

Higher-Order Non-Smooth Optimization on Manifolds



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Oberwolfach Mini-Workshop on Computational Optimization on Manifolds
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Institute of Mathematics and
Image Computing



UNIVERSITÄT ZU LÜBECK

Setting

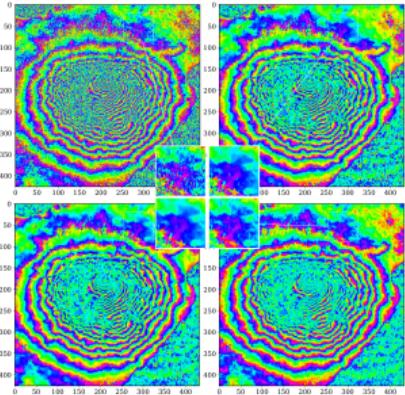
Problem

Find the minimizer of

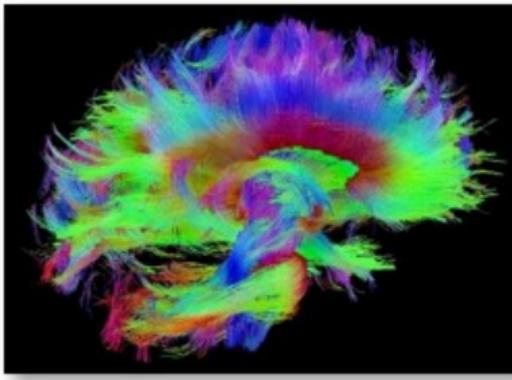
$$\inf_{x \in \mathcal{M}} F(x)$$

- ▶ \mathcal{M} Riemannian manifold
- ▶ objective $F : \mathcal{M} \rightarrow \mathbb{R}$ is non-smooth

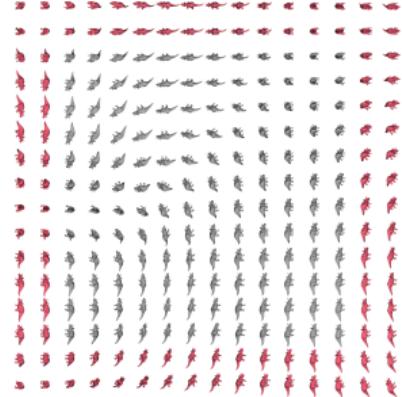
Why?



InSAR
 $\mathcal{S}(1)$



DW-MRI
 $\mathcal{P}(3)$



Orientations
 $SO(3)$

- Typical in function space: Given $b : \Omega \rightarrow \mathcal{M}$, find minimizer $u^* : \Omega \rightarrow \mathcal{M}$ of

$$\inf_{u: \Omega \rightarrow \mathcal{M}} \left\{ \int_{\Omega} d_{\mathcal{M}}(u(x), b(x))^p + \lambda \text{TV}_{\mathcal{M}}(u) \right\}$$

Higher-order Non-smooth Optimization on Manifolds

Higher-order **Non-smooth Optimization** on Manifolds

The Euclidean Convex Case

Euclidean model

$$\inf_{x \in \mathbb{R}^n} \{f(x) + g(Ax)\}$$

- $A : \mathbb{R}^n \rightarrow \mathbb{R}^m$ linear operator, often discretizes derivatives
- $f : \mathbb{R}^n \rightarrow \bar{\mathbb{R}}, g : \mathbb{R}^m \rightarrow \bar{\mathbb{R}}$ convex but non-smooth

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Saddle-point formulation

$$\inf_{x \in \mathbb{R}^n} \sup_{y \in \mathbb{R}^m} \{f(x) + \langle y, Ax \rangle - g^*(y)\}$$

g^* Legendre-Fenchel conjugate: $g^*(y) := \sup_{y' \in \mathbb{R}^m} \{ \langle y', y \rangle - g(y') \}$

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Dual problem

$$\sup_{y \in \mathbb{R}^m} \{-g^*(y) - f^*(-A^\top y)\}$$

Optimality Conditions

Saddle-point formulation

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Primal-dual optimality conditions

$$\begin{aligned} 0 &\in A^\top y^* + \partial f(x^*) \\ 0 &\in -Ax^* + \partial g^*(y^*) \end{aligned}$$

Optimality Conditions

Saddle-point formulation

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Primal-dual optimality conditions

$$0 \in A^\top y^* + \partial f(x^*)$$

$$0 \in -Ax^* + \partial g^*(y^*)$$

- ▶ For non-smooth f, g^* this is a system of **inclusions** – non-unique, hard to manage

Proximal map

Proximal map

$$\text{prox}_{\sigma f}(x) := \arg \min_{x' \in \mathbb{R}^n} \left\{ \frac{1}{2} \|x' - x\|_2^2 + \sigma f(x') \right\}, \quad \sigma > 0.$$

Important property:

$$0 \in z + \partial f(x) \iff 0 = x - \text{prox}_{\sigma f}(x - \sigma z)$$

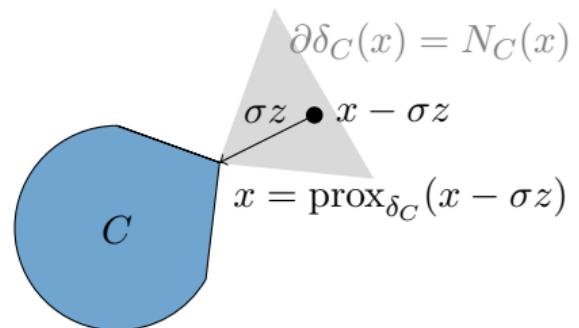
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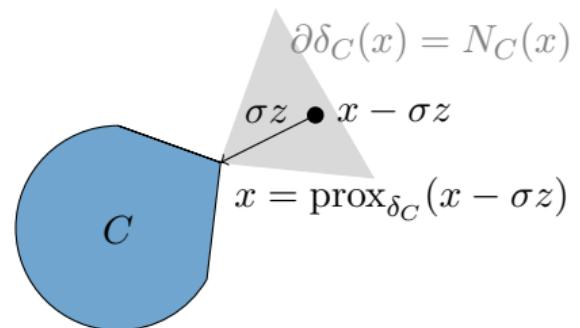
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Important property:

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This turns an **inclusion** into an **equality**!



Optimality conditions II

Primal-dual optimality conditions, inclusion form

$$\begin{aligned} 0 &\in A^\top y^* + \partial f(x^*) \\ 0 &\in -Ax^* + \partial g^*(y^*) \end{aligned}$$

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Primal-dual optimality conditions, equality form

$$\begin{aligned} 0 &= x - \text{prox}_{\sigma f}(x - \sigma A^\top y) \\ 0 &= y - \text{prox}_{\tau g^*}(y + \tau Ax) \end{aligned}$$

First-Order Methods

Primal-dual optimality conditions, equality form

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$$\begin{aligned} 0 &= x - \text{prox}_{\sigma f}(x - \sigma A^\top y) \\ 0 &= y - \text{prox}_{\tau g^*}(y + \tau Ax) \end{aligned}$$

Fixed-point iteration

$$\begin{aligned} x^{k+1} &:= \text{prox}_{\sigma f}(x^k - \sigma A^\top y^k) \\ y^{k+1} &:= \text{prox}_{\tau g^*}(y^k + \tau Ax^k) \end{aligned}$$

First-Order Methods

Primal-dual optimality conditions, equality form

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Primal-dual optimality conditions, equality form

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Fixed-point iteration + Gauss-Seidel + overrelaxation = Primal-Dual-Hybrid-Gradient

$$\begin{aligned} y^{k+1} &:= \text{prox}_{\tau^k g^*}(y^k + \tau^k A(\textcolor{blue}{x^k} + \theta^k(x^k - x^{k-1}))) \\ x^{k+1} &:= \text{prox}_{\sigma^k f}(x^k - \sigma^k A^\top \textcolor{blue}{y^{k+1}}) \end{aligned}$$

Extensions: non-linear A , acceleration schemes for $\theta^k, \tau^k, \sigma^k$ for strong convexity, preconditioning (non-scalar τ, σ), ...

Higher-order **Non-smooth Optimization** on Manifolds

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Manifold Setting

Problem

$$\inf_{p \in \mathcal{M}} \{f(p) + g(\Lambda(p))\},$$

- ▶ \mathcal{M}, \mathcal{N} smooth Riemannian manifolds
- ▶ $\Lambda : \mathcal{M} \rightarrow \mathcal{N}$ (non-linear!) mapping
- ▶ $f : \mathcal{M} \rightarrow \bar{\mathbb{R}}, g : \mathcal{N} \rightarrow \bar{\mathbb{R}}$ functions, **non-smooth**

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Saddle-Point Problem [Bergmann et al.'19]

For a fixed base point $n \in \mathcal{N}$ and cotangent space $T_n^*\mathcal{N}$:

$$\inf_{p \in \mathcal{M}} \sup_{\xi_n \in T_n^*} \{f(p) + \langle \log_n \Lambda(p), \xi_n \rangle - g_n^*(\xi_n)\},$$

where $g_n^*(\xi_n) := \sup_{X \in \mathcal{L}_{\mathcal{C},n}} \{\langle \xi_n, X \rangle - g(\exp_n X)\}$ is the n -conjugate.

- ▶ For proper lsc convex g , we get $g_{nn}^{**} = g$ and Fenchel: $f(p) + f_m^*(\xi_m) \geq \langle \xi_m, \log_m p \rangle$.

Linearized optimality system

Saddle-Point

$$\inf_{p \in \mathcal{M}} \sup_{\xi_n \in T_n^*} \{f(p) + \langle \log_n \Lambda(p), \xi_n \rangle - g_n^*(\xi_n)\},$$

- Disadvantage: No good concept of adjoint for Λ .

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Linearized Saddle-Point

Around base point m , approximate $\Lambda(p) \approx \exp_{\Lambda(m)} D_m \Lambda[\log_m p]$, where $D_m F[v]$ differential of F at $m \in \mathcal{M}$ applied to $v \in T_p \mathcal{M}$. Then for $n := \Lambda(m)$,

$$\inf_{p \in \mathcal{M}} \sup_{\xi_n \in T_n^*} \{f(p) + \langle \textcolor{blue}{D}_m \Lambda[\log_m p], \xi_n \rangle - g_n^*(\xi_n)\}.$$

Linearized optimality system

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- Can show weak duality on Hadamard manifolds for proper, lsc, convex problems
- Saddle point solves linearized problem

Optimality by Equality on Manifolds

Primal-dual optimality conditions on manifolds [Bergmann et al.'19]

Manifold case: $p \in \mathcal{M}$, $\xi_n \in T_n^*$, fixed base point $n \in \mathcal{N}$, linearized version:

$$\begin{aligned} p &= \text{prox}_{\sigma f} \left(\exp_p \left(\mathcal{P}_{m \rightarrow p} \left(-\sigma (D_m \Lambda)^* [\mathcal{P}_{n \rightarrow \Lambda(m)} \xi_n] \right)^\sharp \right) \right) \\ \xi_n &= \text{prox}_{\tau g_n^*} \left(\xi_n + \tau (\mathcal{P}_{\Lambda(m) \rightarrow n} D_m \Lambda [\log_m p])^\flat \right) \end{aligned}$$

Compare Euclidean case: $x \in \mathbb{R}^n$, $y \in \mathbb{R}^m$:

$$\begin{aligned} 0 &= x - \text{prox}_{\sigma f}(x - \sigma A^\top y) \\ 0 &= y - \text{prox}_{\tau g^*}(y + \tau Ax) \end{aligned}$$

Requires linearization of primal problem around m , but...

- ▶ Can construct first-order Linearized Riemannian Chambolle-Pock method (IRCPA)
- ▶ IRCPA converges to saddle point for proper, convex, lsc problems on Hadamard manifolds

Other Non-Smooth First-Order Methods on Manifolds

- ▶ Subgradient descent, gradient sampling
- ▶ Primal proximal steps:
 - ▶ Cyclic Proximal Point Algorithm (CPPA)
 - ▶ Iteratively Reweighted Least Squares (IRLS)
 - ▶ Parallel Douglas-Rachford (PDR)
- ▶ Specialized/exact algorithms/dynamic programming

Convergence generally for Hadamard manifolds, but also seem to work on manifolds with positive sectional curvature.

Higher-order **Non-smooth Optimization on Manifolds**

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Higher-Order Methods

- ▶ First-order methods converge **sublinearly** or **linearly** (strongly convex primal & dual problems) – very slow tail convergence
- ▶ **Goal:** apply higher-order methods for superlinear convergence. Choices:
 - ▶ Extrinsic approach & use Euclidean solver
 - ▶ Smooth energy & use Riemannian (Quasi-)Newton-type method/Trust region/CG
 - ▶ Here: **Semismooth Newton**

Euclidean Semismooth Newton

Problem

Solve non-linear system equation

$$X(x) = 0,$$

where $X : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is (Lipschitz-)continuous but **not** C^1 .

Typical application:

$$\begin{aligned} x^* &\in \arg \min_{x \in \mathbb{R}^n} F(x) \\ \text{s.t. } x &\leqslant 0 \end{aligned}$$

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$$\begin{array}{l} x^* \in \arg \min_{x \in \mathbb{R}^n} F(x) \\ \text{s.t. } x \leq 0 \end{array} \iff \begin{array}{l} 0 = \nabla F(x^*) + \lambda \\ x \leq 0, \lambda \geq 0, \lambda x = 0 \end{array}$$

Euclidean Semismooth Newton

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Typical application:

$$\begin{array}{lcl} x^* \in \arg \min_{x \in \mathbb{R}^n} F(x) & \iff & 0 = \nabla F(x^*) + \lambda \\ \text{s.t. } x \leq 0 & & x \leq 0, \lambda \geq 0, \lambda x = 0 \end{array} \iff \begin{array}{l} 0 = \nabla F(x^*) + \lambda \\ 0 = \lambda - \max\{0, \lambda + \sigma x\} \end{array}$$

Euclidean Semismooth Newton

Algorithm 1 Semismooth Newton

Initialization: $x^0 \in \mathbb{R}^n$

for $k = 0, 1, \dots$ **do**

 Choose any $V(x^k) \in \partial_C X(x^k)$

 Solve $V(x^k)d^k = -X(x^k)$

$x^{k+1} := x^k + d^k$

end for

Theorem (consequence of [Qi, Sun'93])

Assume that x^* satisfies $X(x^*) = 0$, X is locally Lipschitz and semismooth at x^* and all $V \in \partial_C X(x^*)$ are nonsingular. Then the iteration in Alg. 1 is well-defined and converges superlinearly to x^* in a neighborhood of x^* . If in addition X is μ -order semismooth at x^* , then the convergence is of order $1 + \mu$.

Euclidean Semismoothness

Definition

Let $X : U \rightarrow \mathbb{R}^n$ be defined on the open set $U \subset \mathbb{R}^n$. Then, for $0 < \mu \leq 1$, X is called μ -order semismooth at $x \in U$ if X is locally Lipschitz at x , all one-sided directional derivatives $X'(x, \cdot)$ exist, and, for every $V \in \partial_C X(x + d)$ in the generalized Clarke differential,

$$\|Vd - X'(x, d)\| = \mathcal{O}(\|d\|^{1+\mu}) \quad \text{as } d \rightarrow 0.$$

If X is μ -order semismooth at all $x \in U$, then we call X μ -order semismooth (on U).

Semismoothness

Equivalent: X is locally Lipschitz continuous at x , $X'(x, \cdot)$ exist, and, for every $V \in \partial_C X(x + d)$ it holds

$$\|X(x + d) - (X(x) + Vd)\| = \mathcal{O}(\|d\|^{1+\mu}) \quad \text{as } d \rightarrow 0.$$

Compare definition of differentiability in smooth case, where $V = \nabla X(x)$.

- ▶ Often fulfilled: norms, convex functions, piecewise C^1 , piecewise affine

Non-Smooth Euclidean SSN

Optimality Conditions

$$\begin{array}{l} x^* \in \arg \min_{x \in \mathbb{R}^n} F(x) \\ \text{s.t. } x \leq 0 \end{array} \Leftrightarrow \begin{array}{l} 0 = \nabla F(x^*) + \lambda \\ x \leq 0, \lambda \geq 0, \lambda x = 0 \end{array} \Leftrightarrow \begin{array}{l} 0 = \nabla F(x^*) + \lambda \\ 0 = \lambda - \max\{0, \lambda + \sigma x\} \end{array}$$

Non-Smooth Euclidean SSN

Optimality Conditions

$$0 \stackrel{!}{=} X(x, y) := \begin{pmatrix} x - \text{prox}_{\sigma f}(x - \sigma A^\top y) \\ y - \text{prox}_{\tau g^*}(y + \tau Ax) \end{pmatrix}$$

Non-Smooth Euclidean SSN

Optimality Conditions

$$0 \stackrel{!}{=} X(x, y) := \begin{pmatrix} x - \text{prox}_{\sigma f}(x - \sigma A^\top y) \\ y - \text{prox}_{\tau g^*}(y + \tau Ax) \end{pmatrix}$$

Newton system

$$\begin{pmatrix} I - K & \sigma K A^\top \\ -\tau H A & I - H \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = -X(x, y)$$

where $K \in \partial_C \text{prox}_{\sigma f}(x - \sigma A^\top y)$, $H \in \partial_C \text{prox}_{\tau g^*}(y + \tau Ax)$.

- ▶ Lipschitz continuous, positive semidefinite at solution [Rust'17]
- ▶ Semismoothness not clear in general, but relatively straightforward to check
- ▶ Invertibility can be an issue – for TV, dual regularization helps [Diepeveen'20]
- ▶ Globalization not finally solved [XLWZ18]

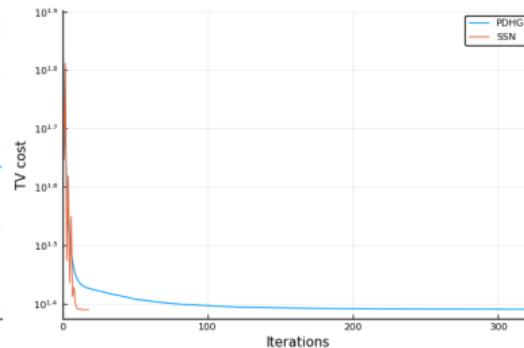
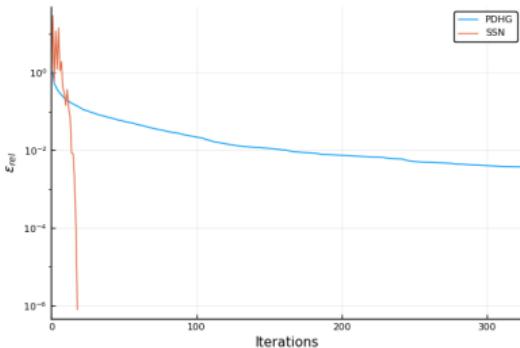
Euclidean Case ℓ^2 – TV Runtimes



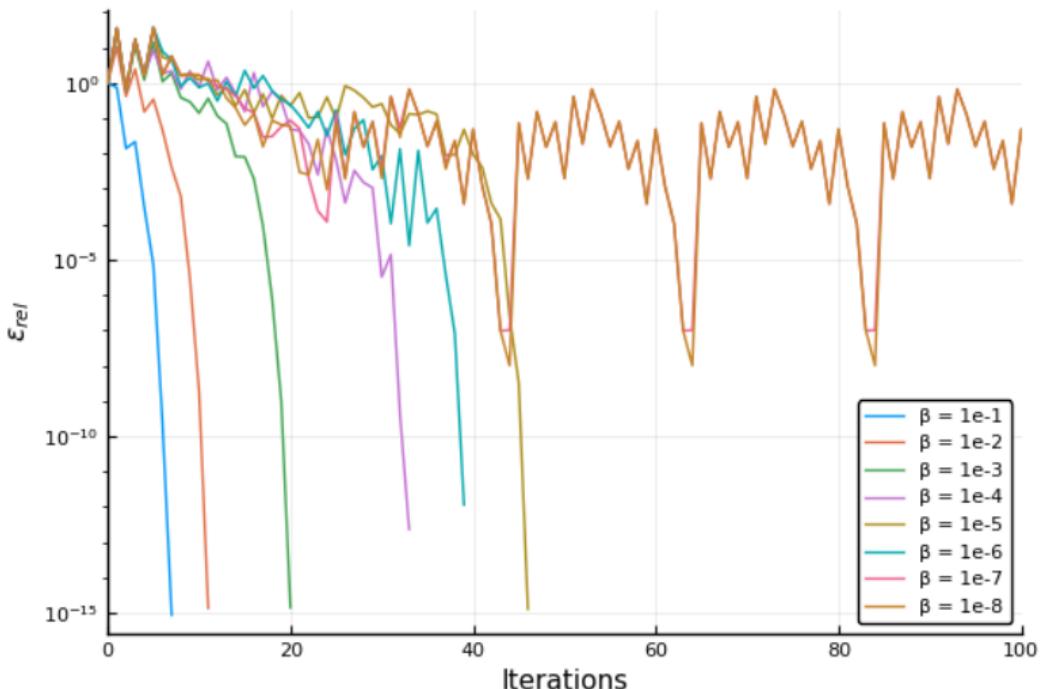
(a) Noisy image

(b) Result PDHG

(c) Result SSN



Dual regularization



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Semismooth Newton on Manifolds

Goal

Find $p \in \mathcal{M}$ that solves

$$X(p) = 0,$$

where X is a locally Lipschitz continuous **vector field** on \mathcal{M} .

Algorithm 2 Riemannian Semismooth Newton

Initialization: $p^0 \in \mathcal{M}$

for $k = 0, 1, \dots$ **do**

 Choose any $V(p^k) \in \partial_{\mathcal{M}, C} X(p^k)$

 Solve $V(p^k)d^k = -X(p^k)$ in the vector space $\mathcal{T}_{p^k}\mathcal{M}$

$p^{k+1} := \exp_{p^k}(d^k)$

end for

Convergence of Semismooth Newton on Manifolds for general X

Theorem (Oliveira, Ferreira'20)

Let X be a *locally Lipschitz continuous vector field* on \mathcal{M} and $p^* \in \mathcal{M}$ be a solution of problem

$$X(p) = 0,$$

Assume that X is *semismooth* at p^* and all $V_{p^*} \in \partial_{\mathcal{M},C} X(p^*)$ are invertible. Then, there exists a $\delta > 0$ such that for each $p^0 \in B_\delta(p^*) \setminus \{p^*\}$, $(p^k)_{k \geq 0}$ generated by RSSN is well-defined, belongs to $B_\delta(p^*)$ and *converges superlinearly* to p^* . Additionally, if X is μ -order semismooth at p^* , then the convergence of $(p^k)_{k \geq 0}$ to p^* is of order $1 + \mu$.

General formulation for vector field equations.

Semismooth Newton on Manifolds – Nonsmooth Case

Riemannian Semismooth Newton [Diepeveen'20]

$$\begin{aligned} p &= \text{prox}_{\sigma f} \left(\exp_p \left(\mathcal{P}_{m \rightarrow p} \left(-\sigma (D_m \Lambda)^* [\mathcal{P}_{n \rightarrow \Lambda(m)} \xi_n] \right)^\sharp \right) \right) \\ \xi_n &= \text{prox}_{\tau g_n^*} \left(\xi_n + \tau \left(\mathcal{P}_{\Lambda(m) \rightarrow n} D_m \Lambda [\log_m p] \right)^\flat \right) \end{aligned}$$

Semismooth Newton on Manifolds – Nonsmooth Case

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$$\begin{aligned} p &= \text{prox}_{\sigma f} \left(\exp_p \left(\mathcal{P}_{m \rightarrow p} \left(-\sigma (D_m \Lambda)^* [\mathcal{P}_{n \rightarrow \Lambda(m)} \xi_n] \right)^\sharp \right) \right) \\ \xi_n &= \text{prox}_{\tau g_n^*} \left(\xi_n + \tau \left(\mathcal{P}_{\Lambda(m) \rightarrow n} D_m \Lambda [\log_m p] \right)^\flat \right) \end{aligned}$$

Unfortunately not a vector field...

Semismooth Newton on Manifolds – Nonsmooth Case

Riemannian Semismooth Newton [Diepeveen'20]

$$\begin{aligned} 0 &= -\log_p \text{prox}_{\sigma f} \left(\exp_p \left(\mathcal{P}_{m \rightarrow p} \left(-\sigma (D_m \Lambda)^* [\mathcal{P}_{n \rightarrow \Lambda(m)} \xi_n] \right)^\sharp \right) \right) \\ 0 &= \xi_n - \text{prox}_{\tau g_n^*} \left(\xi_n + \tau (\mathcal{P}_{\Lambda(m) \rightarrow n} D_m \Lambda [\log_m p])^\flat \right) \end{aligned}$$

Semismooth Newton on Manifolds – Nonsmooth Case

Riemannian Semismooth Newton [Diepeveen'20]

$$0 = X(p, \xi_n) := \begin{pmatrix} -\log_p \text{prox}_{\sigma f} \left(\exp_p \left(\mathcal{P}_{m \rightarrow p} (-\sigma (D_m \Lambda)^* [\mathcal{P}_{n \rightarrow \Lambda(m)} \xi_n])^\sharp \right) \right) \\ \xi_n - \text{prox}_{\tau g_n^*} \left(\xi_n + \tau (\mathcal{P}_{\Lambda(m) \rightarrow n} D_m \Lambda [\log_m p])^\flat \right) \end{pmatrix}$$

- ▶ find zero of vector field $X : \mathcal{M} \times T_n^* \mathcal{M} \rightarrow T \mathcal{M} \times T_n^* \mathcal{M}$
- ▶ prox steps are still non-smooth

Implementation

- ▶ By W. Diepeveen'20, based on `manopt.jl`
- ▶ Chain rule for covariant derivative
- ▶ Jacobi fields for evaluating parts in chain rule/derivatives of $d_{\mathcal{M}}$, \log_p , \exp_p
- ▶ Pole ladder approximation for differentiating parallel transport, exact on symmetric manifolds

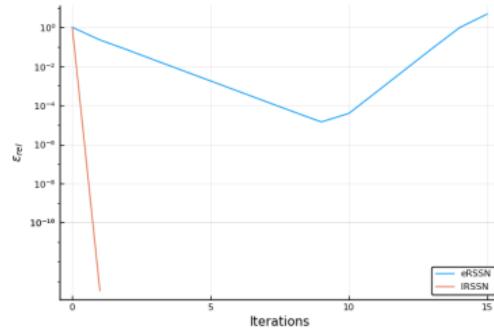
Case 1b: $\mathcal{P}(3)$ Signals with Known Minimizer



(a) Original

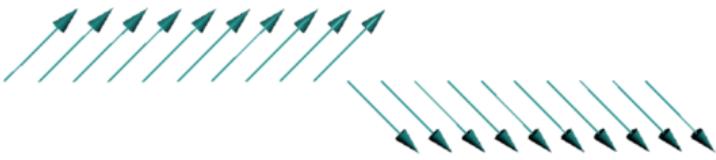


(b) RSSN solution



(c) Progression of relative error

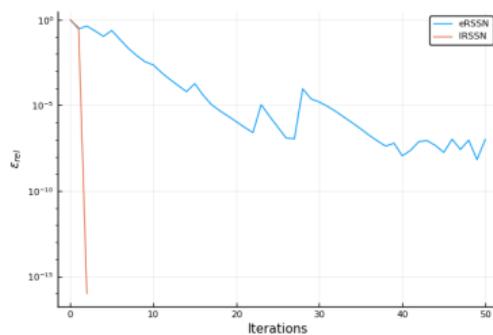
Case 1a: S^2 Signals with Known Minimizer



(a) Original

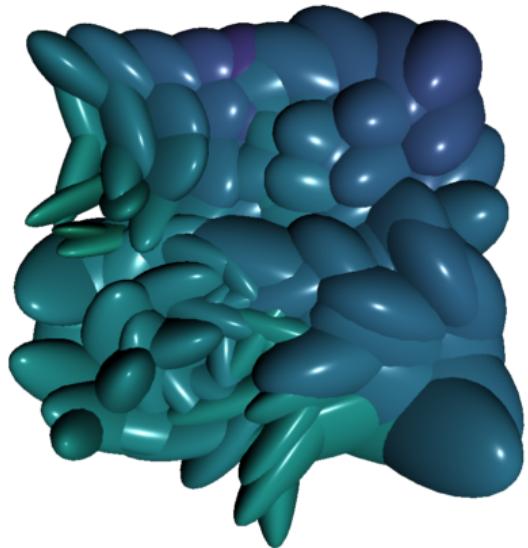


(b) RSSN solution

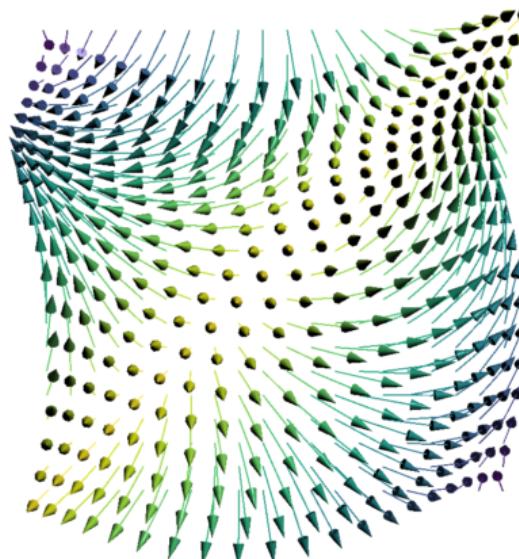


(c) Progression of relative error

Case 2: Manifold-valued Images

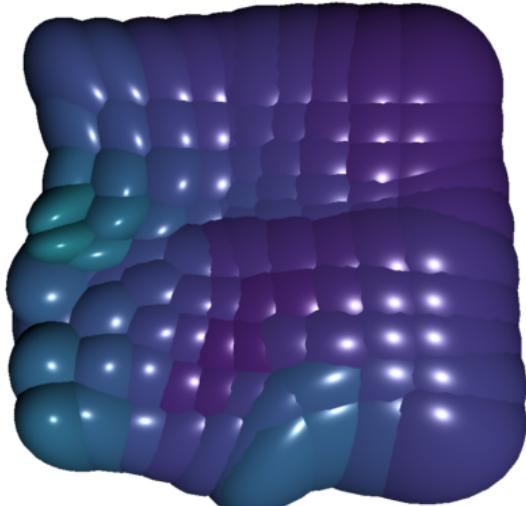


(a) Original $\mathcal{P}(3)$ data

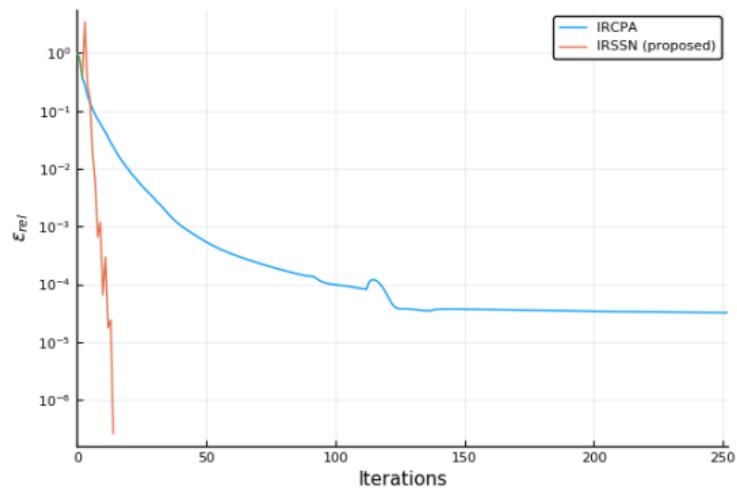


(b) Original S^2 data

Case 2a: $\mathcal{P}(3)$

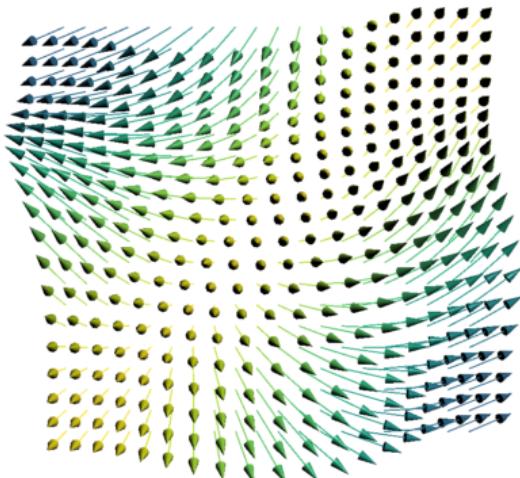


(a) Solution RSSN

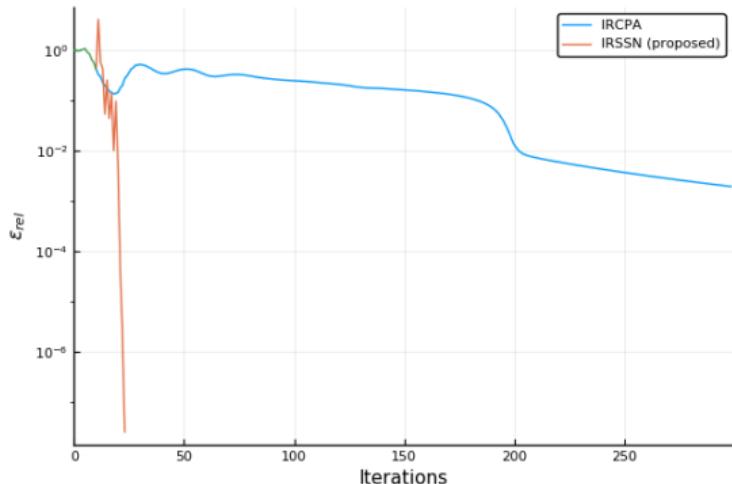


(b) Progression of relative error

Case 2b: S^2



(a) Solution RSSN



(b) Progression of relative error

Inexact Semismooth Newton on Manifolds

Algorithm 3 Inexact Semismooth Newton

Initialization: $p^0 \in \mathcal{M}$, $a^0 \geq 0$

for $k = 0, 1, \dots$ **do**

 Choose $V_k(p^k) \in \partial_{\mathcal{M}, C} X(p^k)$

 Solve $V_k(p^k)d^k = -X(p^k) + r^k$ in $T_{p^k}\mathcal{M}$ where $\|r^k\|_{(p^k)} \leq a^k \|X(p^k)\|_{(p^k)}$

$p^{k+1} := \exp_{p^k}(d^k)$

 Choose $a^{k+1} \geq 0$

end for

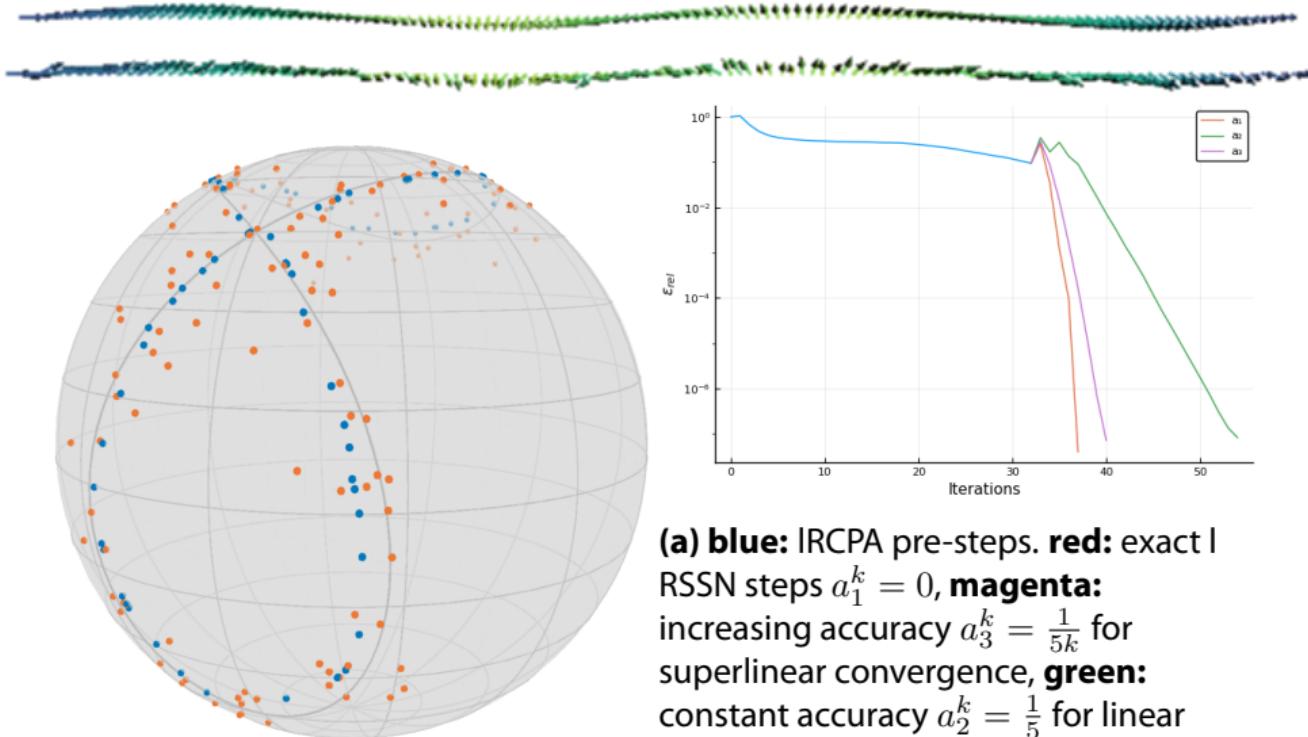
Convergence for Inexact RSSN

Theorem (Thesis [Diepeveen, L.'20])

Let X be locally Lipschitz continuous vector field on \mathcal{M} and $p^* \in \mathcal{M}$ be a solution of problem the $X(p) = 0$. Assume that X is semismooth at p^* and that all $V_{p^*} \in \partial_{\mathcal{M},C} X(p^*)$ are invertible. Then the following statements hold:

- (i) There exist $a > 0$ and $\delta > 0$ such that for every $p^0 \in B_\delta(p^*)$ and $a^k \leq a$, the sequence $(p^k)_{k \geq 0}$ generated by Alg. 3 is well-defined, is contained in $B_\delta(p^*)$ and converges Q-linearly to the solution p^* .
- (ii) If the sequence $(p^k)_{k \geq 0}$ generated by Alg. 3 converges to the solution p^* and further $\|r^k\|_{(p^k)} \in o\left(\|X(p^k)\|_{(p^k)}\right)$, then the rate of convergence is Q-superlinear.
- (iii) If the sequence $(p^k)_{k \geq 0}$ generated by Alg. 3 converges to the solution p^* , X is μ -order semismooth at p^* , and $\|r^k\|_{(p^k)} \in O\left(\|X(p^k)\|_{(p^k)}^{1+\mu}\right)$, then the rate of convergence is Q-order $1 + \mu$.

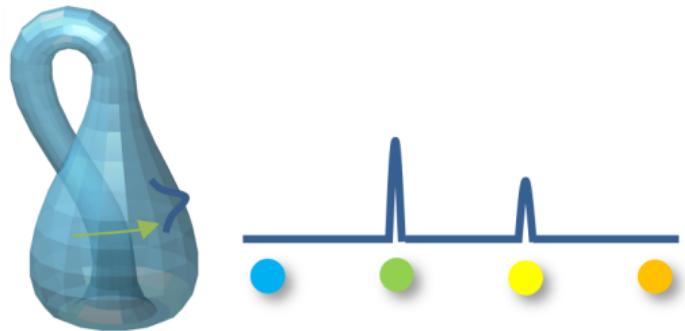
Lemniscate using Inexact RSSN



(a) blue: IRCPA pre-steps. **red:** exact RSSN steps $a_1^k = 0$, **magenta:** increasing accuracy $a_3^k = \frac{1}{5k}$ for superlinear convergence, **green:** constant accuracy $a_2^k = \frac{1}{5}$ for linear convergence.

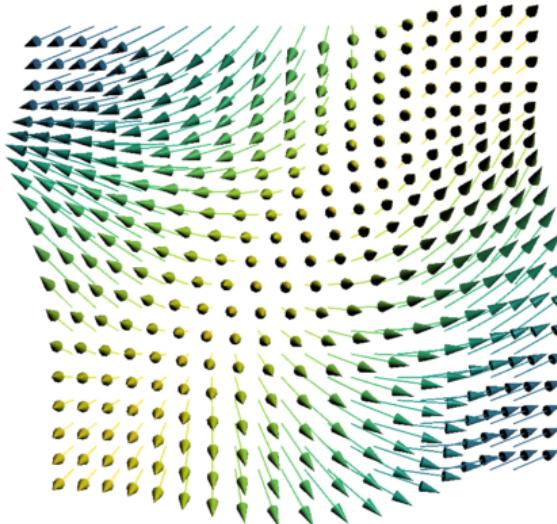
Lifting Approaches

- ▶ “Lift” problem to space of probability measures over \mathcal{M}
- ▶ Higher-dimensional but convex – global optimality possible
- ▶ Works on discrete spaces
- ▶ Also in \mathbb{R}^n to handle non-convexity
- ▶ Connections to dynamical optimal transport



Summary

- ▶ Non-smooth problem
 - prox-optimality system
 - Semismooth Newton
- ▶ Inexact Semismooth Newton with local convergence proof also for non-Hadamard case
- ▶ Implementation in `manopt.jl`
- ▶ Faster convergence confirmed in practice



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