VRDI TDA Breakout Session: Applications of Topological Data Analysis

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Voting Rights Data Institute
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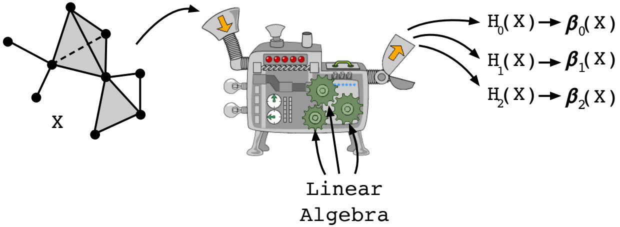
Quick Review of TDA

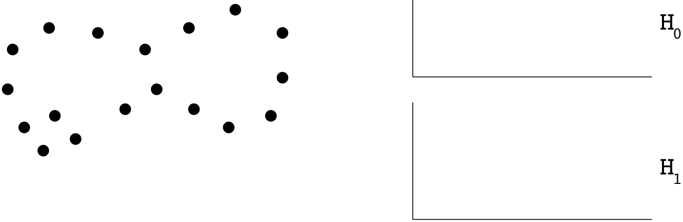
Topology studies geometrical objects (called spaces) up to a loose notion of equivalence.

Algebraic topology distinguishes spaces by computing invariants; e.g., Betti numbers $\beta_k(X)$ count k-dimensional holes in a space X.

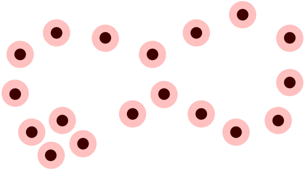

X
$H_0(X) \rightarrow \beta_0(X)$
$H_1(X) \rightarrow \beta_1(X)$
$H_2(X) \rightarrow \beta_2(X)$
Linear Algebra

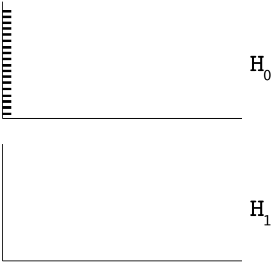
Topological Data Analysis explores the shape of a dataset (e.g. a point cloud in $\mathbb{R}^d$) by computing invariants across a family of spaces generated from the dataset.

Persistent Homology - An Example



Persistent Homology - An Example





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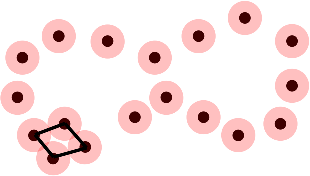

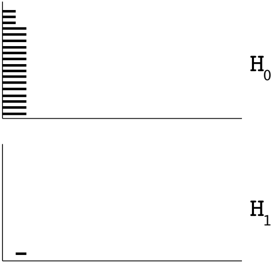

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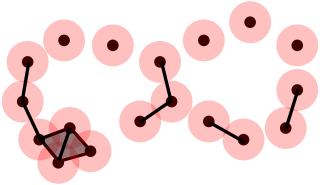
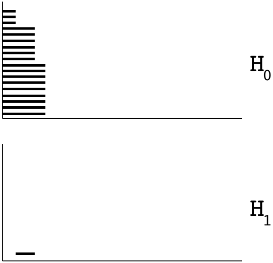
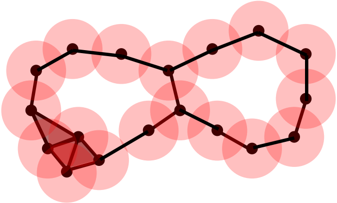
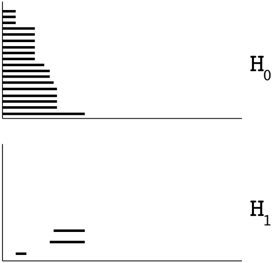


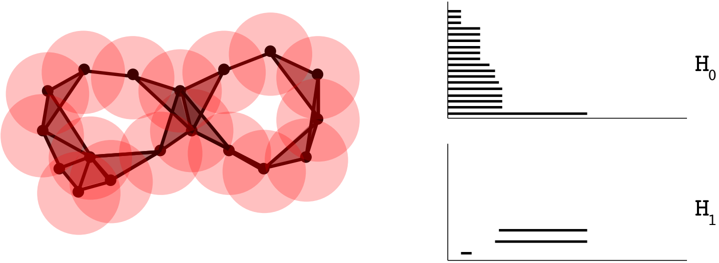


Persistent Homology - An Example

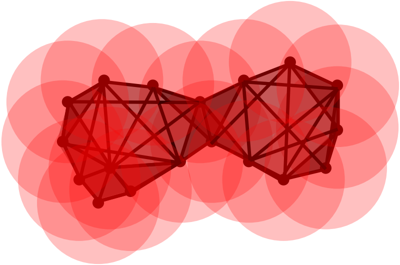


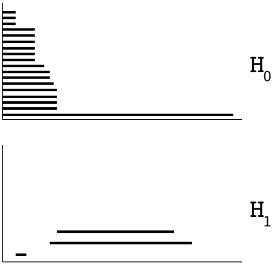


Persistent Homology - An Example



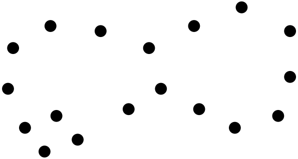
Persistent Homology - An Example



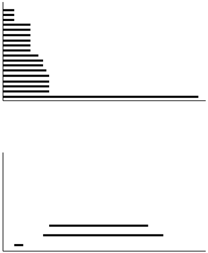


Terminology

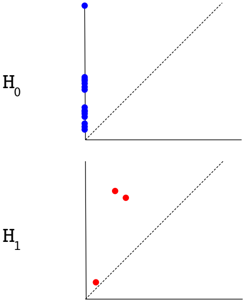
We can record the "birth time" and "death time" of each topological feature to get a barcode or a persistence diagram.



Dataset X



Barcodes for X



Persistence Diagrams for X

Distance Between Diagrams

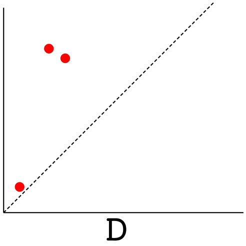
Important piece of the story: comparing persistence diagrams.

Each diagram D is a set[1] of points

$$D = \{(b_i, d_i)\}_{i=1}^{N}$$

with each $b_i < d_i$. Each point in D represents a topological feature of a dataset.

Let $\mathcal{D}$ denote the set of all diagrams.



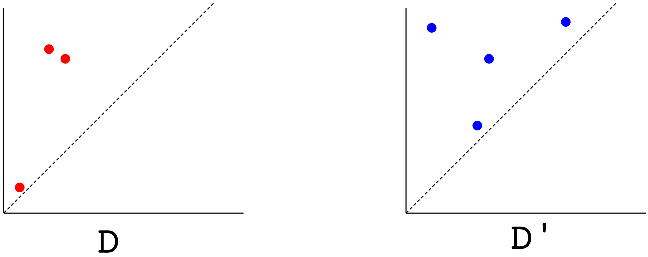
[1] Actually it's a multiset, but let's ignore that...

Metric on Diagrams

We wish to define a metric on $\mathcal{D}$.

This is a function $d : \mathcal{D} \times \mathcal{D} \to \mathbb{R}_{\geq 0}$ satisfying:

- (Positivity) $d(D, D') = 0 \Leftrightarrow D = D'$
- (Symmetry) $d(D, D') = d(D', D)$
- (Triangle Inequality) $d(D, D'') \leq d(D, D') + d(D', D'')$.



How "close"?

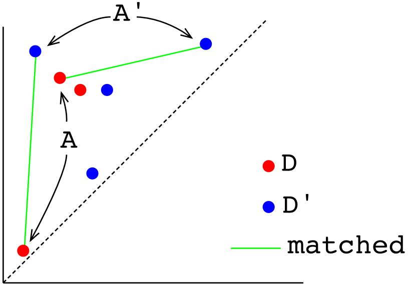
Idea: Match Features

Given diagrams D, D', we want to match points as best as possible.

Problem: diagrams might have a different number of points! So we can't expect a perfect matching.

Let $\phi : A \to A'$ be a bijection, where $A \subset D$ and $A' \subset D'$.

This is called a partial matching.



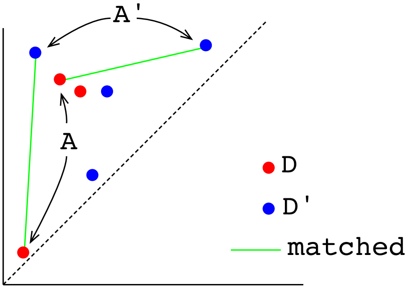
Idea: Match Features

Pick a matching cost c_m (TBD).

For each $p = (b, d) \in A$, we evaluate $c_m(p, \phi(p))$.

Pick a cost for unmatched points c_u (TBD).

For each $p \in D \setminus A$ and each $p' \in D' \setminus A'$, we evaluate $c_u(p)$ and $c_u(p')$.



Idea: Match Features

For a partial matching ϕ, we evaluate the total cost:

$$\mathrm{TC}(\phi) = \max\left\{\max_{p \in A} c_m(p, \phi(p)), \max_{p \notin A} c_u(p), \max_{p' \notin A'} c_u(p')\right\}.$$

Define a metric as min over all partial matchings

$$d(D, D') = \min_{\phi} \mathrm{TC}(\phi).$$

For theoretical reasons, choose costs for $p = (b, d)$ and $p' = (b', d')$ as

$$c_m(p, p') = \max\{|b' - b|, |d' - d|\}, \quad c_u(p) = \frac{d - b}{2}.$$

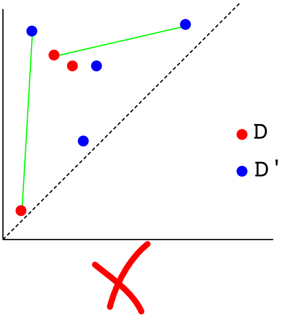
Bottleneck Distance

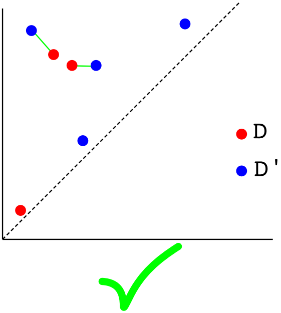
The bottleneck distance between persistence diagrams D and D' is

$$d_b(D, D') = \min_{\phi} \max \left\{ \max_{p \in A} c_m(p, \phi(p)), \max_{p \notin A} c_u(p), \max_{p' \notin A'} c_u(p') \right\}$$

with min over partial matchings and

$$c_m(p, p') = \max\{|b' - b|, |d' - d|\}, \quad c_u(p) = \frac{d - b}{2}.$$





Applications

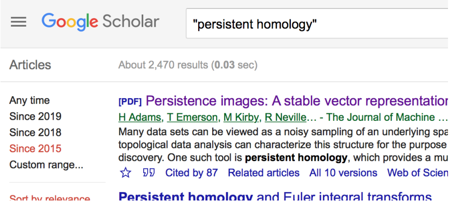
Question

So what is this actually good for?

Let’s look at some interesting examples of TDA “in action".

Disclaimer

This is very far from an exhaustive list!



About 2,470 results (**0.03** sec)

[PDF] Persistence images: A stable vector representatior

H Adams, T Emerson, M Kirby, R Neville… - The Journal of Machine …

Many data sets can be viewed as a noisy sampling of an underlying spa
topological data analysis can characterize this structure for the purpose
discovery. One such tool is **persistent homology**, which provides a mu

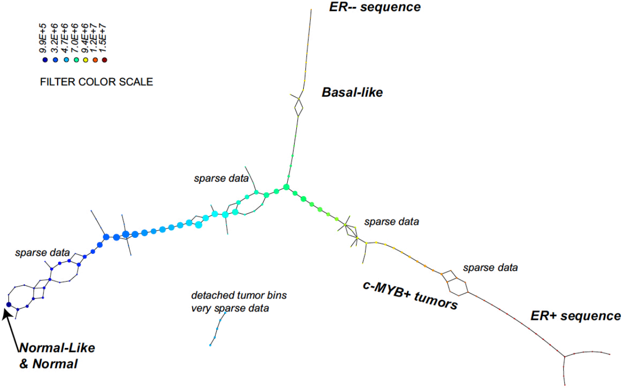
Persistent homology and Euler integral transforms

The applications are skewed toward my own interests and things which I think might be relevant to the districting problem.

Biomedicine

Topology based data analysis identifies a subgroup of breast cancers with a unique mutational profile and excellent survival

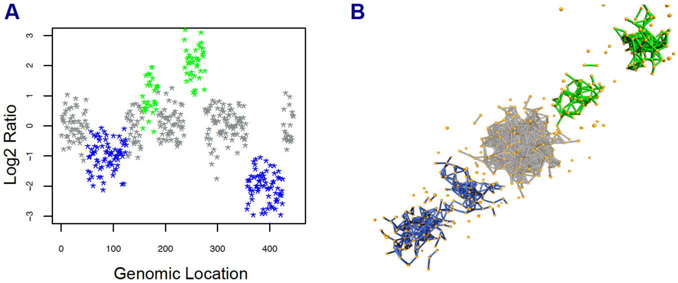
Nicolau, Levine, Carlsson, 2011.



Biomedicine

Identification of Copy Number Aberrations in Breast Cancer Subtypes Using Persistence Topology

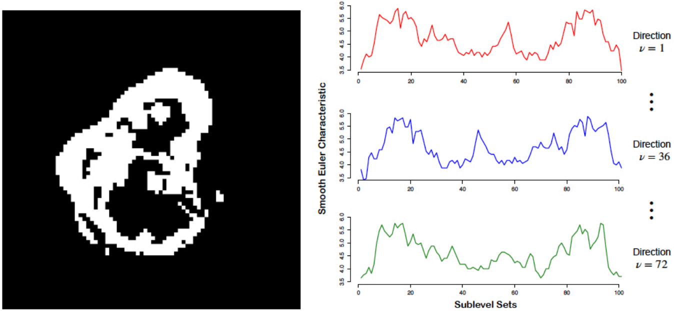
Arsuaga, Borrman, Cavalcante, Gonzalez, Park, 2015



Biomedicine

Functional Data Analysis using a Topological Summary Statistic: the Smooth Euler Characteristic Transform

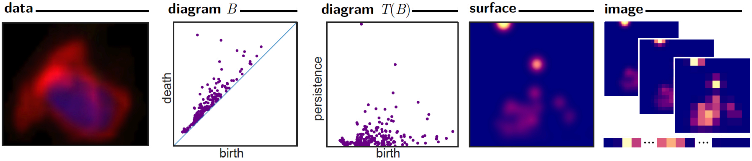
Crawford, Monod, Chen, Mukherjee, Rabadán, 2019



Machine Learning

Extracting Feature Vectors with TDA

- Persistence Landscapes, Bubenik, 2015
- Persistence Images, Adams et. al. 2016



TDA Layers in Neural Networks

- Brüel-Gabrielsson et. al. 2019
- Carrieère et. al. 2019

Studying the Structure of Neural Networks

- Guss, Salakhutdinov, 2018
- Rieck et. al. 2019

Shape Analysis

Persistent Homology Transform for Modeling Shapes and Surfaces

Turner, Mukherjee, Boyer, 2013

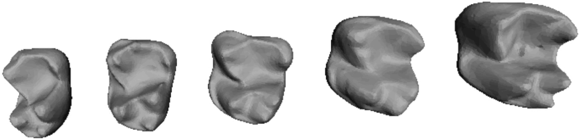


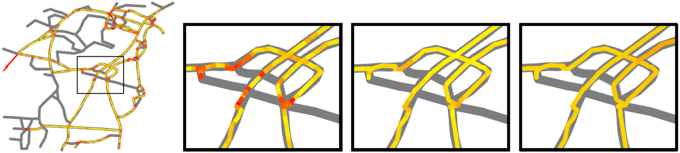
Figure 1: Images of the meshes of five teeth. A common problem in morphology is to measure distances between these five teeth.

Continued in:
Curry, Mukherjee, Turner, 2018
Ghrist, Levanger, Mai, 2018

Shape Analysis

Local Persistent Homology Based Distance Between Maps

Ahmed, Fasy, Wenk, 2014



(a) Local Homology (b) LH Detailed View (c) Hausdorff (d) Fréchet

Shape Analysis

Gromov-Hausdorff Stable Signatures for Shapes using Persistence

Chazal, Cohen-Steiner, Guibas, Mémoli and Oudot, 2009

Theorem

Let (X, d_X) and (Y, d_Y) be finite metric spaces. Let $D_k(X)$ and $D_k(Y)$ be the persistence diagrams for the k-dimensional persistent homology of their Vietoris-Rips complexes. Then

$$d_b(D_k(X), D_k(Y)) \leq d_{GH}(X, Y),$$

where d_{GH} denotes Gromov-Hausdorff distance.