

The Riemannian Difference of Convex Algorithm in Manopt.jl

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joint work with

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Introduction



Optimization on Manifolds

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

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

This especially includes

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



The Rayleigh Quotient

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

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

- \triangle 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, IP Newton, ...)

Today Utilize the geometry of the sphere



unconstrained optimization

$$\arg\min_{p\in\mathbb{S}^{n-1}}p^{\mathsf{T}}Ap$$

adapt unconstrained optimization to Riemannian manifolds.



The Generalized Rayleigh Quotient

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

$$\underset{X \in \mathsf{St}(n,k)}{\mathsf{arg \, min} \, \mathsf{tr}(X^\mathsf{T} A X)}, \qquad \mathsf{St}(n,k) \coloneqq \big\{ X \in \mathbb{R}^{n \times k} \, \big| \, X^\mathsf{T} X = I \big\},$$

- \triangle a problem on the Stiefel manifold St(n, k)
- \bigwedge Invariant under rotations within a k-dim subspace.
- Tind the best subspace!

$$\underset{\mathsf{span}(X) \in \mathsf{Gr}(n,k)}{\mathsf{arg}\,\mathsf{min}}\,\mathsf{tr}(X^\mathsf{T}\!AX), \qquad \mathsf{Gr}(n,k) \coloneqq \big\{\mathsf{span}(X)\,\big|\,X \in \mathsf{St}(n,k)\big\},$$



 \triangle a problem on the Grassmann manifold Gr(n,k) = 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, Sepulchre, 2008]



A Riemannian Manifold ${\mathcal M}$

Notation.

- lacksquare Logarithmic map $\log_{
 ho}q=\dot{\gamma}(0;
 ho,q)$
- ightharpoonup Exponential map $\exp_{\rho} X = \gamma_{\rho,X}(1)$
- Geodesic $\gamma(\cdot; p, q)$
- ► Tangent space $\mathcal{T}_p\mathcal{M}$
- ▶ inner product $(\cdot, \cdot)_p$
- ▶ parallel transport $\mathcal{P}_{q \leftarrow p} X$

$\mathcal{T}_{p}\mathcal{M}$ X $\gamma(\cdot; p, q)$

Numerics.

- \triangle exp_p and log_p may not be available efficiently / in closed form
- use a retraction and its inverse

 \mathcal{M}



(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 $f: \mathcal{C} \to \overline{\mathbb{R}}$ 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 Difference of Convex Algorithm



Difference of Convex

We aim to solve

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

where

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

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

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



The Riemannian Subdifferential

Let \mathcal{C} be a convex set.

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

$$\partial_{\mathcal{M}} f(p) := ig\{ \xi \in \mathcal{T}_p^* \mathcal{M} \, ig| f(q) \geq f(p) + \langle \xi \, , \log_p q
angle_p \; ext{ for } q \in \mathcal{C} ig\},$$

where

- $ightharpoonup \mathcal{T}_p^*\mathcal{M}$ is the dual space of $\mathcal{T}_p\mathcal{M}$, also called cotangent space
- $lackbox{} \langle \cdot \, , \cdot \rangle_p$ 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 Fenchel Conjugate

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

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

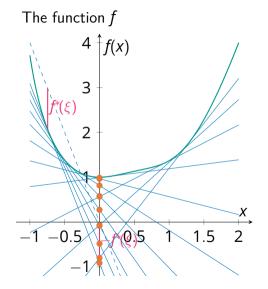
- lacktriangle given $\xi \in \mathbb{R}^n$: maximize the distance between ξ^T and f
- can also be written in the epigraph

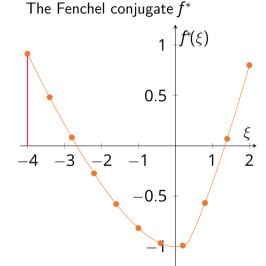
The Fenchel biconjugate reads

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



Illustration of the Fenchel Conjugate







The Euclidean DCA

Idea 1. At $x^{(k)}$, approximate h(x) by its affine minorization

$$h_k(x) := h(x^{(k)}) + \langle x - x^{(k)}, y^{(k)} \rangle$$
 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

$$y^{(k)} \in rg \min_{y \in \mathbb{R}^n} \Bigl\{ h^*(y) - g^*(y^{(k-1)}) - \langle y - y^{(k-1)}, x^{(k)}
angle \Bigr\}$$

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

In the Euclidean case, all three models are equivalent.



A Fenchel Duality on a Hadamard Manifold

Let

- $ightharpoonup T_{\mathcal{P}} T_{\mathcal{P}} \mathcal{M}$ denote the tangent bundle
- ightharpoonup analogously $T^*\mathcal{M}$ denotes the cotangent bundle
- \triangleright \mathcal{M} be a Hadamard manifold (non-positive sectional curvature).

Definition

[Silva Louzeiro, RB, 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

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



The Dual Difference of Convex Problem

Given the Difference of Convex problem

$$rg \min_{p \in \mathcal{M}} g(p) - h(p)$$

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

[RB, Ferreira, Santos, Souza, 2024]

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

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

Theorem.

[RB, Ferreira, Santos, Souza, 2024]

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



The Dual Difference of Convex Problem

The primal and dual Difference of Convex problem

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

are equivalent in the following sense.

Theorem.

[RB, Ferreira, Santos, Souza, 2024]

If p^* is a solution of the primal problem, then $(p^*, \xi^*) \in \mathcal{T}^*\mathcal{M}$ 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

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

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.

$$h_k(q) \le h(q)$$
 locally around $p^{(k)}$

$$\Rightarrow$$
 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.

The Riemannian DC Algorithm

[RB, Ferreira, Santos, Souza, 2024]

Input: An initial point $p^{(0)} \in \text{dom}(g)$, 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

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

- 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 $grad g \Rightarrow Gradient descent.$



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, Ferreira, Santos, Souza, 2024]

If \bar{p} is a cluster point of $\{p^{(k)}\}_{k\in\mathbb{N}}$, then $\bar{p}\in \text{dom}(g)$ 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, Ferreira, Santos, Souza, 2024]

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

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

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



Optimization on Manifolds in Julia



Goals of the Software – 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?

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



julialang.org



ManifoldsBase.jl



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



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 $M1 = \mathbb{R}^3$ and 2-sphere M2 = Sphere(2)
- ► their product manifold M3 = M1 × M2
- ► A signal of rotations M4 = Rotations(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) ⇒ 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.





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





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





Implementing Gradient Descent

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

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

$$\operatorname{cost} f(p) = p^{\mathsf{T}} A p$$
, and gradient $\nabla f(p) = 2 A p$.

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  \begin{tabular}{lll} M = Sphere(2); & A = Matrix(reshape(1.0:9.0, 3, 3)); \\ f(M,p) = p'*A*p; \\ \nabla f(M,p) = 2A*p; \\ p0 = [1.0, 0.0, 0.0]; \\ q = gradient_descent(M, f, <math>\nabla f, p0; objective_type=:Euclidean) \\ \end{tabular}
```



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

- 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], return_objective=true



The Difference of Convex Algorithm in Manopt.jl

The algorithm is implemented and released in Julia using Manopt.jl¹. It can be used with any manifold from Manifolds.jl

A solver call looks like

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

where one has to implement f(M, p), g(M, p), and $\partial h(M, p)$.

- ▶ 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

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



A Numerical Example



Rosenbrock and First Order Methods

Problem. We consider the classical Rosenbrock example²

$$\underset{x \in \mathbb{R}^2}{\arg \min} \, \alpha (x_1^2 - x_2)^2 + (x_1 - b)^2,$$

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

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

²available online in ManoptExamples.il



A "Rosenbrock-Metric" on \mathbb{R}^2

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

$$\textit{G}_{\textit{p}} \coloneqq \begin{pmatrix} 1 + 4p_1^2 & -2p_1 \\ -2p_1 & 1 \end{pmatrix}, \text{ with inverse } \textit{G}_{\textit{p}}^{-1} = \begin{pmatrix} 1 & 2p_1 \\ 2p_1 & 1 + 4p_1^2 \end{pmatrix}.$$

We obtain $(X, Y)_p = X^T G_p Y$

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 $MetricManifold(\mathbb{R}^2)$, RosenbrockMetric()).



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

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

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

While we could implement this denoting $abla f(p) = ig(f_1'(p) \ f_2'(p)ig)^{\mathsf{T}}$ using

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

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

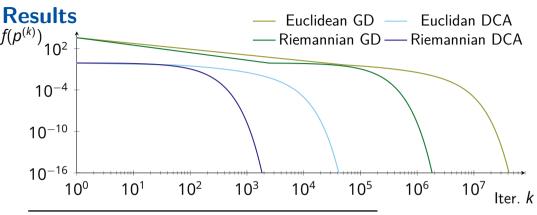
$$g(x) = a(x_1^2 - x_2)^2 + 2(x_1 - b)^2$$
 and $h(x) = (x_1 - b)^2$.

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

Stopping Criterion.

$$d_{\mathcal{M}}(p^{(k)}, p^{(k-1)}) < 10^{-16} \text{ or } \|\text{grad } f(p^{(k)})\|_p < 10^{-16}.$$





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
- Manifolds that are also groups: LieGroups.jl
- ▶ What is (Fenchel) duality on manifolds?



Selected References



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