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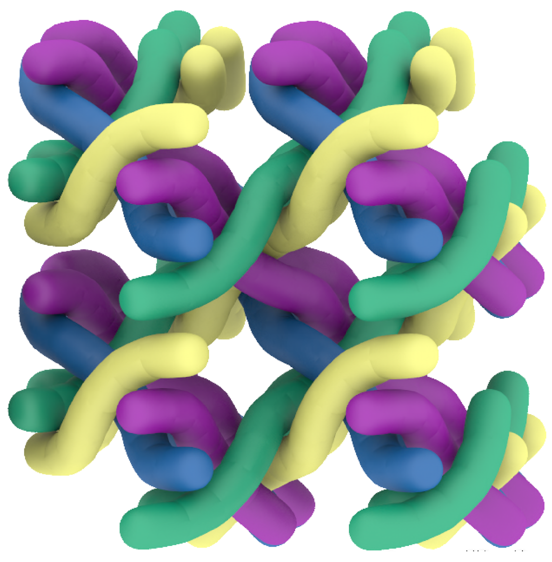
SFB TRR 109 Discretization in Geometry and Dynamics

Berlin Mathematical School BMS

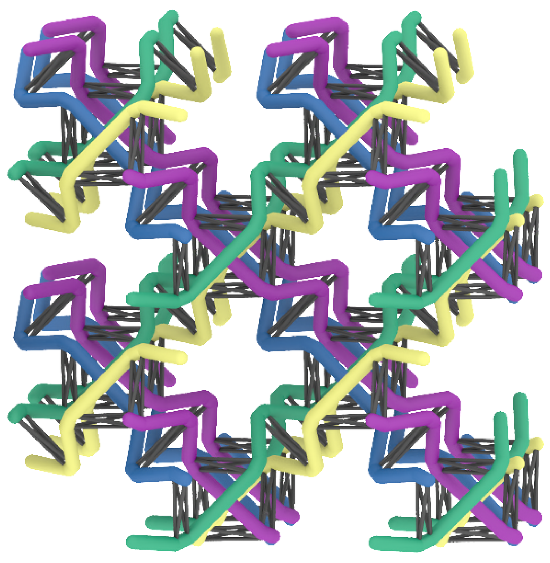
Riemannian Optimization and Algebraic Varieties – a Contradiction?†

Motivation

Curvilinear cylinder packings have been discussed extensively in relation to metal-organic frameworks, with some exhibiting fascinating expansive behavior under deformation[1]. They can be modeled using tensegrity frameworks[2], leading to a nonlinear optimization problem with algebraic constraints.



However, even in the simplest cases, these frameworks' variables live in $\mathbb{R}^{150}$, making global methods infeasible. Since we were unable to provide a suitable initialization for existing local methods, developing a new technique for equilibrating these structures becomes necessary.



Riemannian Geometry[3]

A **Riemannian manifold** is a pair $(\mathcal{M}, g)$ consisting of a smooth manifold $\mathcal{M}$ together with a smoothly varying symmetric positive definite bilinear form $g_x : T_x\mathcal{M} \times T_x\mathcal{M} \to \mathbb{R}$ for each $x \in \mathcal{M}$.

Any embedded submanifold $\iota : \mathcal{S} \hookrightarrow \mathcal{M}$ becomes Riemannian by inheriting the pullback metric $\iota^* g$. The **normal space** is

$$N_x(\mathcal{S}, \mathcal{M}) = \{v \in T_x\mathcal{M} \ : \ g_x(v, w) = 0 \ \forall w \in T_x\mathcal{S}\}.$$

We call a smooth curve $\gamma : I \to \mathcal{S}$ a **geodesic**, if its acceleration $\ddot{\gamma}(t) \in N_{\gamma(t)}(\mathcal{S}, \mathcal{M})$ for all $t \in I$. The corresponding **exponential map** is $Exp_p(v) = \gamma(1)$ for the unique geodesic with $\gamma'(0) = v$.

Moving on Manifolds

Definition: *Let $\mathcal{S} \hookrightarrow \mathcal{M}$ be an embedded Riemannian manifold and $x \in \mathcal{M}$. A **retraction** at x is a smooth map $R_x : T_x\mathcal{M} \to \mathcal{M}$ such that each curve $c(t) = R_x(tv)$ satisfies*

$$c(0) = x \text{ and } \dot{c}(0) = v.$$

*If additionally $\ddot{c}(0) \in N_x(\mathcal{S}, \mathcal{M})$, it is called 2^{nd}**-order**.*

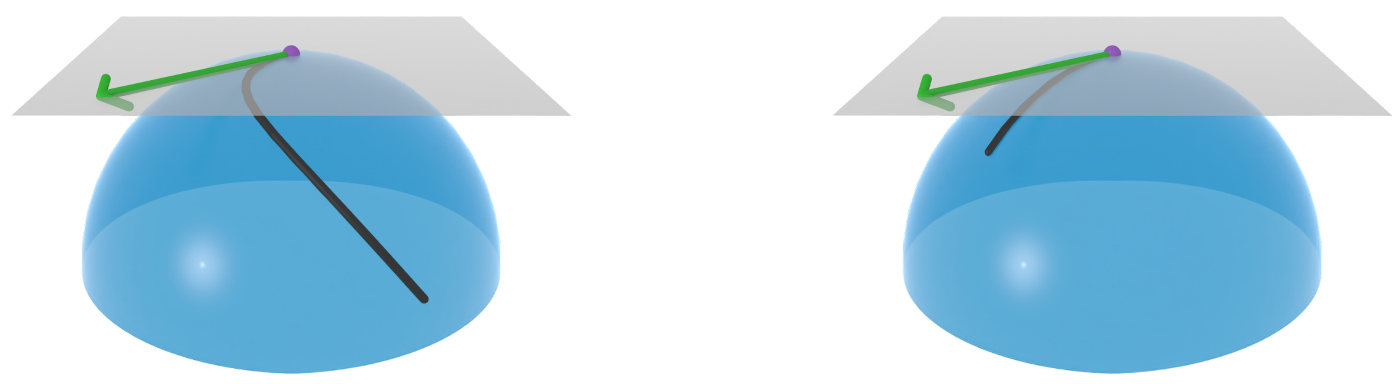


Figure: A first-order (l.) and a second-order retraction (r.) on a sphere.

Theorem[4]**:** *Let $\mathcal{M} \subset \mathbb{R}^n$ be a smooth manifold. For any point $p \in \mathcal{M}$, define the relation $R_p \subset T_p\mathcal{M} \times \mathcal{M}$ by*

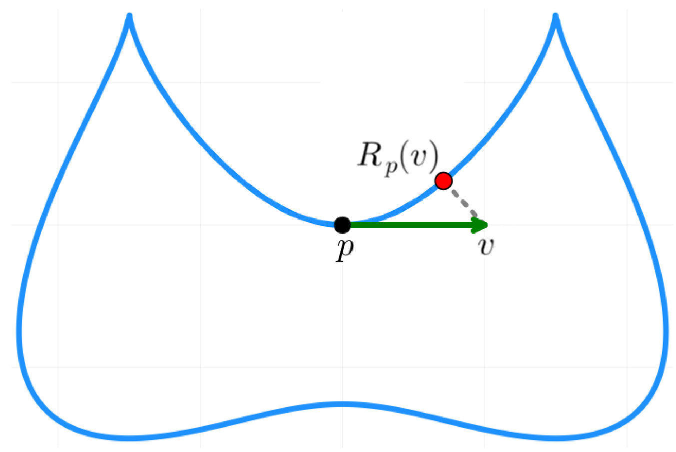
$$R_p = \{(v, u) \in \mathbb{R}^n \times \mathbb{R}^n \ : \ u \in \text{argmin}_{y \in \mathcal{M}} |p + v - y|\}.$$

There exists a neighborhood U of 0 in $T_p\mathcal{M}$ such that R_p defines a local, second-order retraction. I.e., the curve $t \mapsto R_p(tv)$ matches the geodesic at p corresponding to v up to second-order.

Implicit Formulation and Path-Tracking

The closest point problem:
For a smooth $\mathcal{M} = g^{-1}(0)$ in $\mathbb{R}^n$ and a fixed point $u \in \mathbb{R}^n$, the closest point problem can be expressed as

$$\min_x \frac{1}{2}|x - u|^2 \quad \text{s.t.} \ g(x) = 0.$$



In terms of Lagrange multipliers, this problem can be rewritten as

$$\mathcal{L}(x, \lambda; u) = \frac{1}{2}\sum_{i=1}^{n}(x_i - u_i)^2 + \lambda^T g(x).$$

We can "track" the known solution $x = p$ with a path $u : [0,1] \to \mathbb{R}^n$ from $u_1 = p$ to $u_0 = p + v$ via the straight-line homotopy

$$H(x, \lambda; t) = \nabla \mathcal{L}_{x,\lambda}(x, \lambda, (1-t)u_0 + tu_1),$$

using the predictor-corrector scheme of homotopy continuation[5].

Theorem[6]**:** *If g is C^3, $\mathcal{M} = g^{-1}(0)$ is smooth, dg_x has full rank and $u(t)$ is a smooth path staying within an explicitly defined tubular neighborhood of $\mathcal{M}$, then there exists a partition of $[0,1]$ that ensures convergence of the path-tracking method on each subinterval and outputs the correct critical point $R_p(v)$.*

Riemannian Optimization

Consider the constrained optimization problem

$$\min_{x \in \mathcal{M}} f(x) \quad \text{for a smooth} \quad f : \mathcal{M} \to \mathbb{R}.$$

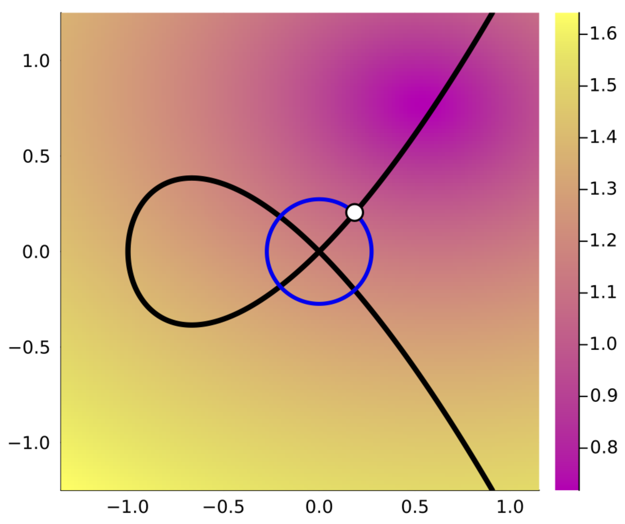
In order to solve the problem, similar to unconstrained optimization, local methods such as gradient descent can be employed[7]: Given a **descent direction** v_k satisfying the conditions from Zoutendijk's theorem[8] and a step size α_k satisfying the Wolfe conditions[8], the retraction is consecutively applied until f's Riemannian gradient is smaller than a given tolerance $\tau > 0$:

$$x_{k+1} = R_{x_k}(\alpha_k v_k) \quad \text{until} \quad ||\text{grad} f(x_k)|| < \tau.$$

Resolving the Contradiction: Algebraic Sets

Given an algebraic variety V, it is known that $V \setminus \text{Sing}(V)$ defines a smooth manifold. Therefore, the described methods work everywhere outside the singular locus. Still, in singularities all kinds of issues occur, the least of which is that the (Riemannian) tangent space is not properly defined.

Drawing inspiration from Hironaka's resolution of singularities, where each singularity is blown up and replaced by a $\mathbb{CP}^k$, we intersect V with a sphere of radius ε centered in the singularity. An intersection with codim -1 random hyperplanes results in finitely many points.



We choose the "best" point to continue the process, for instance, the point with the lowest objective function value. Finally, this results in the development of `HomotopyOpt.jl`[9], a software package for solving nonlinear optimization problems on algebraic sets.

†This project is joint work with Alexander Heaton, Lawrence University, Wisconsin.

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