

Manopt.jl

Optimization on Riemannian Manifolds

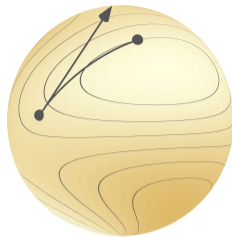
Ronny Bergmann

 @ronnybergmann_

Norwegian University of Science and Technology, Trondheim, Norway.

Lightning Talk

JuliaCon 2022, online and everywhere



Optimization

(Constrained) Optimization aims to find for a function $f: \mathbb{R}^m \rightarrow \mathbb{R}$ a point

$$\arg \min_{x \in \mathbb{R}^m} f(x)$$

Challenges:

- ▶ constrained to some $\mathcal{C} \subset \mathbb{R}^m$, e. g. unit vectors
- ▶ symmetries / invariances

Geometric Optimization aims to find

$$\arg \min_{p \in \mathcal{M}} F(p)$$

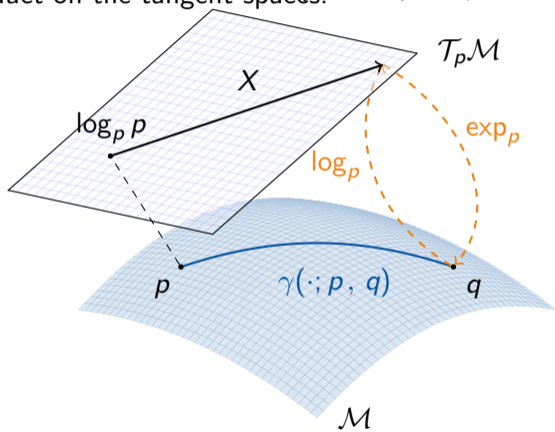
where F is defined on a Riemannian manifold \mathcal{M} , e. g. the sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$.
 \Rightarrow the problem is unconstrained (again).

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 $(\cdot, \cdot)_p$



ManifoldsBase.jl & Manifolds.jl

`ManifoldsBase.jl` is an interface for Riemannian manifolds M

- ▶ `inner(M, p, X, Y)` $(X, Y)_p$
- ▶ `exp(M, p, X)` and `log(M, p, q)`,
- ▶ more general:
`retract(M, p, X, m)`,
where `m` is a retraction method
- ▶ embeddings as decorator
- 😊 mutating variants, e. g.
`exp!(M, q, p, X)`
works in place of `q`

 [juliamanifolds.github.io/ManifoldsBase.jl/](https://github.com/JuliaManifolds/ManifoldsBase.jl)
 [juliamanifolds.github.io/Manifolds.jl/](https://github.com/JuliaManifolds/Manifolds.jl/)

`Manifolds.jl` is a Library of manifolds

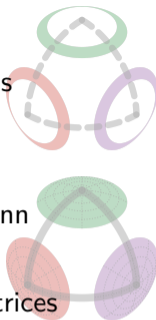
- ▶ Circle, (unit) Sphere & Torus
- ▶ Fixed Rank Matrices
- ▶ (Symplectic) Stiefel & Grassmann
- ▶ Hyperbolic space & Rotations
- ▶ Symmetric positive definite matrices
- ▶ ...and many more

as well as generically

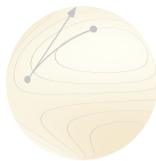
- ▶ power & product manifold
- ▶ tangent & vector bundles
- ▶ Lie groups, connections, metrics,...

[Axen, Baran, RB, and Rzecki 2021]

 JuliaCon 2020 youtu.be/md-FnDGCh9M



Manopt.jl – Structure



Manopt.jl depends **only** on `ManifoldsBase.jl` and consists of

- ▶ a `Problem P` to specify **static properties**:
the manifold \mathcal{M} , the cost F , its (Riemannian) gradient $\text{grad } F$, ...
 - ▶ some `Options O` to specify a solver and containing **dynamic data**:
the current iterate, the current gradient, a stopping criterion, ...
 - ▶ **implement**
 1. `initialize_solver!(P, O)` to initialise a solver run
 2. `step_solver!(P, O, i)` to perform the i th step
- ⇒ call `solve(P,O)` to run the solver **or** use a high-level interface

Furthermore one can

- ▶ specify a `Stepsize s`, that is for example a `LineSearch l`
- ▶ include a `StoppingCriterion sc`, a functor `sc(P, O, i)` returning true/false
- 😊 `sc1 | sc2` and `sc1 & sc2` to build more advanced criteria
- ▶ `DebugOptions` and `RecordOptions` decorate `Options` with print/record

Manopt.jl – Available Solvers

Currently the following solvers are available

- ▶ Gradient Descent
CG, Stochastic, Momentum, Alternating, Average, Nesterov, ...
- ▶ Quasi-Newton
(L-)BFGS, DFP, Broyden, SR1, ...
- ▶ Nelder-Mead, Particle Swarm
- ▶ Subgradient Method
- ▶ Trust Regions
- ▶ Chambolle-Pock (PDHG)
- ▶ Douglas-Rachford
- ▶ Cyclic Proximal Point

The Manopt Family.

 manoptjl.org [RB 2022]

 manopt.org
[Boumal, Mishra, Absil, and Sepulchre 2014]

 pymanopt.org
[Townsend, Koep, and Weichwald 2016]

Example – A Riemannian Center of Mass

The mean of N data points $x_1, \dots, x_N \in \mathbb{R}^n$ is

$$x^* = \frac{1}{N} \sum_{i=1}^N x_i \Leftrightarrow x^* = \arg \min_{x \in \mathbb{R}^m} \frac{1}{2N} \sum_{i=1}^N \|x - x_i\|_2^2$$

\Rightarrow the minimizer of sum of squared distances

For $p_1, \dots, p_N \in \mathcal{M}$:

Riemannian center(s) of mass are

[Karcher 1977]





$$\arg \min_{p \in \mathcal{M}} \frac{1}{2N} \sum_{i=1}^N d_{\mathcal{M}}^2(p, p_i),$$

- ▶ (in general) neither closed form nor unique
- ▶ For $F(p) = \frac{1}{2} d_{\mathcal{M}}^2(p, p_i)$
we have $\text{grad } F(p) = -\log_p p_i$

\Rightarrow use gradient descent

```
using LinearAlgebra
using Manopt, Manifolds
M = Sphere(2)
N = 100
pts = [randn(3) for _ in 1:N]
pts ./= norm.(pts)
F(M, p) = sum(
    pi -> distance(M, pi, p)^2/2N,
    pts,
)
gF(M, p) = sum(
    pi -> grad_distance(M, pi, p)/N,
    pts,
)
# compute a center of mass
# in place of m
m = copy(M, pts[1])
gradient_descent!(M, F, gF, m)
```

References

-  Absil, P.-A., R. Mahony, and R. Sepulchre (2008). *Optimization Algorithms on Matrix Manifolds*. Princeton University Press. DOI: [10.1515/9781400830244](https://doi.org/10.1515/9781400830244).
-  Axen, S. D., M. Baran, RB, and K. Rzecki (2021). *Manifolds.jl: An Extensible Julia Framework for Data Analysis on Manifolds*. arXiv: [2106.08777](https://arxiv.org/abs/2106.08777).
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-  Karcher, H. (1977). “Riemannian center of mass and mollifier smoothing”. In: *Communications on Pure and Applied Mathematics* 30.5, pp. 509–541. DOI: [10.1002/cpa.3160300502](https://doi.org/10.1002/cpa.3160300502).
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 ronnybergmann.net/talks/2022-JuliaCon-Manoptjl.pdf