Point Clouds of Varieties and Persistent Homology

Mikael Vejdemo-Johansson (St. Andrews)
Jon Hauenstein (Texas A&M)
David Eklund (KTH)
Martina Scolamiero (KTH)
Chris Peterson (Colorado State)
Primoz Skraba (Jožef Stefan Institute)

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Outline

Generating point clouds on varieties

Homotopy methods yield points of varieties by numerical solution of the defining equations.

Explicit implementation in `Bertini`, by Dan Bates, Jon Hauenstein, Andrew Sommese and Charles Wampler.

By intersecting variety with random hyperplanes, sample points on complementary dimensional components can be guaranteed.

Most important fact here

We can generate point clouds from varieties.

Topology of point clouds

Basic problem

Given a finite point sample X from a metric space $\mathbb{X}$, infer topological properties of $\mathbb{X}$ using only the data in X.

There is a method to approach this problem: *persistence*.

Topology of point clouds

Fundamental pipeline

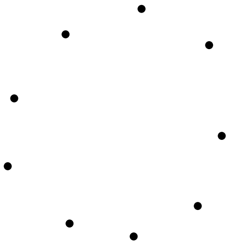
$$\boxed{\text{Point sample } X} \xrightarrow{\text{Čech or Vietoris-Rips complex}} \boxed{\text{Filtered simplicial complex } S_*X} \xrightarrow{\text{Persistence algorithm}} \boxed{\text{Persistent homology } H_*^{pers}(S_*X)}$$

Filtered simplicial complex construction

Definition

The Vietoris-Rips complex is an abstract simplicial complex $VR_\epsilon(X)$ for $\epsilon \in \mathbb{R}_+$ and X a finite metric space:

- Contains one vertex for each element in X.
- Contains a simplex $(x_0, \ldots, x_k)$ exactly when $d(x_i, d_j) < \epsilon$ for all $i, j \in [k]$.



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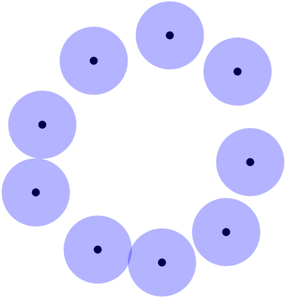

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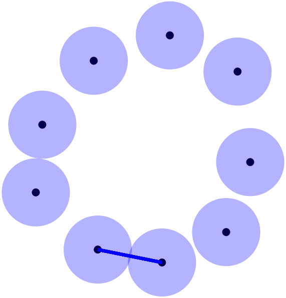

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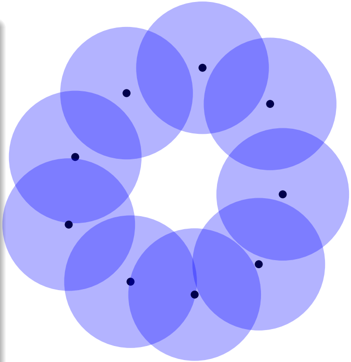

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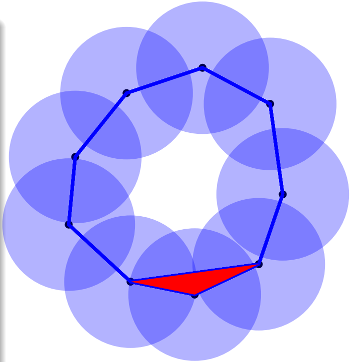


Persistent homology

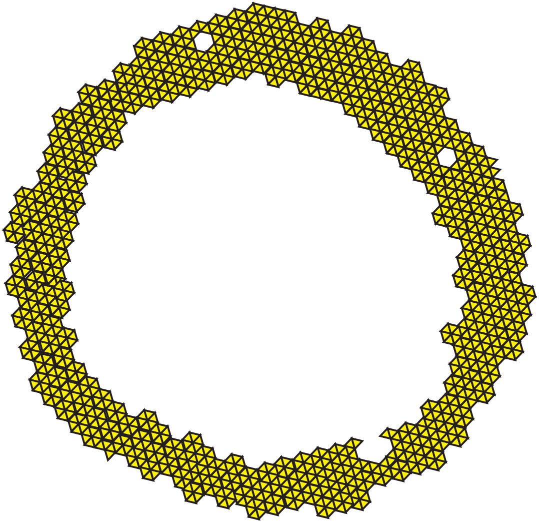
S_* a filtered simplicial complex: $\cdots \subseteq S_i \subseteq S_{i+1} \subseteq \ldots$

Apply homology to each S_n; produces a diagram:
$\cdots \to H_*S_i \to H_*S_{i+1} \to \ldots.$

In the resulting diagram, we can track basis elements as long as they remain independent.

Algorithm originally described by Edelsbrunner–Letscher–Zomorodian.

Basis elements that survive long are important



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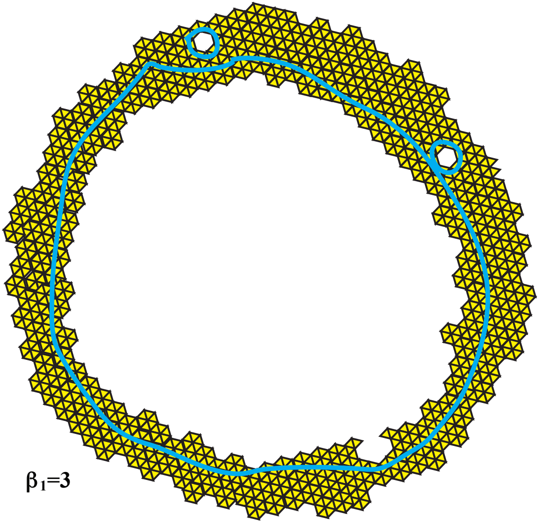

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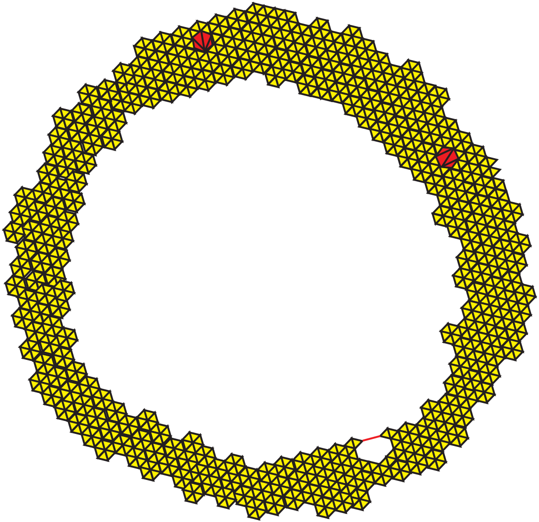

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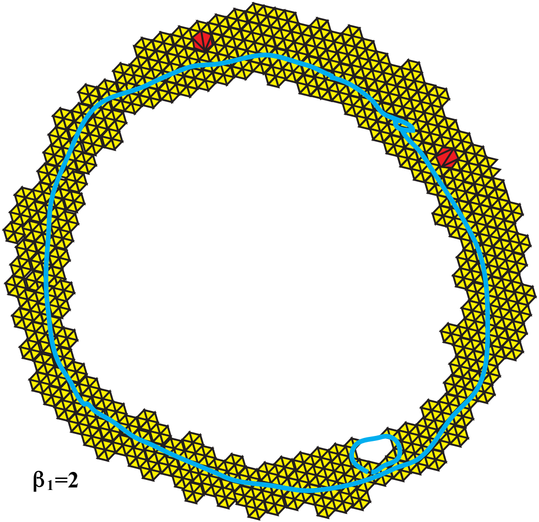


First failures

First attempts at explicit computation had several failure points:

- Large computation: only managed to finish computations on the large-memory clusters at Texas A&M. Consumption running up to 30-40G.
- Sampling conditions: even with this much memory, we still couldn't get the right homological signature on known data, likely due to uneven sampling.

Outline

Decompose the variety

We can easily compute both $V(f)$ and $V_{Sing}(f)$.

If the singularities have codimension 1, they decompose the smooth points into several components.

- Compute points on $V(f)$ and on $V_{Sing}(f)$. Let $C = \{x \in V(f), d(x, V_{Sing}(f)) < \varepsilon\}$.
- Cluster the points in $V(f) \setminus C$.
- For each cluster X_i from above:
  - Cluster $C \cup X_i$.
  - Form patches from clusters of $C \cup X_i$ that do not include into C.
- Compute homology on each patch, and each patch intersection. Patch intersections are all contained in C by construction.

This data suffices to reconstruct $H_*(V(f))$.

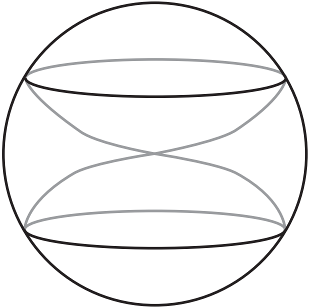
Worked example: Cyclo-octane configurations

Working to replicate an analysis in *Topology of cyclo-octane energy landscape* (Martin, Thompson, Coutsias, Watson; J. Chem. Phys. **132**, 234115 (2010)), we consider cyclo-octane as a linkage. Martin-Thompson-Coutsias-Watson established the topology of this to be a sphere and a Klein bottle, fused along two circles. They also computed the Betti numbers to be $\beta_0 = 1$, $\beta_1 = 1$, and $\beta_2 = 2$.

Requiring rest-state distances between atoms, and rest-state planar angles for carbon-carbon bonds, the resulting linkage has only rotational joints at each carbon atom.

We sampled 34k points from the resulting variety, and are using this as a test-case for a systematic method for the computation.

Decomposing the space



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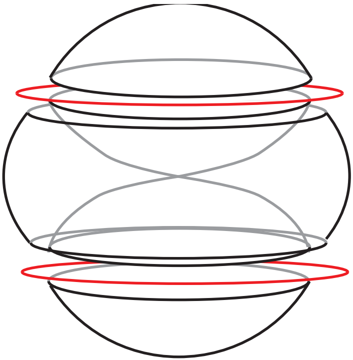

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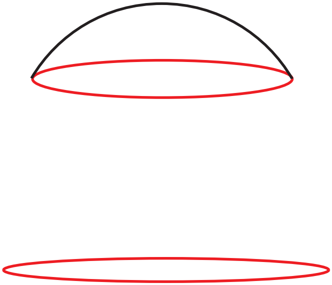

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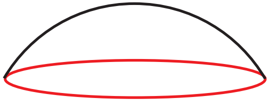
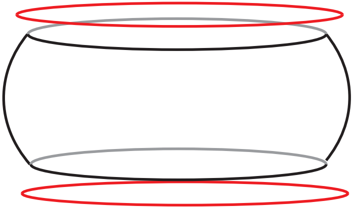


P_1

Decomposing the space



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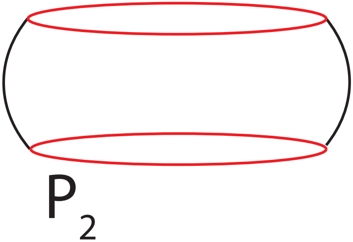

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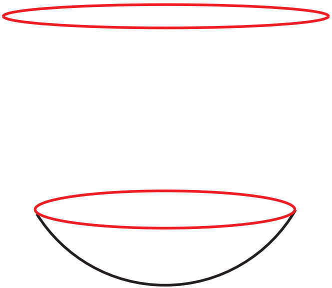
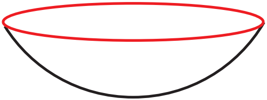


Decomposing the space

P_3



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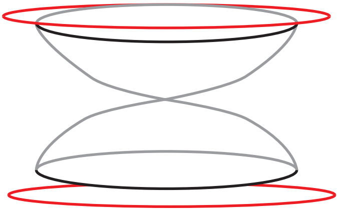

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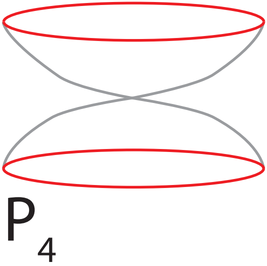

Spectral sequences to the rescue

We can glue these pieces together. We use the topological techniques of *spectral sequences* to generalize Mayer-Vietoris to several pieces.

Ongoing research with Primoz Skraba on building parallelization techniques from this approach.

Mayer-Vietoris spectral sequence

E^0:

$$\begin{array}{ccc}
\bigoplus_{i,j,k} C_2 P_i \cap P_j \cap P_k & \bigoplus_{i,j} C_2 P_i \cap P_j & \bigoplus_i C_2 P_i \\
\downarrow & \downarrow & \downarrow \\
\bigoplus_{i,j,k} C_1 P_i \cap P_j \cap P_k & \bigoplus_{i,j} C_1 P_i \cap P_j & \bigoplus_i C_1 P_i \\
\downarrow & \downarrow & \downarrow \\
\bigoplus_{i,j,k} C_0 P_i \cap P_j \cap P_k & \bigoplus_{i,j} C_0 P_i \cap P_j & \bigoplus_i C_0 P_i
\end{array}$$

Mayer-Vietoris spectral sequence

E^1:

$$\bigoplus_{i,j,k} H_2 P_i \cap P_j \cap P_k \longrightarrow \bigoplus_{i,j} H_2 P_i \cap P_j \longrightarrow \bigoplus_i H_2 P_i$$

$$\bigoplus_{i,j,k} H_1 P_i \cap P_j \cap P_k \longrightarrow \bigoplus_{i,j} H_1 P_i \cap P_j \longrightarrow \bigoplus_i H_1 P_i$$

$$\bigoplus_{i,j,k} H_0 P_i \cap P_j \cap P_k \longrightarrow \bigoplus_{i,j} H_0 P_i \cap P_j \longrightarrow \bigoplus_i H_0 P_i$$

Mayer-Vietoris spectral sequence

E^2:

$$\begin{tikzcd}
0 & 0 & 0 \\
0 \arrow[urr] & \mathbb{k}^2 & 0 \\
0 \arrow[urr] & \mathbb{k} & \mathbb{k}
\end{tikzcd}$$

Mayer-Vietoris spectral sequence

E^2:

$$
\begin{array}{cccc}
 & & & H_2 = \Bbbk^2 \\
0 & 0 & 0 & \\
 & & & H_1 = \Bbbk \\
0 & \Bbbk^2 & 0 & \\
 & & & H_0 = \Bbbk \\
0 & \Bbbk & \Bbbk &
\end{array}
$$

Questions?

In summary:

- Numerical algebraic geometry produces point clouds from varieties.
- Persistent homology produces Betti number estimates from point clouds.
- Computations end up being large and difficult.
- Classical topology techniques might save the day.