

Manopt.jl

Numerical Optimization on Riemannian Manifolds in Julia

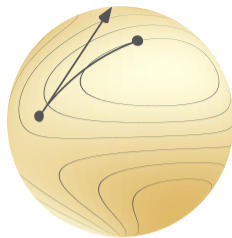
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Software for Optimization on Manifolds

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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}

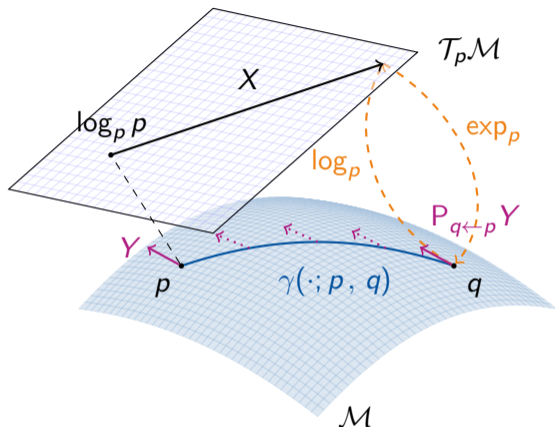
A d -dimensional Riemannian manifold can be informally defined as a set \mathcal{M} covered with a 'suitable' collection of charts, that identify subsets of \mathcal{M} with open subsets of \mathbb{R}^d and a continuously varying inner product on the tangent spaces.

[Absil, Mahony, and Sepulchre 2008]

A d -dimensional Riemannian manifold \mathcal{M}

Notation.

- ▶ Geodesic $\gamma(\cdot; p, q)$
- ▶ Tangent space $\mathcal{T}_p\mathcal{M}$
- ▶ inner product $(\cdot, \cdot)_p$
- ▶ Logarithmic map $\log_p q = \dot{\gamma}(0; p, q)$
- ▶ Exponential map $\exp_p X = \gamma_{p,X}(1)$
where $\gamma_{p,X}(0) = p$ and $\dot{\gamma}_{p,X}(0) = X$
- ▶ Parallel transport $P_{q \leftarrow p} Y$ “move”
tangent vectors from $\mathcal{T}_p\mathcal{M}$ to $\mathcal{T}_q\mathcal{M}$



Example I: The Sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$

The set of unit vectors or the **Sphere**

$$\mathbb{S}^d := \{p \in \mathbb{R}^{d+1} \mid \|p\|_2 = 1\}$$

is a Riemannian manifold. A tangent space is of the form

$$T_p \mathbb{S}^d := \{X \in \mathbb{R}^{d+1} \mid \langle X, p \rangle = 0\}$$

The exponential map is given by “following great arcs” from p in direction X we get

$$\exp_p X = \cos(\|X\|_2)p + \sin(\|X\|_2) \frac{X}{\|X\|_2},$$

But the inverse $\log_p q$ is only locally defined, for example if $p = -q$ are opposite points, there are infinitely many tangent vectors such that $\exp_p X = q$.

Example II: Stiefel & Grassmann

The **Stiefel** manifold consists of all orthonormal bases (ONB) for k -dimensional subspaces of \mathbb{R}^n

$$\text{St}(n, k) := \{p \in \mathbb{R}^{n \times k} \mid p^T p = I_k\},$$

If we are only interested in the **subspace**, we obtain the **Grassmann** manifold

$$\text{Gr}(n, k) := \{\text{span}(p) \mid p \in \mathbb{R}^{n \times k}, p^T p = I_k\},$$

\Rightarrow All ONBs $p \in \text{St}(n, k)$ of one subspace are the same point $q \in \text{Gr}(n, k)$.
Formally we obtain sets of equivalence classes or a quotient structure

$$\text{Gr}(n, k) = \text{St}(n, k) / O(k),$$

Implementing a Riemannian manifold



`ManifoldsBase.jl` introduces a manifold type with its field $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}, \mathbb{H}\}$ as parameter 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, which is a `subtype` of `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/](https://github.com/juliamanifolds/ManifoldsBase.jl)

Manifolds.jl – A library of manifolds in Julia

Manifolds.jl is based on the 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
- ▶ Embedded manifolds
- ▶ perform statistics
- ▶ well-documented, including formulae and references
- ▶ well-tested, >98% code cov.

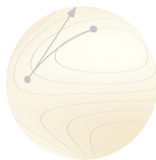
Manifolds. For example

- ▶ (unit) Sphere
- ▶ Circle & Torus
- ▶ Fixed Rank Matrices
- ▶ (Generalized) Stiefel & Grassmann
- ▶ Hyperbolic space
- ▶ Rotations, $O(n)$, $SO(n)$, $SU(n)$
- ▶ Symmetric positive definite matrices
- ▶ Symplectic & Symplectic Stiefel
- ▶ ...

[juliamanifolds.github.io/Manifolds.jl/](https://github.com/axen/manifolds.jl)

[JuliaCon 2020 youtu.be/md-FnDGCh9M](https://www.youtube.com/watch?v=md-FnDGCh9M)

Manopt.jl – Internal Structure



Manopt.jl is implemented depending **only** on `ManifoldsBase.jl`.

A **solver** for an **optimization problem** consists of three ingredients

- ▶ a `Problem P` that specifies **static** properties
 - ▶ the manifold \mathcal{M}
 - ▶ a cost function $F: \mathcal{M} \rightarrow \mathbb{R}$
 - ▶ (maybe) a gradient $\text{grad } F: \mathcal{M} \rightarrow T\mathcal{M}$
 - ▶ (maybe) a Hessian $\text{Hess } F$
 - ▶ ...
- ▶ some `Options O` containing **dynamic** data
 - ▶ the current iterate p_i
 - ▶ a `StoppingCriterion`
 - ▶ any parameter required during an iteration
- ▶ implementation of
 1. `initialize_solver!(P, O)` to initialise a solver run
 2. `step_solver!(P, O, i)` to perform the i th step

Running a solver & high level Interfaces

Running a solver consists of

1. generating a `Problem P`
2. generating some `Options O`
3. calling `solve(P,O)`

These steps are usually provided by a high level interface.

Example. For a gradient descent algorithm on a Riemannian manifold one can use

```
gradient_descent(M, F, gradF, p0)
```

which performs

1. create
 - ▶ `PG = GradientProblem(M, F, gradF)`
 - ▶ `OG = GradientOptions(p0, gradF(M, p0))`
2. runs the algorithm by calling `solve(PG,OG)`
3. returns the resulting last iterate (calling `get_solver_result(OG)`)

Stopping criteria

The `Options` usually include a `StoppingCriterion sc`. This is accessed via `stop_solver!(P,0,i)` at every iteration `i`

A `StoppingCriterion sc` should

- ▶ be a functor `sc(P,0,i)` returning `true/false`
- ▶ implement `get_reason(sc)` returning a string with the reason when `true` was returned
- 😊 Combine stopping criteria using `sc1 | sc2` or `sc1 & sc2`

Examples.

- ▶ `StopAfterIteration(N)` - stop after `N` iterations.
- ▶ `StopAfterIteration(N) | StopWhenGradientLess(1e-8)`
... or when the gradient is small

Within a step: Stepsize & Line search

In many algorithms, after determining a `direction` “to walk into”, e. g.

$$X = -\text{grad } F(p)$$

there is a `Stepsize` `s` left to determine, which is modelled (again) as a functor `sk = s(p,o,i)`. It can be e. g.

- ▶ a `ConstantStepsize(c)`
- ▶ an `ArmijoLineSearch(M)`
- ▶ a `NonmonotoneLineSearch(M)`

Options `O` often contain a `AbstractRetractionMethod` in `O.retraction_method`
⇒ line search along the curve given by

```
t -> retract(P.M, O.x, t * X, O.retraction_method)
```

Printing debug output & Record values

Every solver has a `debug=` keyword using `DebugActions`, Strings and Symbols, e. g.

```
debug=[:Iteration, DebugCost(), (:Change, "change: %1.9f\n"), :Stop]
```

prints

- ▶ the iteration number and the cost $F(p_k)$ (in default format, also `:Cost`),
- ▶ the change $d_{\mathcal{M}}(p_{k-1}, p_k)$ in a specific format (and a line break)
- ▶ the reason the algorithm stopped at the end

The same with the keyword `record=` to record values, for example

```
record=[:Iteration, :Cost, :Iterate]
```

and set `return_options=true`

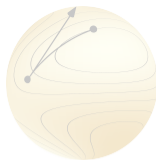
⇒ final state (options `fin0`) are returned.

⇒ use `get_record(fin0)` to get a vector of `(i, cost, point)` tuples

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)
- ▶ Inexact Semismooth Newton Method
- ▶ 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 Problem: The 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 $F(p) = \frac{1}{2} d_{\mathcal{M}}^2(p, p_i)$ the gradient is given by $\text{grad } F(p) = -\log_p p_i$
- \Rightarrow use gradient descent

Example Codes: The Riemannian center of mass

```
using Manopt, Manifolds, LinearAlgebra
M = Sphere(2)
N = 100

# generate N unit vectors
pts = [normalize(randn(3)) for _ in 1:N]

# define cost and gradient
F(M, p) = sum(pi -> distance(M, pi, p)^2 / 2N, pts)
grad_F(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, grad_F, m)

# Alternatively: Use a set of proximal maps and cyclic proximal point
proxes = Function[(M,λ,q) -> prox_distance(M,λ/N,p,q,1) for p in pts]
cyclic_proximal_point(M, F, proxes, pts[1])
```


Summary

`Manopt.jl` is a Julia package that provides

- ▶ a framework for optimization algorithms on manifolds
- ▶ a library of optimization algorithms within this framework
- ▶ includes generic step size / line search functions, debug & record.

based on `ManifoldsBase.jl`, so it can be used with all manifolds from `Manifolds.jl`.

Also included. cost functions, gradients, differentials and proximal maps.
...as well as several tutorials at manoptjl.org








Soon. Constrained optimisation algorithms on manifolds,

- ▶ Augmented Lagrangian Method, Exact Penalty Method
- ▶ Frank-Wolfe Method

[Liu and Boumal 2019]

[Weber and Sra 2022]

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).
-  RB (2022). “Manopt.jl: Optimization on Manifolds in Julia”. In: *Journal of Open Source Software* 7.70, p. 3866. DOI: [10.21105/joss.03866](https://doi.org/10.21105/joss.03866).
-  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>.
-  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).
-  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>.
-  Weber, M. and S. Sra (July 2022). “Riemannian Optimization via Frank-Wolfe Methods”. In: *Mathematical Programming*. DOI: [10.1007/s10107-022-01840-5](https://doi.org/10.1007/s10107-022-01840-5).

 ronnybergmann.net/talks/2022-ICCOPT-Manoptjl.pdf