Topological Data Analysis: An Introduction to Persistent Homology

Part 1: Inference and Stability

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TUM

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Machine learning summer school 2019
Skoltech, Moscow

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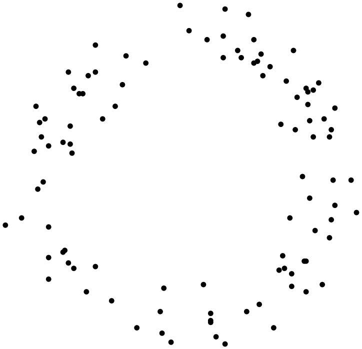
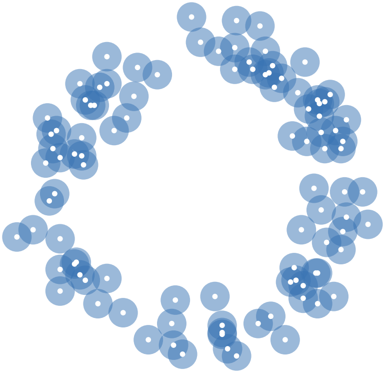
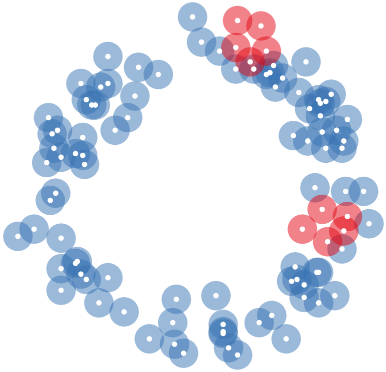
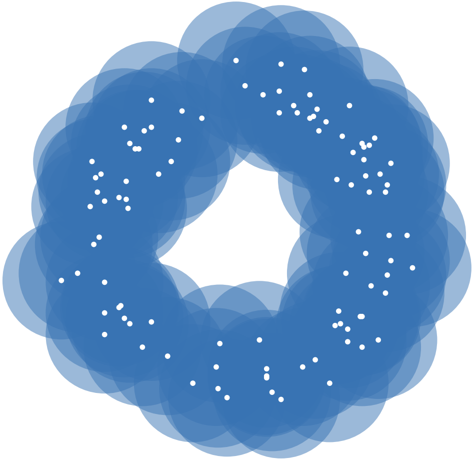
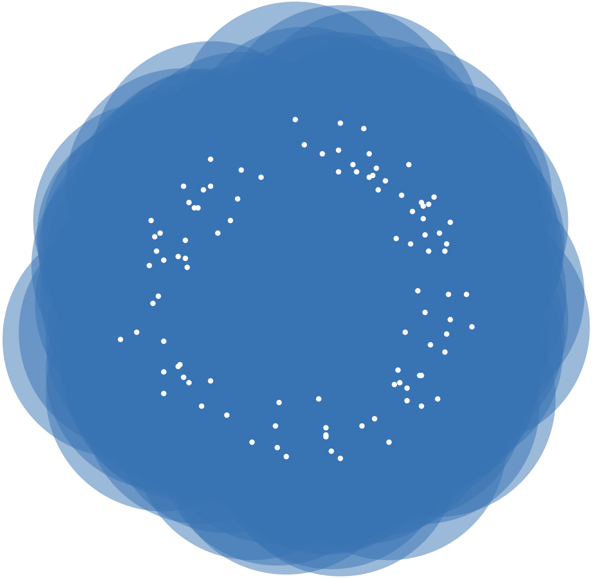
Persistent homology

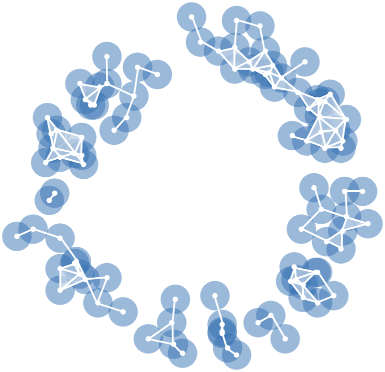


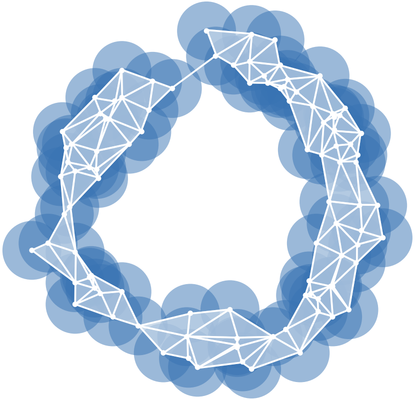


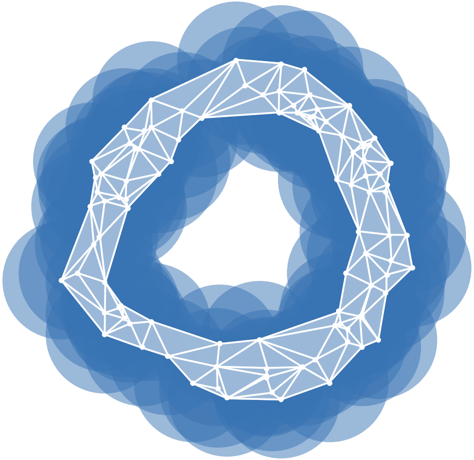


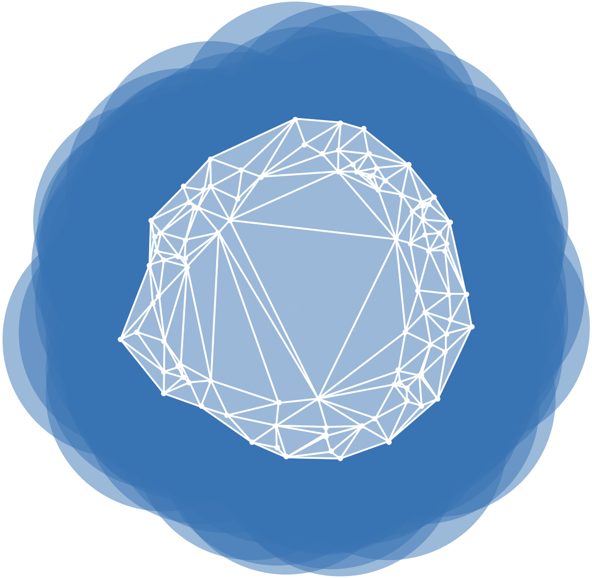




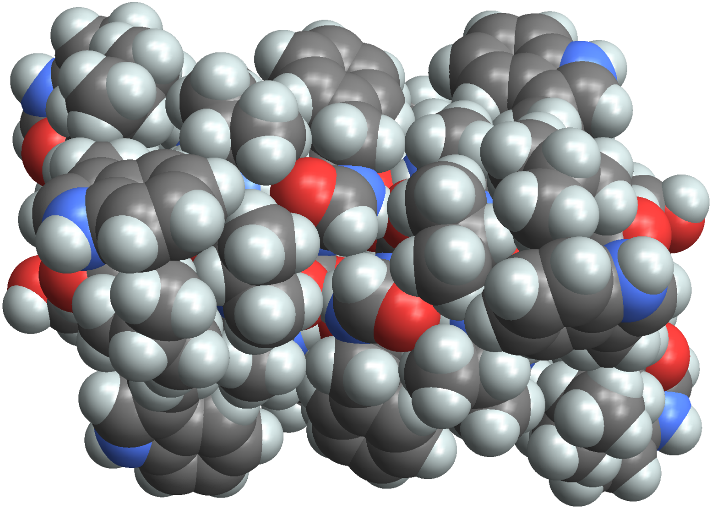








Gramicidin: an antibiotic functioning as ion channel



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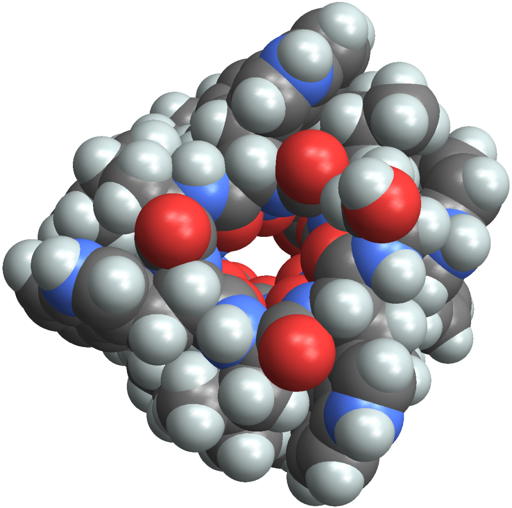

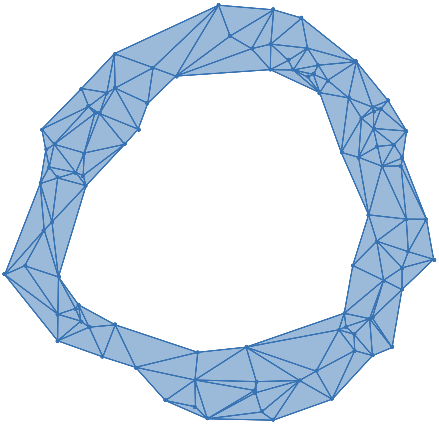

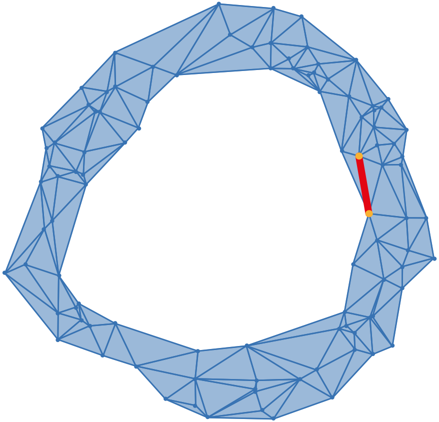

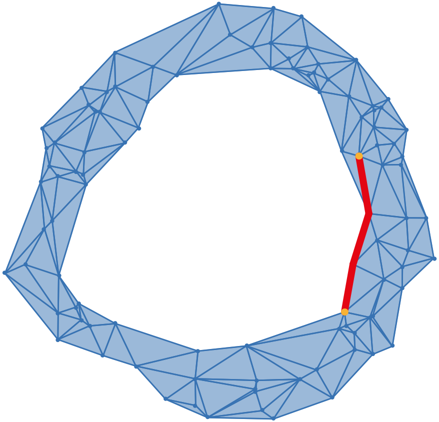

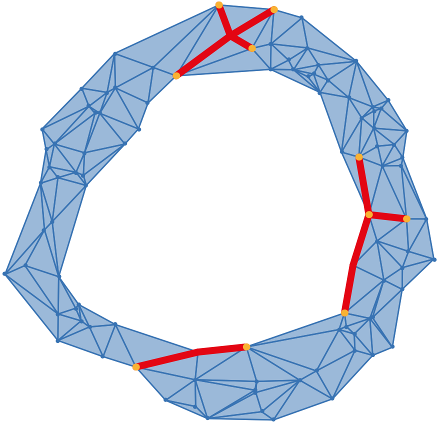

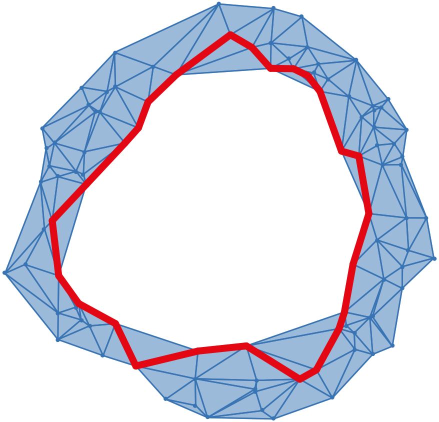

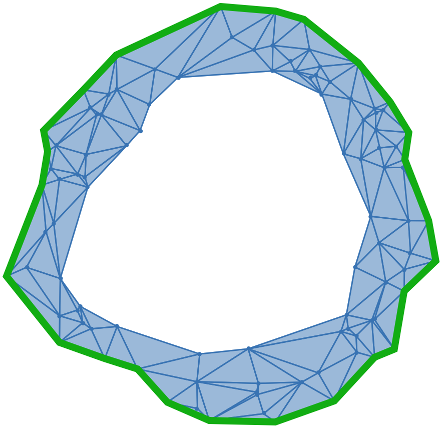

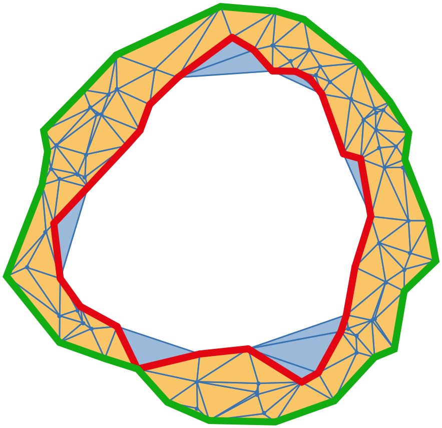

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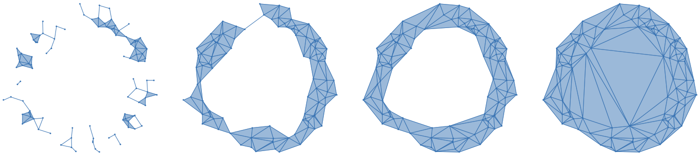

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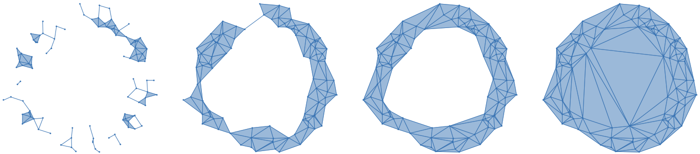

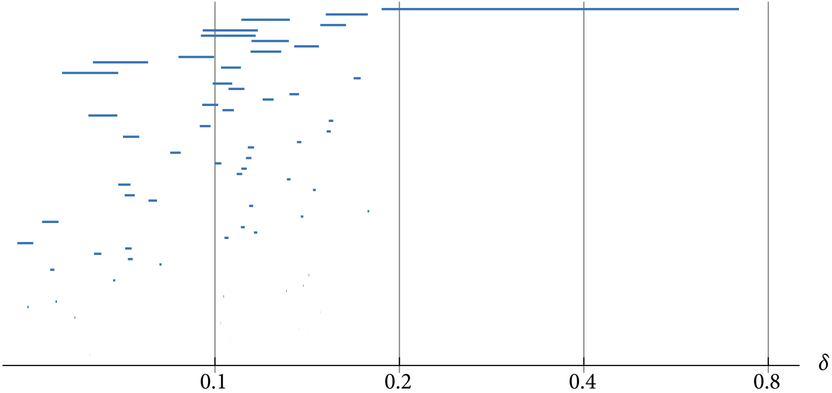

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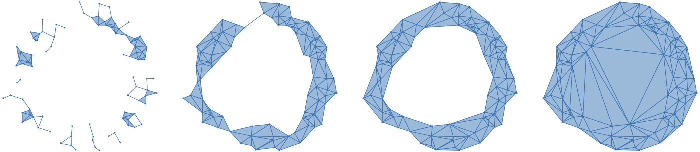

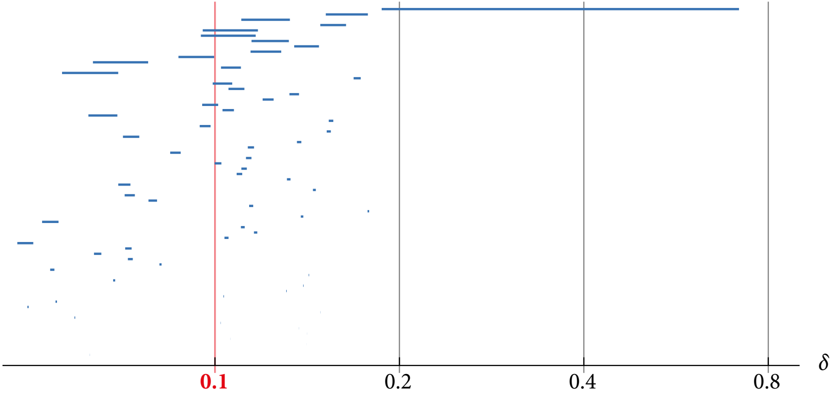

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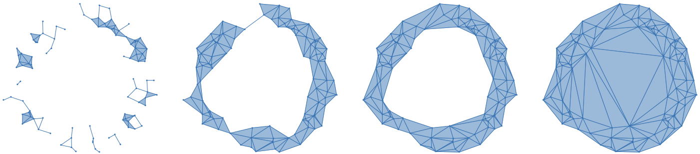

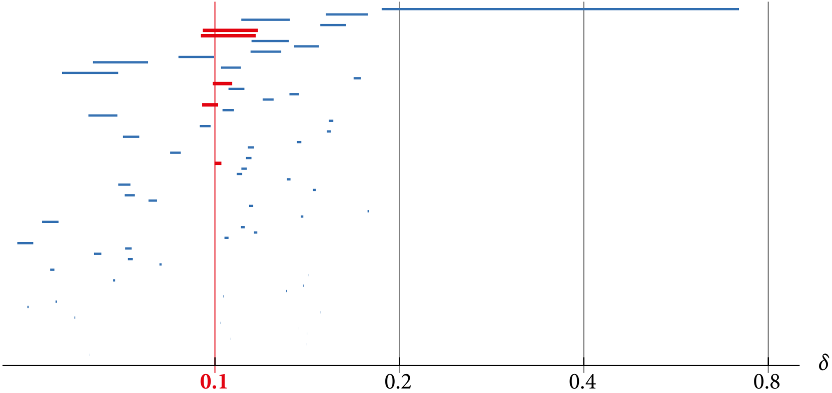

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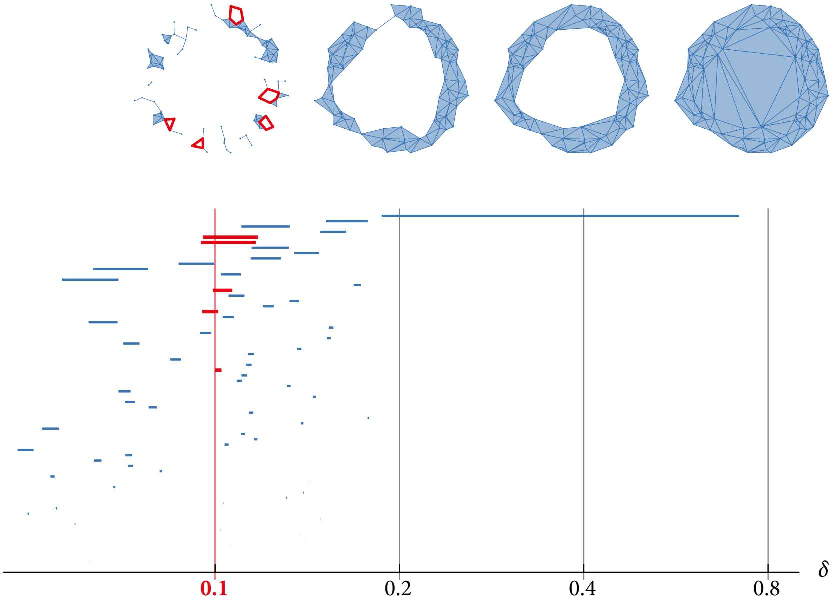

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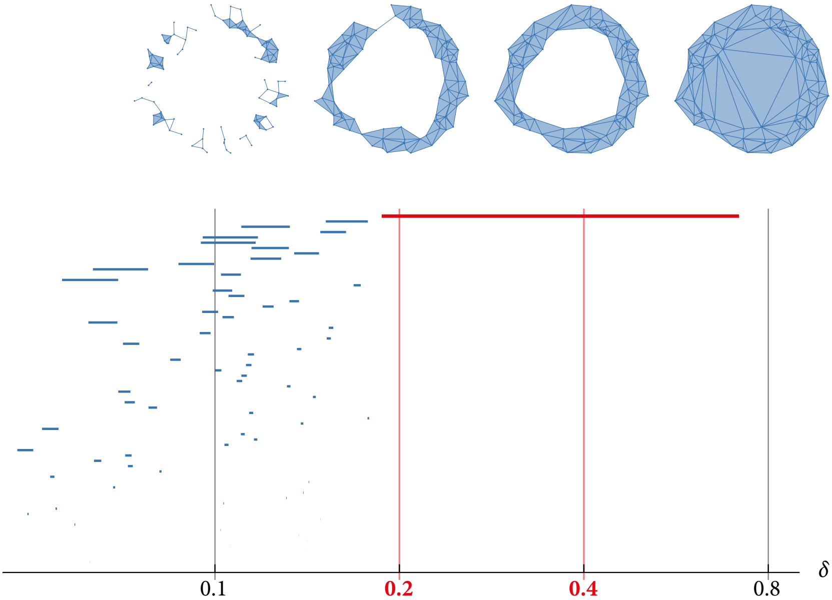

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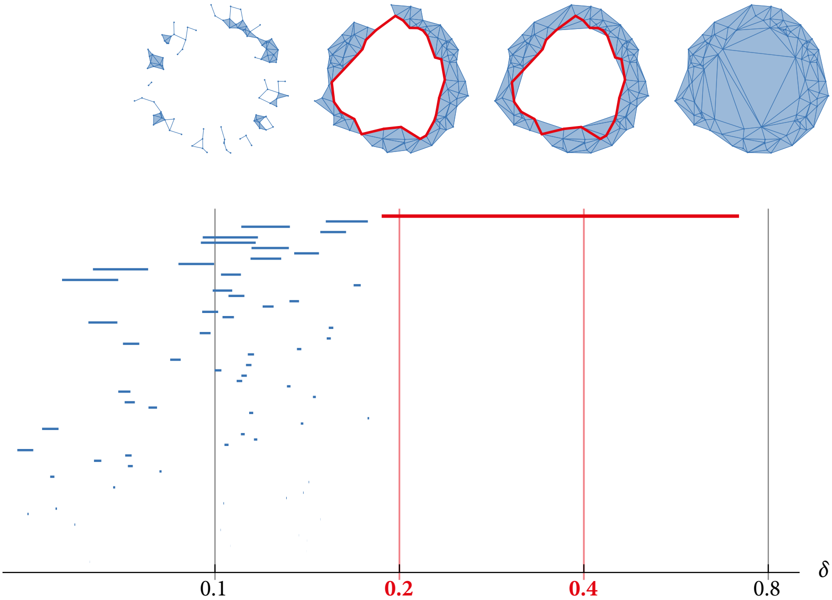

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- A filtration is a certain diagram $K : \mathbb{R} \to \mathbf{Top}$ of topological spaces, indexed over the reals:

$$\cdots\cdots\dashrightarrow K_s \hookrightarrow K_t \dashrightarrow\cdots\cdots$$

  - a topological space K_t for each $t \in \mathbb{R}$
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- Apply homology $H_* : \mathbf{Top} \to \mathbf{Vect}$
- Persistent homology is a diagram $M : \mathbb{R} \to \mathbf{Vect}$ *(persistence module)*.

In this talk, all vector spaces will be finite dimensional.

Persistence modules

A *persistence module* M is a diagram $M : \mathbb{R} \to \mathbf{vect}$ of vector spaces, indexed over the reals:

$$\cdots\cdots\to M_s \longrightarrow M_t \cdots\cdots\to$$

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The maps (*morphisms*) between persistence modules are *natural transformations*:

$$\begin{tikzcd} \cdots \arrow[r, dotted] & M_s \arrow[r] \arrow[d, "f_s"'] & M_t \arrow[r, dotted] \arrow[d, "f_t"] & \cdots \\ \cdots \arrow[r, dotted] & N_s \arrow[r] & N_t \arrow[r, dotted] & \cdots \end{tikzcd}$$

- a linear map $f_t : M_t \to N_t$ for each $t \in \mathbb{R}$
- horizontal and vertical maps commute (for all $s \leq t$)

Barcodes: the structure of persistence modules

Theorem (Crawley-Boevey 2015)

Any persistence module $M : \mathbb{R} \to \mathbf{vect}$ *(of finite dim. vector spaces over some field* $\mathbb{F}$*) decomposes as a direct sum of* interval modules

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- The barcode completely describes the persistence module (up to isomorphism).
- This is why we use homology with coefficients in a field.
- We rarely have a similarly clean structure for other parameter spaces, like $\mathbb{R}^2 \to \mathbf{vect}$ (two-parameter persistence modules)

Stability

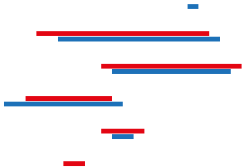
Stability of persistence barcodes for functions

Theorem (Cohen-Steiner, Edelsbrunner, Harer 2005)

Let $f, g : X \to \mathbb{R}$ with $\|f - g\|_\infty = \delta$ (and some regularity assumptions).

Consider the persistence barcodes of (sublevel set filtrations of) f and g.

Then there exists a matching between their intervals such that



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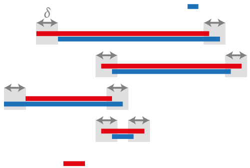

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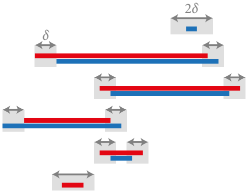

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Requires strong assumptions:

Homology reconstruction by thickening

Theorem (Niyogi, Smale, Weinberger 2006)

Let X *be a submanifold of* $\mathbb{R}^d$*. Let* $P \subset X$ *and* $\delta > 0$ *be such that*

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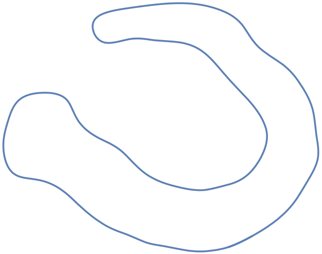

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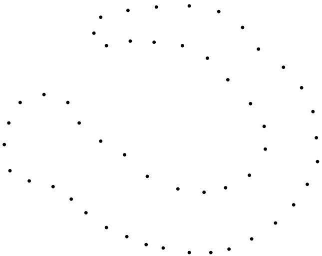

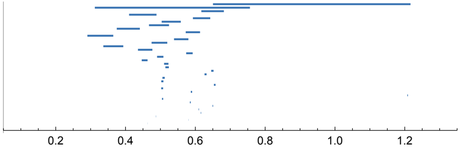

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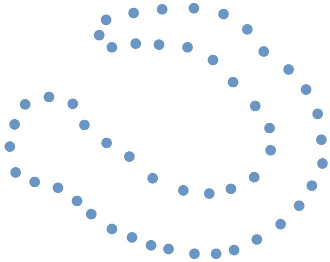

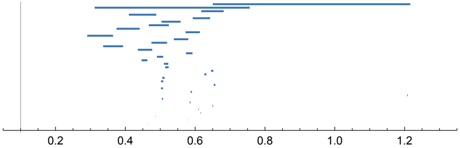

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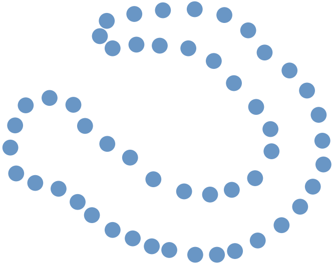

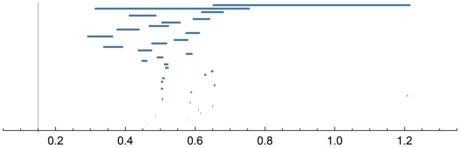

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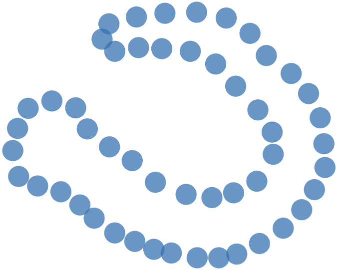

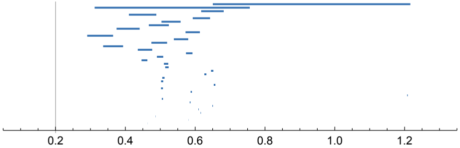

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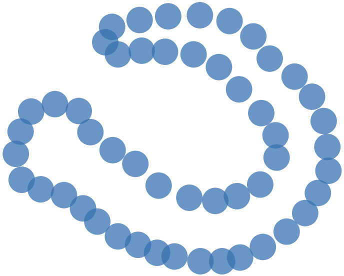

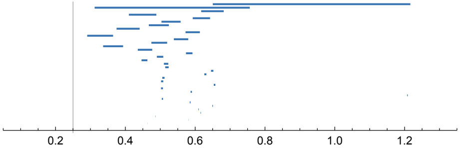

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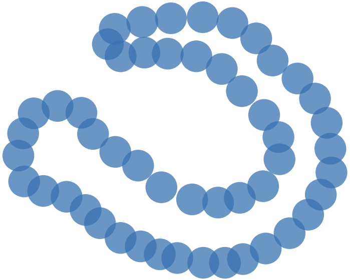

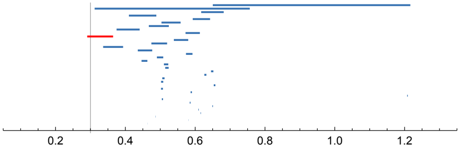

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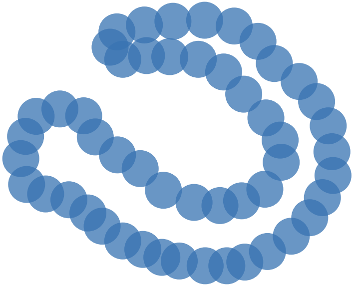

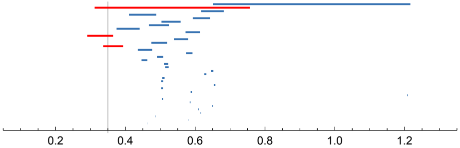

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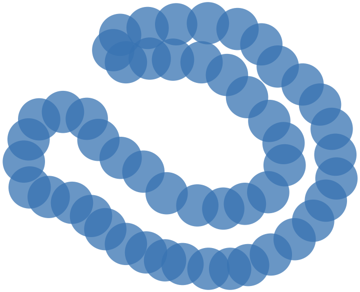

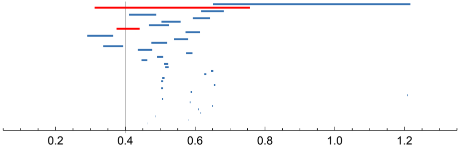

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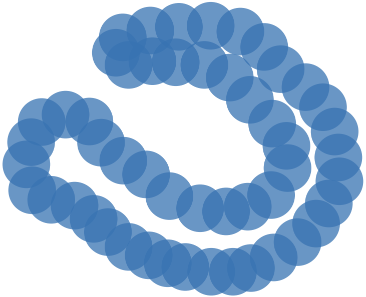

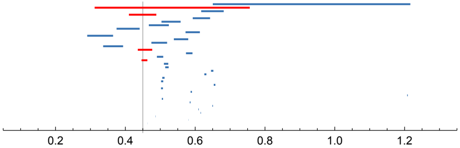

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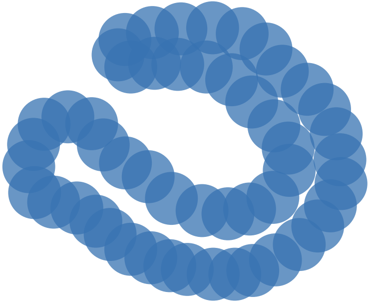

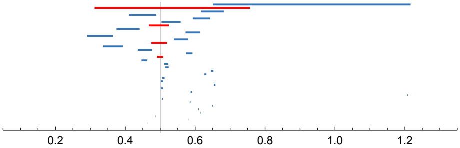

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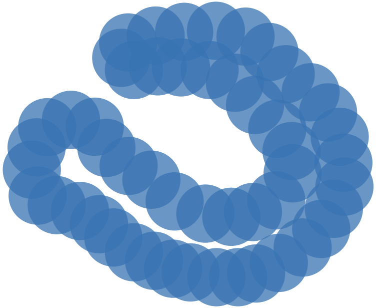

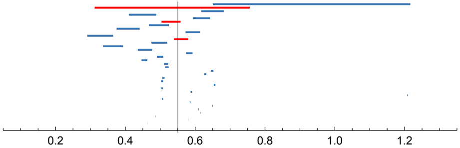

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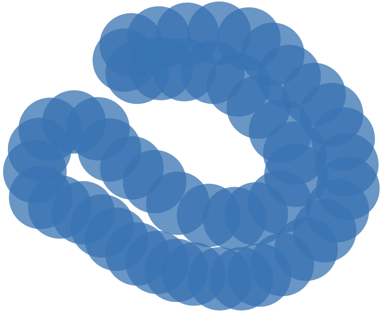

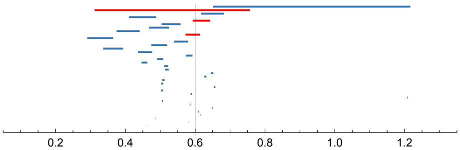

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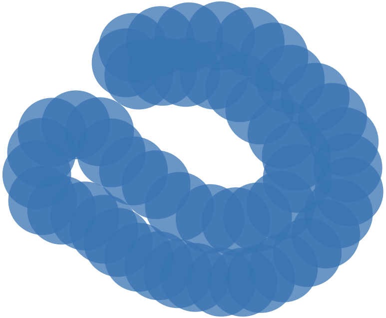

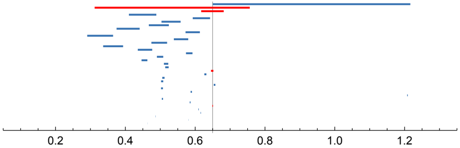

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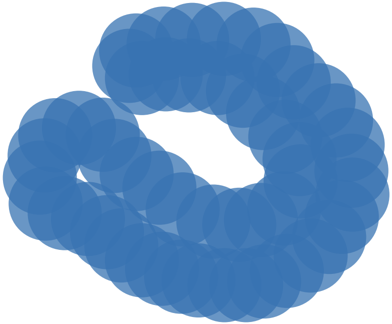

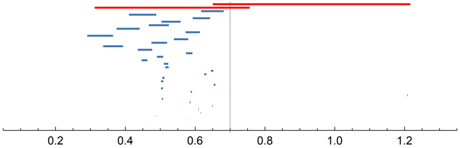

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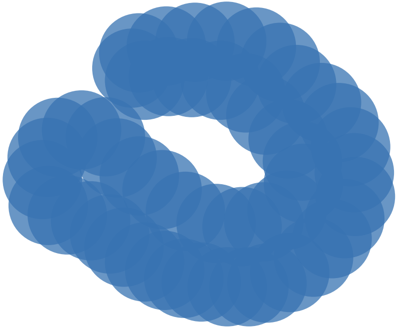

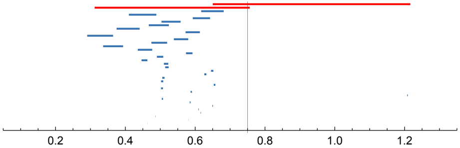

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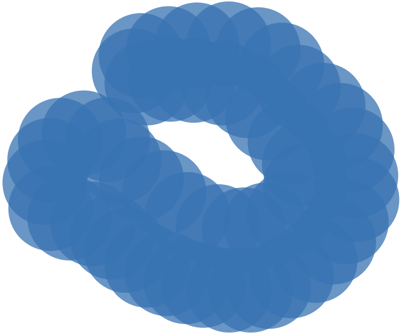

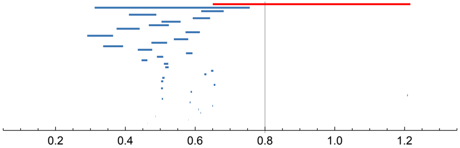

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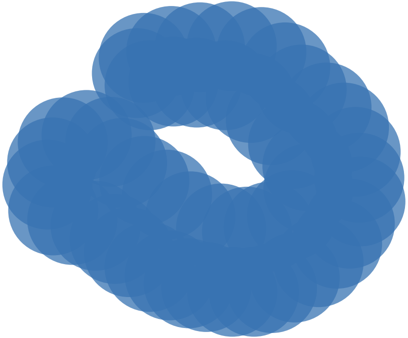

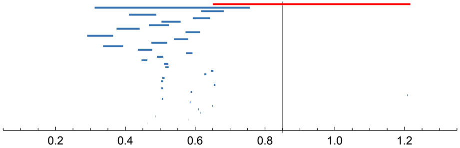

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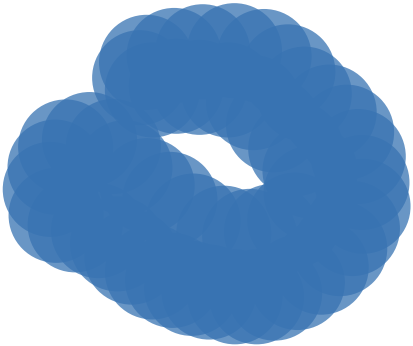

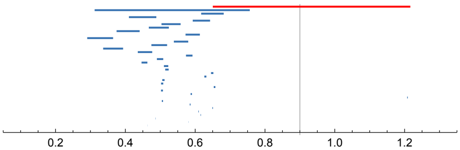

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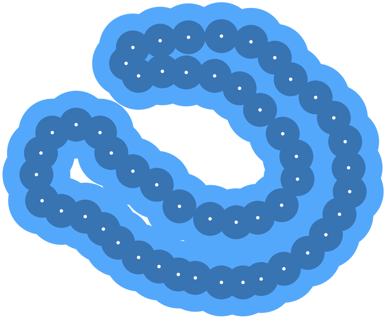

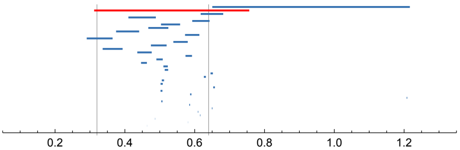

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This motivates the *homological realization problem*:

Problem

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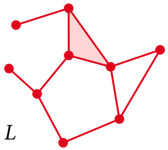

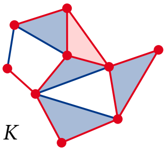

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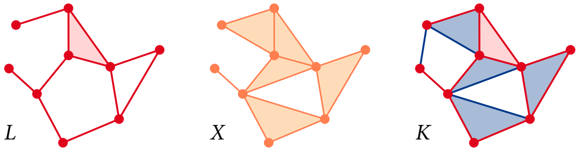

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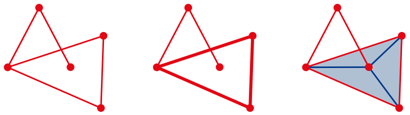

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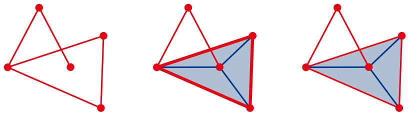

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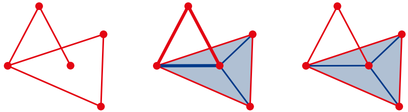

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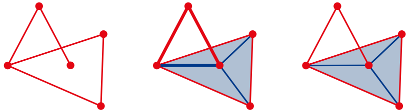

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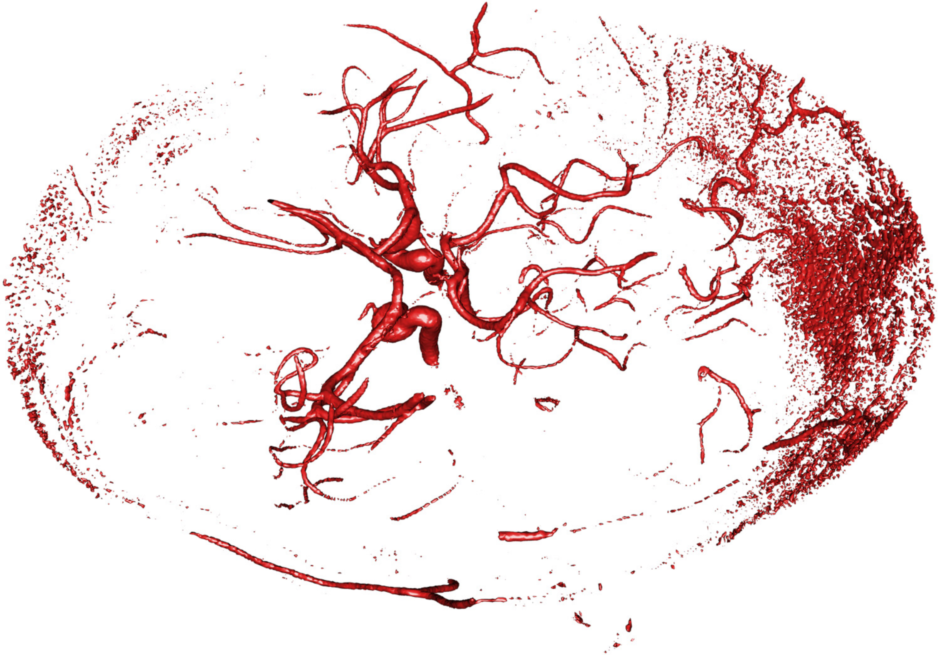
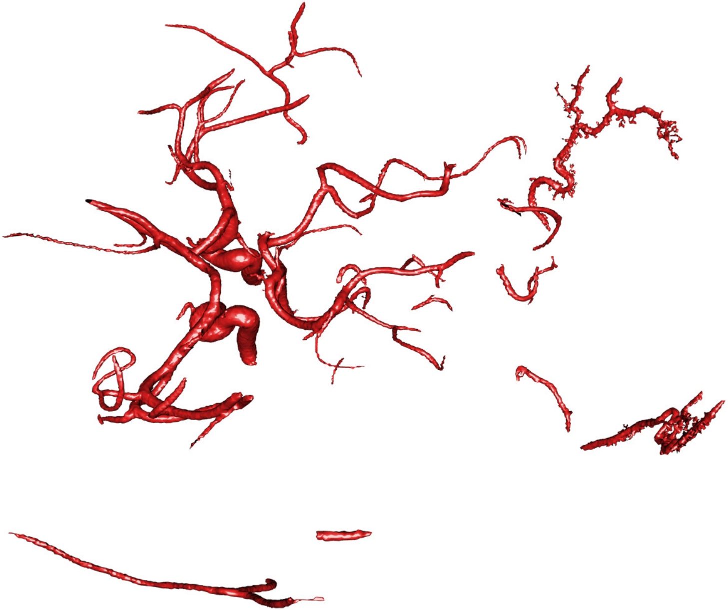
Theorem (Attali, B, Devillers, Glisse, Lieutier 2013)

The homological realization problem is NP-hard, even in $\mathbb{R}^3$.

Simplification





Sublevel set simplification

Let $F_t = f^{-1}(-\infty, t]$ denote the t-sublevel set of f.

Problem (Sublevel set simplification)

Given a function $f : X \subset \mathbb{R}^3 \to \mathbb{R}$ *and* $t \in \mathbb{R}$, $\delta > 0$,
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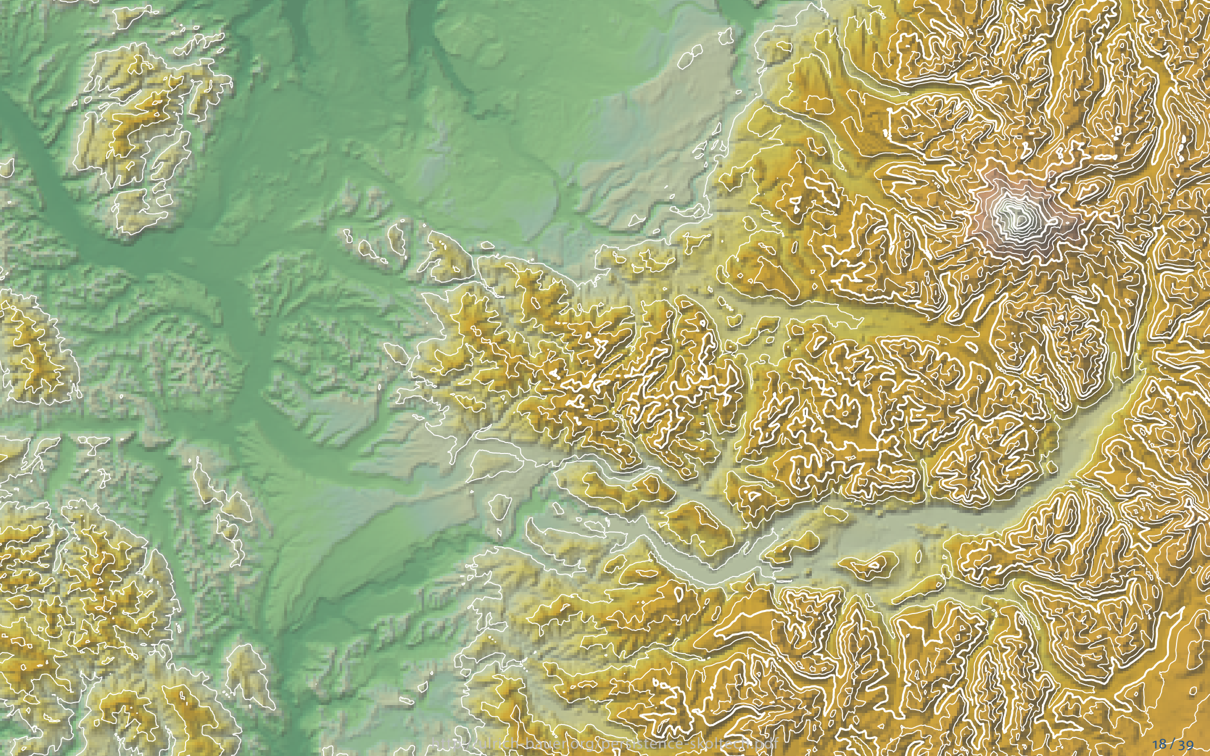
Theorem (Attali, B, Devillers, Glisse, Lieutier 2013)

Sublevel set simplification in $\mathbb{R}^3$ is NP-hard.



Topological simplification of functions

Consider the following problem:

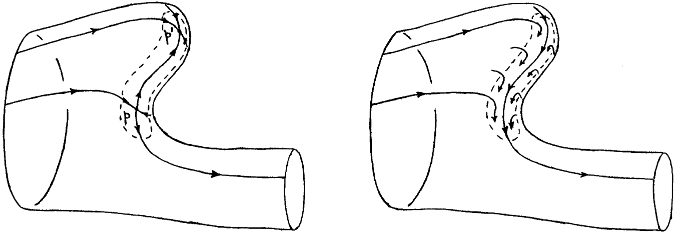
Problem (Topological simplification)

Given a function f and a real number $\delta \geq 0$, find a function f_δ subject to $\|f_\delta - f\|_\infty \leq \delta$ with the minimal number of critical points.

Persistence and Morse theory

Morse theory (smooth or discrete):

- Relates critical points to homology of sublevel sets
- Provides a method for *canceling* pairs of critical points



(from Milnor: *Lectures on the h-cobordism theorem*, 1965)

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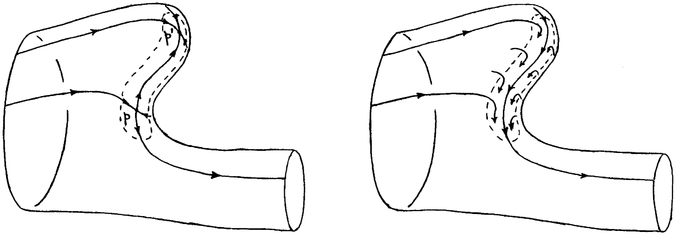

(from Milnor: *Lectures on the h-cobordism theorem*, 1965)

Persistent homology:

- Relates homology of different sublevel set
- Identifies pairs of critical points (birth and death of homological feature) and quantifies their *persistence*

Persistence and discrete Morse theory

By stability of persistence barcodes:

Proposition

The intervals in the barcode of f with persistence $> 2\delta$ provide a lower bound on the number of critical points of any function g with $\|g - f\|_\infty \leq \delta$.

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Theorem (B, Lange, Wardetzky, 2011)

Let f be a function on a surface and let $\delta > 0$.
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- Does not generalize to higher-dimensional manifolds!

Persistence and stability: the big picture

Data	point cloud	$P \subset \mathbb{R}^d$

Persistence and stability: the big picture

$$\begin{array}{ccc}
\text{Data} & \text{point cloud} & P \subset \mathbb{R}^d \\
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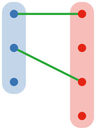
The category of matchings

Consider the category **Mch** with

- objects: sets,
- morphisms: matchings (bijections between subsets).



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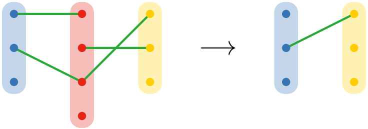
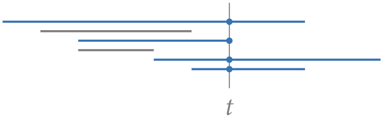
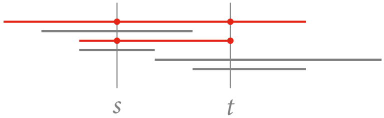


From barcodes to matching diagrams (and back)

- A barcode (collection of intervals) defines a diagram $\mathbf{R} \to \mathbf{Mch}$:



$t \mapsto \{\text{intervals in barcode containing } t\}$



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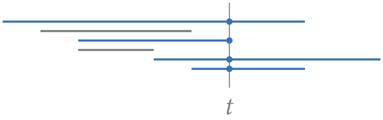

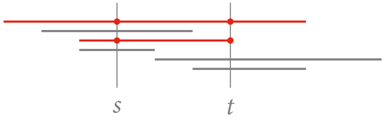

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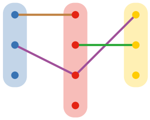
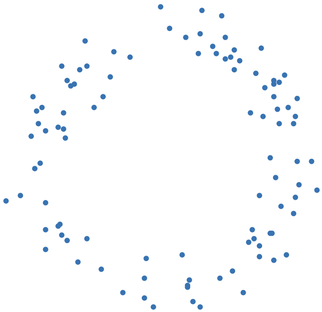
- A matching diagram defines a barcode:



  - intervals are formed by equivalence classes of matched elements

Geometric interleavings



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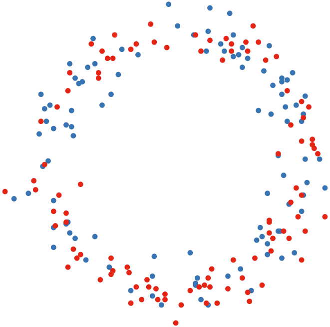

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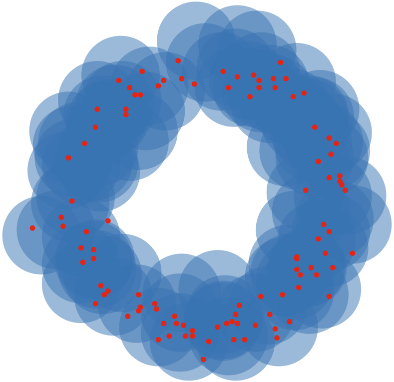

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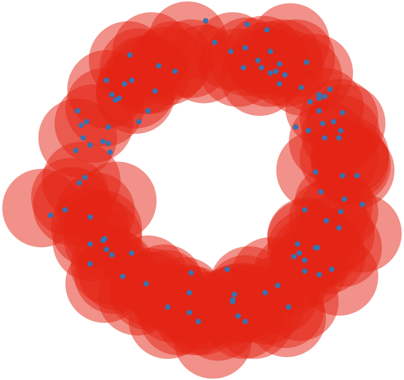

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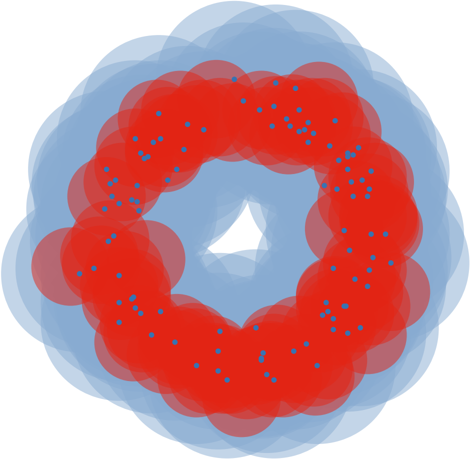

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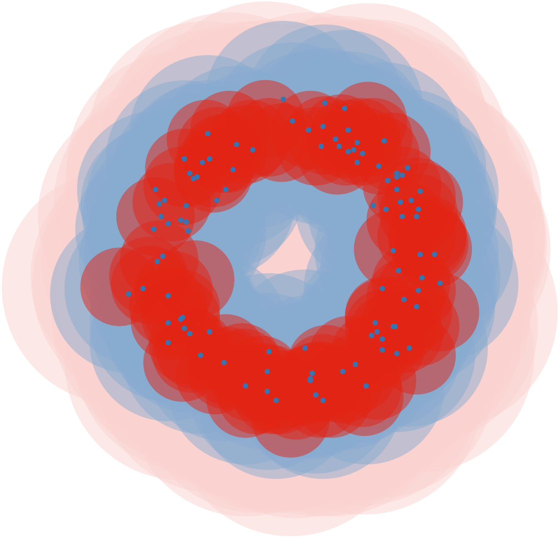

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$$\begin{tikzcd}
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- Applying homology yields a δ-interleaving of persistent homology (functors preserve commutativity):

$$\begin{tikzcd}
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Algebraic stability of persistence barcodes

Theorem (Chazal et al. 2009, 2012; B, Lesnick 2015)

If two persistence modules are δ-interleaved,
then there exists a δ-matching of their barcodes:

- matched intervals have endpoints within distance $\leq \delta$,
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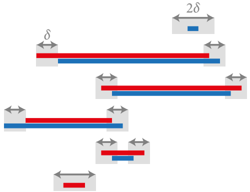

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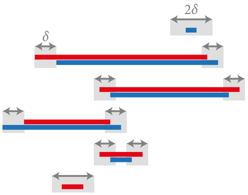

Equivalently: there exists a δ-interleaving of their barcodes (as diagrams $\mathbf{R} \to \mathbf{Mch}$).

Non-functoriality of persistence barcodes

Can a persistence module M be mapped to its barcode $B(M)$ by a functor $B : \mathbf{vect} \to \mathbf{Mch}$?

- This would preserve δ-interleavings, and thus yield stability of persistence barcodes.

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- In other words, there is no canonical way of assigning a basis to a vector space.

Structure of persistence sub-/quotient modules

Proposition

Let $f : M \twoheadrightarrow N$ *be an* epimorphism *of persistence modules:*

- *a surjective map* $f_t : M_t \twoheadrightarrow N_t$ *for each* $t \in \mathbb{R}$ *(commuting with horizontal maps)*

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Then there is an injection of barcodes $\chi(f): B(N) \hookrightarrow B(M)$.

If $\chi(f)$ *maps* J *to* I*, then*

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Dually, there is an injection $B(M) \hookrightarrow B(N)$ for monomorphisms $M \hookrightarrow N$.

Induced matchings

For $f : M \to N$ a morphism of pfd persistence modules, we always have a factorization through the image,

$$M \twoheadrightarrow \operatorname{im} f \hookrightarrow N.$$

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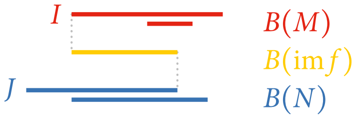
- compose the injections $B(M) \hookleftarrow B(\operatorname{im} f) \hookrightarrow B(N)$ for epimormpisms and monomorphisms to a matching

$$\chi(f) : B(M) \nrightarrow B(N).$$



Algebraic stability via induced matchings

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{} \arrow[r, dotted] & N_{t-\delta} \arrow[uur, "g_{t-\delta}"] \arrow[r, two heads] & \operatorname{im} n_{t-\delta,t+\delta} \arrow[ur, hook] \arrow[rr, hook] & & N_{t+\delta} \arrow[r, dotted] \arrow[uur, dotted] & {}
\end{tikzcd}
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Induced δ-matching of barcodes:

$B(N)$

- Left endpoints of matched intervals in $B(M), B(N)$ are within distance δ.

Algebraic stability via induced matchings

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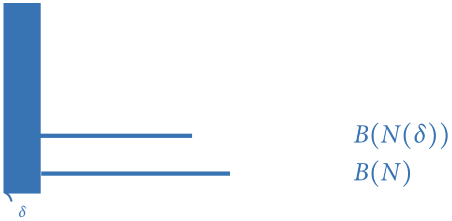

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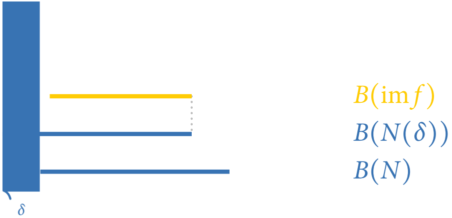

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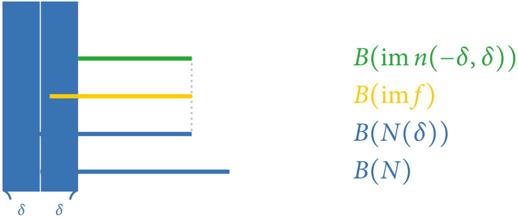

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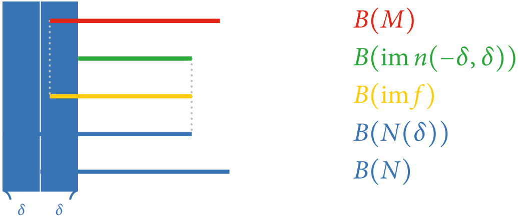

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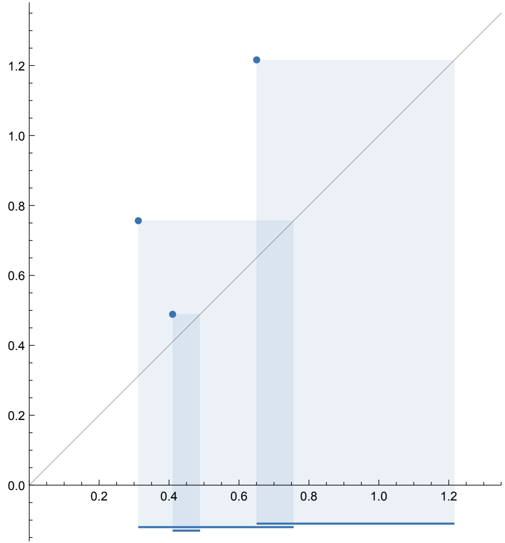
Machine learning with persistence diagrams

Extending the TDA pipeline

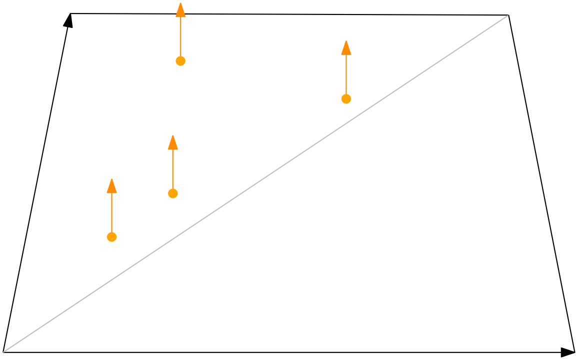
Mapping barcodes into a Hilbert space:

- desirable for machine learning methods (kernel methods, neural network) and statistics
- stability (Lipschitz continuity): important for reliable predictions
- inverse stability (bi-Lipschitz): avoid loss of information

Persistence barcodes and persistence diagrams



Persistence scale space kernel



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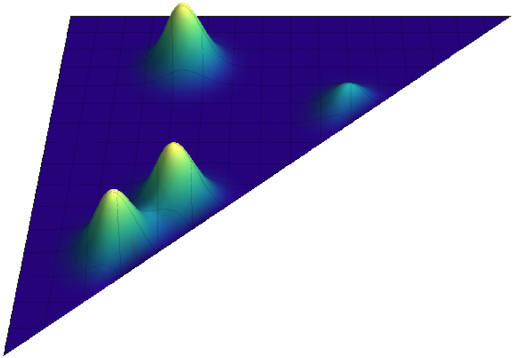

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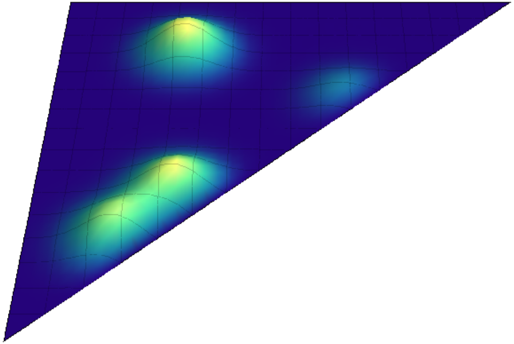

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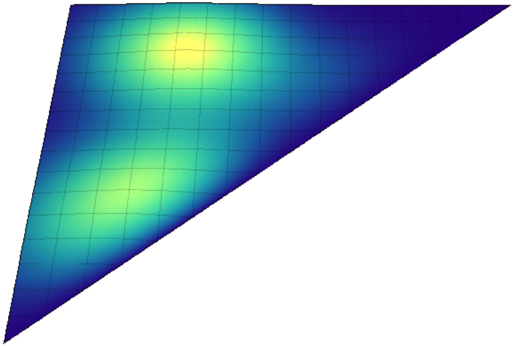

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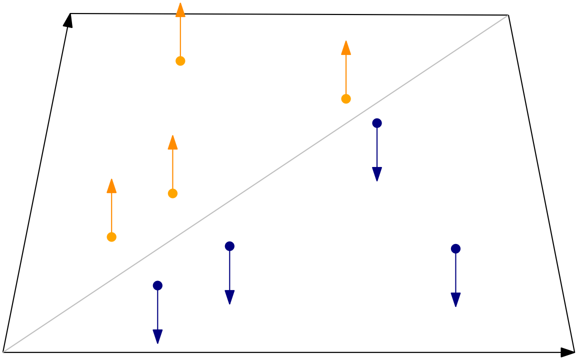

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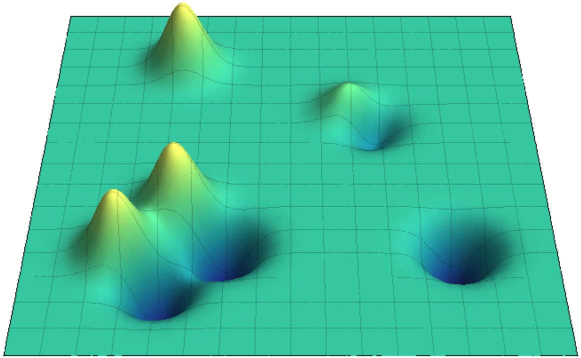

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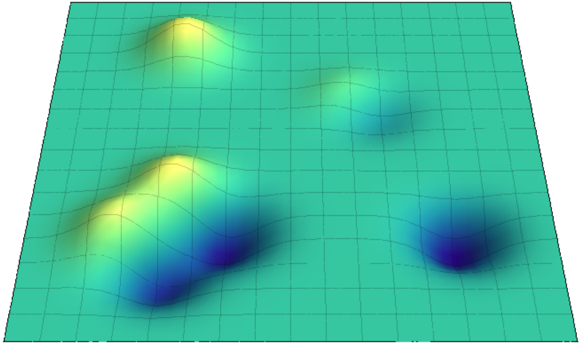

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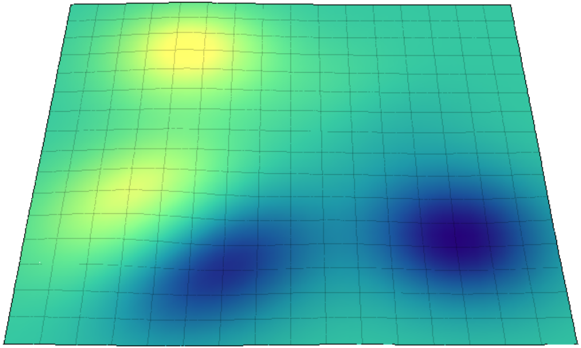

Metric distortion of the PSS kernel

Let $d_{\text{PSS}}(D_f, D_g)$ be the L^2 distance between smoothings of the persistence diagrams D_f, D_g (i.e., a *kernel distance*).

Theorem (Reininghaus, Huber, B, Kwitt 2015)

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- Here: stability with respect to *Wasserstein distance*:

$$d_p(D_f, D_g) = \Big(\inf_{\mu: D_f \leftrightarrow D_g} \sum_{x \in D_f} \|x - \mu(x)\|_\infty^p \Big)^{\frac{1}{p}}$$

- Note: bottleneck distance $d_B(D_f, D_g) = \lim_{p \to \infty} d_p(D_f, D_g)$

No bi-Lipschitz feature maps for persistence

Existing kernels for persistence diagrams in the literature:

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Theorem (B, Carrière 2018)

If there was such a bi-Lipschitz map into any Hilbert space, the Lipschitz constant would have to go to ∞ when the restrictions on the bars are lifted.

Ripser

Vietoris–Rips complexes

Consider a finite metric space (X, d) (given as a distance matrix).
The *Vietoris–Rips complex* is the simplicial complex

$$\mathrm{Rips}_t(X) = \{S \subseteq X \mid \operatorname{diam} S \leq t\}$$

- all edges with pairwise distance $\leq t$
- all possible higher simplices

An example computation

Example data set:

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- persistent homology barcodes up to dimension 2
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- Ripser: 1.2 seconds, 160 MB

Another example data set

(Columbia Object Image Library)