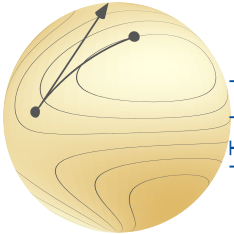

Manopt.jl

Optimization on Riemannian Manifolds

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Optimization

(Constrained) Optimization aims to find for a function $f\colon \mathbb{R}^m \to \mathbb{R}$ 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).

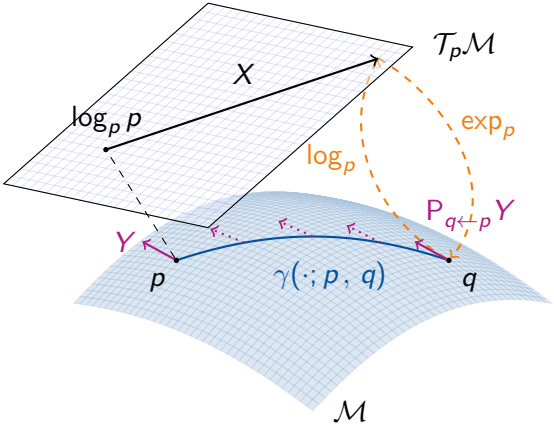
A Riemannian manifold $\mathcal{M}$

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 $\mathrm{P}_{q\leftarrow p} Y$ "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

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

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

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

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

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

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 $\mathbb{R}^n$

$$\mathrm{St}(n,k) := \left\{ p \in \mathbb{R}^{n\times k} \;\middle|\; p^\mathsf{T} p = I_k \right\},$$

For one k-dimensional subspace, there are several ONBs.
Construction: Rotate one ONB such that no vector leaves the subspace
If we are only interested in the subspace, we obtain the Grassmann manifold

$$\mathrm{Gr}(n,k) := \left\{ \mathrm{span}(p) \;\middle|\; p \in \mathbb{R}^{n\times k}, p^\mathsf{T} p = I_k \right\},$$

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

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

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/

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 & SO(n)
- Symmetric positive definite matrices
- Symplectic & Symplectic Stiefel
- ...

juliamanifolds.github.io/Manifolds.jl/

JuliaCon 2020 youtu.be/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 $F\colon \mathcal{M} \to \mathbb{R}$
  - (maybe) a gradient $\operatorname{grad} F\colon \mathcal{M} \to T\mathcal{M}$
  - (maybe) a Hessian $\operatorname{Hess} F$
  - ...
- 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 ith 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 like

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, po))`
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,O,i)` at every iteration `i`

A `StoppingCriterion sc` should

- be a functor `sc(P,O,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 & Linesearch

In many algorithms, after determining a direction "to walk into", e. g.

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

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)`

usually the `Options O` then also have a `AbstractRetractionMethod` for example as `O.retraction_method` to perform the actual (gradient) step as

```
retract!(P.N, O.x, O.x, sk * X, O.retraction_method)
```

and the curve `t -> retract(P.M, o.x, t*X)` is also used for line search methods.

Printing debug output

Approach. `D = DebugOptions(O,dA)` where `dA` is a `DebugAction`.

$\Rightarrow$ These options "act like" the original `Options O` But

- in the beginning (overwriting `initialize_step!(P, D)`)
- after each step (overwriting `solver_step!(P, D)`)
- in the end (when the `StoppingCriterion` returns true)

High level interface. 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
- a line break (after each iteration)
- the reason the algorithm stopped at the end

Recording values

Approach. Analogously `R = RecordOptions(O,rA)` where `rA` is a `RecordAction`.
⇒ These options (also) "act like" the original `Options O` but records

- in the beginning (overwriting `initialize_step!(P, R)`)
- after each step (overwriting `solver_step!(P, R)`)
- in the end (when the `StoppingCriterion` returns true)

High level interface. use the keyword `record=` for example

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

and set `return_options=true` ⇒ final state (options `finO`) are returned.

- `get_record(finO)` yields a vector of `(i, cost, point)` tuples
- long form: `get_record(finO, :Iteration, [:Iteration, :Cost, :Iterate])`
- `get_record(finO, :Iteration, :Cost)` yields the vector of recorded `:Cost`s

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 Problem: The Riemannian center of mass

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

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

$\Rightarrow$ the minimizer of sum of squared distances

For $p_1, \dots, p_N \in \mathcal{M}$: Riemannian center(s) of mass are [Karcher 1977]

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

- (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 $\operatorname{grad} F(p) = -\log_p p_i$

$\Rightarrow$ 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

and includes generic step size / line search functions, debug & record.

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

References

Absil, P.-A., R. Mahony, and R. Sepulchre (2008). *Optimization Algorithms on Matrix Manifolds*. Princeton University Press. DOI: 10.1515/9781400830244.

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