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The Riemannian Difference of Convex Algorithm in Manopt.jl

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joint work with
O. P. Ferreira, E. M. Santos, and J. C. O. Souza.

Optimization Techniques in Quantum Chemistry

Aachen, June 5, 2024.

Difference of Convex

We aim to solve

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

where

- $\mathcal{M}$ is a Riemannian manifold
- $f\colon \mathcal{M} \to \mathbb{R}$ is a difference of convex function, i. e. of the form

$$f(p) = g(p) - h(p)$$

- $g, h\colon \mathcal{M} \to \overline{\mathbb{R}}$ are convex, lower semicontinuous, and proper

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A Riemannian Manifold $\mathcal{M}$

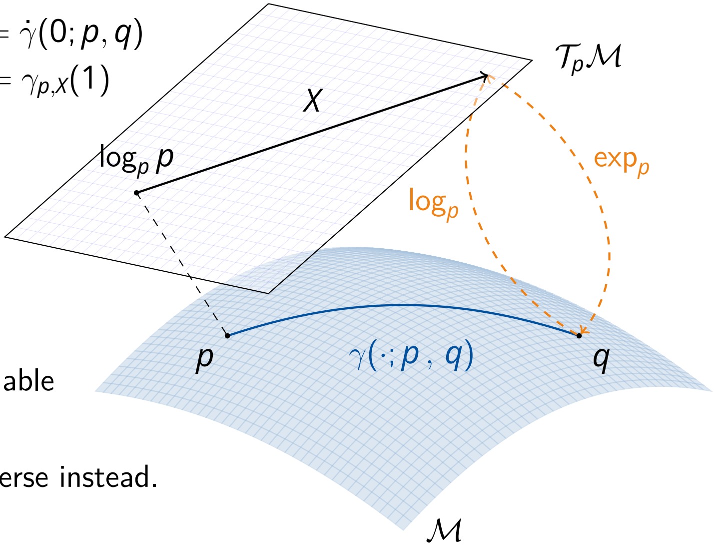
A d-dimensional Riemannian manifold can be informally defined as a set $\mathcal{M}$ covered with a "suitable" collection of charts, that identify subsets of $\mathcal{M}$ with open subsets of $\mathbb{R}^d$ and a continuously varying inner product on the tangent spaces.

[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.

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 $\mathcal{T}_p^* \mathcal{M} \times \mathcal{T}_p \mathcal{M}$

The Fenchel Conjugate

The Fenchel conjugate of a function $f\colon \mathbb{R}^n \to \overline{\mathbb{R}}$ is given by

$$f^*(\xi) := \sup_{x\in\mathbb{R}^n} \langle \xi, x\rangle - f(x) = \sup_{x\in\mathbb{R}^n} \begin{pmatrix} \xi \\ -1 \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} x \\ f(x) \end{pmatrix}$$

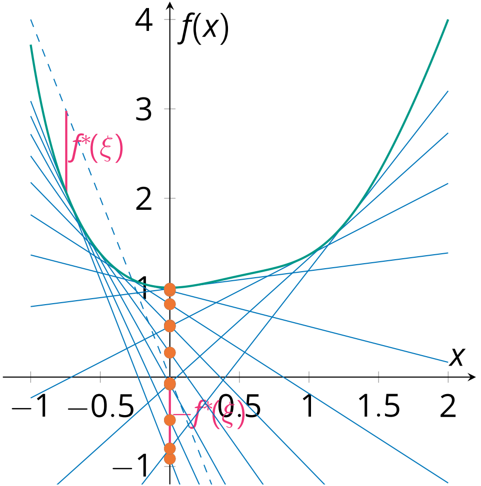
- given $\xi \in \mathbb{R}^n$: maximize the distance between $\xi^{\mathrm{T}}\cdot$ and f
- can also be written in the epigraph

The Fenchel biconjugate reads

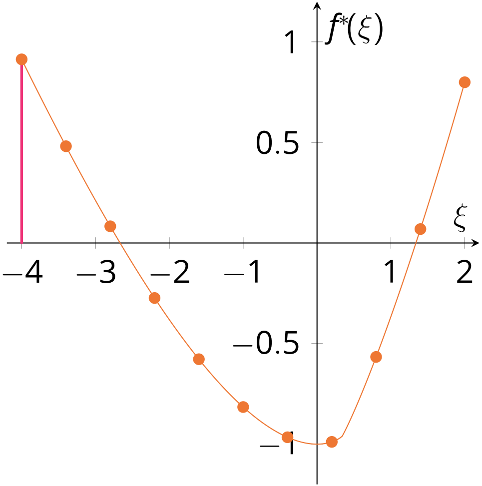
$$f^{**}(x) = (f^*)^*(x) = \sup_{\xi\in\mathbb{R}^n} \langle \xi\,, x\rangle - f^*(\xi).$$

Illustration of the Fenchel Conjugate

The function f



The Fenchel conjugate f^*



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The Riemannian Difference of Convex Algorithm

The Euclidean DCA

Idea 1. At x_k, approximate $h(x)$ by its affine minorization

$$h_k(x) := h(x^{(k)}) + \langle x - x^{(k)}, y^{(k)} \rangle \text{ for some } y^{(k)} \in \partial h(x^k)$$

$\Rightarrow$ iteratively minimize $g(x) - h_k(x) = g(x) - h(x^{(k)}) - \langle x - x^{(k)}, y^{(k)} \rangle$

Idea 2. Using duality theory finding a new $y^{(k)} \in \partial h(x^{(k)})$ is equivalent to

$$y^{(k)} \in \operatorname*{arg\,min}_{y \in \mathbb{R}^n} \Bigl\{ h^*(y) - g^*(y^{(k-1)}) - \langle y - y^{(k-1)}, x^{(k)} \rangle \Bigr\}$$

Idea 3. Reformulate 2 using a proximal map $\Rightarrow$ DCPPA
on manifolds this was done in [Almeida, Neto, Oliveira, and Souza 2020; Souza and Oliveira 2015]

In the Euclidean case, all three models are equivalent.

A Fenchel Duality on a Hadamard Manifold

Let

- $T\mathcal{M} = \dot{\bigcup}_p T_p\mathcal{M}$ denote the tangent bundle
- analogously $T^*\mathcal{M}$ denotes the cotangent bundle
- $\mathcal{M}$ be a Hadamard manifold (non-positive sectional curvature).

Definition [Silva Louzeiro, RB, and Herzog 2022]

Let $f\colon \mathcal{M} \to \overline{\mathbb{R}}$.
The Fenchel conjugate of f is the function $f^*\colon \mathcal{T}^*\mathcal{M} \to \overline{\mathbb{R}}$ defined by

$$f^*(p,\xi) := \sup_{q\in\mathcal{M}} \Bigl\{ \langle \xi, \log_p q \rangle - f(q) \Bigr\}, \qquad (p,\xi) \in \mathcal{T}^*\mathcal{M}.$$

The Dual Difference of Convex Problem

Given the Difference of Convex problem

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

and the Fenchel duals g^* and h^*,
we can state the dual difference of convex problem as

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

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

On $\mathcal{M} = \mathbb{R}^n$ this indeed simplifies to the classical dual problem.

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

$$\inf_{(q,X)\in\mathcal{T}^*\mathcal{M}} \Bigl\{ h^*(q,X) - g^*(q,X) \Bigr\} = \inf_{p\in\mathcal{M}} \{ g(p) - h(p) \}\,.$$

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The Dual Difference of Convex Problem

The primal and dual Difference of Convex problem

$$\operatorname*{arg\,min}_{p \in \mathcal{M}} g(p) - h(p) \qquad \text{and} \qquad \operatorname*{arg\,min}_{(p,\xi) \in T^*\mathcal{M}} h^*(p,\xi) - g^*(p,\xi)$$

are equivalent in the following sense.

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

If p^* is a solution of the primal problem, then $(p^*, \xi^*) \in T^*\mathcal{M}$ is a solution for the dual problem for all $\xi^* \in \partial_{\mathcal{M}} h(p^*) \cap \partial_{\mathcal{M}} g(p^*)$.

If $(p^*, \xi^*) \in T^*\mathcal{M}$ is a solution of the dual problem for some $\xi^* \in \partial_{\mathcal{M}} h(p^*) \cap \partial_{\mathcal{M}} g(p^*)$, then p^* is a solution of the primal problem.

Derivation of the Riemannian DCA

We consider the first order Taylor approximation of h at some point $p^{(k)}$:
With $\xi \in \partial h(p^{(k)})$ we set

$$h_k(p) := h(p^{(k)}) + \langle \xi \,, \log_{p^{(k)}} p \rangle_{p^{(k)}}$$

Using musical isomorphisms we identify $X = \xi^\sharp \in T_p\mathcal{M}$,
where we call X a subgradient. Locally h_k minorizes h, i. e.

$$h_k(q) \leq h(q) \quad \text{locally around} \quad p^{(k)}$$

$\Rightarrow$ Use $-h_k(p)$ as upper bound for $-h(p)$ in $f = g - h$.

Note. On $\mathbb{R}^n$ the function h_k is linear.
On a manifold h_k is nonlinear and not even necessarily convex, even on a Hadamard manifold.

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The Riemannian DC Algorithm

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

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

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

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

Note. In general the subproblem $(*)$ can not be solved in closed form. But an approximate solution yields a good candidate.

For example: Given g, $p^{(k)}$, and $X^{(k)}$ and $\operatorname{grad} g \Rightarrow$ Gradient descent.

Convergence of the Riemannian DCA

Let $\{p^{(k)}\}_{k\in\mathbb{N}}$ and $\{X^{(k)}\}_{k\in\mathbb{N}}$ be the iterates and subgradients of the RDCA.

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

If $\bar{p}$ is a cluster point of $\{p^{(k)}\}_{k\in\mathbb{N}}$, then $\bar{p} \in \operatorname{dom}(g)$ and there exists a cluster point $\bar{X}$ of $\{X^{(k)}\}_{k\in\mathbb{N}}$ s. t. $\bar{X} \in \partial g(\bar{p}) \cap \partial h(\bar{p})$.

$\Rightarrow$ Every cluster point of $\{p^{(k)}\}_{k\in\mathbb{N}}$, if any, is a critical point of f.

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

Let g be σ-strongly (geodesically) convex. Then

$$f(p^{(k+1)}) \leq f(p^{(k)}) - \frac{\sigma}{2} d^2(p^{(k)}, p^{(k+1)})$$

and $\displaystyle\sum_{k=0}^{\infty} d^2(p^{(k)}, p^{(k+1)}) < \infty$, so in particular $\displaystyle\lim_{k\to\infty} d(p^{(k)}, p^{(k+1)}) = 0$.

Software

Manifolds.jl & Manopt.jl – Why Julia?

Goals.

- abstract definition of manifolds

⇒ implement abstract solvers on a generic manifold

- well-documented and well-tested
- fast.

⇒ "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
  ⇒ "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.

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

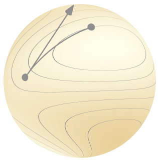
Load packages with `using Manifolds` and

- 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.

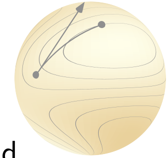
Manopt family.

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 `reocord=[: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 Difference of Convex Algorithm in Manopt.jl

The algorithm is implemented and released in Julia using `Manopt.jl`[1].
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

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

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A Numerical Example

Rosenbrock and First Order Methods

Problem. We consider the classical Rosenbrock example[2]

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

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

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

[2] 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 $\nabla f(p) = \begin{pmatrix} f_1'(p) & f_2'(p)\end{pmatrix}^{\mathrm{T}}$ 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 $\mathcal{M}$.

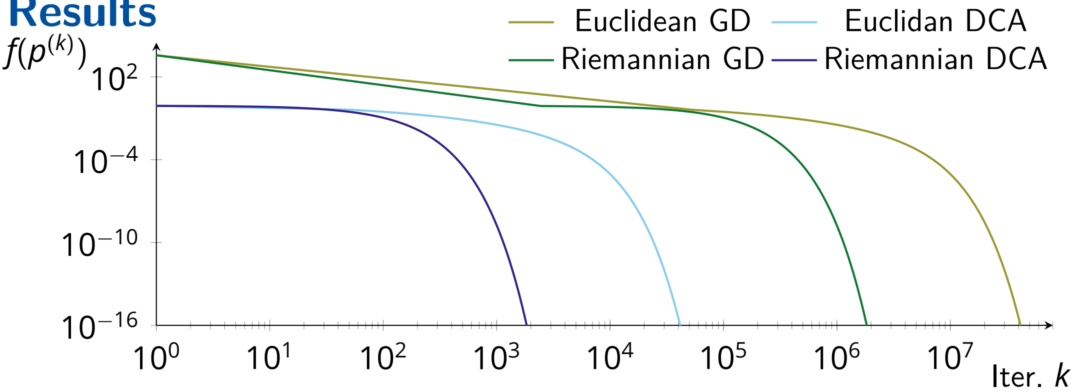
For DCA third we split f into $f(x) = g(x) - h(x)$ with

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

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 $\|\operatorname{grad} f(p^{(k)})\|_p < 10^{-16}$.

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

- Nonsmooth, nonconvex problems on manifold: difference of convex

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

- The Difference of Convex Algorithm
- ➜ Relation to Fenchel Duality on Hadamard manifolds
- ➜ Convergence on Hadamard manifolds
- `Manifolds.jl` and `Manopt.jl`
- ➜ Numerically solve optimization problems on Riemannian manifolds

Outlook.

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

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Selected References

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