



New tools from applied topology for data analysis and signal processing

Physics & Astronomy Colloquium

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Mathematics Department

February 22, 2024



Part I

Persistent homology

Points clouds and multi-scale approximation

| 1



Western

Points clouds and multi-scale approximation

| 1

Data sets are often encountered as point clouds in \mathbb{R}^n

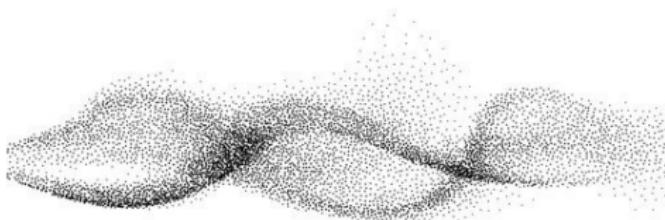


Western

Points clouds and multi-scale approximation

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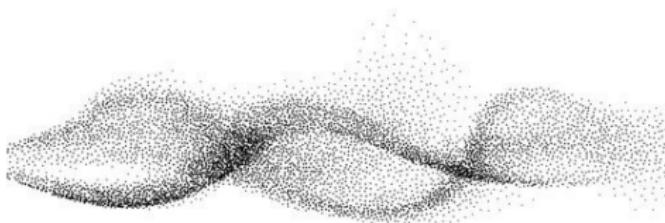


Western

Points clouds and multi-scale approximation

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Underlying probability dist. concentrated on a subspace.

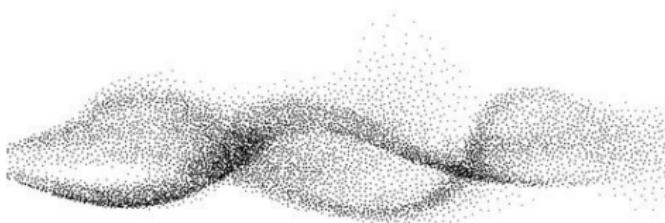


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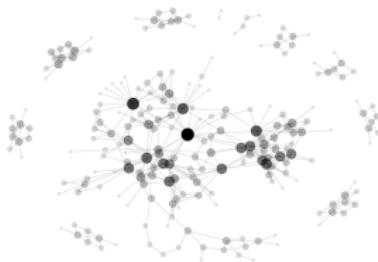
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Given a scale $t \in \mathbb{R}_{\geq 0}$ construct a graph X_t



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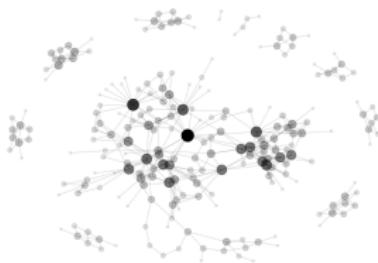
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approximating it. [What is the “right” scale?](#)



Western

Points clouds and multi-scale approximation

| 2



Western

Points clouds and multi-scale approximation

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Consider all scales and obtain a family of nested graphs

$$X_{t_0} \subset X_{t_1} \subset \cdots \subset X_{t_n}$$

with t_i a value where the graph changes.



Western

Points clouds and multi-scale approximation

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From these we can track connected components of X_t as t varies.



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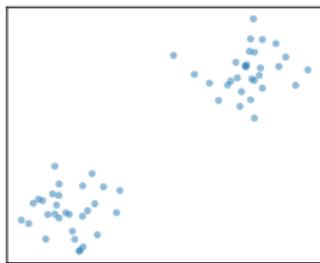
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Points clouds and multi-scale approximation

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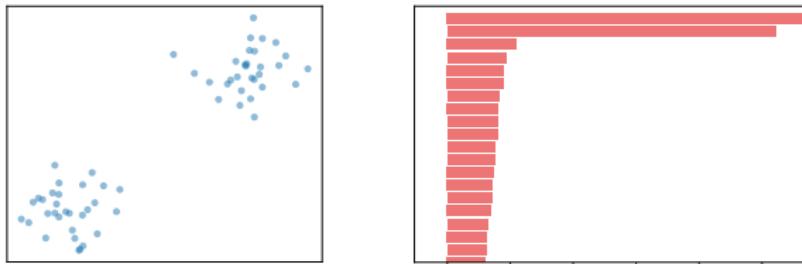
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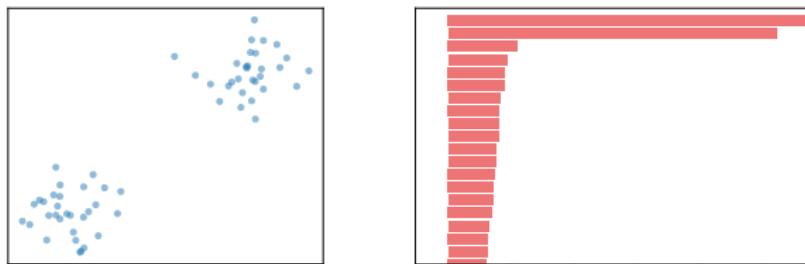
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Example:



Longer bars correspond to features that persist.

Points clouds and multi-scale approximation

| 3

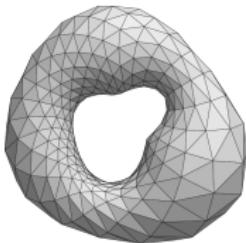


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Points clouds and multi-scale approximation

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A **simplicial complex** is a generalization of a graph



with higher dimensional “edges” termed **simplices**.

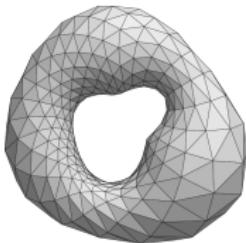


Western

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$$distance(v, w) \leq t.$$

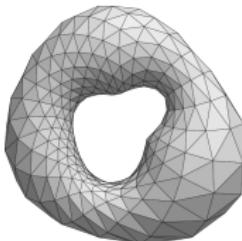


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The simplicial complex X_t has an n -simplex $[v_0, v_1, \dots, v_n]$ if

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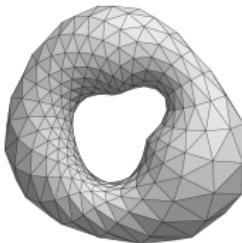


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Obtain **filtered simplicial complex**

$$X_{t_0} \subset X_{t_1} \subset \dots \subset X_{t_n}$$



Western

Robust/stable invariants

| 4



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We want invariants of the underlying space/shape not of the simplicial complex approximating it.

E.g. Alternative point cloud samples should give the same or “similar” invariants.



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Bad ideas: count number of simplices, measure incidence angles, record volumes,...

All of these depend on the simplicial complex.



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Bad ideas: count number of simplices, measure incidence angles, record volumes,...

All of these depend on the simplicial complex.

Basic example: (Euler characteristic)

$$\chi = \# \text{vertices} - \# \text{edges} + \cdots + (-1)^n \#(\text{n-simplices}).$$



Finer features: Homology

| 5

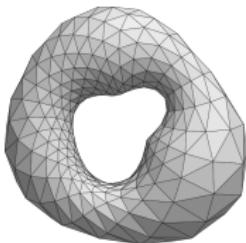


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Finer features: Homology

| 5

Given a simplicial complex X



the [homology](#) construction produces $\forall d \in \mathbb{N}$ a vector space $H_d(X)$ whose dimension $\beta_d(X)$ counts the “ d -dim'l components” or “ d -cavities” of X .

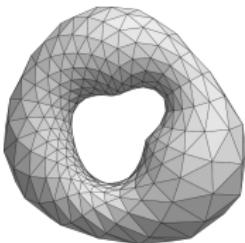


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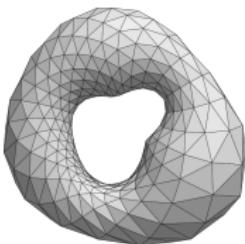


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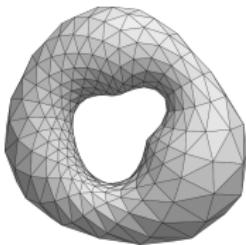
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Finer features: Homology

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Example if T is the above space

$$\beta_0(T) = 1, \quad \beta_1(T) = 2, \quad \beta_2(T) = 1, \quad \beta_i(T) = 0.$$

It is connected, has two independent loops,
and one 2-dimensional cavity.



Western

Persistence homology

| 6



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Persistence homology

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Applying homology to the multi-scale approximation

$$X_0 \subset X_1 \subset \cdots \subset X_n$$

gives a family of vector spaces and linear maps

$$H_d(X_0) \rightarrow H_d(X_1) \rightarrow \cdots \rightarrow H_d(X_n).$$



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Persistence homology

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The way their dimensions β_d “fit together” defines the d^{th} barcode.



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Persistence homology

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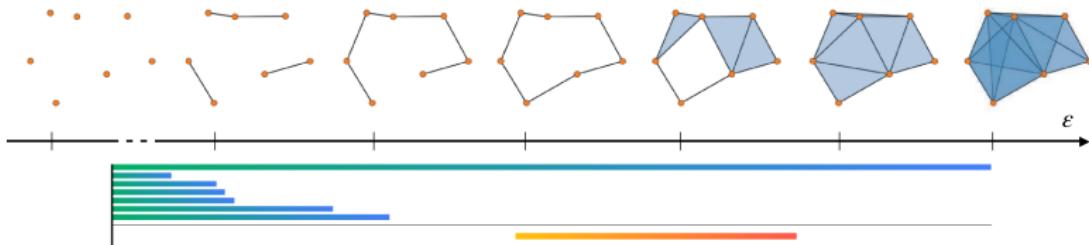
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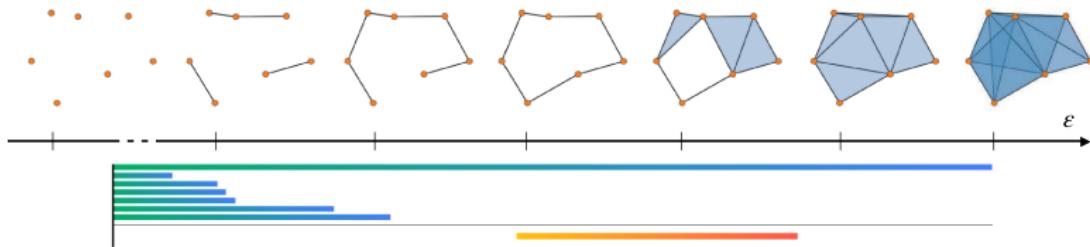
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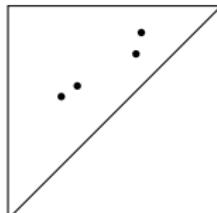
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Abstractly, a barcode is a collection of pairs $(a, b) \in \mathbb{R}^2$ with multiplicity.



Why are barcodes useful?

| 7



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Why are barcodes useful?

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1. **Stability**: The passage from point clouds to barcodes preserves distances.



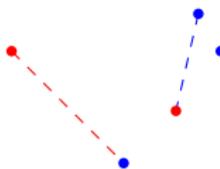
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Point cloud distance is Gromov–Hausdorff:

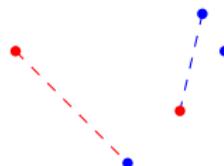


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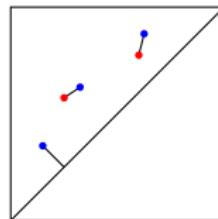
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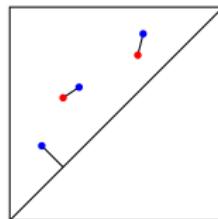
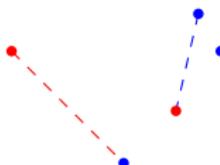


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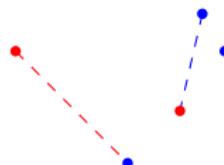
$$d_{GH}(X, Y) \leq d_b(\mathcal{B}_X, \mathcal{B}_Y)$$

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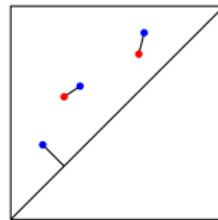
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2. **Computability:** Based on matrix reduction algorithms, its complexity is

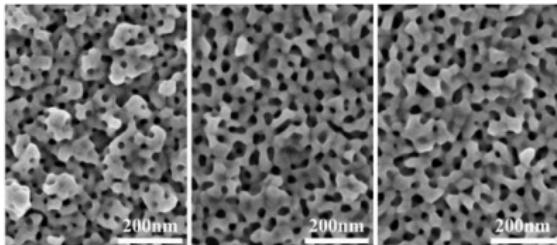
$$\sim O(\#\text{simplices}^3).$$



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Exemplar - Nanoporous materials (Lee et al.)

| 8

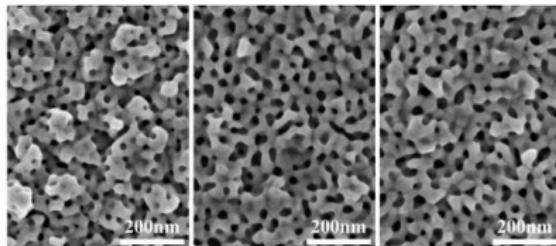


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Comparing geometries
directly, impossible,
over 3M structures.

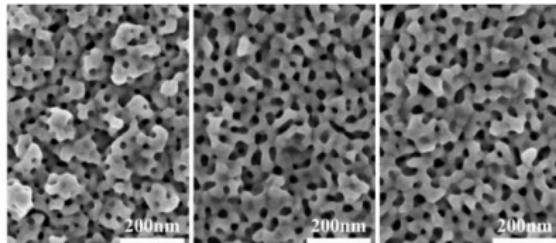


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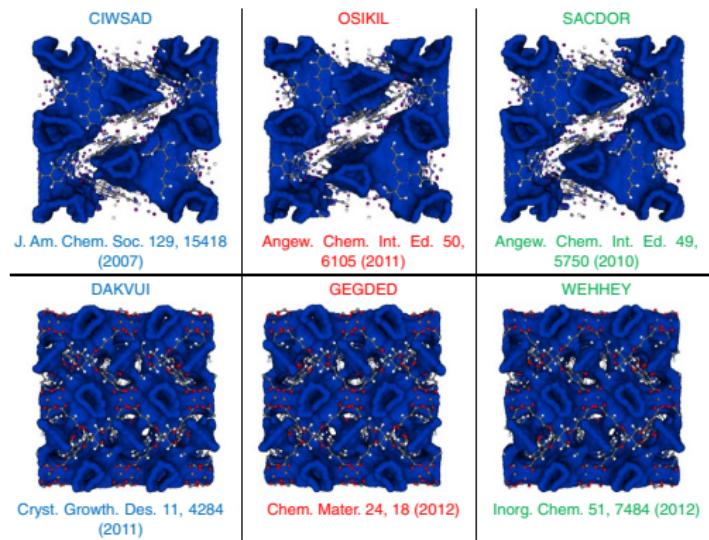
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Comparing Barcodes
is done fast
and faithfully
by stability.



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Where to find these tools? giotto-tda

| 9



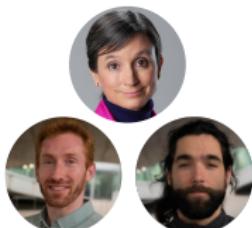
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Where to find these tools? giotto-tda

| 9

Integration of persistence algorithms into scikit-learn.

The *giotto-tda* team



EPFL



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Part II

Steenrod barcodes

Goal: introduce Steenrod barcodes

| 10



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Goal: introduce Steenrod barcodes

| 10

These generalize usual barcodes, and are also



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Goal: introduce Steenrod barcodes

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These generalize usual barcodes, and are also **stable**,



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These generalize usual barcodes, and are also **stable**, **computable**,



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Goal: introduce Steenrod barcodes

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These generalize usual barcodes, and are also [stable](#), [computable](#), and present in [real-data](#).

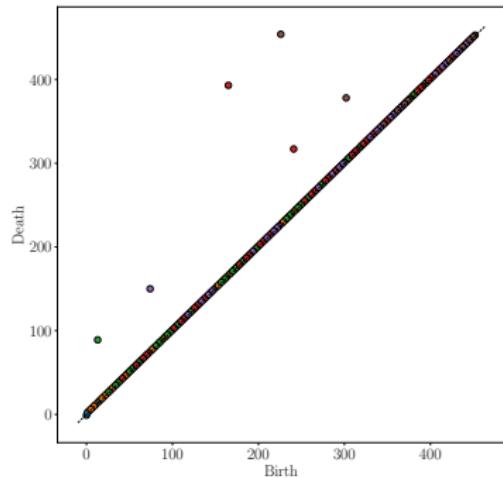


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(a) $C\Sigma(S^2 \vee S^4)$

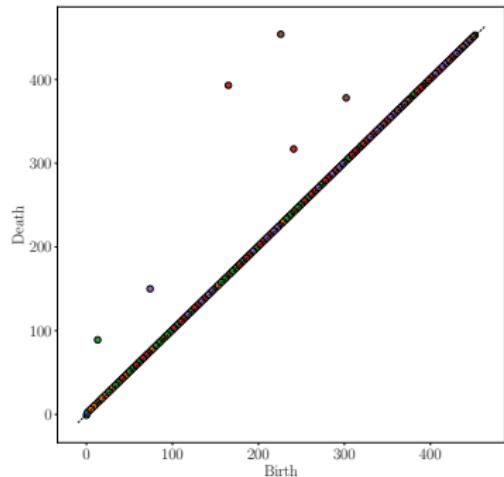


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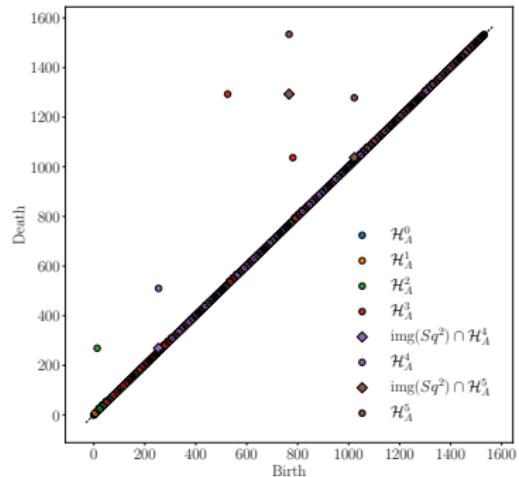
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(b) $C\Sigma \mathbb{C}\mathbb{P}^2$

Shortcomings of Betti numbers

| 11



Western

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Barcodes are based on the **Betti numbers** of spaces, the β_d 's.



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But these **forget** much information.



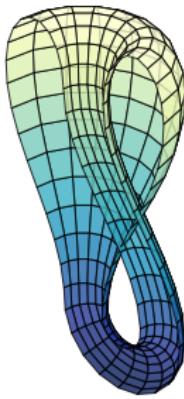
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Shortcomings of Betti numbers

| 11

Barcodes are based on the [Betti numbers](#) of spaces, the β_d 's.

But these [forget](#) much information. For [example](#), if K is the Klein bottle



over the field with two elements \mathbb{F}_2 we have

$$\beta_0(K) = 1, \quad \beta_1(K) = 2, \quad \beta_2(K) = 1, \quad \beta_i(K) = 0.$$

The same as the torus T .



Western

Steenrod squares

| 12



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Steenrod squares

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For each k there are natural maps

$$\text{Sq}^k : H^d(X; \mathbb{F}_2) \rightarrow H^{d+k}(X, \mathbb{F}_2).$$



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Steenrod squares

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Sq^1 distinguishes the torus and the Klein bottle



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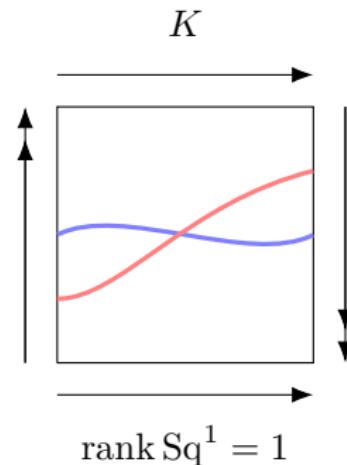
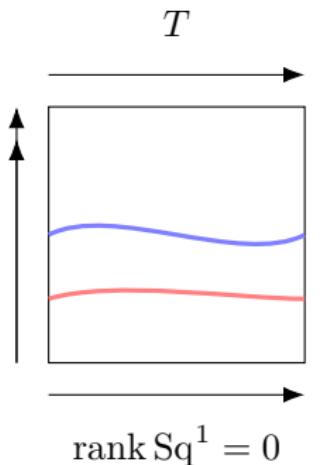
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Computing Steenrod squares

| 13



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Computing Steenrod squares

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Contribution (Med.): A faster way to compute Sq^k for simplicial complexes.



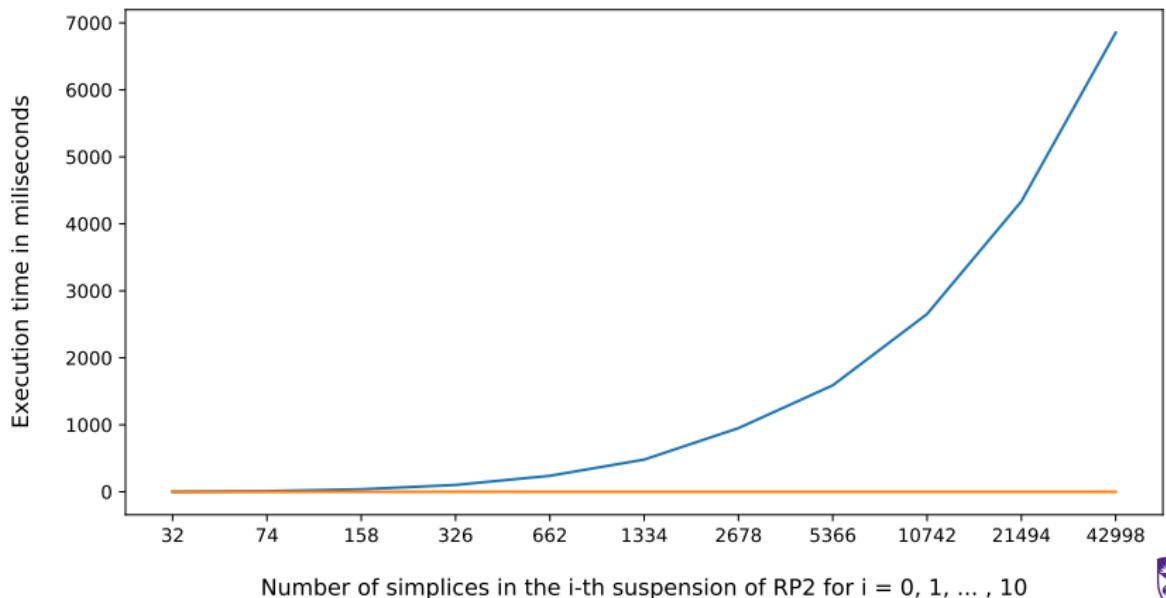
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Computing Steenrod squares

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Contribution (Med.): A faster way to compute Sq^k for simplicial complexes.

Example: Clocking the computation of Sq^1 , the old and new ways.



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Persistent Steenrod squares

| 14



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Persistent Steenrod squares

| 14

Given a filtered simplicial complex

$$(1) \quad X_0 \subset X_1 \subset \cdots \subset X_n,$$



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Persistent Steenrod squares

| 14

Given a filtered simplicial complex

$$(1) \quad X_0 \subset X_1 \subset \cdots \subset X_n,$$

For each k and d , Sq^k induces a family of compatible linear maps

$$\begin{array}{ccccccc} H^d(X_n; \mathbb{F}_2) & \longrightarrow & \cdots & \longrightarrow & H^d(X_{n-1}; \mathbb{F}_2) & \longrightarrow & H^d(X_0; \mathbb{F}_2) \\ \downarrow \text{Sq}^k & & & & \downarrow \text{Sq}^k & & \downarrow \text{Sq}^k \\ H^{d+k}(X_n; \mathbb{F}_2) & \longrightarrow & \cdots & \longrightarrow & H^{d+k}(X_{n-1}; \mathbb{F}_2) & \longrightarrow & H^{d+k}(X_0; \mathbb{F}_2). \end{array}$$



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Definition (Lupo–Med.–Tauzin)

The Sq^k barcode of (1) is defined as the barcode of $\text{img } \text{Sq}^k$.



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$$\begin{array}{ccccccc} H^d(X_n; \mathbb{F}_2) & \longrightarrow & \cdots & \longrightarrow & H^d(X_{n-1}; \mathbb{F}_2) & \longrightarrow & H^d(X_0; \mathbb{F}_2) \\ \downarrow \text{Sq}^k & & & & \downarrow \text{Sq}^k & & \downarrow \text{Sq}^k \\ H^{d+k}(X_n; \mathbb{F}_2) & \longrightarrow & \cdots & \longrightarrow & H^{d+k}(X_{n-1}; \mathbb{F}_2) & \longrightarrow & H^{d+k}(X_0; \mathbb{F}_2). \end{array}$$

Definition (Lupo–Med.–Tauzin)

The Sq^k barcode of (1) is defined as the barcode of $\text{img } \text{Sq}^k$.

Theorem (Ling Zhou–Med.–Mémoli)

These barcodes are stable.



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Persistent Steenrod squares

| 14

Given a filtered simplicial complex

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Computable?



Western

A ready-to-use package for computing Steenrod barcodes.



Developed with *U. Lupo* and *G. Tuzin* from  **Giotto-tda**.

github.com/Steenroder/steenroder

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Question: Are these finer invariants out there in the real world?

Space of conformations of C₈H₁₆

| 16



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Space of conformations of C₈H₁₆

| 16

Points in \mathbb{R}^{24} (positions of 8 carbons in \mathbb{R}^3)



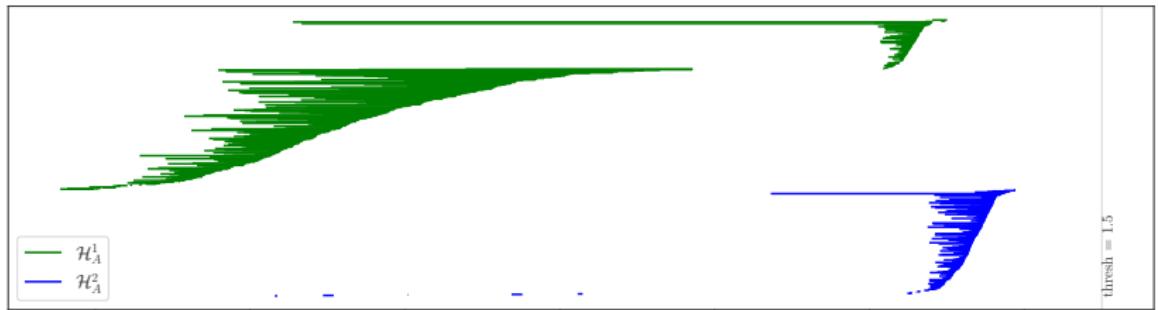
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Space of conformations of C₈H₁₆

| 16

Points in \mathbb{R}^{24} (positions of 8 carbons in \mathbb{R}^3)

H^1 (green) and H^2 (blue) barcodes of (part of) this point cloud



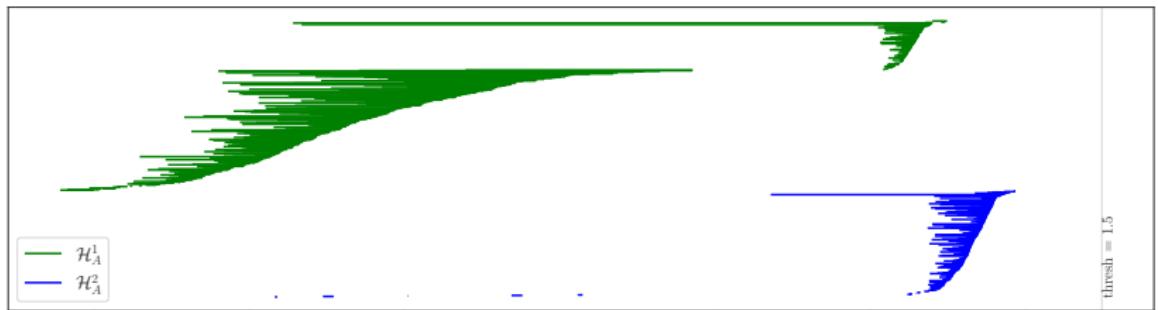
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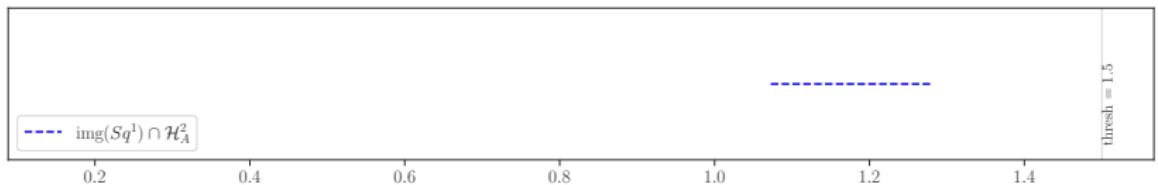
| 16

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Sq¹ barcode



Consistent with a Klein bottle.



Western

Persistent homology and their Steenrod generalization are principled tools for feature extraction.



Persistent homology and their Steenrod generalization are principled tools for feature extraction.

- ▶ They capture the primitive **shape** of data.
- ▶ They are relevant at **multiple scales**.
- ▶ Their output, barcodes, form a **metric space**.
- ▶ They are **robust** to noise.
- ▶ They are **computable** in practice: giotto-tda - steenroder.
- ▶ They are useful in the study **real-world data**.



Part III

(time-permitting)

Hyperharmonic analysis

Complex systems

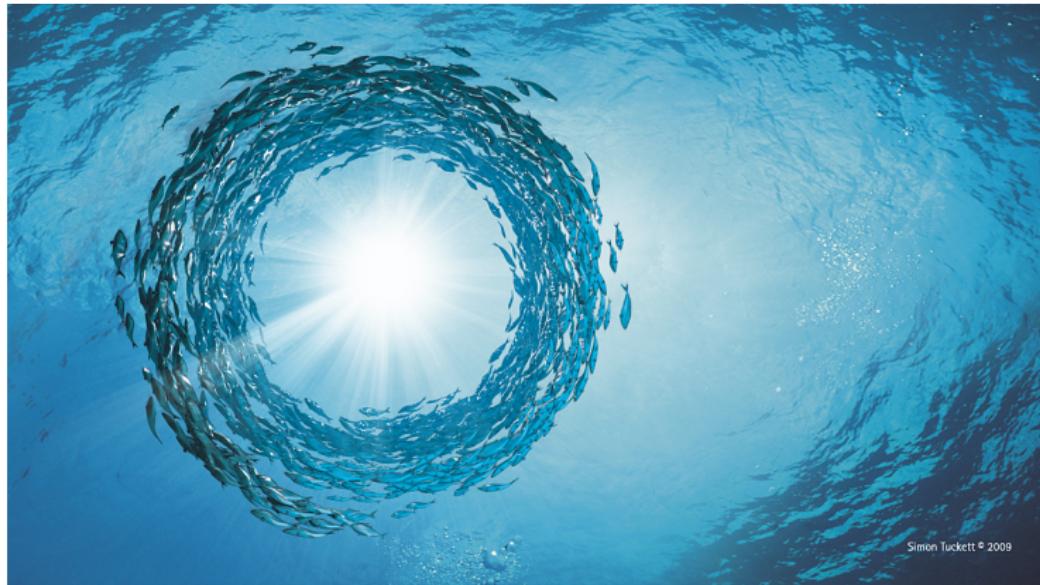
| 18



The whole is greater than the sum of its parts.



Western



The whole is greater than the sum of its parts.

Question: How to **quantify** this slogan?



Information signals

| 19



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Information signals

| 19

Let X_0, \dots, X_N be probability distributions



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Information signals

| 19

Let X_0, \dots, X_N be probability distributions

- ▶ The **entropy** of each

$$H(X_i) = -\sum_{x_i} p(x_i) \log p(x_i).$$



Western

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- ▶ The **mutual information** of pairs

$$I(X;Y) = H(X,Y) - H(X \mid Y) - H(Y \mid X).$$

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- ▶ The **interaction information** of triples

$$\begin{aligned} I(X;Y;Z) &= H(X) + H(Y) + H(Z) \\ &\quad - H(X,Y) - H(X,Z) - H(Y,Z) \\ &\quad + H(X,Y,Z). \end{aligned}$$

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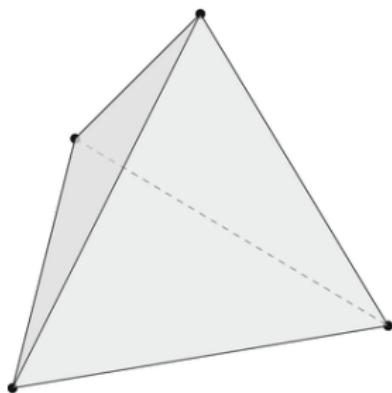
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- ▶ Analogues for higher cardinality subsets.

Problem: Number of subsets grows exponentially with N .

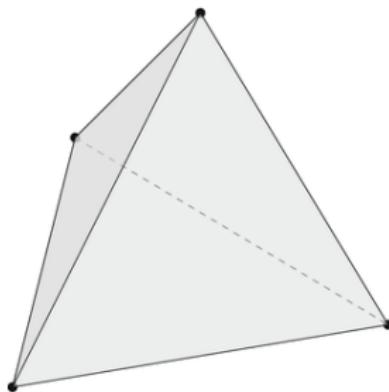
Signals on a simplex

| 20



Signals on a simplex

| 20



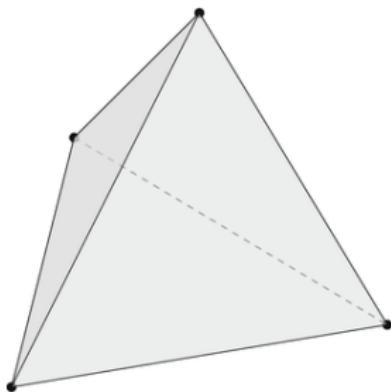
Weighted with **structural** information. (e.g. EEG node positions)



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Signals on a simplex

| 20



Weighted with **structural** information. (e.g. EEG node positions)

Signals are the same as \mathbb{R} -valued functions on simplices. E.g.

Entropy : 0-simplices

Mutual information : 1-simplices

Interaction information : 2-simplices

Higher order signals : d -simplices



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Hyperharmonic analysis

| 21

Analogy: Listen to a few harmonics to tell a guitar and a piano apart.



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Contribution (Med.-Rosas-Rodríguez-Cofré)

A principled method to compress high-order information signals based on Fourier analysis and combinatorial topology.



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Fourier basis: Eigenvectors of the discrete Laplacian

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How to measure compressibility?

Given signal α , let $\{\alpha_i\}$ be its coeff's in a basis with $\alpha_1^2 \geq \alpha_2^2 \geq \dots$

$$\text{EV}_\alpha(k) = \frac{\alpha_k^2}{\sum_i \alpha_i^2} \quad \text{and} \quad \text{CEV}_\alpha(k) = \sum_{1 \leq i \leq k} \text{EV}_\alpha(i),$$



Proof of concept: Haydn's symphonies

| 22



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Proof of concept: Haydn's symphonies

| 22

Music as a probability distribution.



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Proof of concept: Haydn's symphonies

| 22

Music as a probability distribution.

We analyzed two high-order information signals across four dimensions:



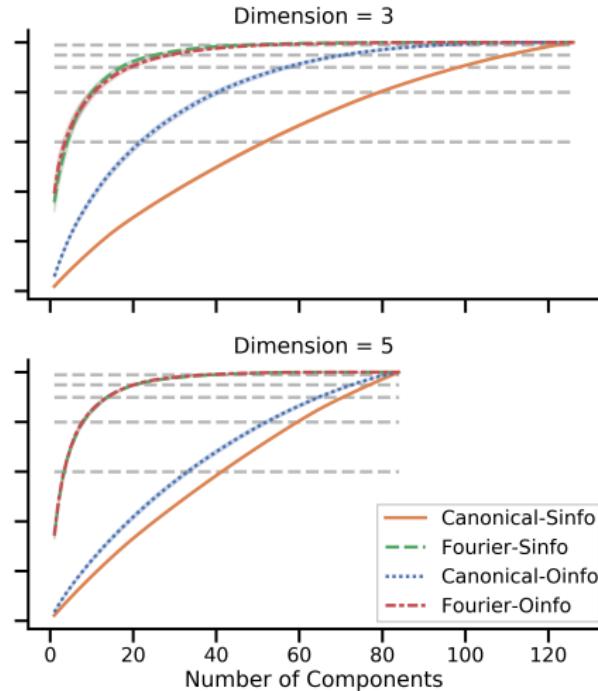
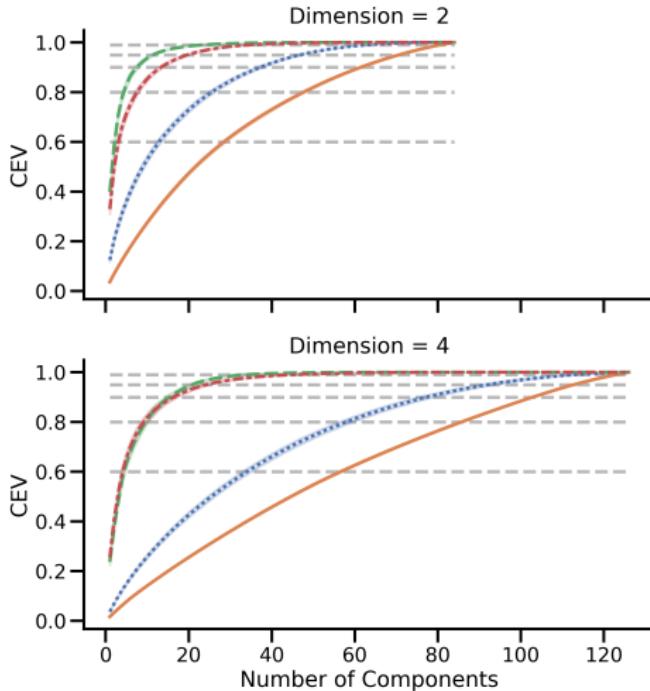
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| 22

Music as a probability distribution.

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Thank you!

1. Guillaume Tazuin et al. **giotto-tda: A Topological Data Analysis Toolkit for Machine Learning and Data Exploration**. *Journal of Machine Learning Research* 22.39 (2021).
2. Yongjin Lee et al. **Quantifying similarity of pore-geometry in nanoporous materials**. *Nature communications* 8.1 (2017).
3. Anibal M. Medina-Mardones. **New formulas for cup- i products and fast computation of Steenrod squares**. *Comput. Geom.* 109 (2023).
4. Umberto Lupo, Anibal M. Medina-Mardones, and Guillaume Tazuin. **Persistence Steenrod modules**. *J. Appl. Comput. Topol.* 6.4 (2022).
5. Anibal M. Medina-Mardones et al. **Hyperharmonic analysis for the study of high-order information-theoretic signals**. *Journal of Physics: Complexity* 2.3 (2021).

