Point Clouds of Varieties and Persistent Homology

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Running problem

Can we find topological properties of algebraic varieties?

Given defining equations, can we find Betti numbers? Euler characteristic? Homology or cohomology representatives?

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Given defining equations, can we find Betti numbers? Euler characteristic? Homology or cohomology representatives?

Turns out to be hard algebraically. There are Gröbner basis methods, but they are only feasible in low ambient and intrinsic dimension.

Point cloud computation

Algebraic geometry

Numerical methods generate points on varieties. Repeat many times yields point clouds on varieties.

- Homotopy continuation
- Gradient descent methods

Algebraic topology

Persistence techniques estimate topological features from point clouds.

- Persistent Betti numbers
- Representatives

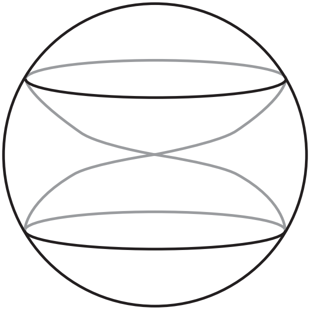
Worked example: Cyclo-octane configurations

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.

Worked example: Cyclo-octane configurations



- Sphere
- Klein bottle
- Intersect in disjoint, unlinked pair of circles.

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

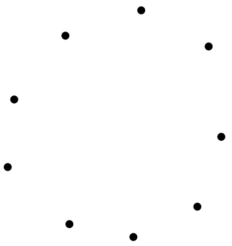
Point sample X → (Čech or Vietoris-Rips complex) → Filtered simplicial complex S_*X → (Persistence algorithm) → Persistent homology $H_*^{pers}(S_*X)$

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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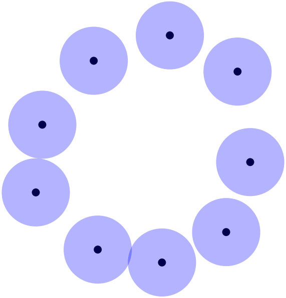

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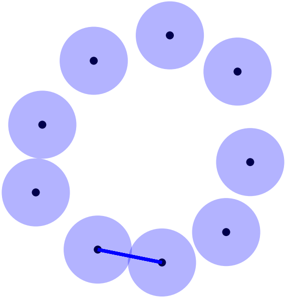

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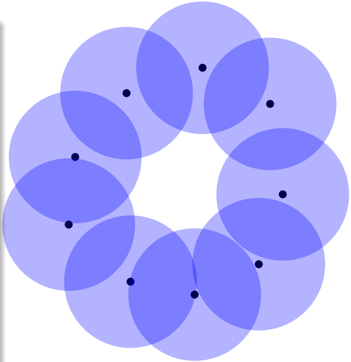

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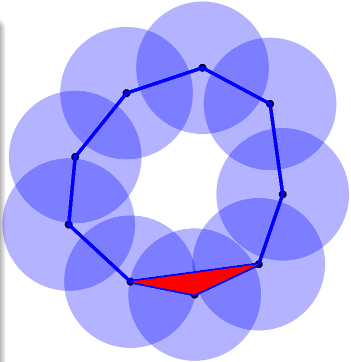


Persistent homology

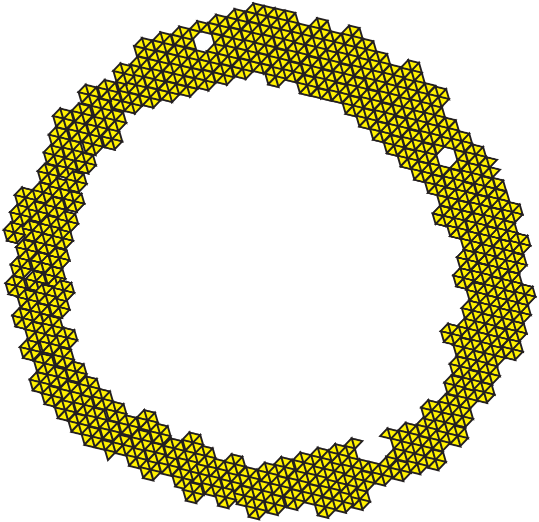
S_* a filtered simplicial complex: $\cdots \subseteq S_i \subseteq S_{i+1} \subseteq \dots$

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

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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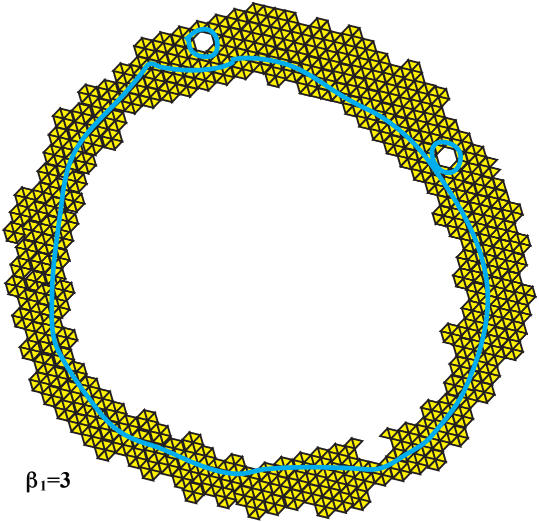

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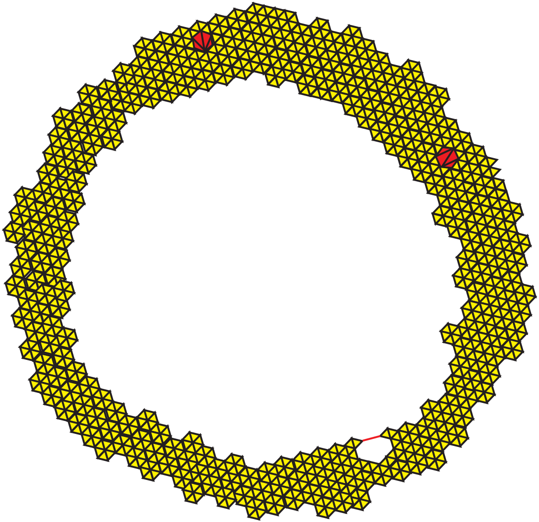

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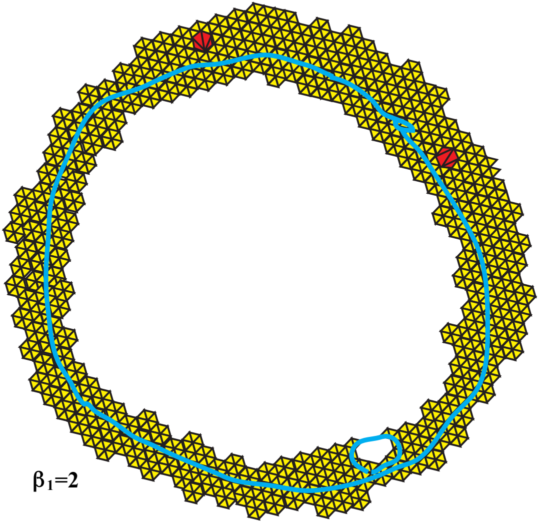


First failures

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

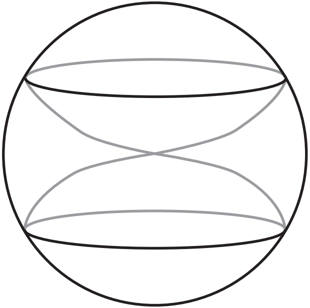
We can easily compute both $V(f)$ and $V_{Sing}(f)$.

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 $H_*(V(f))$.

Decomposing the space



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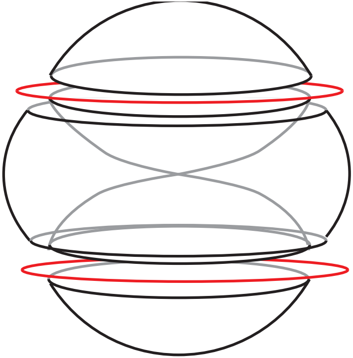

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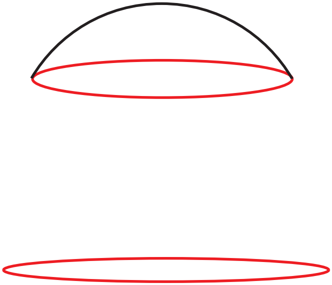

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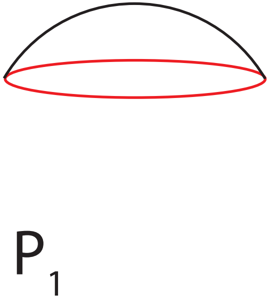

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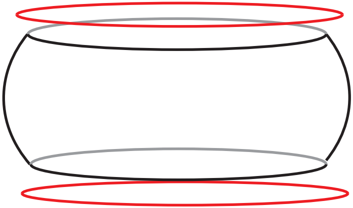

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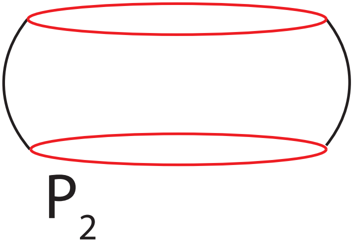

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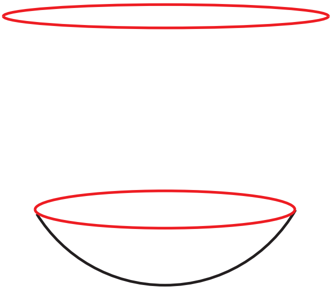
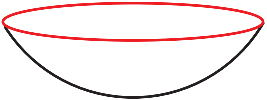


Decomposing the space

P_3



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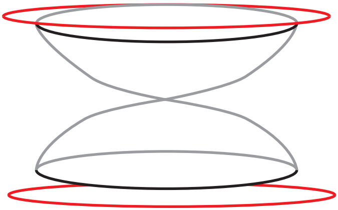

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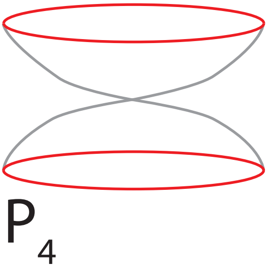
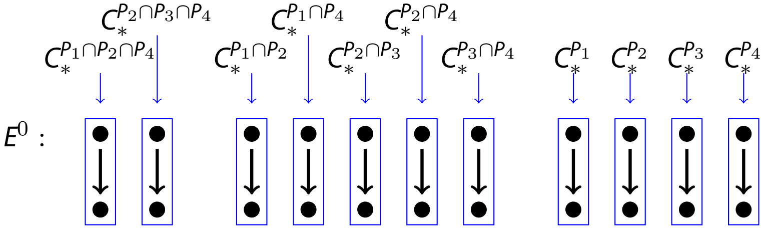


Mayer-Vietoris Spectral Sequence



Arrows are differentials in each chain complex.

Mayer-Vietoris Spectral Sequence

$$E^1: \quad \boxed{k \quad k} \longrightarrow \boxed{k \quad k \quad k \quad k^2 \quad k} \longrightarrow \boxed{0 \quad k \quad 0 \quad k}$$

$$\boxed{k \quad k} \longrightarrow \boxed{k \quad k \quad k \quad k^2 \quad k} \longrightarrow \boxed{k \quad k \quad k \quad k}$$

Arrows are induced maps from the inclusion maps on intersections.

Mayer-Vietoris Spectral Sequence

$$E^1: \quad k \quad k \longrightarrow \boxed{k \quad k \quad k \quad k^2 \quad k} \longrightarrow \boxed{0 \quad k \quad 0 \quad k}$$

$$k \quad k \longrightarrow \boxed{k \quad k \quad k \quad k^2 \quad k} \longrightarrow \boxed{k \quad k \quad k \quad k}$$

Red arrows are injections, so homology vanishes.

Mayer-Vietoris Spectral Sequence

$$E^1: \quad 0 \quad 0 \quad \boxed{k \quad k \quad k \quad k^2 \quad k} \longrightarrow \boxed{0 \quad k \quad 0 \quad k}$$

$$0 \quad 0 \quad \boxed{k \quad k \quad k \quad k^2 \quad k} \longrightarrow \boxed{k \quad k \quad k \quad k}$$

Top map is given by:

$$\begin{pmatrix} -1 & 0 \\ 0 & -1 \\ 1 & 0 \\ 1 & -1 \\ 1 & -1 \\ 0 & -1 \end{pmatrix}$$

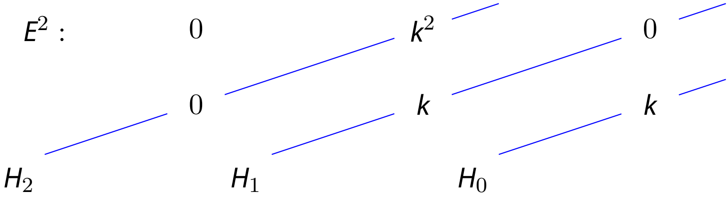
Bottom map is given by:

$$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix}$$

Mayer-Vietoris Spectral Sequence

E^2 :	0	k^2	0
	0	k	k

Mayer-Vietoris Spectral Sequence



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.