NTNU

Norwegian University of Science and Technology

Nonsmooth Optimization on Riemannian Manifolds in Manopt.jl

Ronny Bergmann

Analysis and PDE Seminar, University of Bergen

Bergna, May 9, 2023

The Setting

Task. We aim to solve

$$\operatorname*{arg\,min}_{p \in \mathcal{M}} f(p)$$

where

- $\mathcal{M}$ is a Riemannian manifold
- $f\colon \mathcal{M} \to \mathbb{R}$ is nonsmooth and possibly high-dimensional

Roadmap.

1. Motivation
2. Algorithms
3. Numerical examples in `Manopt.jl`

Intuition: Embedded Manifolds

Consider $h\colon \mathbb{R}^n \to \mathbb{R}^k$, $1 \leq k \leq n$ as an equality constraint $h(p) = 0$.
If $\operatorname{rank} Dh(p) = k$ for all p with $h(p) = 0$, then

$$\mathcal{M} := \left\{ p \in \mathbb{R}^n \,\middle|\, h(p) = 0 \right\}$$

is a (smooth embedded sub-)manifold of $\mathbb{R}^n$ of dimension $m = n - k$,
cf. Definition 3.10. [Boumal 2023]

Example. The Sphere $\mathbb{S}^m \subset \mathbb{R}^n$ has $h(p) = \|p\| - 1 = 0$
$\Rightarrow$ We have $k = 1$ and $m = n - 1$.

Actually. It is enough to find such a function h locally around every p.

Intuition: Retractions – “Walking on Manifolds”

Interpretation. With $\operatorname{rank} Dh(p) = k$ we get $\dim\ker Dh(p) = m = n - k$
$\Rightarrow$ we have m “different directions”, where $Dh(p)[X] = 0$.

We call the set of these “directions” the Tangent space $T_p\mathcal{M}$.
The (disjoint) union of all tangent spaces is called the tangent bundle $T\mathcal{M}$.

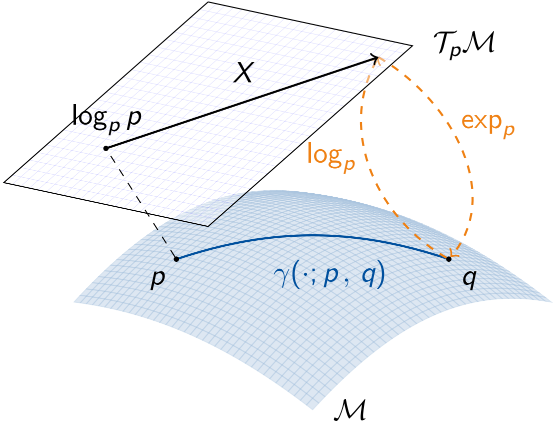
Goal. We would like to “walk” into these directions while staying on the manifold.

Definition. A function $R\colon T\mathcal{M} \to \mathcal{M}$, also denoted by $R_p\colon T_p\mathcal{M} \to \mathcal{M}$ for each $p \in \mathcal{M}$, is called a retraction
if each curve $c(t) = R_p(tX)$ satisfies $c(0) = p$ and $c'(0) = X$.

A Riemannian Manifold $\mathcal{M}$

A d-dimensional Riemannian manifold can be informally defined as a set $\mathcal{M}$ covered with a 'suitable' collection of charts, that identify subsets of $\mathcal{M}$ with open subsets of $\mathbb{R}^d$ and a continuously varying inner product on the tangent spaces.

[Absil, Mahony, and Sepulchre 2008]



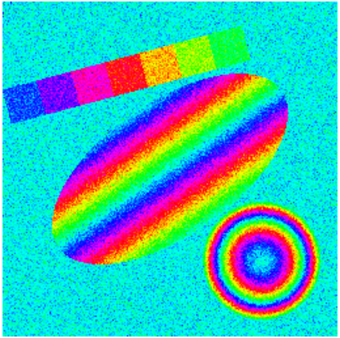
Notation.

- Logarithmic map $\log_p q = \dot\gamma(0; p, q)$
- Exponential map $\exp_p X = \gamma_{p,X}(1)$
- Geodesic $\gamma(\cdot; p, q)$
- Tangent space $\mathcal{T}_p\mathcal{M}$
- inner product $(\cdot, \cdot)_p$

Manifold-valued Signal & Image Processing

Tasks in image processing are often phrased as an optimisation problem.
Here. The pixel take values on a manifold

- phase-valued data ($\mathbb{S}^1$)
- wind-fields, GPS ($\mathbb{S}^2$)
- DT-MRI ($\mathcal{P}(3)$)
- EBSD, (grain) orientations ($\mathrm{SO}(n)$)



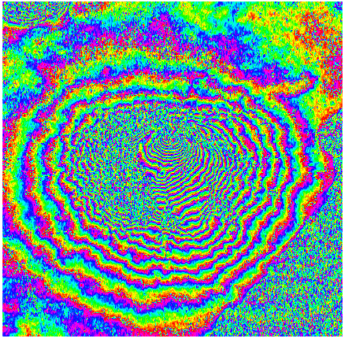
Artificial noisy phase-valued data.

Tasks. Denoising, Inpainting, labeling (classification), deblurring,...

Manifold-valued Signal & Image Processing

Tasks in image processing are often phrased as an optimisation problem.
Here. The pixel take values on a manifold

- phase-valued data ($\mathbb{S}^1$)
- wind-fields, GPS ($\mathbb{S}^2$)
- DT-MRI ($\mathcal{P}(3)$)
- EBSD, (grain) orientations ($\mathrm{SO}(n)$)



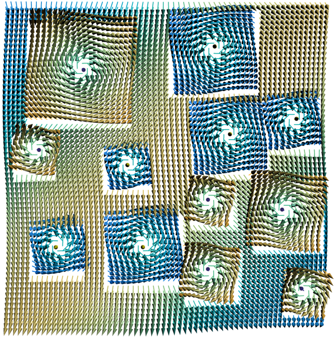
InSAR-Data of Mt. Vesuvius.
[Rocca, Prati, and Guarnieri 1997]

Tasks. Denoising, Inpainting, labeling (classification), deblurring,...

Manifold-valued Signal & Image Processing

Tasks in image processing are often phrased as an optimisation problem.
Here. The pixel take values on a manifold

- phase-valued data ($\mathbb{S}^1$)
- wind-fields, GPS ($\mathbb{S}^2$)
- DT-MRI ($\mathcal{P}(3)$)
- EBSD, (grain) orientations ($\mathrm{SO}(n)$)



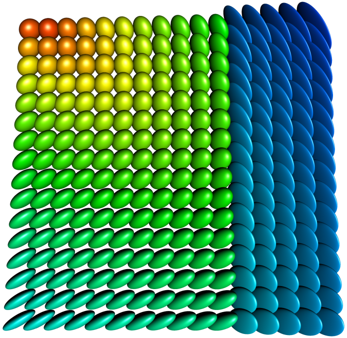
Artificial noisy data on the sphere $\mathbb{S}^2$.

Tasks. Denoising, Inpainting, labeling (classification), deblurring,...

Manifold-valued Signal & Image Processing

Tasks in image processing are often phrased as an optimisation problem.
Here. The pixel take values on a manifold

- phase-valued data ($\mathbb{S}^1$)
- wind-fields, GPS ($\mathbb{S}^2$)
- DT-MRI ($\mathcal{P}(3)$)
- EBSD, (grain) orientations ($\mathrm{SO}(n)$)



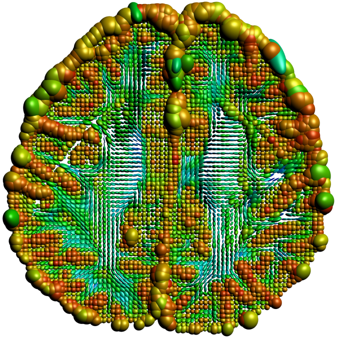
Artificial diffusion data,
each pixel is a symmetric positive matrix.

Tasks. Denoising, Inpainting, labeling (classification), deblurring,...

Manifold-valued Signal & Image Processing

Tasks in image processing are often phrased as an optimisation problem.
Here. The pixel take values on a manifold

- phase-valued data ($\mathbb{S}^1$)
- wind-fields, GPS ($\mathbb{S}^2$)
- DT-MRI ($\mathcal{P}(3)$)
- EBSD, (grain) orientations ($\mathrm{SO}(n)$)



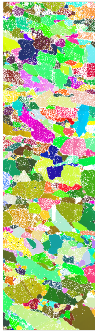
DT-MRI of the human brain.
Camino Profject: cmic.cs.ucl.ac.uk/camino

Tasks. Denoising, Inpainting, labeling (classification), deblurring,...

Manifold-valued Signal & Image Processing

Tasks in image processing are often phrased as an optimisation problem.
Here. The pixel take values on a manifold

- phase-valued data ($\mathbb{S}^1$)
- wind-fields, GPS ($\mathbb{S}^2$)
- DT-MRI ($\mathcal{P}(3)$)
- EBSD, (grain) orientations ($\mathrm{SO}(n)$)



Grain orientations in EBSD data.
MTEX toolbox: mtex-toolbox.github.io

Tasks. Denoising, Inpainting, labeling (classification), deblurring,...

Why Manifolds?

- A constrained problem on $\mathbb{R}^n \Rightarrow$ an unconstrained problem on $\mathcal{M}$
- The “type of convexity” changes: Convexity is defined along geodesics γ
- If we can omit “working” in the embedding $\Rightarrow$ dimension reduction

! we need efficient ways to compute e. g. retractions.

The Smooth Case & Gradient Descent

For a smooth function $f\colon \mathcal{M} \to \mathbb{R}$ we have

- The differential $Df\colon T\mathcal{M} \to \mathbb{R}$, or phrased differently $Df(p)\colon T_p\mathcal{M} \to \mathbb{R}$
- the gradient $\operatorname{grad} f(p) \in T_p\mathcal{M}$ is the Riesz representer defined by the property

$$Df(p)[X] = (\operatorname{grad} f(p)\,,\, X)_p, \qquad \text{for all } X \in T_p\mathcal{M}$$

$\Rightarrow$ Like in $\mathbb{R}^n$: $Y = -\operatorname{grad} f(p)$ is the direction of steepest descent.

Algorithm. Gradient descent.
Given f and a retraction R we perform

$$p_{k+1} = R_{p_k}(-s_k \operatorname{grad} f(p))$$

for some step size(s) s_k – e. g. an Armijo backtracking line-search, cf. Ch. 4.1
[Absil, Mahony, and Sepulchre 2008]

Proximal Map

For $f\colon \mathcal{M} \to \overline{\mathbb{R}}$ and $\lambda > 0$ we define the Proximal Map as
[Moreau 1965; Rockafellar 1970; Ferreira and Oliveira 2002]

$$\operatorname{prox}_{\lambda f}(p) := \operatorname*{arg\,min}_{u \in \mathcal{M}} d_{\mathcal{M}}(u,p)^2 + \lambda f(u).$$

! For a minimizer u^* of f we have $\operatorname{prox}_{\lambda f}(u^*) = u^*$.

- For f proper, convex, lsc:
  - the proximal map is unique.
  - Proximal-Point-Algorithm:
    $p_k = \operatorname{prox}_{\lambda f}(p_{k-1})$ converges to $\operatorname{arg\,min} f$

The Cyclic Proximal Point Algorithm

NTNU

If we can split our nonsmooth $f(p) = \sum_{i=1}^{c} g_i(p)$, we can use the Cyclic Proximal Point-Algorithmus (CPPA): [Bertsekas 2011; Bačák 2014]

$$p_{k+\frac{i+1}{c}} = \operatorname{prox}_{\lambda_k g_i}(p_{k+\frac{i}{c}}), \quad i = 0, \ldots, c-1, \ k = 0, 1, \ldots$$

On a Hadamard manifold $\mathcal{M}$:
convergence to a minimizer of f if

- all g_i proper, convex, lower semi-continuous
- $\{\lambda_k\}_{k\in\mathbb{N}} \in \ell_2(\mathbb{N})\backslash\ell_1(\mathbb{N})$.

! no convergence rate

The Exact Riemannian Chambolle–Pock Algorithm

[RB, Herzog, Silva Louzeiro, Tenbrinck, and Vidal-Núñez 2021; Chambolle and Pock 2011]

Assume. $f(p) = F(p) + G(\Lambda(p))$, with $\Lambda\colon \mathcal{M} \to \mathcal{N}$.

Input: m, $p^{(0)} \in \mathcal{C} \subset \mathcal{M}$, $n = \Lambda(m)$, $\xi_n^{(0)} \in \mathcal{T}_n^*\mathcal{N}$, and parameters σ, τ, $\theta > 0$

1: $k \leftarrow 0$

2: $\bar{p}^{(0)} \leftarrow p^{(0)}$

3: **while** not converged **do**

4: $\quad\xi_n^{(k+1)} \leftarrow \operatorname{prox}_{\tau G_n^*}\Bigl(\xi_n^{(k)} + \tau\bigl(\log_n \Lambda(\bar{p}^{(k)})\bigr)^\flat\Bigr)$

5: $\quad p^{(k+1)} \leftarrow \operatorname{prox}_{\sigma F}\Bigl(\exp_{p^{(k)}}\Bigl(\mathrm{P}_{p^{(k)}\leftarrow m}\bigl(-\sigma D\Lambda(m)^*[\xi_n^{(k+1)}]\bigr)^\sharp\Bigr)\Bigr)$

6: $\quad\bar{p}^{(k+1)} \leftarrow \exp_{p^{(k+1)}}\bigl(-\theta \log_{p^{(k+1)}} p^{(k)}\bigr)$

7: $\quad k \leftarrow k + 1$

8: **end while**

Output: $p^{(k)}$

Beyond Nonsmooth I: Constrained Optimisation

One can consider problems like

[Liu and Boumal 2019; RB and Herzog 2019]

$$\begin{aligned} &\operatorname*{arg\,min}_{p\in\mathcal{M}} f(p) \\ &\text{subject to } g_i(p) \leq 0, \quad i = 1,\ldots,m \\ &\phantom{\text{subject to }} h_j(p) = 0, \quad j = 1,\ldots,p \end{aligned}$$

where $g_i, h_j \colon \mathcal{M} \to \mathbb{R}$ describe constraints to p.

$\Rightarrow$ Classical algorithms (ALM, EPM) adapted

We can choose our own trade-off between geometry and constraint.

Beyond Nonsmooth II: Difference of Convex

One can consider problems like

[RB, Ferreira, Santos, and J. C. O. Souza 2023; J. C. d. O. Souza and Oliveira 2015]

$$\operatorname*{arg\,min}_{p\in\mathcal{M}} f(p), \qquad f(p) = g(p) - h(p)$$

where $g, h\colon \mathcal{M} \to \mathbb{R}$ are geodesically convex.

$\Rightarrow$ Far more flexible – especially new feature: geodesic convexity

Still efficient algorithms available for this broad class, basede on ∂h and either $\operatorname{prox}_{\lambda g}$ or $\operatorname{grad} g$.

Implementing Manifolds & Optimisation – in Julia.

Goals.

- abstract definition of manifolds and properties thereon
  e. g. different metrics, retractions, embeddings
- $\Rightarrow$ implement abstract algorithms for generic manifolds
- easy to implement own manifolds & easy to use
- well-documented and well-tested
- fast.

Why Julia?

- high-level language, properly typed
- multiple dispatch (cf. `f(x)`, `f(x::Number)`, `f(x::Int)`)
- just-in-time compilation, solves two-language problem
- I like the language – and the community.

Implementing a Riemannian Manifold

`ManifoldsBase.jl` uses a `AbstractManifold{𝔽}` with type parameter $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}, \mathbb{H}\}$ to provide an interface for implementing functions like

- `inner(M, p, X, Y)` for the Riemannian metric $(X, Y)_p$
- `exp(M, p, X)` and `log(M, p, q)`,
- more general: `retract(M, p, X, m)`, where `m` is a retraction method
- similarly: `parallel_transport(M, p, X, q)` and `vector_transport_to(M, p, X, q, m)`

for your manifold `M` a subtype of the abstract manifold `Manifold{𝔽}`.

☺ mutating version `exp!(M, q, p, X)` works in place in `q`

➜ basis for generic algorithms working on any `Manifold` and generic functions like `norm(M,p,X)`, `geodesic(M, p, X)` and `shortest_geodesic(M, p, q)`

🔗 juliamanifolds.github.io/ManifoldsBase.jl/

Manifolds.jl – A Library of Manifolds in Julia

`Manifolds.jl` is build upon `ManifoldsBase.jl` interface. [Axen, Baran, RB, and Rzecki 2021]

Features.

- different metrics
- Lie groups
- Build manifolds using
  - Product manifold $\mathcal{M}_1 \times \mathcal{M}_2$
  - Power manifold $\mathcal{M}^{n \times m}$
  - Tangent bundle
- Quotient manifolds
- Embedded manifolds
- perform statistics
- well-documented, including formulae and references
- well-tested, $>98\,\%$ code cov.

Manifolds. For example

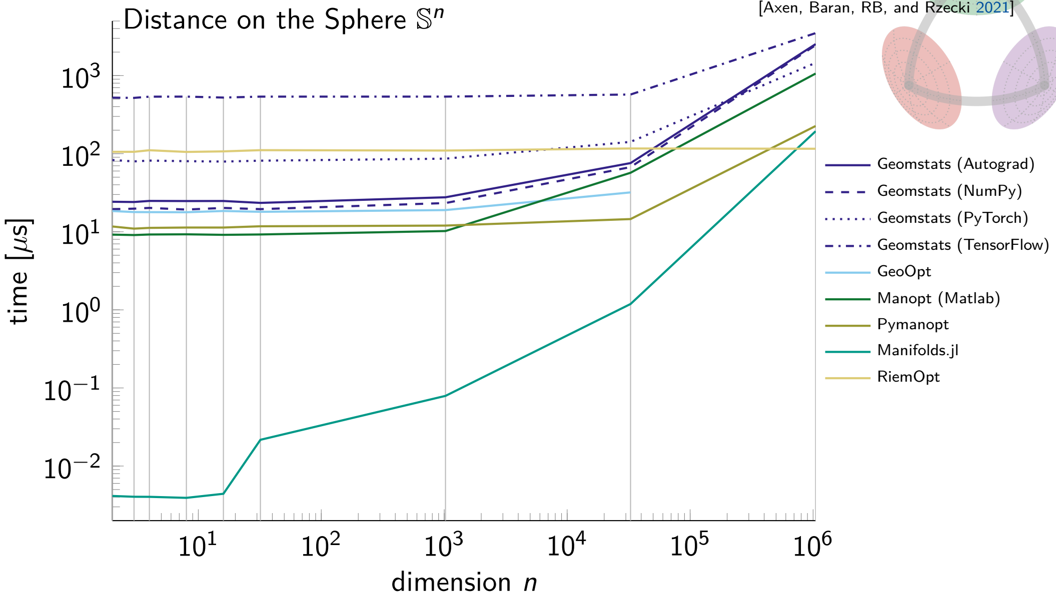
- (unit) Sphere, Circle & Torus
- Fixed Rank Matrices
- (Generalized) Stiefel & Grassmann
- Hyperbolic space
- Rotations, $\mathrm{O}(n)$, $\mathrm{SO}(n)$, $\mathrm{SU}(n)$
- several further Lie groups
- Symmetric positive definite matrices
- Symplectic & Symplectic Stiefel
- Kendall's shape space
- …

juliamanifolds.github.io/Manifolds.jl/

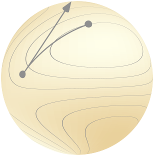
JuliaCon 2020 youtu.be/md-FnDGCh9M

Manifolds.jl – An Example comparison in speed

[Axen, Baran, RB, and Rzecki 2021]



Manopt.jl: Optimisation on Manifolds in Julia



Goal. Optimisation algorithms on Riemannian manifolds, based on `ManifoldsBase.jl` $\Rightarrow$ works with any manifold from `Manifolds.jl`.

Features.

- generic algorithm framework:
  With `Problem p` and a `SolverState s`
  - `initialize_solver!(p, s)`
  - `step_solver!(p, s, i)`: ith step
- run algorithm: call `solve(p, s)`
- generic debug and recording
- step sizes and stopping criteria.

Manopt Family.

- manoptjl.org [RB 2022]
- manopt.org [Boumal, Mishra, Absil, and Sepulchre 2014]
- pymanopt.org [Townsend, Koep, and Weichwald 2016]

Algoirthms.

- Nelder-Mead, Particle Swarm
- Subgradient Method
- Gradient Descent
  CG, Stochastic, Momentum, ...
- Quasi-Newton
  BFGS, DFP, Broyden, SR1, ...
- Trust Regions
- Chambolle-Pock
- Douglas-Rachford, CPPA
- ALM, EPM, Frank-Wolfe,...
- Difference of Convex
  DCA, DCPPA

Software packages – An Overview

We[1] founded the `JuliaManifolds`, GitHub Community for manifold related packages in Julia

Currently our main packages are (ordered by age)

Manopt.jl Optimisation on Riemannian manifolds, based on `ManifoldsBase.jl` [RB 2022]

Manifolds.jl A library of Riemannian manifolds and Lie groups [Axen, Baran, RB, and Rzecki 2021]

ManifoldsBase.jl A lightweight interface to implement and work on manifolds

ManifoldDiff.jl (automatic) differentiation on Riemannian manifolds and a function library of differentials, gradients,...

ManifoldDiffEq.jl differential equations on Riemannian manifolds Combining the interfaces `ManifoldsBase.jl` and `OrdinaryDiffEq.jl`

ManoptExamples.jl A collection of examples and benchmarks for `Manopt.jl`

[1] Seth Axen, U Tübingen; Mateusz Baran, AGH Krakow; RB, NTNU

NTNU

Selected References

- Axen, S. D., M. Baran, RB, and K. Rzecki (2021). *Manifolds.jl: An Extensible Julia Framework for Data Analysis on Manifolds*. arXiv: 2106.08777.
- Bačák, M. (2014). "Computing medians and means in Hadamard spaces". In: *SIAM Journal on Optimization* 24.3, pp. 1542–1566. DOI: 10.1137/140953393.
- RB (2022). "Manopt.jl: Optimization on Manifolds in Julia". In: *Journal of Open Source Software* 7.70, p. 3866. DOI: 10.21105/joss.03866.
- RB, R. Herzog, M. Silva Louzeiro, D. Tenbrinck, and J. Vidal-Núñez (Jan. 2021). "Fenchel duality theory and a primal-dual algorithm on Riemannian manifolds". In: *Foundations of Computational Mathematics*. DOI: 10.1007/s10208-020-09486-5. arXiv: 1908.02022.
- Boumal, N., B. Mishra, P.-A. Absil, and R. Sepulchre (2014). "Manopt, a Matlab toolbox for optimization on manifolds". In: *The Journal of Machine Learning Research* 15, pp. 1455–1459. URL: https://www.jmlr.org/papers/v15/boumal14a.html.
- Chambolle, A. and T. Pock (2011). "A first-order primal-dual algorithm for convex problems with applications to imaging". In: *Journal of Mathematical Imaging and Vision* 40.1, pp. 120–145. DOI: 10.1007/s10851-010-0251-1.
- Townsend, J., N. Koep, and S. Weichwald (2016). "Pymanopt: A Python Toolbox for Optimization on Manifolds using Automatic Differentiation". In: *Journal of Machine Learning Research* 17.137, pp. 1–5. URL: http://jmlr.org/papers/v17/16-177.html.

ronnybergmann.net/talks/2023-Bergen-Nonsmooth-Optim.pdf

NTNU