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Manopt.jl

Optimization on Riemannian Manifolds in Julia

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Julia for numerical problems in quantum and solid-state physics
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Optimization on Manifolds

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

- $f\colon \mathcal{M} \to \mathbb{R}$ is a (smooth) function
- $\mathcal{M}$ is a Riemannian manifold
- ➜ Riemannian optimization

This especially includes

- nonsmooth problems: f is (only) lower semicontinuous
- ➜ splitting methods $f(p) = g(p) + h(p)$, where g is smooth
- Difference of Convex problems $f(p) = g(p) - h(p)$
- constraints $p \in \mathcal{C} \subset \mathcal{M}$

The Rayleigh Quotient

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

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

- 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 $\lVert x\rVert = 1$!

classic constrained optimization (ALM, EPM, IP Newton, …)

Today Utilize the geometry of the sphere

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

The Generalized Rayleigh Quotient

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

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

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

Invariant under rotations within a k-dim subspace.

Find the best subspace!

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

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

A Riemannian Manifold $\mathcal{M}$

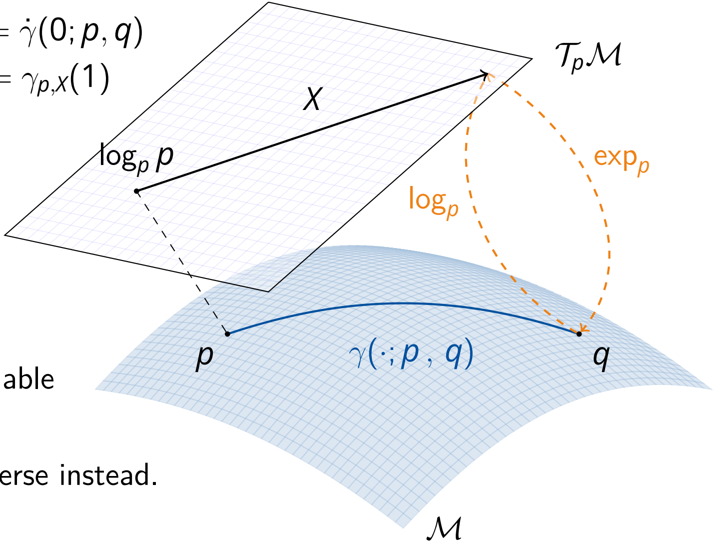
A d-dimensional Riemannian manifold can be informally defined as a set $\mathcal{M}$ covered with a "suitable" collection of charts, that identify subsets of $\mathcal{M}$ with open subsets of $\mathbb{R}^d$ and a continuously varying inner product on the tangent spaces.

[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.

(Geodesic) Convexity

[Sakai 1996; Udriște 1994]

A set $\mathcal{C} \subset \mathcal{M}$ is called (strongly geodesically) convex if for all $p, q \in \mathcal{C}$ the geodesic $\gamma(\cdot; p, q)$ is unique and lies in $\mathcal{C}$.

A function $f\colon \mathcal{C} \to \overline{\mathbb{R}}$ is called (geodesically) convex if for all $p, q \in \mathcal{C}$ the composition $f(\gamma(t; p, q)), t \in [0, 1]$, is convex.

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)`

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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, …

Concrete Manifold Examples.

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

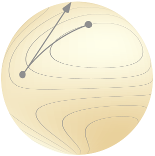
Load packages with `using Manifolds` and

- 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.

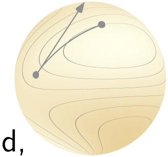
Manopt family.

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, Interior Point Newton

nonconvex Difference of Convex Algorithm, DCPPA

manoptjl.org/stable/solvers/

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Gradient Descent

For the Rayleigh quotient on $\mathbb{S}^{n-1}$ we have for $p \in \mathbb{S}^{n-1}$

$$\text{cost } f(p) = p^{\mathrm{T}}Ap, \qquad \text{and gradient } \nabla f(p) = 2Ap.$$

But this is not the Riemannian one. For example: $\nabla f(p) \notin T_p\mathcal{M}$.
Formally: We need the Riesz representer $Df(p)[X] = \langle \operatorname{grad} f(p), X\rangle_p$.

Easier: Let `Manopt.jl` convert the Euclidean into a Riemannian gradient:

```
using Manopt, Manifolds
M = Sphere(2); A = Matrix(reshape(1.0:9.0, 3, 3));
f(M,p) = p'*A*p;
∇f(M,p) = 2A*p;
p0 = [1.0, 0.0, 0.0];
q = gradient_descent(M, f, ∇f, p0; objectiv_type=:Euclidean)
```

Works as well if you have a Hessian $\nabla^2 f$ is required.

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Illustrating a few Keyword Arguments

Given a manifold `M`, a cost `f(M,p)`, its Riemannian gradient `grad_f(M,p)`, 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`)

The Riemannian Subdifferential

Let $\mathcal{C}$ be a convex set.

The subdifferential of f at $p \in \mathcal{C}$ is given by [O. Ferreira and Oliveira 2002; Lee 2003; Udriște 1994]

$$\partial_{\mathcal{M}} f(p) := \bigl\{\xi \in \mathcal{T}_p^*\mathcal{M} \,\big|\, f(q) \geq f(p) + \langle \xi \,, \log_p q \rangle_p \text{ for } q \in \mathcal{C}\bigr\},$$

where

- $\mathcal{T}_p^*\mathcal{M}$ is the dual space of $\mathcal{T}_p\mathcal{M}$, also called cotangent space
- $\langle \cdot \,, \cdot \rangle_p$ denotes the duality pairing on $\mathcal{T}_p^*\mathcal{M} \times \mathcal{T}_p\mathcal{M}$
- numerically we use musical isomorphisms $X = \xi^\flat \in \mathcal{T}_p\mathcal{M}$ to obtain a subset of $\mathcal{T}_p\mathcal{M}$

The Riemannian DCA in `Manopt.jl`

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

To solve a problem of a difference of convex (DC) functions

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

where g is convex and smooth and h is convex but not necessarily smooth:

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

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

1: **for** $k = 1, 2, \ldots$ until convergence **do**

2: Take $X^{(k)} \in \partial_{\mathcal{M}} h(p^{(k)})$

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

4: **end for**

- implement `f(M, p)`, `g(M, p)`, and `∂h(M, p)`.
- efficient sub solver used if `grad_g=` is set (implement `grad_g(M, p)`)
- `sub_state=` to specify a solver or `sub_problem=` for closed-form solution

Summary

`Manifolds.jl` & `Manifolds.jl`

- provide a high-level interface for defining manifolds
- offer a library of manifolds and functions defined thereon

`Manopt.jl`

- provides an interface to define solvers
- offers a library of algorithms for optimization on manifolds
- offers several tools to
  - state stopping criteria, debug, record, caching
  - (re)use Euclidean gradients and Hessians

Future work.

- What is a Fenchel conjugate on Manifolds?
  Friday 10.15 in the MathICSE seminar.
- `GroupManifolds` are currently reworked ⇒ `LieGroups.jl`.

Selected References

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

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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Boumal, N. (2023). *An introduction to optimization on smooth manifolds*. Cambridge University Press. URL: https://www.nicolasboumal.net/book.

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ronnybergmann.net/talks/2024-Lausanne-Manopt.pdf