An Invitation to Hadamard Space

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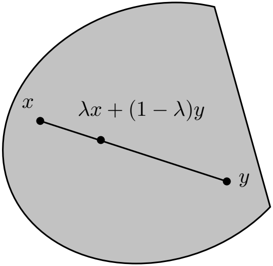
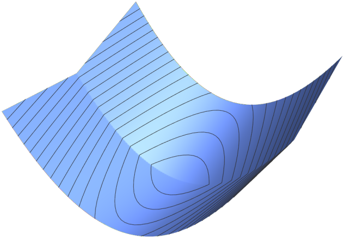
Applied Mathematics Student Colloquium

November 13th 2024

Convexity

$C \subseteq \mathbb{E}$ is **convex** if $\lambda x + (1-\lambda)y \in C$ for $x, y \in C, \lambda \in (0,1)$





$f(x,y) = |x| + y^2$

$f : \mathbb{E} \to (-\infty, +\infty]$ is **convex** if

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda) f(y) \quad \forall x, y \in \mathbb{E}, \lambda \in (0,1)$$

Convex Optimization

$$\min_{x \in C} f(x)$$

$f : \mathbb{E} \to (-\infty, +\infty]$ and $C \subseteq \mathbb{E}$ are both convex

Examples:

1. Linear programming (network flow)
2. Convex quadratic programming (regularized least squares)
3. Semidefinite programming (approximations for NP-hard problems)
4. Lagrangian relaxation (lower bounds for nonconvex problems)

Many **smooth** problems can be solved efficiently. . .

. . . and can use **subgradient** methods for structured **nonsmooth** problems

Euclidean Space is Nice

Euclidean spaces benefit from **duality**; (sub)gradients are dual objects
$v \in \mathbb{E}$ is a **subgradient** of $f : \mathbb{E} \to (-\infty, +\infty]$ at x if

$$f(y) \geq f(x) + \langle v, y - x \rangle \quad \text{for all } y \in \mathbb{E}$$

Inner product: convex functions and optimization problems come in pairs

Riemannian manifolds: inner product on tangent space $\Rightarrow$ subgradients

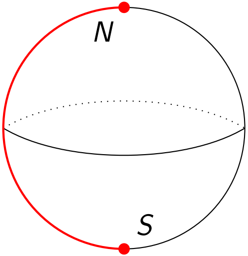
Can we succeed in spaces **without local linearity**?

Structure for Convex Optimization

Nonlinear spaces occur naturally in modeling various phenomena

Suppose (X, d) is a metric space.

1. What does convexity mean in X, and what functions are convex?
2. What structure should X have to sustain convex optimization?



$\mathbb{S}^n$ with *angular metric*:

$$\cos(d(x, y)) = \langle x, y \rangle$$

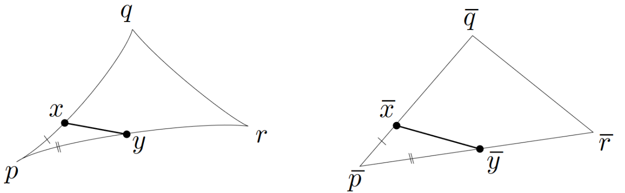
Hadamard Space

A **complete** metric space (X, d) where points connect via **geodesics** (isometries of compact intervals into X) that is **CAT(0)**, meaning $d(\cdot, y)^2$ is strongly convex for all $y \in X$, i.e.

$$t \mapsto d(\gamma(t), y)^2 - t^2 \text{ is convex for any geodesic } \gamma$$

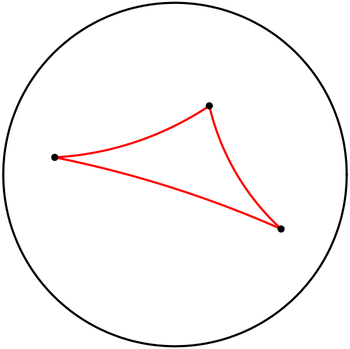
- CAT(κ) = "curvature bounded above by κ"
- Triangles in CAT(0) spaces are **skinny**
- Cosine law: $a = d(p, q), b = d(p, r), c = d(q, r)$,

$$c^2 \geq a^2 + b^2 - 2ab\cos(\angle([p, q], [p, r]))$$



Hyperbolic Space $\mathbb{H}^n$

The open unit ball $B^n \subseteq \mathbb{R}^n$ with $\cosh(d(x,y)) = 1 + \frac{2\|x-y\|^2}{(1-\|x\|^2)(1-\|y\|^2)}$

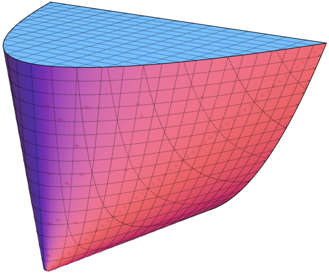


Geodesics are **circular arcs** intersecting boundary at right angles

Applications: Hierarchical data embedding (De Sa…'18), large-margin classification (Cho…'18)

Positive Definite Cone S^n_{++}

$n \times n$ positive definite matrices with $d(X, Y) = \| \log(X^{-1/2} Y X^{-1/2}) \|_{\text{Frob}}$



$$\begin{bmatrix} x & y \\ y & z \end{bmatrix} \succ 0$$

$$\Updownarrow$$

$$x + z > 0 \text{ and } xz - y^2 > 0$$

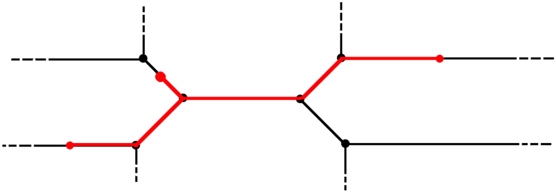
Why not **Euclidean metric**? Can also add $\det(X) = 1$ constraint

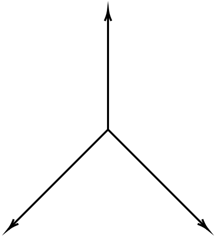
Applications: Matrix means (Bhatia. . . '12), diffusion tensor imaging (Pennec. . . '06)

Real Trees

Geodesic space where every triangle is a **tripod**

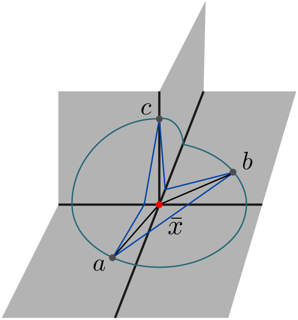
Ex: Trees (connected acyclic graphs) with positive real edge lengths

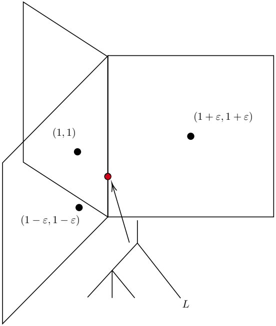




Applications: Facility location (Hansen. . . '87)

A **complex** X of **cells** – Euclidean cubes and their faces – each pair of cells sharing at most one face – is **CAT(0)** $\iff$ simply connected and **link condition** holds (Gromov '81)





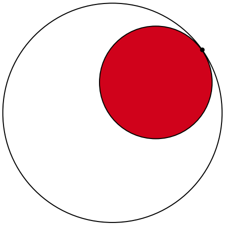
Applications: Phylogenetics (Billera-Holmes-Vogtmann '01), robot configurations (Ardila-Mantilla '20)

Basic Notions in Hadamard Space

- $C \subseteq X$ is **convex** if it contains all geodesics between its points
- The **convex hull** of $A \subseteq X$ is the smallest convex set containing A
- A function is **convex** if it is convex along every geodesic
- Any two points are connected by a **unique geodesic**

Q: Convex hull of $\{x, y\}$?

A: The **geodesic segment** $[x, y]$



A geodesically convex set in $\mathbb{H}^n$

Pulse Check

- Projections onto closed convex subsets exist uniquely **(Yes)**
- The closed convex hull of finitely many points is compact **(?)**
- The convex hull of n points is at most $n-1$ dimensional **(No)**
- Real-valued convex functions are continuous **(No)**
- Balls are convex **(Yes)**
- $C \subseteq X$ is *Chebyshev* if each $x \in X$ has a unique closest point in C. Are closed Chebyshev sets convex? **(? in Hilbert, No in Hadamard)**
- Geodesics extend uniquely to rays **(No)**

Weighted Means in Hadamard Space

Natural Questions

Let (X, d) be a Hadamard space, and let $A = \{a_1, \ldots, a_m\} \subseteq X$.

1. What does the convex hull of A look like?
2. Can we compute **weighted means** of A, defined by

$$\operatorname*{argmin}_{x \in X} \sum_a w_a d(x, a)^2$$

   where $w \geq 0$?

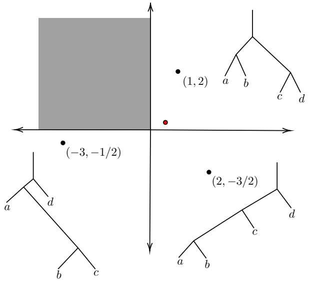
3. How quickly can we solve these problems?

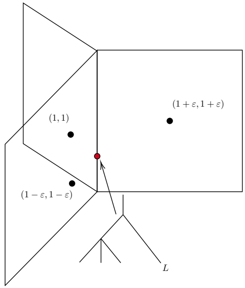
Medians of Phylogenetic Trees

Given several **binary trees**, how to compare or average them?

The **BHV Tree Space** $\mathcal{T}_n$ is a metric space whose points are binary trees on n (labelled) leaves, with $n-2$ non-negative internal edge lengths

$\mathcal{T}_n$ is Hadamard – it's a CAT(0) cubical complex





Geodesics are computable in **polynomial time** (Owen-Provan '12)

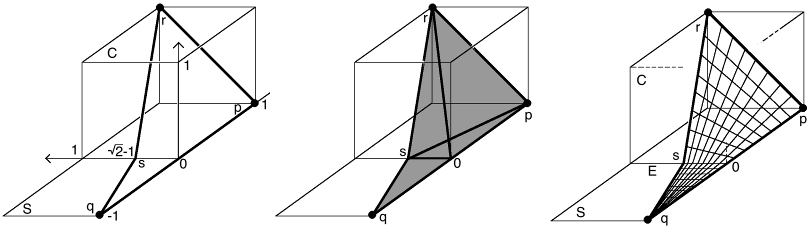
Averaging Finite Sets

In **Euclidean space**, can characterize convex hulls of finite sets:

$$x \in \operatorname{conv} A \iff \text{there exists } 0 \neq w \geq 0 : x \text{ minimizes } \sum_a w_a d(\cdot, a)^2$$

Theorem 1 (Weighted averages vs convex combinations)

A point $\bar{x}$ minimizes $\sum_a w_a d(\cdot, a)^2$ for some weight vector $0 \neq w \geq 0$ if and only if $\bar{x}$ minimizes the **test function** $\max_a \{d(\cdot, a) - d(\bar{x}, a)\}$. *In that case $\bar{x} \in \operatorname{conv} A$ (but the converse fails outside $\mathbb{R}^n$).*

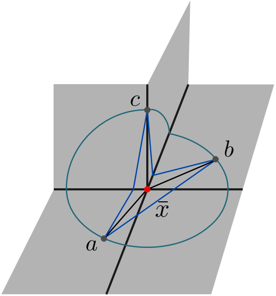


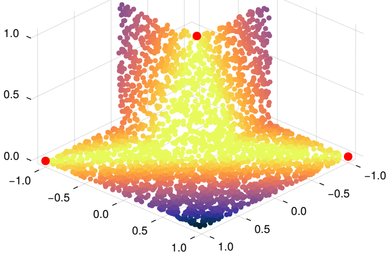
Recognizing Weighted Means

Strategy: Quantify whether $\bar{x}$ is a mean of A by computing an *optimality measure* of the convex test function $\max_a \{d(\cdot, a) - d(\bar{x}, a)\}$

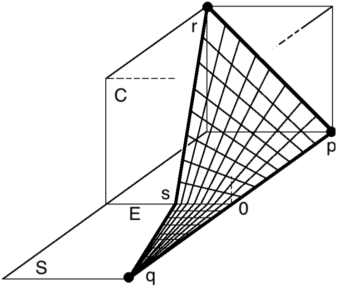
Assume geodesics $[\bar{x}, a]$ extend to rays. These rays, traversed at speed $d(\bar{x}, a)$, give rise to "cone of tangents" $T_{\bar{x}}X$ ($\underline{[\bar{x}, a]}$ is a **tangent**). If $T_{\bar{x}}X \cong \mathbb{R}^n$ (e.g. X is a manifold) then the test function has **slope**

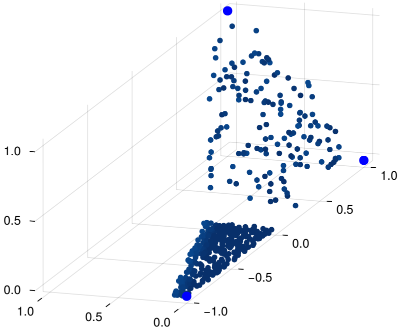
$$\operatorname{dist}\left(0, \operatorname{conv}\left\{\underline{[\bar{x}, a]} \mid a \in A\right\}\right)$$





Detecting Mean Sets





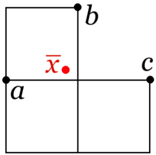
Convex Optimization on Cubical Complexes

Computing Means

Mean of A: $\bar{x} = \text{argmin}_{y \in X} \sum_a d(y,a)^2 =: \phi(y)$

Restrict ourselves to CAT(0) cubical complexes. Can we compute means?
Yes, but very **slowly**... cyclic algorithm (Bačák '14)

for $k = 1, 2, \ldots$ $x \in \frac{k}{k+1} x + \frac{1}{k+1} \{a, b, c\}$



Geodesics are **polynomial time** (Hayashi '21)

Cells are typically **low-dimensional**

Algorithm: Given current point x and list Ω of optimized cells
repeat

- Choose cell $P \notin \Omega$ containing x
- $x = \text{argmin}_P \, \phi$ **???**

A Single Subgradient

Strategy: Solve a Euclidean optimization problem on each cell using good subgradient algorithms **(cutting plane methods)**

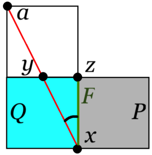
In CAT(0) cubical complex, consider points $a \neq x \in$ cell $P \subseteq \mathbb{R}^n$

Idea: at x, find a (Euclidean) **subgradient** for the function

$$z \in \mathbb{R}^n \mapsto \begin{cases} d(z,a), & z \in P \\ +\infty, & z \notin P \end{cases}$$

Solution: Suppose geodesic $[x,a]$ has initial segment $[x,y]$ in cell Q. Project y onto its nearest point z in the face F shared by P and Q. Then one subgradient at x is

$$\cos(\angle yxz)\frac{x-z}{\|x-z\|}$$

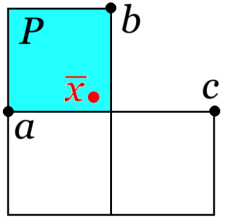


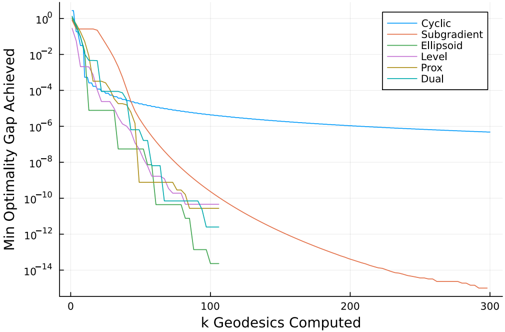
Fast Mean Computation

Minimize over cell P

$$d(\cdot, a)^2 + d(\cdot, b)^2 + d(\cdot, c)^2$$

Compare cutting planes vs cyclic





For the Curious

For those interested in. . .

- **Optimization:** *Convex Analysis and Optimization on Hadamard Spaces*, M. Bačák
- **Geometric Group Theory, Topology:** *Metric Spaces of Non-Positive Curvature*, M. Bridson and A. Haefliger
- **Probability:** *Probability Measures on Metric Spaces of Nonpositive Curvature*, K.-T. Sturm

Recent work with A.S. Lewis, G. López-Acedo, and A. Nicolae:

- Recognizing weighted means in geodesic spaces (arXiv:2406.03913)
- Convex optimization on CAT(0) cubical complexes (arXiv:2405.01968)