#### Bounding Geometric Penalties in First-Order Riemannian Optimization

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#### Collaborators



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Christopher Criscitiello (EPFL)

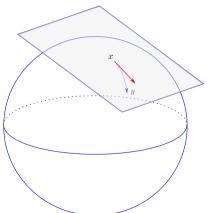


Sebastian Pokutta (ZIB, TU Berlin)

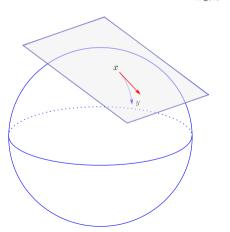
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For a Riemannian manifold  $\mathfrak{M}$ :





#### For a Riemannian manifold $\mathfrak{M}$ :



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

- Spheres, hyperbolic spaces.
- ► SPD matrices.
- ▶ SO(n) (real orthogonal matrices with det(A) = 1).
- Stiefel manifold  $V_k(\mathbb{R}^n)$  (ordered orthonormal basis of a k-dim vector space).
- **>** ...

#### Riemannian Optimization - Applications

- ▶ Principal Components Analysis (Jolliffe et al., 2003; Genicot et al., 2015; Huang and Wei, 2019).
- ▶ Low-rank matrix completion (Cambier and Absil, 2016; Heidel and Schulz, 2018; Mishra and Sepulchre, 2014; Tan et al., 2014; Vandereycken, 2013).
- Dictionary learning (Cherian and Sra, 2017; Sun et al., 2017).
- ➤ Optimization under orthogonality constraints (Edelman et al., 1998).
  - ► Some applications to RNNs (Lezcano-Casado and Martínez-Rubio, 2019).
- ▶ Robust covariance estimation in Gaussian distributions (Wiesel, 2012).
- Gaussian mixture models (Hosseini and Sra, 2015).
- ▶ Operator scaling (Allen-Zhu et al., 2018).
- Wasserstein Barycenters (Hosseini and Sra, 2020).
- ► Many more...

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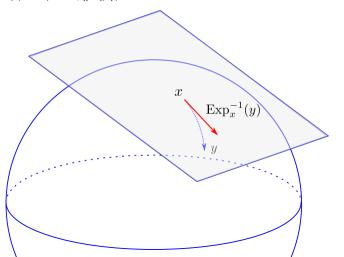
- ightharpoonup Constrained ightharpoonup unconstrained.
- **▶ Sometimes:** Euclidean non-convex → Riemannian geodesically convex.

#### Many first-order methods have analogous Riemannian counterparts:

- ▶ **Deterministic** (de Carvalho Bento et al., 2017; Zhang and Sra, 2016).
- ▶ Stochastic (Hosseini and Sra, 2017; Khuzani and Li, 2017; Tripuraneni et al., 2018).
- Variance reduced (Sato et al., 2017, 2019; Zhang et al., 2016).
- ► Adaptive (Kasai et al., 2019).
- ▶ Saddle-point escaping (Criscitiello and Boumal, 2019; Sun et al., 2019; Zhang et al., 2018; Zhou et al., 2019; Criscitiello and Boumal, 2020).
- Projection-free (Weber and Sra, 2017, 2019).
   Accelerated (Zhang and Sra, 2018; Ahn and Sra, 2020; Kim and Yang, 2022).
- Min-max (Zhang et al., 2022; Jordan et al., 2022).

#### Geodesic Convexity

**Notation:** Let  $\mathcal{M}$  be a Riemannian manifold. Given  $x, y \in \mathcal{M}$  and  $v \in T_x \mathcal{M}$  we use  $\langle v, y - x \rangle \stackrel{\text{def}}{=} -\langle v, x - y \rangle \stackrel{\text{def}}{=} \langle v, \operatorname{Exp}_v^{-1}(y) \rangle_x$ .



#### Geodesic Convexity

# **Notation:** Let $\mathcal{M}$ be a Riemannian manifold. Given $x, y \in \mathcal{M}$ and $v \in \mathcal{T}_x \mathcal{M}$ we use $\langle v, y - x \rangle \stackrel{\text{def}}{=} -\langle v, x - y \rangle \stackrel{\text{def}}{=} \langle v, \operatorname{Exp}_x^{-1}(y) \rangle_x$ .

ightharpoonup  $\mu$ -strongly geodesic convexity of  $F: \mathcal{M} \to \mathbb{R}$ :

$$F(y) \ge F(x) + \langle \nabla F(x), y - x \rangle + \frac{\mu}{2} d(x, y)^2$$
, for  $\mu > 0, \forall x, y \in \mathcal{M}$ .

If  $\mu = 0$ , F is geodesically convex (g-convex).

$$\mu = 0$$
,  $F$  is geodesically convex (g-c)  $I$ -smoothness:

$$F(y) \le F(x) + \langle \nabla F(x), y - x \rangle + \frac{L}{2} d(x, y)^2, \quad \forall x, y \in \mathcal{M}.$$

► *G*-Lipschitzness:

$$\|\nabla F(y)\| \leq G$$
 for all  $y \in \mathcal{M}$ .

lackbox A set  ${\mathfrak X}$  is uniquely geodesically convex if there is one and only one geodesic between two points, and it remains in  ${\mathfrak X}$ .

#### Distance squared and cosine inequalities

- ▶ Sectional curvature in  $[K_{min}, K_{max}]$ . Assume wlog  $|K_{min}| = 1$ .
- $\blacktriangleright$   $\mathfrak{X} \subset \mathfrak{M}$  compact, g-convex set of diameter D.

$$\nabla \Phi_{x}(y) = -\operatorname{Exp}_{y}^{-1}(x) \qquad \text{and} \qquad \delta \left\| v \right\|^{2} \leq \operatorname{Hess} \Phi_{x}(y)[v,v] \leq \zeta \left\| v \right\|^{2} \ \text{for all} \ x,y \in \mathfrak{X}.$$

where

$$\zeta \stackrel{\text{def}}{=} D\sqrt{|K_{\text{min}}|} \coth(D\sqrt{|K_{\text{min}}|}) = \Theta(D\sqrt{|K_{\text{min}}|} + 1) \qquad \text{if } K_{\text{min}} < 0 \text{ else } 1.$$
 
$$\delta \stackrel{\text{def}}{=} D\sqrt{K_{\text{max}}} \cot(D\sqrt{K_{\text{max}}}) \qquad \text{if } K_{\text{max}} > 0 \text{ else } 1.$$

### Distance squared and cosine inequalities

- ▶ Sectional curvature in  $[K_{min}, K_{max}]$ . Assume wlog  $|K_{min}| = 1$ .
- $\Phi_{x}(y) \stackrel{\text{def}}{=} \frac{1}{2}d(x,y)^{2}$ .

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where

$$\delta \stackrel{ ext{ iny def}}{=} D\sqrt{K_{\sf max}}\cot(D\sqrt{K_{\sf max}})$$

**Cosine inequalities:** Let 
$$x, y, z \in \mathcal{X}$$
. We have:

 $\zeta \stackrel{\text{def}}{=} D\sqrt{|K_{\text{min}}|} \coth(D\sqrt{|K_{\text{min}}|}) = \Theta(D\sqrt{|K_{\text{min}}|} + 1)$ 

$$2\langle \mathsf{Exp}_{\mathsf{x}}^{-1}(y), \mathsf{Exp}_{\mathsf{x}}^{-1}(z) \rangle \geq \delta d(x,y)^2 + d(x,z)^2 - d(y,z)^2.$$

In neg. curvature: minimum condition number of any L-smooth  $\mu$ -strongly convex function is  $\approx \zeta_D!!$ 

 $2\langle \mathsf{Exp}^{-1}(y), \mathsf{Exp}^{-1}(z) \rangle < \zeta d(x, y)^2 + d(x, z)^2 - d(y, z)^2$ 

if  $K_{\min} < 0$  else 1.

if  $K_{max} > 0$  else 1.

#### Bound what's gotta be bounded!

"Showing that a method converges assuming iterates remain bounded is compatible with the algorithm **diverging**."

A. Matthem Attishen

Ha ha ha!
I proved
convergence!



Bound what's gotta be bounded!

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Even worse, if you assume your algorithm knows the bound **a priori**, uses its value and the **iterates depend on it**. Circularity!

Let's do better than that.

Bound what's gotta be bounded!

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Let's do better than that.

Aim of papers in my talk: Show convergence without unreasonable assumptions.

Techniques to guarantee iterates are bounded, to deal with in-manifold constraints, new rates are discovered, some times very different algorithms, etc.

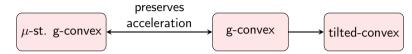
You won't Believe these 7 Techniques to Bound your Riemannian Iterates!

#5 will blow up your mind!



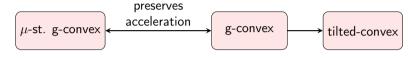
### 1. Mapping to Euclidean space (I): Constant curvature solution (Ref.)

We reduce the problem to a non-convex, Euclidean *constrained* problem.



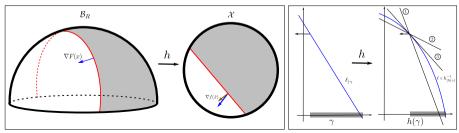
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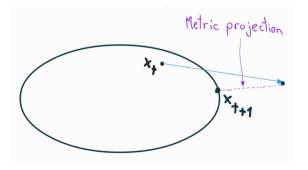
A function  $f: \mathbb{R}^d \to \mathbb{R}$  is tilted-convex if  $\exists \ \gamma_n, \gamma_p \in (0, 1]$  such that:

$$\begin{split} f(\tilde{x}) + \frac{1}{\gamma_{\mathsf{n}}} \langle \nabla f(\tilde{x}), \tilde{y} - \tilde{x} \rangle &\leq f(\tilde{y}) \quad \text{if } \langle \nabla f(\tilde{x}), \tilde{y} - \tilde{x} \rangle \leq 0, (\text{grey area}) \\ f(\tilde{x}) + \gamma_{\mathsf{p}} \langle \nabla f(\tilde{x}), \tilde{y} - \tilde{x} \rangle &\leq f(\tilde{y}) \quad \text{if } \langle \nabla f(\tilde{x}), \tilde{y} - \tilde{x} \rangle \geq 0. \end{split}$$



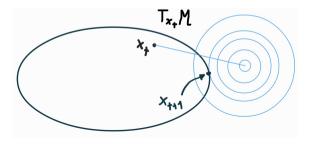
#### 2. Metric-Projected Riemannian Gradient Descent (Ref.)

- ▶ PRGD works in **Hadamard**:  $x_{t+1} = \Pi_{\mathfrak{X}}(\mathsf{Exp}_{\mathsf{x}_t}(-\eta \nabla f(x_t))).$
- ▶ Metric projection:  $\Pi_{\mathcal{X}}(x) \leftarrow \operatorname{argmin}_{v \in \mathcal{X}} \{d(y, x)\}$  for closed g-convex  $\mathcal{X}$ .
- Easy to implement if the constraint is a ball.
- Convergence for Lipschitz functions: easy.
- For **smooth** problems: not so easy.
- ▶ We show convergence and pay a  $\zeta_R$  factor, where R = G/L (Lipschitzness over smoothness).



### 3. Another Projected Riemannian Gradient Descent (Ref.)

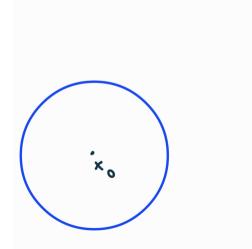
- ▶ Minimize, in  $T_{x_r}M$ , the quadratic upper model given by smoothness.
- Works regardless of the curvature.
- Possibly a non-convex problem. Implementable at least in constant curvature.
- Gives better information theoretical upper bound wrt number of gradient oracle queries.



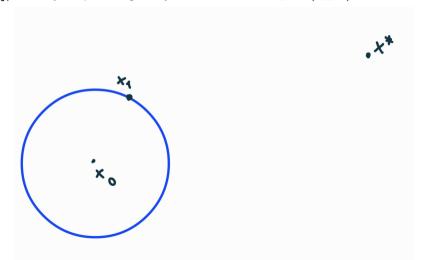
### 4. Proximal point algorithm (Ref.)

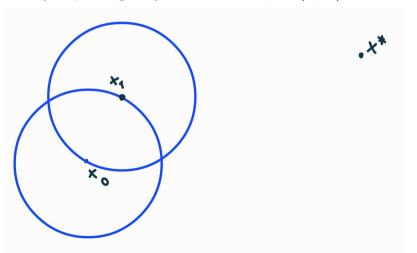
- 1. Known: nonexpansive operator in Hadamard manifolds.
- 2. We showed: quasi-nonexpansive, i.e., for minimizers  $x^*$  it is  $d(x_t, x^*) \le d(x_{t-1}, x^*)$  in the general Riemannian case.
- 3. Approximate versions of this algorithm work and are almost quasi-nonexpansive.
- 4. For *L*-smooth functions and  $\lambda = 1/L$  we get a condition number of  $\zeta_{R_0}$  in  $B(x, R_0)$ . Only depends on the geometry!

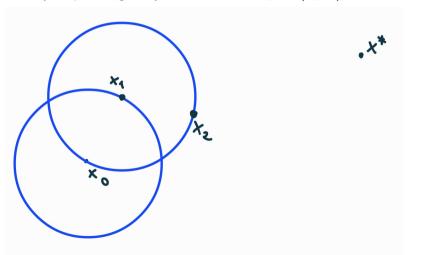
$$x_t \leftarrow \operatorname{argmin} \left\{ f(x) + \frac{1}{\lambda} d(x, x_{t-1})^2 \right\}$$

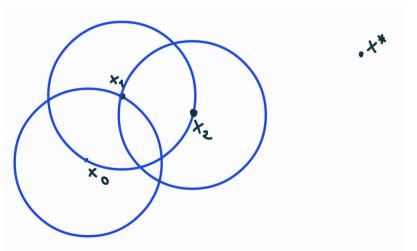


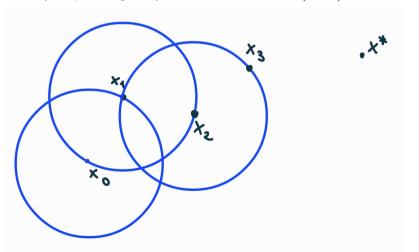












## 6. Mapping to Euclidean space (II) (Ref.)

**Manifold:** Locally symmetric space (all applications satisfy this). Actually it works slightly more broadly. For f L-smooth and  $\mu$ -strongly convex in a ball of center  $x_0$ , and diameter  $\approx \min\{\sqrt{\frac{\mu}{L}}, \frac{\mu}{G}\}$ , pulling back:

$$\hat{f}: \mathbb{R}^d o \mathbb{R}, \quad \hat{f}(\hat{x}) = f(\mathsf{Exp}_{\mathsf{x_0}}(\hat{x})),$$

results in  $\Theta(L)$ -smooth,  $\Theta(\mu)$ -strongly convex Euclidean function.

This technique is not ours, it is from (CB20), but we use it with the proximal method for an  $\it L$ -smooth function with  $\it \lambda=1/\it L$ :

$$\min\left\{f(x)+\frac{L}{2}d(x,x_0)^2\right\}$$

**Condition number**:  $\zeta_D$ . Thus, we just need diameter  $D \leq \zeta_D$  if  $x^* \in \text{the ball}$ . Holds for a D = O(1). This relaxes the required diameter from  $O(\sqrt{\mu/L})$  to O(1).

# 7. Showing naturally-ocurring iterate boundedness (Ref.)

- 1. Monotonous methods stay in the level set. But this is too bad.
- 2. Subproblems of proximal methods have much smaller level sets.
- 3. Mirror descent approaches can give us natural boundedness.
  - ► Euclidean step-size: we stay in a bigger ball of diameter  $O(R_0\zeta_{R_0})$ .
  - ► Smaller step size by a  $\frac{1}{\zeta_{R_0}}$  factor: We stay in a ball of diameter  $O(R_0)$ .
  - ▶ In the hyperbolic space we can do much better. Can this be generalized?

### Projected Riemannian Gradient Descent & Prox Subproblems

 $D \stackrel{\text{def}}{=} \operatorname{diam}(\mathfrak{X}), R \stackrel{\text{def}}{=} \operatorname{Lips}(F,\mathfrak{X})/L, \lambda \stackrel{\text{def}}{=} 1/L.$ 

Metric projection. Efficient steps.

$$x_{t+1} \leftarrow \mathcal{P}_{\mathcal{X}}\left(\mathsf{Exp}_{x_t}\left(-\frac{1}{L+\zeta/\lambda}\nabla F(x_t)\right)\right).$$

**Rates:** 
$$\widetilde{O}(\zeta_R\zeta_D)$$
, where  $F(x) = f(x) + \frac{1}{2\lambda}d(x,\hat{x})^2$ .

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**Rates:**  $\widetilde{O}(\zeta_R\zeta_D)$ , where  $F(x) = f(x) + \frac{1}{2\lambda}d(x,\hat{x})^2$ .

► Quadratic upper model in the tangent space. ¿Efficient steps?

$$x_{t+1} \leftarrow \operatorname{argmin}_{y \in \mathcal{X}} \{ \langle \nabla F(x_t), \operatorname{Exp}_{x_t}^{-1}(y) \rangle_{x_t} + \frac{L + \zeta/\lambda}{2} d(x_t, y)^2 \}.$$

**Rates:** 
$$\widetilde{O}(\zeta_D)$$
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**Rates:**  $\widetilde{O}(\zeta_R \zeta_D)$ , where  $F(x) = f(x) + \frac{1}{2\lambda} d(x, \hat{x})^2$ . Quadratic upper model in the **tangent space**. i Efficient steps?

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**Rates:**  $\widetilde{O}(\zeta_D)$ , where  $F(x) = f(x) + \frac{1}{2\lambda}d(x,\hat{x})^2$ .

 $x_{t+1} \leftarrow \operatorname{argmin}_{y \in \mathcal{X}} \{ \langle \nabla F(x_t), \operatorname{\mathsf{Exp}}_{x_t}^{-1}(y) \rangle_{x_t} + \frac{L}{2} d(x_t, y)^2 + g(y) \}.$ 

**Rates:** 
$$\widetilde{O}(1)$$
, where  $F(x) = f(x)$  and  $g(x) = \frac{1}{2\lambda}d(x,\hat{x})^2$ .

### Different Results and Trade-Offs in Smooth G-Convex Riem. Optimization

 $R\stackrel{\mathrm{def}}{=} d(x_0,x^*),\ \zeta_D=\Theta(D\sqrt{|K_{\min}|}+1)\ \mathrm{if}\ K_{\min}<0\ \mathrm{else}\ 1.\ K_{\min}\stackrel{\mathrm{def}}{=} \min\{\mathrm{sectional}\ \mathrm{curv.}\},\ \kappa=L/\mu.$ 

|   | Result    | g-convex   | $\mu$ -st. g-cvx                                  | K?           | C/NC?  | D?            | Needs R?  |
|---|-----------|--|---|--------------|--------|---------------|-----------|
| 0 | (Nes05)   | $O(\sqrt{\frac{LR^2}{arepsilon}})$   | $\widetilde{O}(\sqrt{\kappa})$                    | 0            | NC     | O(R)          | No   No   |
| 1 | (Mar22)   | $\widetilde{O}(\zeta^{\frac{3}{2}}\sqrt{\zeta+\frac{LR^2}{\varepsilon}})$                  | $\widetilde{O}(\zeta^{\frac{3}{2}}\sqrt{\kappa})$ | ctant.≠ 0    | С      | O(R)          | Yes   Yes |
| 2 | (CB22)    | ,<br>-   | $\widetilde{\Omega}(\zeta)$                       | $\leq c < 0$ | -      | -             | -         |
| 3 | (MP23)    | $\widetilde{O}(\zeta^2\sqrt{\zeta+\frac{LR^2}{\varepsilon}})$                              | $\widetilde{O}(\zeta^2\sqrt{\kappa})$             | Hadamard*    | C & NC | O(R)          | Yes   No  |
| 4 | (MRCP23)  | $\widetilde{O}(\zeta\sqrt{\zeta+\frac{LR^2}{\varepsilon}})$                                | $\widetilde{O}(\sqrt{\zeta\kappa}+\zeta)$         | Hadamard     | C & NC | O(R)          | Yes   No  |
| 5 | (CB23)    | $\widetilde{\Omega}(\zeta + rac{LR^2}{\zeta\sqrt{arepsilon}}) \ O(rac{LR^2}{arepsilon})$ | $\widetilde{\Omega}(\sqrt{\kappa}+\zeta)$         | ctant < 0    | -      | -             | -         |
| 6 | (MRP24).1 | $O(\frac{LR^2}{\varepsilon})$  | $\widetilde{O}(\kappa)$                           | ctant < 0    | NC     | O(R)          | No   No   |
| 7 | (MRP24).2 | $O(\zeta \frac{LR^2}{\varepsilon})$  | $\widetilde{O}(\kappa)$                           | bounded      | NC     | $O(R\zeta_R)$ | No   No   |
| 8 | (MRP24).3 | $O(\zeta \frac{LR^2}{\varepsilon})$  | $\widetilde{O}(\zeta\kappa)$                      | bounded      | NC     | O(R)          | Yes   Yes |
| 9 | (MRP24).4 | $O(\frac{LR^2}{\varepsilon})$  | $\widetilde{O}(\kappa)$                           | Hadamard     | С      | O(R)          | Yes   Yes |