Semi-Riemannian Manifold Optimization

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Outline

Motivation

- Riemannian Manifold Optimization
- Barrier Functions and Interior Point Methods

Semi-Riemannian Manifold Optimization

- Optimality Conditions
- Descent Direction
- Semi-Riemannian First Order Methods
- Metric Independence of Second Order Methods

Optimization on Semi-Riemannian Submanifolds

Joint work with **Lek-Heng Lim (The University of Chicago)** and **Ke Ye (Chinese Academy of Sciences)**

Riemannian Manifold Optimization

- Optimization on manifolds:

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

  where $(\mathcal{M}, g)$ is a (typically nonlinear, non-convex) Riemannian manifold, $f : \mathcal{M} \to \mathbb{R}$ is a smooth function on $\mathcal{M}$
- Difficult constrained optimization; handled as unconstrained optimization from the perspective of manifold optimization
- Key ingredients: tangent spaces, geodesics, exponential map, parallel transport, gradient ∇f, Hessian $\nabla^2 f$

Riemannian Manifold Optimization

- **Riemannian Steepest Descent**

$$x_{k+1} = \mathrm{Exp}_{x_k}\left(-t\nabla f\left(x_k\right)\right), \quad t \geq 0$$

- **Riemannian Newton's Method**

$$\begin{aligned} \left[\nabla^2 f\left(x_k\right)\right]\eta_k &= -\nabla f\left(x_k\right) \\ x_{k+1} &= \mathrm{Exp}_{x_k}\left(-t\eta_k\right), \quad t \geq 0 \end{aligned}$$

- Riemannian trust region
- Riemannian conjugate gradient
- ......

Gabay (1982), Smith (1994), Edelman et al. (1998), Absil et al. (2008), Adler et al. (2002), Ring and Wirth (2012), Huang et al. (2015), Sato (2016), etc.

Riemannian Manifold Optimization

- Applications: Optimization problems on matrix manifolds
  - Stiefel manifolds
  $$V_k(\mathbb{R}^n) = O(n)/O(k)$$
  - Grassmannian manifolds
  $$\mathrm{Gr}(k,n) = O(n)/(O(k) \times O(n-k))$$
  - Flag manifolds: for $n_1 + \cdots + n_d = n$,
  $$\mathrm{Flag}_{n_1,\cdots,n_d} = O(n)/(O(n_1) \times \cdots \times O(n_d))$$
  - Shape Spaces
  $$\left(\mathbb{R}^{k\times n} \setminus \{0\}\right)/O(n)$$
  - ......

From Riemannian to Semi-Riemannian

Motivation 1: Question from a Geometer

How does optimization depend on the choice of metrics?

- Critical points $\{x \in \mathcal{M} \mid \nabla f(x) = 0\}$ are metric independent
- Gradients, Hessians, Geodesics are metric dependent
- *Index* of Hessian becomes metric independent at a critical point; Morse theory
- Optimization trajectories are obviously metric dependent
- Newton's equation is metric independent

$$\left[\nabla^2 f(x_k)\right] \eta_k = -\nabla f(x_k) \quad \Leftrightarrow \quad \left[\widetilde{\nabla}^2 f(x_k)\right] \eta_k = -\widetilde{\nabla} f(x_k)$$

- Does it still work if the metric structure is more general than Riemannian? (E.g. Semi-Riemannian, Finsler, etc.)

Barrier Functions and Interior Point Methods

$f : Q \to \mathbb{R}$ strictly convex, defined on an open subset $Q \subset \mathbb{R}^d$.

- $\nabla^2 f(x) \succ 0$ on any $x \in Q$
- $\nabla^2 f(x)$ defines a Riemannian metric on Q
- gradient under this Riemannian metric: $\left[\nabla^2 f(x)\right]^{-1} \nabla f(x)$
- Newton's method for f is exactly the gradient descent under the Riemannian metric defined by $\nabla^2 f(x)$!
- Nesterov and Todd (2002): primal-dual central path are "close to" geodesics under this Riemannian metric

• Nesterov, Yurii E., and Michael J. Todd. *On the Riemannian geometry defined by self-concordant barriers and interior-point methods*. Foundations of Computational Mathematics 2, no. 4 (2002): 333-361.

• Duistermaat, Johannes J. *On Hessian Riemannian structures*. Asian Journal of Mathematics 5, no. 1 (2001): 79-91.

From Riemannian to Semi-Riemannian

Motivation 2: Nonconvex objectives for interior point methods

- What if $f : Q \to \mathbb{R}$ is not strictly convex?
- What happens to Newton's method if the Hessian is not positive semi-definite? (Newton's method with modified Hessian)

Semi-Riemannian Geometry

- **Scalar product**: $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R}$ symmetric bilinear form on vector space V, not necessarily positive (semi-)definite
- **Non-degeneracy**: $\langle v, w \rangle = 0$ for all $w \in V \quad \Leftrightarrow \quad v = \vec{0}$
- A **semi-Riemannian manifold** is a differentiable manifold M with a scalar product $\langle \cdot, \cdot \rangle_x$ defined on $T_x M$, and $\langle \cdot, \cdot \rangle_x$ varies smoothly with respect to $x \in M$
- A semi-Riemannian manifold is **non-degenerate** if $\langle \cdot, \cdot \rangle_x$ is non-degenerate for all $x \in M$
- **Non-degeneracy needs not be inherited by subspaces**!
- Semi-Riemannian submanifold, geodesic, parallel transport, gradient, Hessian, ... all well-defined if non-degenerate
- Of great interest to general relativity as a spacetime model (Lorentzian geometry)

Semi-Riemannian Geometry

A Simplest Degenerate Subspace Example

- Consider $\mathbb{R}^2$ equipped with the Lorentzian metric of signature $(-,+)$, i.e., for $x=(x_1,x_2)\in\mathbb{R}^2$ and $y=(y_1,y_2)\in\mathbb{R}^2$, define the scalar product as $\langle x,y\rangle=-x_1y_1+x_2y_2$
- Let $W=\operatorname{span}\{(1,1)\}$, which is a degenerate subspace of $\mathbb{R}^2$
- If we define $W^\perp:=\left\{v\in\mathbb{R}^2 \mid \langle w,v\rangle=0\,\forall w\in W\right\}$, then one has $W=W^\perp$!
- **Take-home message**: If W is a degenerate subspace of a scalar product space $(V,\langle\cdot,\cdot\rangle)$, then in general $W+W^\perp\neq V$, and it may well be the case that $W\cap W^\perp\neq 0$!
- **Nevertheless**: If W is a non-degenerate subspace of V, then it is still true that $V=W\oplus W^\perp$

Examples of Semi-Riemannian Manifolds

- **Minkowski space** $\mathbb{R}^{p,q}$ ($p \geq 0$, $q \geq 0$): vector space $\mathbb{R}^{p+q}$ equipped with scalar product

$$\langle u, v \rangle = u^\top I_{p,q} v$$

where

$$I_{p,q} = \begin{pmatrix} -I_p & 0 \\ 0 & I_q \end{pmatrix}$$

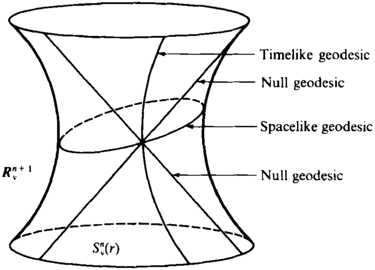
- Square matrices $\mathbb{R}^{n\times n}$, equipped with scalar product

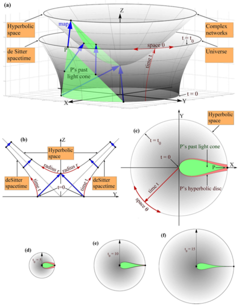
$$\langle A, B \rangle = \mathrm{Tr}\left(A^\top I_{p,q} B\right) = \mathrm{vec}\left(A\right)^\top \left(I_n \otimes I_{p,q}\right) \mathrm{vec}\left(B\right)$$

- Submanifolds of semi-Riemannian manifolds

Examples of Semi-Riemannian Manifolds: Applications

- **Spacetime models**: Lorentzian spaces, de Sitter spaces, anti-de Sitter spaces, ...
- **Network models**: social networks "behave like" spaces of negative Alexandrov curvature





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• Krioukov, Dmitri, Maksim Kitsak, Robert S. Sinkovits, David Rideout, David Meyer, and Marián Boguñá. **Network cosmology.** *Scientific reports* 2 (2012): 793.

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Optimality Conditions

Given a semi-Riemannian manifold with scalar product $\langle \cdot, \cdot \rangle_x$ on $T_x M$, define the *semi-Riemannian gradient* of a smooth function $f \in C^2(M)$ by

$$\langle Df, X \rangle_x = Xf(x), \quad \forall X \in \Gamma(M, T_x M), x \in M$$

and define the *semi-Riemannian Hessian* of f by

$$D^2 f(X, Y) = X(Yf) - (D_X Y) f, \quad \forall X, Y \in \Gamma(M, T_x M)$$

where $D_X Y$ is the *covariant derivative* of Y with respect to X.

Optimality Conditions

Necessary conditions: A local optimum $x \in M$ satisfies

- (First order necessary condition) $Df(x) = 0$ if $f : M \to \mathbb{R}$ is first-order differentiable
- (Second order necessary condition) $Df(x) = 0$ and $D^2 f(x) \succeq 0$ if $f : M \to \mathbb{R}$ is second-order differentiable

Sufficient condition:

- (Second-order sufficient condition) If $x \in M$ is an interior point on a semi-Riemannian manifold M, if $Df(x) = 0$ and $D^2 f(x) \succ 0$, then x is a strict relative minimum of f

Descent Direction

- If general, $-Df(x)$ is not a descent direction at $x \in M$! The main issue is that $\langle -Df(x), Df(x)\rangle_x$ may be negative, so the first-order approximation $f(x - Df(x)) \approx f(x) - \langle Df(x), Df(x)\rangle_x$ needs not be smaller than $f(x)$
- Similar issue exists in Newton's method: When Hessian $\nabla^2 f(x)$ is not positive definite, the Newton direction $-[\nabla f(x)]^{-1} \nabla f(x)$ may not be a descent direction
- Solution for Newton's method: **Modified Hessian Methods**
- For semi-Riemannian optimization: similar idea of modifying $Df(x)$

Descent Direction

Solution: modify $-Df(x)$ to obtain a descent direction on the semi-Riemannian manifold

- For each $T_x M$, use semi-Riemannian Gram-Schmidt to find an orthonormal basis $e_1, \cdots, e_d$ for $T_x M$
- Construct $[Df(x)]^+ = \sum_{i=1}^{n} \langle Df(x), e_i \rangle e_i$
- $-[Df(x)]^+$ is a descent direction, since

$$\left\langle -[Df(x)]^+, Df(x) \right\rangle = -\sum_{i=1}^{n} |\langle Df(x), e_i \rangle|^2 < 0$$

Semi-Riemannian Steepest Descent I/II

Algorithm 3.1 SEMI-RIEMANNIAN STEEPEST DESCENT

Require: Manifold M, semi-Riemannian metric $\langle \cdot, \cdot \rangle$, objective function f, retraction $\mathrm{Retr} : TM \to M$, initial value $x_0 \in M$, parameters for LINESEARCH, gradient Df

$x_0 \leftarrow$ INITIATE
$k \leftarrow 0$
while not converge **do**
  $\eta \leftarrow$ FINDDESCENTDIRECTION$(x_k, M, Df\,(x_k))$ ▷ c.f. Algorithm 3.4
  $0 < t_k \leftarrow$ LINESEARCH(f, x_k, η_k) ▷ t_k is the Armijo step size
  Choose x_{k+1} such that ▷ $c \in (0, 1)$ is a parameter

$$f\,(x_k) - f\,(x_{k+1}) > c\,[f\,(x_k) - f\,(\mathrm{Retr}_{x_k}\,(t_k \eta_k))]$$

  $k \leftarrow k + 1$
end while
return Sequence of iterates $\{x_k\}$

Semi-Riemannian Steepest Descent II/II

Algorithm 3.4 FINDING SEMI-RIEMANNIAN DESCENT DIRECTION

function FINDDESCENTDIRECTION$(x, M, Df(x))$

  $\{e_1, \cdots, e_n\} \leftarrow$FINDONBASIS$(T_xM, \langle \cdot, \cdot \rangle)$

  $\eta \leftarrow -[Df(x)]^+ = -\sum_{i=1}^{n} \langle Df(x), e_i \rangle e_i$

  return η

end function

Semi-Riemannian Conjugate Gradient

Algorithm 3.5 SEMI-RIEMANNIAN CONJUGATE GRADIENT (POLAK-REBIÈRE)

Require: Manifold M, objective function f, retraction Retr, parallel transport P, initial value $x_0 \in M$, parameters for LINESEARCH, gradient Df and Hessian $D^2 f$

$k \leftarrow 0$

$x_0 \leftarrow$ INITIATE

$\eta_0 \leftarrow$FINDDESCENTDIRECTION$(x_0, M, Df(x_0))$ ▷ c.f. Algorithm 3.4

while not converge **do**

  $0 < t_k \leftarrow$ LINESEARCH(f, x_k, η_k) ▷ t_k is the Armijo step size

  $x_{k+1} \leftarrow \mathrm{Retr}_{x_k}(t_k \eta_k)$

  $\xi_{k+1} \leftarrow$FINDDESCENTDIRECTION$(x_{k+1}, M, Df(x_{k+1}))$

  $\eta_{k+1} = \xi_{k+1} + \beta_k P \eta_k$, where ▷ $P : T_{x_k}M \rightarrow T_{x_{k+1}}M$

$$\beta_k := \max\left\{0, \frac{\left\langle Df(x_{k+1}) - P\left[Df(x_k)\right], \left[Df(x_{k+1})\right]^{+}\right\rangle}{\left\langle Df(x_k), \left[Df(x_k)\right]^{+}\right\rangle}\right\}$$

  $k \leftarrow k + 1$

end while

return Sequence of iterates $\{x_k\}$

Semi-Riemannian Second-Order Methods

- **Newton's Method**: Solve $\left[D^2 f(x)\right] \eta = Df(x)$ for a descent direction $\eta \in T_x M$ at $x \in M$. Note that this is exactly the same Newton's equation for Riemannian optimization!
- **Trust Region**: Minimize a local quadratic optimization problem near each $x \in M$. Again same as Riemannian optimization!
- The equivalence between Riemannian and Semi-Riemannian second-order methods is not just a coincidence; it is because these methods build upon local polynomial surrogates, which are always *metric-independent* in the sense of *jets*.

Outline

Joint work with **Lek-Heng Lim (The University of Chicago)** and **Ke Ye (Chinese Academy of Sciences)**

Which manifolds admit semi-Riemannian structures?

- Euclidean spaces and all Riemannian manifolds are particular semi-Riemannian manifolds
- Tangent bundles of manifolds admitting a semi-Riemannian metric that is not Riemannian must admit at least one decomposition into two sub-bundles
- Any manifold with trivial tangent bundle admits semi-Riemannian manifolds, e.g. all matrix Lie groups, Minkowski $\mathbb{R}^{p,q}$
- Unfortunately, almost all matrix Lie groups are either degenerate semi-Riemannian manifolds as submanifolds of the ambient Minkowski space, or do not admit closed-form semi-Riemannian geodesics and/or parallel-transports

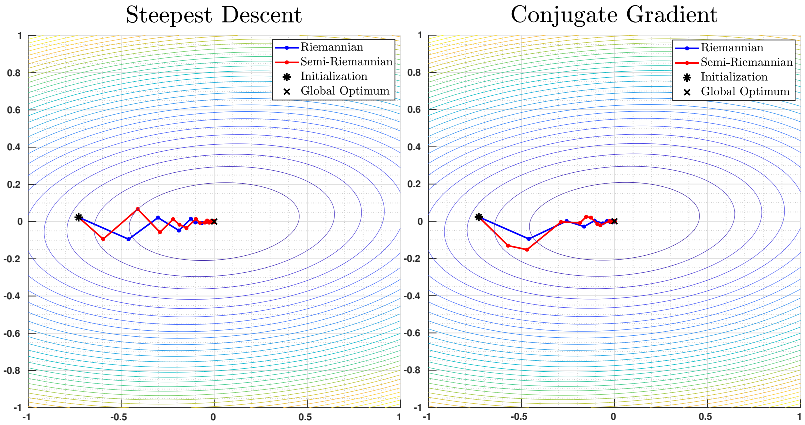
Optimization on Semi-Riemannian Submanifolds

Minkowski Spaces $\mathbb{R}^{p,q}$ ($\cong \mathbb{R}^{p+q}$ as vector spaces)
For all $x, y \in \mathbb{R}^{p,q}$ and $V, W \in T_x\mathbb{R}^{p,q}$:

- Tangent Spaces: $T_x\mathbb{R}^{p,q} = \mathbb{R}^{p,q}$
- Scalar Product: $\langle V, W \rangle_x = -\sum_{i=1}^{p} V_i W_i + \sum_{j=p+1}^{p+q} V_j W_j$
- Geodesics: $\mathrm{Exp}_x(tV) = x + tV$
- Parallel Transport: $P_{x \to y} V = V, \forall V \in T_x\mathbb{R}^{p,q} = T_y\mathbb{R}^{p,q}$
- Semi-Riemannian Gradient: $Df(x) = I_{p,q} \nabla f(x)$
- Semi-Riemannian Hessian: $D^2 f(x) = I_{p,q} \nabla^2 f(x) I_{p,q}$

Example: Minkowski Spaces

$$\min_{x \in \mathbb{R}^{1,1}} x^\top A x, \qquad \text{where } A \succeq 0$$



Optimization on Semi-Riemannian Submanifolds

Euclidean sphere in a Minkowski space $\mathbb{S}^{p+q-1}$

- Tangent Spaces: $T_x\mathbb{S}^{p+q-1} = \{V \in T_x\mathbb{R}^{p,q} \mid \langle V, I_{p,q}x\rangle = 0\}$
- Scalar Product: Inherited from the ambient space $\mathbb{R}^{p,q}$
- The induced scalar product is non-degenerate except for a set of measure zero $\mathcal{Z} := \left\{x \in \mathbb{S}^{p+q-1} \mid x^\top I_{p,q}x = 0\right\}$
- Projection from $T_x\mathbb{R}^{p,q}$ to $T_x\mathbb{S}^{p+q-1}$:

$$\mathrm{Proj}_x(V) = V - \frac{V^\top x}{x^\top I_{p,q}x} I_{p,q}x, \quad \forall x \in \mathbb{S}^{p+q-1} \backslash \mathcal{Z}$$

- Geodesics: No closed-form expression, but can use Riemannian geodesics for optimization purposes
- Parallel Transport: No closed-form expression, but can use Riemannian parallel-transports for optimization purposes

Optimization on Semi-Riemannian Submanifolds

Euclidean sphere in a Minkowski space $\mathbb{S}^{p+q-1}$

- Semi-Riemannian Gradient:

$$Df(x) = \mathrm{Proj}_x(\nabla f(x)), \quad \forall x \in \mathbb{S}^{p+q-1} \backslash \mathcal{Z}$$

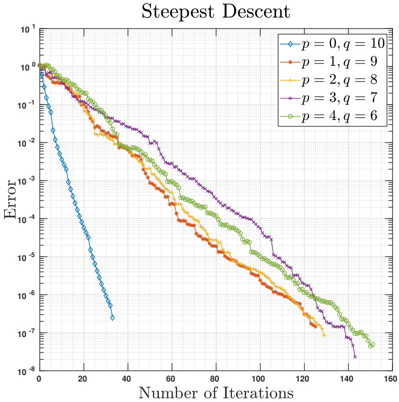
- Semi-Riemannian Hessian:

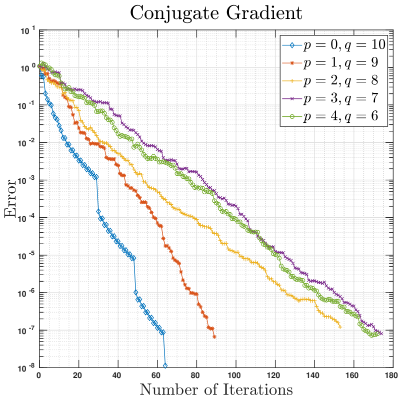
$$D^2 f(x) = \mathrm{Proj}_x \circ \nabla^2 f(x), \quad \forall x \in \mathbb{S}^{p+q-1} \backslash \mathcal{Z}$$

(Viewing $\nabla^2 f(x)$ as a linear map from $T_x\mathbb{R}^{p,q}$ to $T_x\mathbb{R}^{p,q}$, and $D^2 f(x)$ as a linear map from $T_x\mathbb{S}^{p+q-1}$ to $T_x\mathbb{S}^{p+q-1}$)

Example: Euclidean Spheres in Minkowski Spaces

$$\max_{x_1^2+\cdots+x_{p+q}^2=1} x^\top A x, \qquad \text{where } A = A^\top$$





Optimization on Semi-Riemannian Submanifolds

Pseudosphere $\mathbb{S}^{p,q}$ in a Minkowski space $\mathbb{S}^{p+q-1}$

$$\mathbb{S}^{p,q} := \left\{ x \in \mathbb{R}^{p,q} \mid -x_1^2 - \cdots - x_p^2 + x_{p+q}^2 + \cdots + x_{p+q}^2 = 1 \right\}$$

- Tangent Spaces: $T_x\mathbb{S}^{p,q} = \left\{ V \in T_x\mathbb{R}^{p,q} \mid \langle V, x \rangle = 0 \right\}$
- Scalar Product: Inherited from the ambient space $\mathbb{R}^{p,q}$
  Non-degenerate!
- Projection from $T_x\mathbb{R}^{p,q}$ to $T_x\mathbb{S}^{p,q}$:

$$\mathrm{Proj}_x(V) = V - \left(V^\top I_{p,q} x \right) x, \quad \forall x \in \mathbb{S}^{p,q}$$

- Semi-Riemannian Gradient:

$$Df(x) = \mathrm{Proj}_x(\nabla f(x)), \quad \forall x \in \mathbb{S}^{p,q}$$

- Semi-Riemannian Hessian:

$$D^2 f(x) = \mathrm{Proj}_x \circ \nabla^2 f(x), \quad \forall x \in \mathbb{S}^{p,q}$$

Optimization on Semi-Riemannian Submanifolds

Pseudosphere $\mathbb{S}^{p,q}$ in a Minkowski space $\mathbb{S}^{p+q-1}$

$$\mathbb{S}^{p,q} := \left\{ x \in \mathbb{R}^{p,q} \mid -x_1^2 - \cdots - x_p^2 + x_{p+q}^2 + \cdots + x_{p+q}^2 = 1 \right\}$$

- Geodesics: For any $x \in \mathbb{S}^{p,q}$ and $V \in T_x\mathbb{S}^{p,q}$,

$$\mathrm{Exp}_x(tV) = \begin{cases} x\cos(t\|V\|) + \dfrac{V}{\|V\|}\sin(t\|V\|), & \text{if } \langle V, V\rangle > 0, \\ x\cosh(t\|V\|) + \dfrac{V}{\|V\|}\sinh(t\|V\|), & \text{if } \langle V, V\rangle < 0, \\ x + tV, & \text{if } \langle V, V\rangle = 0. \end{cases}$$

where $\|V\| := \sqrt{|\langle V, V\rangle|}$.

Optimization on Semi-Riemannian Submanifolds

Pseudosphere $\mathbb{S}^{p,q}$ in a Minkowski space $\mathbb{S}^{p+q-1}$

- Parallel Transport along geodesics: For any $x \in \mathbb{S}^{p,q}$ and $V \in T_x\mathbb{S}^{p,q}$, the parallel transport of V along a geodesic emanating from x in the direction $X \in T_x\mathbb{S}^{p,q}$ is

$$P_{x\to \mathrm{Exp}_x(tX)}(V) =$$
$$\begin{cases} -\dfrac{\langle V, X\rangle}{\|X\|}\left[x\sin\left(t\|X\|\right) - \dfrac{X}{\|X\|}\cos(t\|X\|)\right], & \\ \qquad\qquad + + \left(V - \langle V, X\rangle X/\|X\|^2\right), & \text{if } \langle X, X\rangle > 0, \\ -\dfrac{\langle V, X\rangle}{\|X\|}\left[x\sinh\left(t\|X\|\right) + \dfrac{X}{\|X\|}\cosh(t\|X\|)\right] & \\ \qquad\qquad + \left(V + \langle V, X\rangle X/\|X\|^2\right), & \text{if } \langle X, X\rangle < 0, \\ -\langle V, X\rangle\left(tx + \dfrac{1}{2}t^2X\right) + V, & \text{if } \langle X, X\rangle = 0. \end{cases}$$

Optimization on Semi-Riemannian Submanifolds

Pseudosphere $\mathbb{S}^{p,q}$ in a Minkowski space $\mathbb{S}^{p+q-1}$

$$\mathbb{S}^{p,q} := \left\{ x \in \mathbb{R}^{p,q} \mid -x_1^2 - \cdots - x_p^2 + x_{p+q}^2 + \cdots + x_{p+q}^2 = 1 \right\}$$

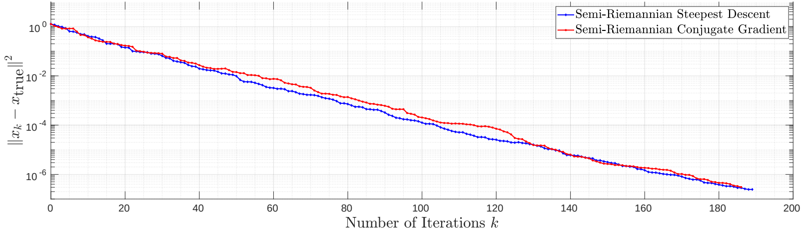
Semi-Riemannian vs. Riemannian optimization on pseudospheres

- Riemannian geodesics and parallel transports are much harder to compute on $\mathbb{S}^{p,q}$, if possible at all
- $\mathbb{S}^{p,q}$ is non-compact

• Fiori, Simone. **Learning by natural gradient on noncompact matrix-type pseudo-Riemannian manifolds.** *IEEE transactions on neural networks* 21, no. 5 (2010): 841-852.

Example: Pseudospheres

$$\min_{x \in \mathbb{S}^{p,q}} \|x - \xi\|_2^2, \qquad \text{where } \xi \notin \mathbb{S}^{p,q}$$



- Tingran Gao, Lek-Heng Lim, and Ke Ye. **Semi-Riemannian Manifold Optimization.** *arXiv:1812.07643* (2018)
- MATLAB code available at `https://github.com/trgao10/SemiRiem`

Matrix Manifolds

- Matrix manifolds are all Lie groups, so their tangent bundles are all trivial. They admit semi-Riemannian metrics of arbitrary index.
- **Unfortunately**, very few matrix manifolds inherit *non-degenerate* semi-Riemannian structures from the ambient Minkowski space; geodesics and parallel-transports for the non-degenerate ones are hard to compute in general

MANIFOLDS	Non-degenerate	GEODESICS	PARAL. TRANSP.
(generic) hyperplane	yes	✓	✓
sphere	no	✗	✗
pseudo-sphere	yes	✓	✓
pseudo-hyperbolic space	yes	✓	✓
indefinite orthogonal group	no	✓	✗
orthogonal group	no	✓	✗
special linear group	yes ($p \neq q$)	✓	✗
symplectic group	no	✓	✗
SPD matrices	no	✓	✗

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Thank you!

Future Work:

- More applications, especially for matrix computation
- Trajectory analysis for non-convex optimization
- **Numerical Differential Geometry**

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