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An Introduction to Optimization on Riemannian Manifolds

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Motivation: Constraint vs Unconstraint Optimization

We want to consider a special case of constrained optimisation

$$\min_{x \in S} f(x) \operatorname*{arg\,min}_{x \in S} f(x),$$

instead of minimal value $f(x^*)$ often minimizer x^* of interest
classical: Constrained Optimization. Describe $S \subset \mathbb{R}^n$ with constraints

$$S = \{x \,|\, g(x) \leq 0 \text{ and } h(x) = 0\}, \qquad g\colon \mathbb{R}^n \to \mathbb{R}^{m_1}, h\colon \mathbb{R}^n \to \mathbb{R}^{m_2}$$

- special algorithms necessary (ALM, EPM)
- g, h might have complicated gradients or be high-dimensional.

today. If $S = \mathcal{M}$ is "nice", i. e. a Riemannian manifold $\mathcal{M}$:

- different notion of e. g. gradient and "means to move around"
- we obtain unconstrained problems on $\mathcal{M}$

$\Rightarrow$ use gradient descent, CG, quasi Newton, trust region,… on $\mathcal{M}$!

Overview

1. A few examples
2. (embedded) Manifolds & Tangent spaces
3. Retractions (moving around on a manifold)
4. First order methods (differentials and gradients)
5. Algorithms & Software

Literature.

- Riemannian Manifolds. do Carmo 1992; Lee 2018
- Optimization on Manifolds. Absil, Mahony, and Sepulchre 2008; Boumal 2023

Example 1: Rayleigh Quotient

Let $A \in \mathbb{R}^{n\times n}$, $A = A^\mathrm{T}$, with eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$ be given.
We can find an eigenvector v_1 by

$$\operatorname*{arg\,min}_{\substack{x\in\mathbb{R}^n\\ x\neq 0}} f(x), \qquad f(x) = \frac{\langle x, Ax\rangle}{\langle x, x\rangle}.$$

- Since $Av_1 = \lambda v_1 \Rightarrow f(v_1) = \lambda_1$
- ⚠ any scaled αv_1, $\alpha \neq 0$ is also a minimizer!
- $\Rightarrow$ Newton iteration might even diverge.

Solution. We rephrase the problem to

$$\operatorname*{arg\,min}_{x\in\mathbb{S}^n} \frac{\langle x, Ax\rangle}{\langle x, x\rangle}\langle x, Ax\rangle, \qquad \mathbb{S}^{n-1} = \left\{x \in \mathbb{R}^n \,\middle|\, \|x\| = 1\right\}$$

An optimisation problem on the $(n-1)$-sphere in $\mathbb{R}^n$.

Example 2: multiple Eigenvectors & The Stiefel manifold

Goal. Find a orthonormal basis $X \in \mathbb{R}^{n\times p}$ for the space spanned by $v_1, \ldots, v_p$ corresponding $\lambda_1 \leq \cdots \leq \lambda_p$.

Then we use columns of X an ONB $\Leftrightarrow X^T X = I_p$, the unit matrix $I_p \in \mathbb{R}^{p\times p}$.

We collect all such matrices representing ONBs for any p-dimensional subspace in

$$\mathrm{St}(n, p) := \{X \in \mathbb{R}^{n\times p} \,|\, X^\mathrm{T} X = I_p\},$$

called the Stiefel manifold.

Our optimization problem to find a best basis reads

$$\operatorname*{arg\,min}_{X\in\mathrm{St}(n,p)} f(X), \qquad f(X) = \mathrm{tr}(X^\mathrm{T} AX)$$

and at a minimizer X^* we have the minimal value $f(X^*) = \sum_{i=1}^{p} \lambda_i$.

Example 3: Subspaces & The Grassmann manifold

Observation. The order of basis vectors in the last example is irrelevant.
Even more. $f(X) = f(Y)$ for $X, Y \in \mathrm{St}(n,p)$ whenever $\mathrm{span}(X) = \mathrm{span}(Y)$

Interpretation. Rotating the basis of the subspace to a new basis of the subspace still yields the same value
$\Rightarrow$ Let's built equivalence classes

$$[X] := \left\{ Y \in \mathrm{St}(n,p) \,\middle|\, \mathrm{span}(X) = \mathrm{span}(Y) \right\}$$

New Goal. Find the subspace

$$\operatorname*{arg\,min}_{[X] \in \mathrm{Gr}(n,p)} g([X]), \qquad g([X]) = \mathrm{tr}(X^{\mathrm{T}} A X)$$

where

$$\mathrm{Gr}(n,p) := \left\{ [X] \,\middle|\, X \in \mathrm{St}(n,p) \right\},$$

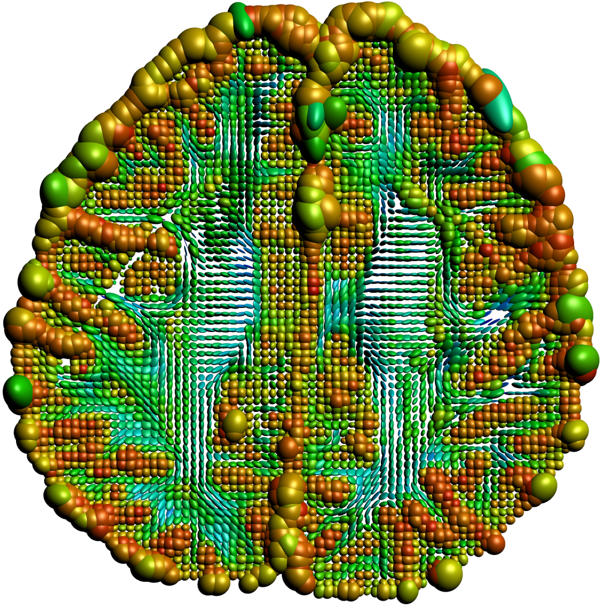
is the Grassmann manifold, i. e. the space of all p-dimensional subspaces of $\mathbb{R}^n$.

Example 4: DT-MRI & Image Denoising

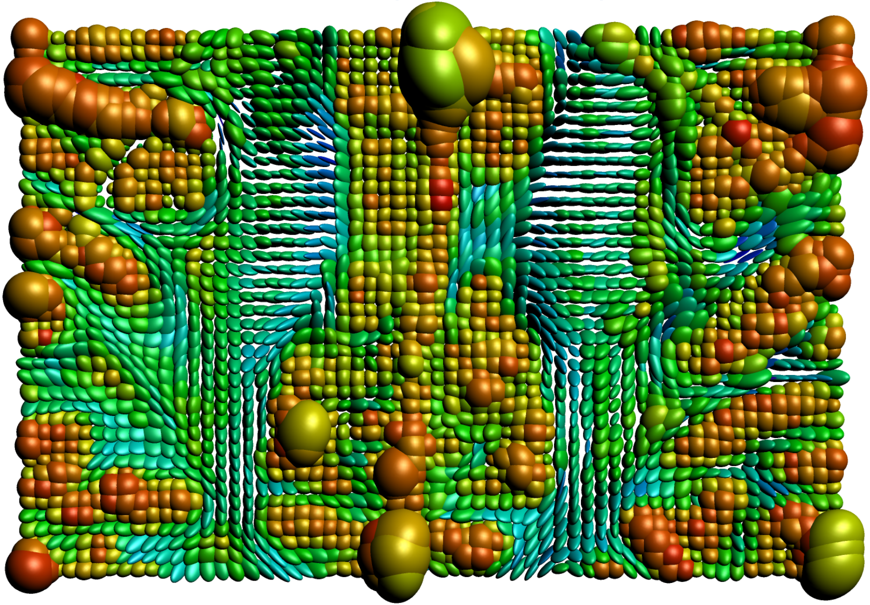
$\mathcal{M} = (\mathcal{P}_3)^{n \times m}$

An image of
"diffusion tensor pixel"
➜ denoising.

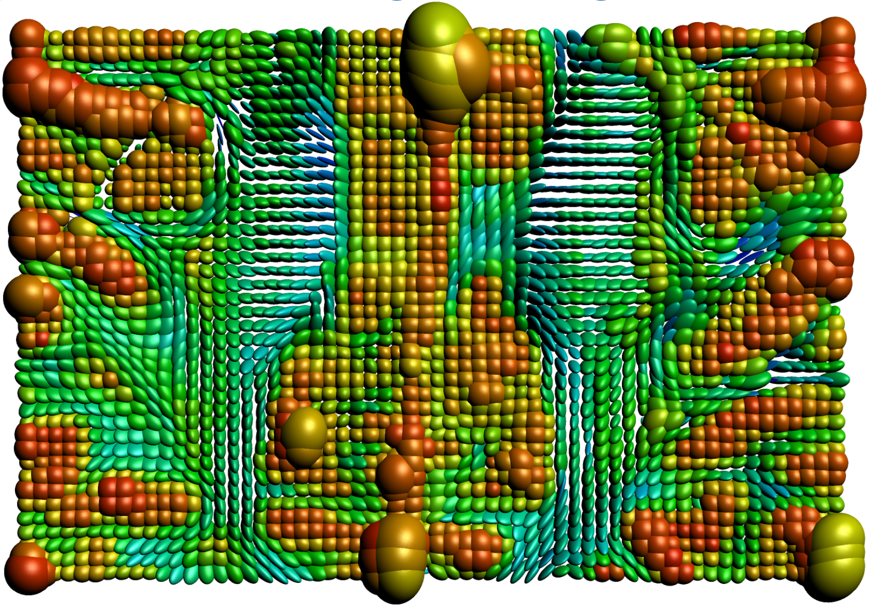
e. g. using ℓ_2–TV



Example 4: DT-MRI & Image Denoising



Example 4: DT-MRI & Image Denoising



Intuition to Tangent space & (sub)manifolds

Intuitive Definition. A (smooth, Riemannian) manifold $\mathcal{M}$ is a set that "locally looks like" $\mathbb{R}^d$
$\Rightarrow$ Collecting all derivatives $c'(0)$ of curves $c\colon I \to \mathcal{M}$ through $c(0) = p$
We obtain a "space of directions"

Example. For the sphere $\mathbb{S}^{n-1} \subset \mathbb{R}^n$ at $c(0) = p$ fulfils $p^\mathrm{T} p = \lVert p \rVert^2 = 1$.
Hence

$$c'(t) \in T_p\mathbb{S}^{n-1} := \{X \in \mathbb{R}^n \,|\, X^\mathrm{T} p + p^\mathrm{T} X = 0\} = \{X \in \mathbb{R}^n \,|\, X^\mathrm{T} p = 0\}$$

is a $(n-1)$-dimensional vector space called the tangent space $T_p\mathbb{S}^{n-1}$ at p.

In general. In order to have a manifold, this "looks like" $\mathbb{R}^d$ always has to be the same dimension d.

Embedded submanifold & Tangent spaces

Definition (Boumal 2023, Def. 3.10,)

Let $\mathcal{E}$ be a linear space of dimension n. A nonempty subset $\mathcal{M}$ of $\mathcal{E}$ is a (smooth) embedded submanifold of $\mathcal{E}$ of dimension d if either

1. $d = n$ and $\mathcal{M}$ is open in $\mathcal{E}$
2. $d = n - k$ for some $k \geq 1$ and for each $p \in \mathcal{M}$ there exists a neighbourhood $\mathcal{U} \subset \mathcal{E}$ and $h\colon \mathcal{U} \to R^k$ such that
   - 2.1 If $y \in \mathcal{U}$ then $h(y) = 0 \Leftrightarrow y \in \mathcal{M}$
   - 2.2 rank $Dh(p) = k$

Tangent space. The rank condition ensures that $\ker Dh(p)$ is d-dimensional. This also forms a vector space, the tangent soace $T_p\mathcal{M}$ at p.

- inherits an inner product by restriction from $\mathcal{E}$, denoted by $\langle \cdot, \cdot \rangle_p$
- the disjoint union of all $\mathcal{T}_p\mathcal{M}$ is the tangent bundle $T\mathcal{M}$ with elements (p, X).

For $\mathbb{S}^{n-1}$ even more: we one global $h(p) = \|p\|^2 - 1$ with $\ker Dh(p) = \{X \in \mathbb{R}^n \,|\, \langle X, p \rangle = 0\}$.

Smooth functions and their Differential

Smooth functions. A function $f\colon \mathcal{M} \to \mathbb{R}$ is called smooth if it is given (locally) as the restriction of a function $\bar{f}\colon \to\mathbb{R}$, i.e. $f = \bar{f}\big|_{\mathcal{M}}$

The (Euclidean) Differential. Classically (for the embedded $\bar{f}$) we have

$$D\bar{f}(x)[v] = \lim_{t\to 0} \frac{\bar{f}(x+tv) - \bar{f}(x)}{t}$$

but for f we have the problem that $x + tv$ is not necessarily on $\mathcal{M}$!

Idea. use as "directions" in the directional derivative
the curves $c\colon I \to \mathcal{M}$ with $c\colon I \to \mathcal{M}, c(0) = p, c'(0) = X$ and define

The Differential of $f\colon \mathcal{M} \to \mathbb{R}$.

$$Df(p)[X] \coloneqq \frac{\mathrm{d}}{\mathrm{d}t} f(c(t)),$$

Fortunately. Both are equivalent, i. e. restricting the Euclidean differential to $T_p\mathcal{M}$ yields the Riemannian one: $Df(p) = D\bar{f}(p)\big|_{T_p\mathcal{M}}$.

Retractions: Moving around on a Manifold.

Iterative Algorithms usually are at some point x, find a (descent) direction v and a step size s and obtain $x^{(k+1)} = x^{(k)} + sv$

How to move on $\mathcal{M}$ given some $p^{(k)}$ and a $X \in T_p\mathcal{M}$?

Definition (Boumal 2023, Def. 3.47)

A retraction on a manifold $\mathcal{M}$ is a smooth map

$$R\colon T\mathcal{M} \to \mathcal{M}, \qquad (p, X) \mapsto R_p(X) \in \mathcal{M}$$

such that each curve $c(t) = R_p(tX)$ satisfies $c(0) = p$, $c'(0) = X$.

Example 1. on $\mathcal{M} = \mathbb{S}^{n-1}$ one can use $R_p(X) = \frac{p+X}{\lVert p+X \rVert}$

Example 2. on $\mathcal{M} = \mathbb{S}^{n-1}$ one can use $R_p(X) = \cos\bigl(\lVert X \rVert_p\bigr)p + \sin\bigl(\lVert X \rVert_p\bigr)\frac{X}{\lVert X \rVert_p}$
$\Rightarrow$ we trace great circles (shortest paths)
This retraction has a special name: the exponential map $\exp_p X$.

The Riemannian Gradient

Definition (Boumal 2023, Def. 3.58)

Let $f\colon \mathcal{M} \to \mathbb{R}$ be smooth on a Riemannian manifold $\mathcal{M}$
The Riemannian gradient of f is the vector field $\operatorname{grad} f$ on $\mathcal{M}$ uniquely defined by the following identities:

$$\text{For all } (p, X) \in T\mathcal{M} \text{ it holds } Df(p)[X] = \langle X, \operatorname{grad} f(p) \rangle_p,$$

where Df denotes the differential.

- $\operatorname{grad} f(p) \in T_p\mathcal{M}$ is the (tangent) direction of steepest ascent
- for the embedded Riemannian submanifolds: $\operatorname{grad} f = \operatorname{proj}_{T_p\mathcal{M}}(\operatorname{grad} \bar{f}(p))$
- (like in $\mathbb{R}^n$:) p is a critical point of $f \Leftrightarrow \operatorname{grad} f(p) = 0 \in T_p\mathcal{M}$.

Gradient Descent

Euclidean Gradient Descent. $x^{(k+1)} = x^{(k)} - \alpha_k \operatorname{grad} f(x^{(k)})$ for some $\alpha_k > 0$.

Riemannian Gradient Descent.
Use the Riemannian gradient and replace "$-$".

Input: $p^{(0)} \in \mathcal{M}$

1: $k \leftarrow 0$
2: **while** not converged **do**
3: Pick a step size $\alpha_k > 0$
4: $p^{(k+1)} = R_{p^{(k)}}\bigl(-\alpha_k s^{(k)}\bigr), \quad s^{(k)} = \operatorname{grad} f(p^{(k)})$
5: $k \leftarrow k+1$
6: **end while**

Output: $p^{(N)}$

Stepsize. For example: Armijo line-search along $\varphi(t) = f\bigl(R_{p^{(k)}}(-ts^{(k)})\bigr)$

Stopping Criteria & the Distance on a manifold

Variant 1. The inner product $\langle\cdot,\cdot\rangle_p$ induces a norm $\|\cdot\|_p$ on any $T_p\mathcal{M}$.

$\Rightarrow$ Given a tolerance $\varepsilon_1 > 0$ stop when $\|\operatorname{grad} f(p^{(k)})\|_{p^{(k)}} < \varepsilon_1$

Variant 2. There is a measure of length for curves $c\colon I \to \mathcal{M}$ induced by $\langle\cdot,\cdot\rangle_p$. Introduce a distance $d_{\mathcal{M}}(p,q)$ as the length of the shortest curve connecting both (a shortest geodesic).

$\Rightarrow$ Given a tolerance $\varepsilon_2 > 0$ stop when $d_{\mathcal{M}}(p^{(k-1)}, p^{(k)}) < \varepsilon_2$

Variant 3. ...as a fallback of course after a maximal number N of iterations.

“Comparing” points and vectors

For Quasi Newton one classically (Euclidean) needs for the secant equation

- $s^{(k)} = x^{(k+1)} - x^{(k)}$
- $y^{(k)} = \operatorname{grad} f(x^{(k+1)}) - \operatorname{grad} f(x^{(k)})$

Problem 1. We do not have a difference of points.
$\Rightarrow$ Interpret $d = z - x$ is the direction pointing from x to z.

We are looking for X such that $R_p(X) = q$ or the inverse retraction $R_p^{-1}(q)$!
For the special case of $R_p = \exp_p$ the inverse is called logarithmic map $\log_p \cdot$.
Obs! the logarithmic map is often not globally defined.

Problem 2. For two gradients $\operatorname{grad} f(p) \in T_p\mathcal{M}$ and $\operatorname{grad} f(q) \in T_q\mathcal{M}$ the difference is not defined, because they live in different spaces

We need a function $T_{q\leftarrow p}$ to “transport” tangent vectors.

Vector Transport

Definition (Absil, Mahony, and Sepulchre 2008, Def. 8.1.1)

Let $\mathcal{M}$ be a manifold, and $p \in \mathcal{M}$ and $X \in T_p\mathcal{M}$.

Then a vector transport $T_{p,X} : T_p\mathcal{M} \to T_q\mathcal{M}$ is a smooth mapping associated to a retraction with $R_p(X) = q$ such that

1. $\mathcal{T}_{p,X} Y \in T_q\mathcal{M}$
2. $\mathcal{T}_{p,0_p} Y = Y$ for all $Y \in T_p\mathcal{M}$,
3. $\mathcal{T}_{p,X}(\alpha Y + \beta Z) = \alpha T_{p,X} Y + \beta T_{p,X} Z$ for all $\alpha, \beta \in \mathbb{R}$, $Y, Z \in T_p\mathcal{M}$

hold.

Alternative Notation. $T_{q\leftarrow p}$ as long as X such that $q = R_p(X)$ is uniquely defined.

Special case. There exists a vector transport that preserves norms $\lVert Y \rVert_p = \lVert T_{p,X} Y \rVert_q$ and angles $\langle Y, Z \rangle_p = \langle T_{p,X} Y, T_{p,X} Z \rangle_q$.
This vector transport is called parallel transport $P_{p,X}$ or $P_{q\leftarrow p}$.

Quasi Newton – Idea

For the Hessian of f we can also start intuitively: How does the gradient $\operatorname{grad} f$ change?

Given a point $p \in \mathcal{M}$ and a direction $X \in T_p\mathcal{M}$ we introduce again a curve $c(t) = R_p(tX)$ to define[1]

$$\operatorname{Hess} f(p)[X] := \lim_{t \to 0} \frac{T_{p \leftarrow c(t)} \operatorname{grad} f(c(t)) - \operatorname{grad} f(p)}{t}$$

Newton equation. We can find a descent direction $X \in T_{p^{(k)}}\mathcal{M}$ by solving

$$\operatorname{Hess} f(p^{(k)})[X] = -\operatorname{grad} f(p^{(k)})$$

Goal. Approximate $\operatorname{Hess} f(p^{(k)}) \approx \mathcal{H}_k \colon T_p\mathcal{M} \to T_p\mathcal{M}$.

[1] formerly done using a connection ∇ which "describes how the metric changes" and then define $\operatorname{Hess} f(p)[X] = \nabla_X \operatorname{grad} f(p)$.

The Riemannian Secant equation

We want to choose $\mathcal{H}_{k+1}$ such that it fulfils the secant equation

$$\mathcal{H}_{k+1}[s^{(k)}] = y^{(k)} \quad \text{or equivalently} \quad \mathcal{B}_{k+1}[y^{(k)}] = s^{(k)}$$

where

- $s^{(k)} = T_{p^{(k+1)} \leftarrow p^{(k)}} R^{-1}_{p^{(k)}} p^{(k+1)}$
- $y^{(k)} = \operatorname{grad} f(p^{(k+1)}) - T_{p^{(k+1)} \leftarrow p^{(k)}} \operatorname{grad} f(p^{(k+1)})$.

Updates similar to the Euclidean case for both $\mathcal{H}_{k+1}$ or $\mathcal{B}_{k+1}$

- BFGS [Huang, Absil, and Gallivan 2018]
- DFP
- Broyden [Huang, Gallivan, and Absil 2015]
- limited memory BFGS
- Symmetric Rank 1 (SR1)

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 $\langle X, Y \rangle_p$
- `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 `AbstractManifold{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

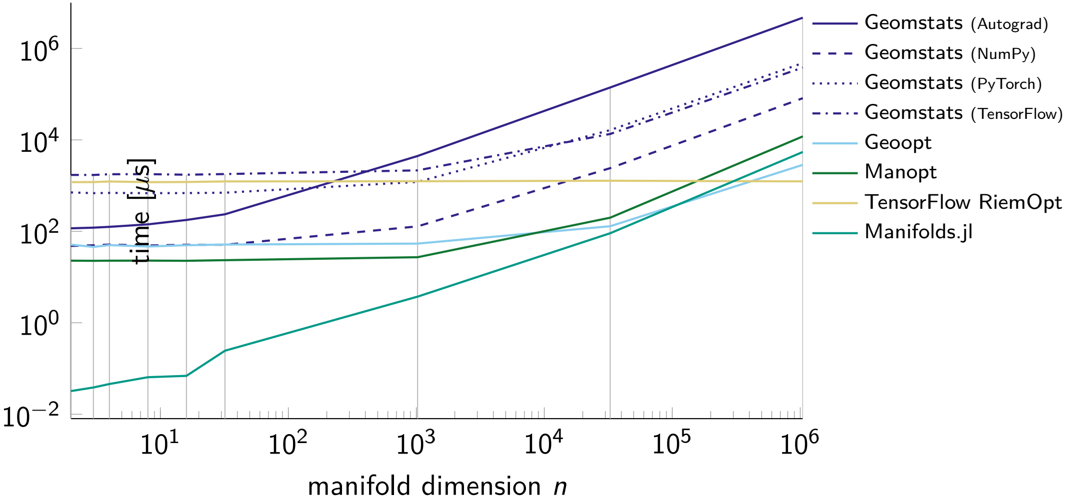
- (unit) Sphere, Circle & Torus
- Fixed Rank Matrices
- (Generalized) Stiefel & Grassmann
- Hyperbolic space
- Rotations, $\mathrm{O}(n)$, $\mathrm{SO}(n)$, $\mathrm{SU}(n)$
- several further Lie groups
- Symmetric positive definite matrices
- Symplectic & Symplectic Stiefel
- Kendall's shape space
-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

juliamanifolds.github.io/Manifolds.jl/

JuliaCon 2020 youtu.be/md-FnDGCh9M

Benchmark of $\log_p$ Hyperbolic space $\mathbb{H}^n$

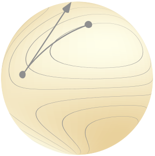
For $n = 2, 3, 2^2, 2^3, 2^4, 2^5, 2^{10}, 2^{15}, 2^{20}$ we compare



➔ For $n > 2^{16}$: PyTorch & TensorFlow based packages faster.

…we could maybe try using `LazyArrays.jl` in Julia.

Manopt.jl – A framework



Goal. Provide optimisation algorithms on Riemannian manifolds, using `ManifoldsBase.jl` to work on any manifold from `Manifolds.jl`.

Generic Framework.

- `AbstractManifoldProblem p` contains static information: $\mathcal{M}$, f, $\operatorname{grad} f$,...
- `AbstractManoptSolverState s` specifies a solver, stores its parameters and values

For your own solver, implement

- `initialize_solver!(p, s)`
- `step_solver!(p, s, i)`

To run an algorithm: `solve!(p, s)`

High level interfaces. E.g.

`gradient_descent(M, f, grad_f, p0)`

setup problem & state, run the algorithm.

Easy access to

- debug, record & status
- step size algorithms
- (modular) stopping criteria.

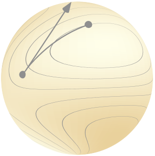
Manopt Family.

manoptjl.org [RB 2022]

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

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

Manopt.jl – Algorithms



Derivative-free

- Nelder-Mead
- Particle Swarm

First order

- Gradient descent:
  Alternating, Conjugate Gradient,
  Momentum, Nesterov, Stochastic
- Subgradient Method
- Quasi Newton
  L-BFGS, BFGS, DFP, Broyden, SR1, …
- Levenberg Marquardt

Proximal map based

- Cyclic Proximal Point Algorithm
- Douglas-Rachford

Primal-Dual

- Chambolle-Pock
- Primal-Dual Semismooth Newton

Second order

- Trust Regions with TCG sub-solver

Constrained

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

manoptjl.org

JuliaCon 2022 youtu.be/thbekfsyhCE

Code Example: Rayleigh Quotient

For the Rayleigh quotient

$$f(p) = p^{\mathrm{T}} A p$$

on the sphere $\mathcal{M} = \mathbb{S}^{n-1}$ we can easily state the Riemannian gradient can also be stated direction (or using the projection)

$$\operatorname{grad} f(p) = 2(I_n - pp^{\mathrm{T}})Ap$$

Let's take a look at the numerics

Outlook: Constrained Optimisation on Manifolds

One can consider problems like

[Liu and Boumal 2019; RB and Herzog 2019]

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

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

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

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

Software packages – An Overview

We[2] 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

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

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

Summary

- constrained optimization turns into unconstraint optimization on a manifold $\mathcal{M}$
- many algorithms can (and have been) generalized to manifolds
- Implementations exist in several languages
- We considered manifolds and algorithms in Julia

Outlook

- manifolds can be defined more general, without an embedding
- numerically we embed somewhere to represent points as arrays
- Riemannian Hessians
- Euclidean AD tools can be used (with some post-processing) to compute Riemannian gradients and Hessians

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