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Nonsmooth Optimization on Riemannian Manifolds in Manopt.jl

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The Rayleigh Quotient

When minimizing the Rayleigh quotient for a symmetric $A \in \mathbb{R}^{n \times n}$

$$\operatorname*{arg\,min}_{x \in \mathbb{R}^n \setminus \{0\}} \frac{x^{\mathsf{T}} A x}{\|x\|^2}$$

- Any eigenvector x^* to the smallest EV λ is a minimizer
- no isolated minima and Newton's method diverges
- Constrain the problem to unit vectors $\|x\| = 1$!

classic constrained optimization (ALM, EPM,...)

Today Utilize the geometry of the sphere

- unconstrained optimization $\displaystyle\operatorname*{arg\,min}_{p \in \mathbb{S}^{n-1}} p^{\mathsf{T}} A p$
- adapt unconstrained optimization to Riemannian manifolds.

The Generalized Rayleigh Quotient

More general. Find a basis for the space of eigenvectors to $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k$:

$$\operatorname*{arg\,min}_{X \in \mathrm{St}(n,k)} \operatorname{tr}(X^\mathsf{T} A X), \qquad \mathrm{St}(n,k) := \left\{X \in \mathbb{R}^{n\times k} \,\middle|\, X^\mathsf{T} X = I\right\},$$

a problem on the Stiefel manifold $\mathrm{St}(n,k)$

Invariant under rotations within a k-dim subspace.

Find the best subspace!

$$\operatorname*{arg\,min}_{\operatorname{span}(X) \in \mathrm{Gr}(n,k)} \operatorname{tr}(X^\mathsf{T} A X), \qquad \mathrm{Gr}(n,k) := \left\{\operatorname{span}(X) \,\middle|\, X \in \mathrm{St}(n,k)\right\},$$

a problem on the Grassmann manifold $\mathrm{Gr}(n,k) = \mathrm{St}(n,k)/O(k)$.

Nonsmooth Optimization on Riemannian Manifolds

We are looking for numerical algorithms to find

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

where

- $\mathcal{M}$ is a Riemannian manifold
- $f\colon \mathcal{M} \to \overline{\mathbb{R}}$ is a function

⚠ f might be nonsmooth and/or nonconvex

⚠ $\mathcal{M}$ might be high-dimensional

A Riemannian Manifold $\mathcal{M}$

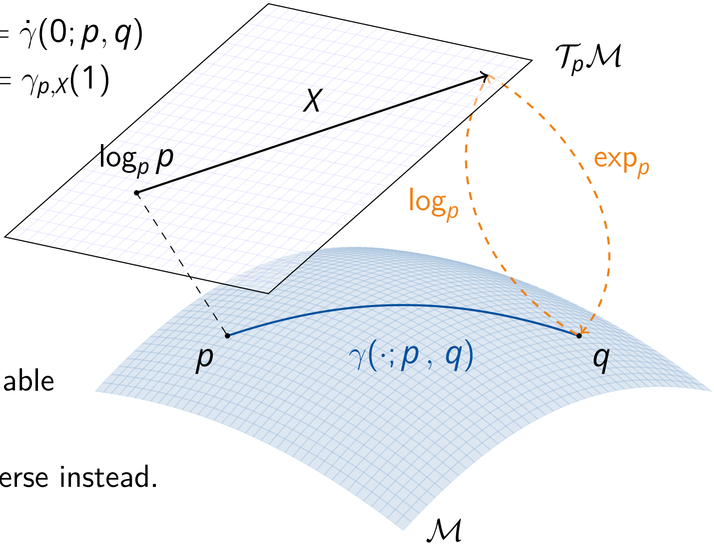
A d-dimensional Riemannian manifold can be informally defined as a set $\mathcal{M}$ covered with a "suitable" collection of charts, that identify subsets of $\mathcal{M}$ with open subsets of $\mathbb{R}^d$ and a continuously varying inner product on the tangent spaces.

[Absil, Mahony, and Sepulchre 2008]

A Riemannian Manifold $\mathcal{M}$

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 $(\cdot\,,\,\cdot)_p$



Numerics.
$\exp_p$ and $\log_p$ maybe not available efficiently/ in closed form

$\Rightarrow$ use a retraction and its inverse instead.

Manifolds.jl & Manopt.jl – Why Julia?

Goals.

- abstract definition of manifolds

$\Rightarrow$ implement abstract solvers on a generic manifold

- well-documented and well-tested
- fast.

$\Rightarrow$ "Run your favourite solver on your favourite manifold".

Why Julia? julialang.org

- high-level language, properly typed
- multiple dispatch (cf. `f(x)`, `f(x::Number)`, `f(x::Int)`)
- just-in-time compilation, solves two-language problem
  $\Rightarrow$ "nice to write" and as fast as C/C++
- I like the community

ManifoldsBase.jl

[Axen, Baran, RB, and Rzecki 2023]

Goal. Provide an interface to implement and use Riemannian manifolds.

Interface `AbstractManifold` to model manifolds

Functions like `exp(M, p, X)`, `log(M, p, X)` or `retract(M, p, X, method)`.

Decorators for implicit or explicit specification of an embedding, a metric, or a group,

Efficiency by providing in-place variants like `exp!(M, q, p, X)`

Manifolds.jl

Goal. Provide a library of Riemannian manifolds, that is efficiently implemented and well-documented

[Axen, Baran, RB, and Rzecki 2023]

Meta. generic implementations for $\mathcal{M}^{n\times m}$, $\mathcal{M}_1 \times \mathcal{M}_2$, vector- and tangent-bundles, esp. $T_p\mathcal{M}$, or Lie groups

Library. Implemented functions for

- Circle, Sphere, Torus, Hyperbolic, Projective Spaces, Hamiltonian
- (generalized, symplectic) Stiefel, Rotations
- (generalized, symplectic) Grassmann, fixed rank matrices
- Symmetric Positive Definite matrices, with fixed determinant
- (several) Multinomial, (skew-)symmetric, and symplectic matrices
- Tucker & Oblique manifold, Kendall's Shape space
- probability simplex, orthogonal and unitary matrices, Rotations, …

Concrete Manifold Examples.

Before first run `] add Manifolds` to install the package.

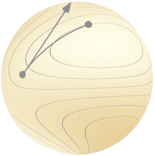
Load packages with `using Manifolds` and

- Euclidean space `M1 = ℝ^3` and 2-sphere `M2 = Sphere(2)`
- their product manifold `M3 = M1 × M2`
- A signal of rotations `M4 = SpecialOrthogonal(3)^10`
- SPDs `M5 = SymmetricPositiveDefinite(3)` (affine invariant metric)
- a different metric `M6 = MetricManifold(M5, LogCholeskyMetric())`

Then for any of these

- Generate a point `p=rand(M)` and a vector `X = rand(M; vector_at=p)`
- and for example `exp(M, p, X)`, or in-place `exp!(M, q, p, X)`

Manopt.jl



Goal. Provide optimization algorithms on Riemannian manifolds.

Features. Given a `Problem p` and a `SolverState s`,
implement `initialize_solver!(p, s)` and `step_solver!(p, s, i)`
$\Rightarrow$ an algorithm in the `Manopt.jl` interface

Highlevel interfaces like `gradient_descent(M, f, grad_f)`
on any manifold `M` from `Manifolds.jl`.

All provide debug output, recording, cache & counting capabilities,
as well as a library of step sizes and stopping criteria.

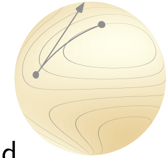
Manopt family.

manoptjl.org [RB 2022]

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

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

List of Algorithms in Manopt.jl



Derivatve Free Nelder-Mead, Particle Swarm, CMA-ES

Subgradient-based Subgradient Method, Convex Bundle Method, Proximal Bundle Method

Gradient-based Gradient Descent, Conjugate Gradient, Stochastic, Momentum, Nesterov, Averaged, …
Quasi-Newton with (L-)BFGS, DFP, Broyden, SR1,…
Levenberg-Marquard

Hessian-based Trust Regions, Adaptive Regularized Cubics (ARC)

nonsmooth Chambolle-Pock, Douglas-Rachford, Cyclic Proximal Point

constrained Augmented Lagrangian, Exact Penalty, Frank-Wolfe

nonconvex Difference of Convex Algorithm, DCPPA

manoptjl.org/stable/solvers/

Illustrating a few Keyword Arguments

Given cost `f(M,p)` and gradient `grad_f(M,p)`, a manifold `M` and a start point `p0`.

- `q = gradient_descent(M, f, grad_f, p0)` to perform gradient descent
- With Euclidean cost `f(E,p)` and gradient `∇f(E, p)`, use for conversion

  ```
  q = gradient_descent(M, f, ∇f, p0; objective_type=:Euclidean)
  ```

- print iteration number, cost and change every 10th iterate

  ```
  q = gradient_descent(M, f, grad_f, p0;
          debug=[:Iteration, :Cost, :Change, 10, "\n"]
      )
  ```

- record `record=[:Iterate, :Cost, :Change], return_state=true`
  Access: `get_solver_result(q)` and `get_record(q)`
- modify stop: `stopping_criterion = StopAfterIteration(100)`
- cache calls `cache=(:LRU, [:Cost, :Gradient], 25)` (uses `LRUCache.jl`)
- count calls `count=[:Cost, :Gradient]` (prints with `return_state=true`)

Numerical Examples

The Riemannian Convex Bundle Method

[RB, Herzog, and Jasa 2024]

- Given $f\colon \mathcal{C} \to \mathbb{R}$ on a (geodesically) convex set $\mathcal{C} \subset \mathcal{M}$
- collect
  - subgradients $X_{q^{(k)}} \in \partial f(q^{(k)})$
  - stabilisation centers $p^{(k)}$ ("best" iterates)
- use this information to
  - determine the next descent direction $d^{(k)} \in \mathcal{T}_{p^{(k)}}\mathcal{M}$ by solving a QP in $\mathcal{T}_{p^{(k)}}\mathcal{M}$
  - where $d^{(k)} \in \partial_{c^{(k)}} f(p^{(k)})$
- we stop when both
  - the approximation $\partial_{c^{(k)}} f(p^{(k)})$ of $\partial f(p^{(k)})$ is "good enough"
  - $\|d^{(k)}\|$ is "small enough"

The Convex Bundle Method in Manopt.jl

In `Manopt.jl` a solver call looks like[1]

```
p = convex_bundle_method(M, f, ∂f, p0;
        diameter = δ, k_max = Ω, m = 10⁻³, kwargs...
    )
```

where

- `M` is a Riemannian manifold
- `f` is the objective function
- `∂f` is a subgradient of the objective function
- `p0` is an initial point on the manifold

The default stopping criterion for the algorithm is set to

$$-\xi^{(k)} \leq 10^{-8}.$$

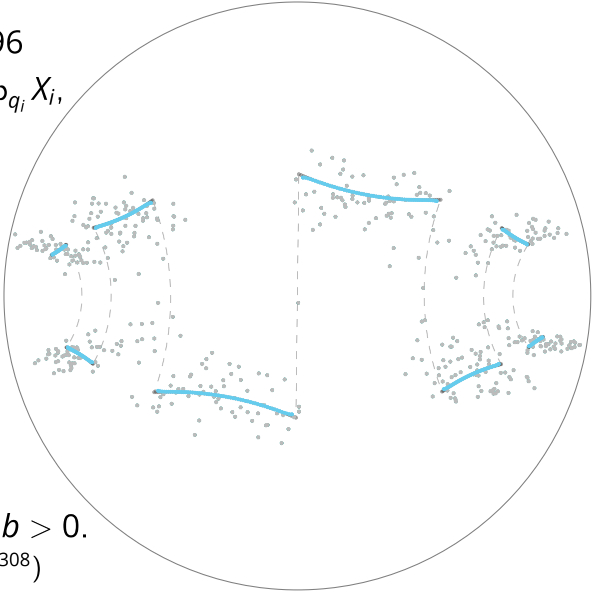
[1] full documentation: manoptjl.org/stable/solvers/convex_bundle_method/

Denoising a Signal on Hyperbolic Space $\mathcal{H}^2$

- signal $q \in \mathcal{M}$, $(\mathcal{H}^2)^n$, $n = 496$
- noisy signal $\bar{q} \in \mathcal{M}$, $\bar{q}_i = \exp_{q_i} X_i$, $\sigma = 0.1$
- ROF Model:

$$\operatorname*{arg\,min}_{p \in \mathcal{M}} \frac{1}{n} d_{\mathcal{M}}(p,q)^2 + \alpha \sum_{i=1}^{n-1} d_{\mathcal{H}^2}(p_i, p_{i+1})$$

- Setting $\alpha = 0.05$ yields reconstruction p^*.
- in RCBM: set $\operatorname{diam}(\operatorname{dom} f) = b > 0$. (in practice: $b =$`floatmax()`$\approx 10^{308}$)



Algorithms for Denoising a Signal

- Riemannian Convex Bundle Method (RCBM) [RB, Herzog, and Jasa 2024]
- Proximal Bundle Algorithm (PBA) [Hoseini Monjezi, Nobakhtian, and Pouryayevali 2021]
- Subgradient Method (SGM) [O. Ferreira and Oliveira 1998]
- Cyclic Proximal Point Algorithm (CPPA) [Bačák 2014]

Algorithm	Iter.	Time (sec.)	Objective	Error
RCBM	3417	51.393	1.7929×10^{-3}	3.3194×10^{-4}
PBA	15 000	102.387	1.8153×10^{-3}	4.3874×10^{-4}
SGM	15 000	99.604	1.7920×10^{-3}	3.3080×10^{-4}
CPPA	15 000	94.200	1.7928×10^{-3}	3.3230×10^{-4}

The Riemannian DC Algorithm

[RB, O. P. Ferreira, Santos, and Souza 2024]

To solve a Difference of Convex problem

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

use

The Riemannian Difference of Convex Algorithm.

Input: An initial point $p^{(0)} \in \operatorname{dom}(g)$, g and $\partial_{\mathcal{M}} h$

1: Set $k = 0$.
2: **while** not converged **do**
3: Take $X^{(k)} \in \partial_{\mathcal{M}} h(p^{(k)})$
4: Compute the next iterate $p^{(k+1)}$ as

$$p^{(k+1)} \in \operatorname*{arg\,min}_{p\in\mathcal{M}} g(p) - \bigl(X^{(k)} , \log_{p^{(k)}} p \bigr)_{p^{(k)}}.$$

5: Set $k \leftarrow k + 1$
6: **end while**

The Difference of Convex Algorithm in Manopt.jl

The algorithm is implemented and released in Julia using `Manopt.jl`[2].
It can be used with any manifold from `Manifolds.jl`

A solver call looks like

```
q = difference_of_convex_algorithm(M, f, g, ∂h, p0)
```

where one has to implement `f(M, p)`, `g(M, p)`, and `∂h(M, p)`.

- a sub problem is generated if keyword `grad_g=` is set
- an efficient version of its cost and gradient is provided
- you can specify the sub-solver using `sub_state=`
  to also set up the specific parameters of your favourite algorithm

[2] see https://manoptjl.org/stable/solvers/difference_of_convex/

Rosenbrock and First Order Methods

Problem. We consider the classical Rosenbrock example[3]

$$\operatorname*{arg\,min}_{x\in\mathbb{R}^2} a\bigl(x_1^2 - x_2\bigr)^2 + \bigl(x_1 - b\bigr)^2,$$

where $a, b > 0$, usually $b = 1$ and $a \gg b$, here: $a = 2 \cdot 10^5$.

Known Minimizer $x^* = \begin{pmatrix} b \\ b^2 \end{pmatrix}$ with cost $f(x^*) = 0$.

Goal. Compare first-order methods, e. g. using the (Euclidean) gradient

$$\nabla f(x) = \begin{pmatrix} 4a(x_1^2 - x_2) \\ -2a(x_1^2 - x_2) \end{pmatrix} + \begin{pmatrix} 2(x_1 - b) \\ 0 \end{pmatrix}$$

[3]available online in ManoptExamples.jl

A “Rosenbrock-Metric” on $\mathbb{R}^2$

In our Riemannian framework, we can introduce a new metric on $\mathbb{R}^2$ as

$$G_p := \begin{pmatrix} 1+4p_1^2 & -2p_1 \\ -2p_1 & 1 \end{pmatrix}, \text{ with inverse } G_p^{-1} = \begin{pmatrix} 1 & 2p_1 \\ 2p_1 & 1+4p_1^2 \end{pmatrix}.$$

We obtain $(X, Y)_p = X^\mathrm{T} G_p Y$

The exponential and logarithmic map are given as

$$\exp_p(X) = \begin{pmatrix} p_1 + X_1 \\ p_2 + X_2 + X_1^2 \end{pmatrix}, \qquad \log_p(q) = \begin{pmatrix} q_1 - p_1 \\ q_2 - p_2 - (q_1 - p_1)^2 \end{pmatrix}.$$

`Manifolds.jl`:
Implement these functions on `MetricManifold(ℝ^2, RosenbrockMetric())`.

The Riemannian Gradient w.r.t. the new Metric

Let $f\colon \mathcal{M} \to \mathbb{R}$. Given the Euclidean gradient $\nabla f(p)$, its Riemannian gradient $\operatorname{grad} f\colon \mathcal{M} \to T\mathcal{M}$ is given by

$$\operatorname{grad} f(p) = G_p^{-1} \nabla f(p).$$

While we could implement this denoting $\nabla f(p) = \begin{pmatrix} f_1'(p) & f_2'(p) \end{pmatrix}^{\mathsf{T}}$ using

$$\Big\langle \operatorname{grad} f(q), \log_q p \Big\rangle_q = (p_1 - q_1) f_1'(q) + (p_2 - q_2 - (p_1 - q_1)^2) f_2'(q),$$

but it is automatically done in `Manopt.jl`.

The Experiment Setup

Algorithms. We now compare

1. The Euclidean gradient descent algorithm on $\mathbb{R}^2$,
2. The Riemannian gradient descent algorithm on $\mathcal{M}$,
3. The Difference of Convex Algorithm on $\mathbb{R}^2$,
4. The Difference of Convex Algorithm on $\mathcal{M}$.

For DCA third we split f into $f(x) = g(x) - h(x)$ with

$$g(x) = a\big(x_1^2 - x_2\big)^2 + 2\big(x_1 - b\big)^2 \quad \text{and} \quad h(x) = \big(x_1 - b\big)^2.$$

Initial point. $p_0 = \frac{1}{10}\begin{pmatrix}1\\2\end{pmatrix}$ with cost $f(p_0) \approx 7220.81$.

Stopping Criterion.
$d_{\mathcal{M}}(p^{(k)}, p^{(k-1)}) < 10^{-16}$ or $\lVert \operatorname{grad} f(p^{(k)}) \rVert_p < 10^{-16}$.

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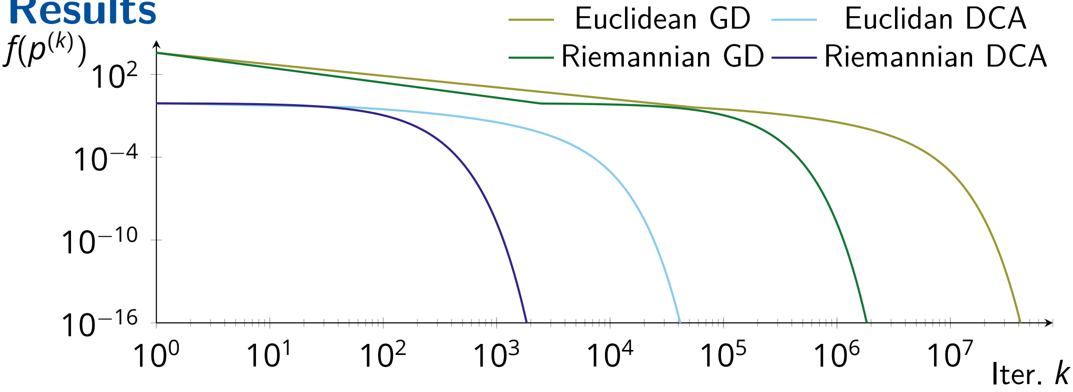
Results



Algorithm	**Runtime** (sec.)	**# Iterations**
Euclidean GD	305.567	53 073 227
Euclidean DCA	58.268	50 588
Riemannian GD	18.894	2 454 017
Riemannian DCA	7.704	2 459

Summary

- `ManifolddsBase.jl` provides an interface to implement a manifold
- `Manifolds.jl` implements a library of manifolds using the interface
- `Manopt.jl` provides optimization algorithms on these manifolds

Outlook.

- couple `Manopt.jl` with (Euclidean) AD tools using `ManifoldDiff.jl`
- What is (Fenchel) duality on manifolds?

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Selected References

Axen, S. D., M. Baran, RB, and K. Rzecki (2023). "Manifolds.jl: An Extensible Julia Framework for Data Analysis on Manifolds". In: *ACM Transactions on Mathematical Software*. Accepted for pulication. DOI: 10.1145/3618296. arXiv: 2106.08777.

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ronnybergmann.net/talks/2024-EURO-Manoptjl.pdf