An SDP relaxation for computing distances between metric spaces

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Ongoing work with:
Afonso Bandeira (MIT, NYU)
Andrew Blumberg (UT Austin)
Rachel Ward (UT Austin)

SIAM Imaging

May 23, 2016

Outline and References

- Gromov-Hausdorff distance.
  - Facundo Mémoli. On the use of Gromov-Hausdorff Distances for Shape Comparison.
- SDP relaxation of Gromov-Hausdorff distance.
  - Ongoing work with Afonso Bandeira, Andrew Blumberg and Rachel Ward.
- Numerical performance on real data.
  - Boyer, Lipman, Daubechies, et al. Algorithms to automatically quantify the geometric similarity of anatomical surfaces.
  - Yang, Sun and Toh. SDPNAL+: a majorized semismooth Newton-CG augmented Lagrangian method for semidefinite programming with nonnegative constraints.
- Future work.

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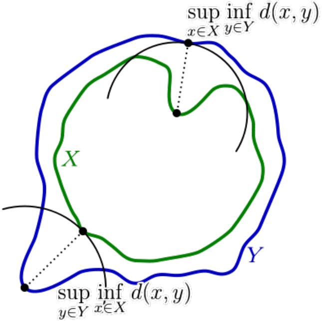
The Hausdorff distance

Let X, Y compact sets of a metric space. Define

$$\begin{aligned} d(x, Y) &= \inf\{d(x,y) : y \in Y\} \\ d(X, Y) &= \sup\{d(x,Y) : x \in X\} \end{aligned}$$



$$d_H(X, Y) = \max\{d(X, Y), d(Y, X)\}$$

The Gromov-Hausdorff distance

Let X, Y compact metric spaces. Define

$$d_{GH}(X, Y) = \inf_{Z,f,g} d_H(f(X), g(Y))$$

where $f : X \to Z, \quad g : Y \to Z$ are isometric embeddings.

Fact: $d_{GH}(X, Y) = 0$ if and only if X, Y are isometric

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Gromov-Hausdorff distance in point clouds

Motivations

- Shape comparison of geometric objects (like surfaces).
- Applications to spaces where geometry is less apparent (like tree spaces, dna sequences, etc).

Quadratic assignment formulation (Mémoli 2007)

Let $X = \{x_1, \ldots, x_n\}$, $Y = \{y_1, \ldots, y_m\}$.

Let $R \subset X \times Y$ and $\delta_{ij} = \begin{cases} 1 & \text{if } (x_i, y_j) \in R \\ 0 & \text{otherwise} \end{cases}$

Let $\Gamma_{ik,jl} = |d_X(x_i, x_k) - d_Y(y_j, y_l)|$

$$d_{GH}(X, Y) = \frac{1}{2} \quad \min_R \quad \max_{ik,jl} \Gamma_{ik,jl} \delta_{ij} \delta_{kl}$$

$$\text{subject to} \quad \delta_{ij} \in \{0, 1\}, \ \sum_{j=1}^{m} \delta_{ij} \geq 1, \ \sum_{i=1}^{n} \delta_{ij} \geq 1$$

Fact: Computing GH distance is NP-hard and also, to approximate it better than a factor of 3 is NP-hard (Agarwal et al 2015).

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Gromov-Wasserstein distance (Mémoli 2007)

$$D_{GW,p}(X,Y) = \frac{1}{2}\left(\inf_{\delta}\sum_{i,j}\sum_{k,l}\Gamma^{p}_{ik,jl}\delta_{ij}\delta_{kl}\right)^{1/p} \quad \sum_{i}\delta_{ij}=1, \sum_{j}\delta_{ij}=1$$

- In this formulation δ's are thought as probability measures on the set of points ($\delta' s$ do not come from a map).
- The max is changed for a sum.
- Mémoli considers a spectral relaxation of the Gromov-Wasserstein distance using heat kernels.

An SDP relaxation of the Gromov-Hausdorff distance

Focus on case $|X| = |Y|$.

$$\tilde{d}(X,Y) = \quad \min_Z \quad \sum_{i,j,k,l} \Gamma_{ik,jl} Z_{ij,kl}$$

$$\text{subject to} \quad \sum_{i=1} X_{ij,ij} = 1 \text{ for all } j$$

$$\sum_{j=1} Z_{ij,ij} = 1 \;\text{ for all } i$$

$$Z_{ij,il} = 0, \text{ for all } i,j,l \text{ with } l \neq j,$$

$$Z_{ij,kj} = 0, \text{ for all } i,j,k \text{ with } i \neq k,$$

$$Z_{ij,kl} \geq 0, \quad Z \succeq 0$$

$$\sum_i Z_{ij,N^2+1} = 1 \text{ for all } j,$$

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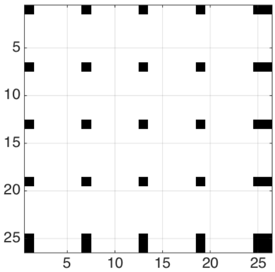
$$Z_{N^2+1,N^2+1} = 1$$



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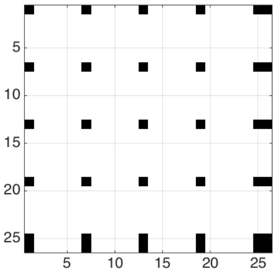

Some properties of $\tilde{d}$

- $\tilde{d}(X, Y)$ is a lower bound for a distance between metric spaces.
- $\tilde{d}(X, Y) \leq \tilde{d}(X, W) + \tilde{d}(W, Y)$
- $\tilde{d}(X, Y) = 0$ if X and Y are isometric, and the SDP finds the isometry.
  - Numerically we observe stability with respect to noise.
- $\tilde{d}(X, Y)$ may be 0 for non isometric X and Y.
  - Graph isomorphism problem can be posed as deciding whether GH distance between graphs is zero.

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Numerical considerations

Computing $\tilde{d}$ involves solving a big SDP!

- Improving SDP solvers is an active research area.
- Work around with sampling, good initializations, etc.
- SDP's and dual certificates can be used to obtain fast algorithms (see Dustin's talk tomorrow).

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Real data application

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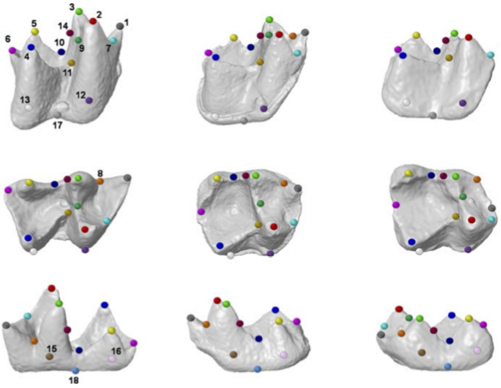

Real data application

Objective: teeth classification.
Two methods:

1. Lipman and Daubechies map the teeth surfaces to the hyperbolic disk and consider a Wesserstein distance that is invariant under conformal transformations.
2. Boyer labels 18 landmarks on each teeth. Then they find the best rigid transformation to match the labeled landmarks.

Assessment: They consider 116 teeth. For each teeth find the closest teeth according to each distance, and see whether they are in the same category.

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Real data application

Our experiments

- Consider $X_i = \{p^i_1, \dots p^i_{18}\}$ $i = 1 \dots 116$.
- Find $\tilde{d}(X_i, X_j)$
- Use their classification scheme

Future work

- Understand topological properties of this SDP-induced distance on the set of finite metric spaces.
  - Convergence
  - Compactness
- Applications to datasets that are not surfaces.
- Understand how the distance behaves with respect to sampling under geometric assumptions.
- Compare with other lower bounds available in the literature.

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Questions?

Tomorrow:
MS22: Convex Signal Recovery from Pairwise Measurements

10:30-10:55. Dustin Mixon. *Probably Certifiably Correct K-Means Clustering*.

11:00-11:25. Soledad Villar. *Efficient Global Solutions to K-Means Clustering Via Semidefinite Relaxation*