @ Generalization Euclidean algorithms to the Riemannian setting;
- Algorithms specialization for applications;
- Library developments;
- Computations on the SPD manifold;
- Computations on the shape space;
- Clustering and graph partitions;
- Beamforming in wireless communication;
- Blind source separation;
- etc

- Manifold recognition, geometry structure analyses and computations;
- @ Generalization Euclidean algorithms to the Riemannian setting;
- Algorithms specialization for applications;
- Library developments;
  - Representation of a manifold and tangent spaces;
- Choose a Riemannian metric;
- Choose a retraction;
- Choose a vector transport;

- Manifold recognition, geometry structure analyses and computations;
- @ Generalization Euclidean algorithms to the Riemannian setting;
- Algorithms specialization for applications;
- Library developments;
  - Representation of a manifold and tangent spaces;
  - Choose a Riemannian metric;
  - Choose a retraction;
  - Choose a vector transport;

Above factors may influence algorithms significantly.

- Manifold recognition, geometry structure analyses and computations;
- @ Generalization Euclidean algorithms to the Riemannian setting;
- Algorithms specialization for applications;
- Library developments;

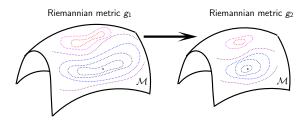


Figure: Changing Riemannian metric may influence the difficulty of a problem.

- Manifold recognition, geometry structure analyses and computations;
- Generalization Euclidean algorithms to the Riemannian setting;
- Algorithms specialization for applications;
- Library developments;
  - Manopt (Matlab library) [Boumal, Mishra, Absil, Sepulchre(2014)]
  - Pymanopt (Python version of Manopt) [Townsend, Koep, Weichwald (2016)]
  - Manoptil (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)]

- Manifold recognition, geometry structure analyses and computations;
- @ Generalization Euclidean algorithms to the Riemannian setting;
- Algorithms specialization for applications;
- Library developments;

## Provide theories to explain behaviors of existing algorithms for particular applications

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

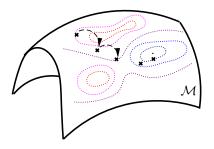
[MBDG2023] P. Mlinaric, C. Beattie, Z. Drmac, and S. Gugercin. IRKA is a Riemannian Gradient Descent Method. arxiv:2311.02031, 2023 [YHAG2020] X. Yuan, W. Huang, P.-A. Absil, K. A. Gallivan. Computing the matrix geometric mean: Riemannian vs Euclidean conditioning, implementation techniques, and a Riemannian BFGS method, *Numerical Linear Algebra with Applications*, 27:5, 1-23, 2020 [BM2006] I. Brace and J. H. Manton. An improved BFGS-on-manifold algorithm for computing weighted low rank approximations.

Proceedings of 17th international Symposium on Mathematical Theory of Networks and Systems, P.1735–1738, 2006

## Comparison with Constrained Optimization

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

- All iterates on the manifold
- Convergence properties of unconstrained optimization algorithms
- No need to consider Lagrange multipliers or penalty functions
- Exploit the structure of the constrained set



## A Non-exhaustive Review

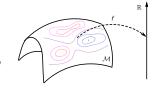
- Smooth unconstrained problems
  - Steepest descent: Smith 1994; Helmke-Moore 1994; lannazzo-Porcelli 2019;
  - Conjugate gradient: Smith 1994; Gallivan-Absil 2010; Ring-Wirth 2012; Sato-Iwai 2015;
  - Quasi-Newton: Ring-Wirth 2012; Huang-Absil-Gallivan 2018; Huang-Gallivan 2022
  - Newton-CG: Absil-Baker-Gallivan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

## A Non-exhaustive Review

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

### **Optimization on Manifolds with Structure:**

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

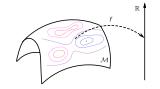


- $\mathcal{M}$  is a finite-dimensional Riemannian manifold;
- f is smooth and may be nonconvex; and
- h(x) is continuous and convex but may be nonsmooth;

Problem statement

### **Optimization on Manifolds with Structure:**

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



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

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

Euclidean proximal gradient/Newton method

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

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

Given 
$$x_0$$
,

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

Euclidean proximal gradient/Newton method

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

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

Given  $x_0$ ,

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

### proximal gradient: $H_k = LI_n$

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

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

- $h \equiv 0 \Rightarrow \text{Newton}$ :
- Superlinear convergence;

Euclidean proximal gradient/Newton method

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

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

Given  $x_0$ ,

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

proximal gradient: $H_k = LI_n$ 

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

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

- $h \equiv 0 \Rightarrow \text{Newton}$ :
- Superlinear convergence;

How to generalize to the Riemannian setting?

Generalizations of proximal gradient method

### **Euclidean Proximal gradient:**

Given 
$$x_0$$
,
$$\begin{cases}
d_k = \arg\min_{p \in \mathbb{R}^n} f(x_k) + \langle \nabla f(x_k), p \rangle + \frac{L}{2} \langle p, p \rangle + h(x_k + p) \\
x_{k+1} = x_k + d_k.
\end{cases}$$

Riemannian generalization 1: (for embedded submanifold)

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

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

Generalizations of proximal gradient method

### **Euclidean Proximal gradient:**

Given 
$$x_0$$
,
$$\begin{cases}
d_k = \arg\min_{p \in \mathbb{R}^n} f(x_k) + \langle \nabla f(x_k), p \rangle + \frac{L}{2} \langle p, p \rangle + h(x_k + p) \\
x_{k+1} = x_k + d_k.
\end{cases}$$

## Riemannian generalization 2: (for general manifold)

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

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

A native generalization

### **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:

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

A native generalization

### **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:

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

Does it converge superlinearly locally?

A native generalization

### **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:

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

Does it converge superlinearly locally?

Not necessarily!

A native generalization

Consider the Sparse PCA over sphere:

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

where 
$$f(x) = -x^{T}A^{T}Ax$$
,  $h(x) = \mu ||x||_{1}$ .

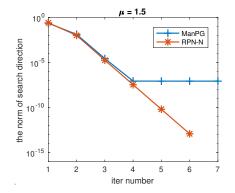


Figure: Comparisons of native generalization (RPN-N) and the proximal gradient method (ManPG) in [CMSZ20].

A native generalization

#### Euclidean version:

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

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

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

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

A native generalization

#### Euclidean version:

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

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

$$\begin{cases} \eta_{k} = \arg\min_{\eta \in \mathcal{T}_{\mathsf{X}_{k}}} \mathcal{M} f(\mathsf{X}_{k}) + \langle \operatorname{grad} f(\mathsf{X}_{k}), \eta \rangle + \frac{1}{2} \langle \eta, \operatorname{Hess} f(\mathsf{X}_{k}) \eta \rangle + h(\mathsf{X}_{k} + \eta) \\ \mathsf{X}_{k+1} = R_{\mathsf{X}_{k}}(\eta_{k}) \end{cases}$$

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

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

A Riemannian proximal Newton method: descripion

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

- **○** Compute the ManPG direction  $v(x_k) = \operatorname{argmin}_{v \in \mathcal{T}_{x_k} \mathcal{M}} f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$
- **③** Find  $u(x_k) \in T_{x_k} \mathcal{M}$  by solving  $J(x_k)[u(x_k)] = -v(x_k),$  where  $J(x_k) = -\left[I_n \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) \mathcal{L}_{x_k})\right]$ ,  $\Lambda_{x_k}$  and  $\mathcal{L}_{x_k}$  are defined later:
- $x_{k+1} = R_{x_k}(u(x_k));$

A Riemannian proximal Newton method: descripion

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

- **②** Compute the ManPG direction  $v(x_k) = \operatorname{argmin}_{v \in \mathcal{T}_{x_k} \mathcal{M}} f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$
- **3** Find  $u(x_k)$  ∈  $T_{x_k}$   $\mathcal{M}$  by solving  $J(x_k)[u(x_k)] = -v(x_k),$  where  $J(x_k) = -\left[I_n \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) \mathcal{L}_{x_k})\right]$ ,  $\Lambda_{x_k}$  and  $\mathcal{L}_{x_k}$  are defined later;
- $x_{k+1} = R_{x_k}(u(x_k));$
- Step 1: compute a Riemannian proximal gradient direction (ManPG)

A Riemannian proximal Newton method: descripion

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

- **○** Compute the ManPG direction  $v(x_k) = \operatorname{argmin}_{v \in \mathcal{T}_{x_k} \mathcal{M}} f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$
- $\text{Find } u(x_k) \in \mathrm{T}_{x_k} \, \mathcal{M} \text{ by solving} \\ J(x_k)[u(x_k)] = -v(x_k), \\ \text{where } J(x_k) = -\left[I_n \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) \mathcal{L}_{x_k})\right], \, \Lambda_{x_k} \text{ and } \mathcal{L}_{x_k} \text{ are defined later;}$
- $x_{k+1} = R_{x_k}(u(x_k));$
- Step 1: compute a Riemannian proximal gradient direction (ManPG)
- **3** 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: descripion

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

- **○** Compute the ManPG direction  $v(x_k) = \operatorname{argmin}_{v \in \mathcal{T}_{x_k} \mathcal{M}} f(x_k) + \langle \nabla f(x_k), v \rangle + \frac{1}{2t} \|v\|_F^2 + h(x_k + v);$
- **3** Find  $u(x_k)$  ∈  $T_{x_k}$   $\mathcal{M}$  by solving  $J(x_k)[u(x_k)] = -v(x_k),$  where  $J(x_k) = -\left[I_n \Lambda_{x_k} + t\Lambda_{x_k}(\nabla^2 f(x_k) \mathcal{L}_{x_k})\right]$ ,  $\Lambda_{x_k}$  and  $\mathcal{L}_{x_k}$  are defined later;
- $x_{k+1} = R_{x_k}(u(x_k));$
- 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  $v(x_k)$ ;
- Step 3: Update iterate by a retraction;

A Riemannian proximal Newton method: local superlinear convergence rate

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  $T_x^{\perp} \mathcal{M}$  at x.

### Assumption:

• 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;

A Riemannian proximal Newton method: local superlinear convergence rate

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  $T_x^{\perp} \mathcal{M}$  at x.

### Assumption:

- 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;
- 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<sup>+</sup>24a]

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 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<sup>+</sup>24b];

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

- 1: **for** k = 0, 1, ... **do**
- 2: Compute a ManPG direction  $v_k$ ;
- 3: If  $||v_k|| \le \epsilon$ , 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

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<sup>+</sup>24b];

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

- 1: **for** k = 0, 1, ... **do**
- 2: Compute a ManPG direction  $v_k$ ;
- 3: If  $||v_k|| \le \epsilon$ , 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

Truncated conjugate gradient

### A Riemannian proximal Newton method (RPN)

Compute the ManPG direction

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

**2** Find  $u(x_k) \in T_{x_k} \mathcal{M}$  by solving

$$J(x_k)[u(x_k)] = -v(x_k);$$

#### Smooth case:

- $v(x_k) = -t \operatorname{grad} f(x_k)$ ;
- $J(x_k) = -t \operatorname{Hess} f(x_k)$ ;
- $J(x_k)[u(x_k)] = -v(x_k) \Longrightarrow$  $\operatorname{Hess} f(x_k)[u(x_k)] = -\operatorname{grad} f(x_k)$ .

truncated conjugate gradient (tCG)

Truncated conjugate gradient

### A Riemannian proximal Newton method (RPN)

Compute the ManPG direction

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

② Find  $u(x_k) \in T_{x_k} \mathcal{M}$  by solving

$$J(x_k)[u(x_k)] = -v(x_k);$$

#### Smooth case:

- $v(x_k) = -t \operatorname{grad} f(x_k)$ ;
- $J(x_k) = -t \operatorname{Hess} f(x_k)$ ;
- $J(x_k)[u(x_k)] = -v(x_k) \Longrightarrow$   $Hess f(x_k)[u(x_k)] = -\operatorname{grad} f(x_k) .$

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

Truncated conjugate gradient

### A Riemannian proximal Newton method (RPN)

Compute the ManPG direction

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

② Find  $u(x_k) \in T_{x_k} \mathcal{M}$  by solving

$$J(x_k)[u(x_k)] = -v(x_k);$$

#### Smooth case:

- $v(x_k) = -t \operatorname{grad} f(x_k)$ ;
- $J(x_k) = -t \operatorname{Hess} f(x_k)$ ;
- $J(x_k)[u(x_k)] = -v(x_k) \Longrightarrow$  $Hess f(x_k)[u(x_k)] = -\operatorname{grad} f(x_k)$ .

  truncated conjugate gradient (tCG)

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!

#### Truncated conjugate gradient

Notation:

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

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

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

$$\implies \bar{u}(x_{k}) = \bar{v}(x_{k}) - \{I_{j_{k}} + (I_{j_{k}} - \bar{B}_{x_{k}}\bar{B}_{x_{k}}^{\dagger})\mathcal{N}_{x_{k}}\}^{-1}(I_{j_{k}} - \bar{B}_{x_{k}}\bar{B}_{x_{k}}^{\dagger})\ell_{x_{k}}$$

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.

Truncated conjugate gradient

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

#### 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

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

Truncated conjugate gradient

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

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

Truncated conjugate gradient

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

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

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

Truncated conjugate gradient

## A Riemannian proximal Newton method (RPN)

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

#### 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;

Truncated conjugate gradient

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

Truncated conjugate gradient

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

### Assumption:

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

Truncated conjugate gradient

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

### Assumption:

- 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;
- **1** 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  $\hat{x} + \hat{v} = 0$ ;
- 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<sub>\*</sub>;
- $\mathcal{B}_{x_*}$  is the Riemannian Hessian of F at  $x_*$  for the submanifold;
- ullet  $\mathcal{B}_{x_*}$  is symmetric positive semidefinite on  $\mathfrak{L}_{x_*}$ ;

Truncated conjugate gradient

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

### Assumption:

- The function f is twice continuously differentiable with a Lipschitz continuous Euclidean Hessian:
- $\bullet$  Let  $B_{\mathbf{x}_*}^T = [\bar{B}_{\mathbf{x}_*}^T, \hat{B}_{\mathbf{x}_*}^T]$ , where  $\bar{B}_{\mathbf{x}_*} \in \mathbb{R}^{j \times d}$  and and  $\hat{B}_{\mathbf{x}_*} \in \mathbb{R}^{(n-j) \times d}$ . It is assumed that j > d and  $\bar{B}_x$  is full column rank;
- **1** 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  $\hat{x} + \hat{v} = 0$ ;
- The linear operator  $\mathcal{B}_{x_*}$  is positive definite on the subspace  $\mathfrak{L}_{\mathbf{x}} = \{ \mathbf{w} \mid \bar{B}_{\mathbf{x}}^T \mathbf{w} = \mathbf{0} \}.$

#### Lemma

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

Truncated conjugate gradient

# Early termination conditions in tCG

### tCG step

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

Truncated conjugate gradient

# Early termination conditions in tCG

### tCG step

$$d(x_k) = \begin{pmatrix} \bar{d}(x_k) \\ \hat{d}(x_k) \end{pmatrix} = \begin{pmatrix} \bar{v}(x_k) + w(x_k) \\ \hat{v}(x_k) \end{pmatrix}, \text{ where } w(x_k) \text{ is an output of }$$
 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:

approximately 
$$\min_{d \in \mathcal{T}_{x_k} \mathcal{M}} \langle \operatorname{grad} f(x_k), d \rangle + \frac{1}{2} \langle \operatorname{Hess} f(x_k)[d], d \rangle$$
, find  $d(x_k)$  such that  $\langle d(x_k), \operatorname{grad} f(x_k) \rangle < 0$ ;

Nonsmooth:

approximately 
$$\min_{\bar{\mathcal{B}}_{y_{k}}^{T}, w=0} \langle \ell_{x_{k}}, w \rangle + \frac{1}{2} \langle w, \mathcal{B}_{x_{k}} w \rangle,$$

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

Truncated conjugate gradient

# Early termination conditions in tCG

### tCG step

$$d(x_k) = \begin{pmatrix} \bar{d}(x_k) \\ \hat{d}(x_k) \end{pmatrix} = \begin{pmatrix} \bar{v}(x_k) + w(x_k) \\ \hat{v}(x_k) \end{pmatrix}, \text{ where } w(x_k) \text{ is an output of }$$
 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:

approximately 
$$\min_{d \in \mathcal{T}_{x_k} \mathcal{M}} \langle \operatorname{grad} f(x_k), d \rangle + \frac{1}{2} \langle \operatorname{Hess} f(x_k)[d], d \rangle$$
, find  $d(x_k)$  such that  $\langle d(x_k), \operatorname{grad} f(x_k) \rangle < 0$ ;

• Nonsmooth:

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

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

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

Truncated conjugate gradient

# 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), status);
 1: if G_{x}(v(x)) > G_{x}(0) then
       return w(x) = 0 and 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
       return w(x) = 0 and 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)
```

### Omit subscript *k* for simplicity

Truncated conjugate gradient

# 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), status);
 1: if G_{x}(v(x)) > G_{x}(0) then
       return w(x) = 0 and 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
       return w(x) = 0 and 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;

Truncated conjugate gradient

# 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), status);
 1: if G_{x}(v(x)) > G_{x}(0) then
       return w(x) = 0 and 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
       return w(x) = 0 and status = ' early 2';
 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)
```

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

Truncated conjugate gradient

# 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), 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 < \vartheta \delta_i then
           return w(x) = w_i and status =' neg';
     end if
 7.
      ..... (Remaining CG iterations)
 9: end for
```

### An existing early termination condition

Truncated conjugate gradient

# Early termination conditions in tCG

```
Algorithm: Truncated conjugate gradient (tCG)
Require: \theta > 0, \gamma > 0, \tau > 0, \theta > 0, and \kappa \in (0,1);
Ensure: (w(x), status);
 1: ..... (See previous slides)
 2: for i = 0, 1, ... do
 3: ..... (See previous slides)
 4: \alpha_i = \frac{\langle r_i, r_i \rangle}{\langle r_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} \overline{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
 6:
             return w(x) = w_i and status =' early3';
         end if
 8:
          ..... (Remaining CG iterations)
10: end for
```

Truncated conjugate gradient

# 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), status);
 1: ..... (See previous slides)
 2: for i = 0, 1, \dots do
 3: ..... (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;
 5: \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)
 6: i = i + 1:
 7: if ||r_i||_F \le ||r_0||_F \min(||r_0||_F^\theta, \kappa) then
            return w(x) = w_i, and status =' \lim_{x \to a} |x_0| \le \kappa and
 8.
            status =' sup' otherwise;
         end if
10: end for
```

RPN-CG: global convergence

### Assumption:

• 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

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

#### RPN-CG: local superlinear convergence

### Assumption:

- 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;
- **1** 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  $\hat{x} + \hat{v} = 0$ ;
- The function F is  $\varsigma$ -geodesically strongly convex at  $x_*$ , i.e., there exists a neighborhood  $\tilde{\mathcal{U}}_{x_*}$  of  $x_*$  in  $\mathcal{M}$  such that

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

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

#### RPN-CG: local superlinear convergence

### Assumption:

- 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;
- **1** 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  $\hat{x} + \hat{v} = 0$ ;
- The function F is  $\varsigma$ -geodesically strongly convex at  $x_*$ , i.e., there exists a neighborhood  $\tilde{\mathcal{U}}_{x_*}$  of  $x_*$  in  $\mathcal{M}$  such that

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

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

#### Lemma

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

#### RPN-CG: local superlinear convergence

### Assumption:

- The function f is twice continuously differentiable with a Lipschitz continuous Euclidean Hessian:
- $\bullet$  Let  $B_{\mathbf{x}_*}^T = [\bar{B}_{\mathbf{x}_*}^T, \hat{B}_{\mathbf{x}_*}^T]$ , where  $\bar{B}_{\mathbf{x}_*} \in \mathbb{R}^{j \times d}$  and and  $\hat{B}_{\mathbf{x}_*} \in \mathbb{R}^{(n-j) \times d}$ . It is assumed that  $j \geq d$  and  $\bar{B}_{x_*}$  is full column rank;
- **1** 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  $\hat{x} + \hat{v} = 0$ ;
- **1** The function F is  $\varsigma$ -geodesically strongly convex at  $x_*$ , i.e., there exists a neighborhood  $\mathcal{U}_{x_*}$  of  $x_*$  in  $\mathcal{M}$  such that

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

holds for any  $v \in \tilde{\mathcal{U}}_{\times}$ .

#### 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.,  $||r_i||_F \leq ||r_0||_F \min(||r_0||_F^\theta, \kappa)$ .

Speaker: Wen Huang

RPN-CG: local superlinear convergence

#### 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  $C_{\mathrm{up}}>0$ .

RPN-CG: local superlinear convergence

#### 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.

RPN-CG: local superlinear convergence

#### 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.

- 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];

RPN-CG: local superlinear convergence

### 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:  $R: T \mathcal{M} \to \mathcal{M}: \eta_x \mapsto x + \eta_x + \begin{pmatrix} 0 \\ 2\eta_x^T \eta_x \end{pmatrix};$
- $R(u(x)) = (1, 2\epsilon^2)^T$ ;
- $F(R_x(u(x))) F(x) = 4\epsilon^4 + \epsilon^2 > 0$ ;
- $\bullet$  Step size one is not acceptable for any  $\epsilon>0;$

RPN-CG: local superlinear convergence

### **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: 
$$R: T \mathcal{M} \to \mathcal{M}: \eta_x \mapsto x + \eta_x + \begin{pmatrix} 0 \\ 2\eta_x^T \eta_x \end{pmatrix};$$

- $R(u(x)) = (1, 2\epsilon^2)^T$ ;
- $F(R_x(u(x))) F(x) = 4\epsilon^4 + \epsilon^2 > 0$ ;
- ullet 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.

RPN-CG: local superlinear convergence

### 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  $\|R_x(d(x)) - x_*\|_F \le C_{\mathrm{up}} \|x - x_*\|_F^{\varkappa}$  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  $x_{++} = R_{x_+}(d(x_+))$ .

RPN-CG: local superlinear convergence

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  $\|R_x(d(x)) - x_*\|_F \le C_{\mathrm{up}} \|x - x_*\|_F^\varkappa$  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

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

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

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

- ullet  $\mathcal{M}_{\textit{sub}}$ : 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

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

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

- ullet  $\mathcal{M}_{\textit{sub}}$ : 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  $\mathcal{M}_{sub}$ ;

# No counterpart in the Euclidean space.

Numerical experiments: sparse PCA

### Sparse PCA problem

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

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

Numerical experiments: sparse PCA

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

$(n, p, \mu)$	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

Numerical experiments: sparse PCA

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

$(n, p, \mu)$	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

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

Numerical experiments: sparse PCA

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

$(n, p, \mu)$	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

- 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  $|(x)_i| \ge ||v(x)||_F$ ;

Numerical experiments: sparse PCA

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

$(n, p, \mu)$	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

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

Numerical experiments: sparse PCA

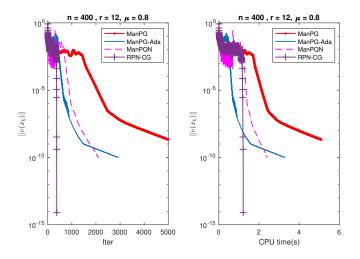


Figure: Sparse PCA: plots of  $||v(x_k)||$  versus iterations and CPU times respectively.

## Numerical Experiments

Compressed modes

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

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

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

Numerical experiments: compressed modes

Table: An average result of 50 random runs for random data. Multiple values of n, p, and  $\mu$  are used. The subscript k indicates a scale of  $10^k$ .

$(n, p, \mu)$	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;

Numerical experiments: compressed modes

Table: An average result of 50 random runs for random data. Multiple values of n, p, and  $\mu$  are used. The subscript k indicates a scale of  $10^k$ .

$(n, p, \mu)$	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  $||v||_F \le 10^{-8}$  and is the most efficient one.

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

Numerical experiments: compressed modes

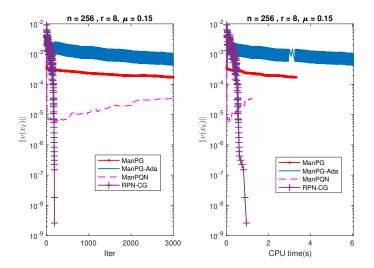


Figure: CM: plots of  $||v(x_k)||$  versus iterations and CPU times respectively.

### Summary

- 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!

### References I



Ognjen Arandjelovic, Gregory Shakhnarovich, John Fisher, Roberto Cipolla, and Trevor Darrell.

Face recognition with image sets using manifold density divergence.

In Computer Vision and Pattern Recognition, 2005. CVPR 2005. IEEE Computer Society Conference on, volume 1, pages 581–588. IEEE, 2005.



Matthias Bollh ofer, Aryan Eftekhari, Simon Scheidegger, and Olaf Schenk.

Large-scale sparse inverse covariance matrix estimation.

SIAM Journal on Scientific Computing, 41(1):A380–A401, 2019.



Shixiang Chen, Shiqian Ma, Anthony Man-Cho So, and Tong Zhang.

Proximal gradient method for nonsmooth optimization over the Stiefel manifold. SIAM Journal on Optimization, 30(1):210–239, 2020.



Haoran Chen, Yanfeng Sun, Junbin Gao, Yongli Hu, and Baocai Yin.

Fast optimization algorithm on riemannian manifolds and its application in low-rank learning. Neurocomputing, 291:59 – 70, 2018.



Guang Cheng, Hesamoddin Salehian, and Baba Vemuri.

Efficient recursive algorithms for computing the mean diffusion tensor and applications to DTI segmentation.

Computer Vision–ECCV 2012, pages 390–401, 2012.



H. Drira, B. Ben Amor, A. Srivastava, M. Daoudi, and R. Slama.

3D face recognition under expressions, occlusions, and pose variations.

Pattern Analysis and Machine Intelligence, IEEE Transactions on, 35(9):2270-2283, 2013.



P. T. Fletcher and S. Joshi.

Riemannian geometry for the statistical analysis of diffusion tensor data. Signal Processing, 87(2):250–262, 2007.



W. Huang, K. A. Gallivan, Anuj Srivastava, and P.-A. Absil.

Riemannian optimization for registration of curves in elastic shape analysis.

Journal of Mathematical Imaging and Vision, 54(3):320–343, 2015.

DOI:10.1007/s10851-015-0606-8.

### References II



Wen Huang, Meng Wei, Kyle A. Gallivan, and Paul Van Dooren.

A Riemannian Optimization Approach to Clustering Problems, 2022.



Zhiwu Huang, Ruiping Wang, Shiguang Shan, and Xilin Chen.

Face recognition on large-scale video in the wild with hybrid Euclidean-and-Riemannian metric learning. Pattern Recognition, 48(10):3113–3124, 2015.



H. Laga, S. Kurtek, A. Srivastava, M. Golzarian, and S. J. Miklavcic.

A Riemannian elastic metric for shape-based plant leaf classification.

2012 International Conference on Digital Image Computing Techniques and Applications (DICTA), pages 1–7, December 2012. doi:10.1109/DICTA.2012.6411702.



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.



Jiwen Lu, Gang Wang, and Pierre Moulin.

Image set classification using holistic multiple order statistics features and localized multi-kernel metric learning.

In Proceedings of the IEEE International Conference on Computer Vision, pages 329–336, 2013.



Vidvuds Ozolinš, Rongjie Lai, Russel Caflisch, and Stanley Osher.

Compressed modes for variational problems in mathematics and physics.

Proceedings of the National Academy of Sciences, 110(46):18368-18373, 2013.



Y. Rathi, A. Tannenbaum, and O. Michailovich.

Segmenting images on the tensor manifold.

In IEEE Conference on Computer Vision and Pattern Recognition, pages 1-8, June 2007.



Wutao Si, P. A. Absil, Wen Huang, Rujun Jiang, and Simon Vary.

A Riemannian Proximal Newton Method, 2024.

arXiv: 2304.04032v3.

### References III



Wutao Si, P.-A. Absil, Wen Huang, Rujun Jiang, and Simon Vary.

A Riemannian Proximal Newton Method.

SIAM Journal on Optimization, 34(1):654-681, 2024,



Gregory Shakhnarovich, John W Fisher, and Trevor Darrell.

Face recognition from long-term observations.

In European Conference on Computer Vision, pages 851-865. Springer, 2002.



Oncel Tuzel, Fatih Porikli, and Peter Meer.

Region covariance: A fast descriptor for detection and classification.

In European conference on computer vision, pages 589–600. Springer, 2006.



Qinsi Wang and Weihong Yang.

Proximal quasi-Newton method for composite optimization over the Stiefel manifold. Journal of Scientific Computing, 95, 5 2023.



Hui Zou, Trevor Hastie, and Robert Tibshirani.

Sparse principal component analysis.



Journal of Computational and Graphical Statistics, 15(2):265-286, 2006,

Y. Zhang, Y. Lau, H.-W. Kuo, S. Cheung, A. Pasupathy, and J. Wright.

On the global geometry of sphere-constrained sparse blind deconvolution.

In Proceedings of IEEE Conference on Computer Vision and Pattern Recognition (CVPR), 2017.