Persistent homology

Theory, computation, and applications

Ulrich Bauer

TUM

Dec 16, 2021

Mathematical Colloquium

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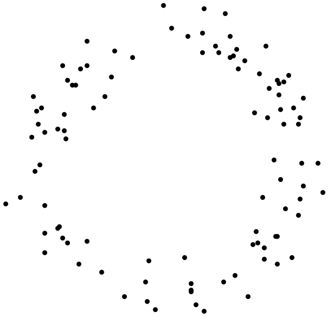
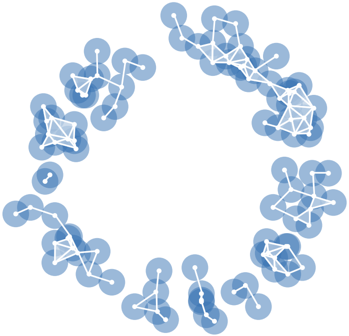
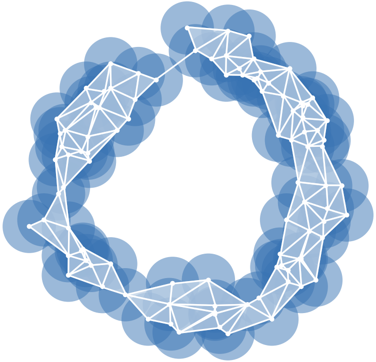
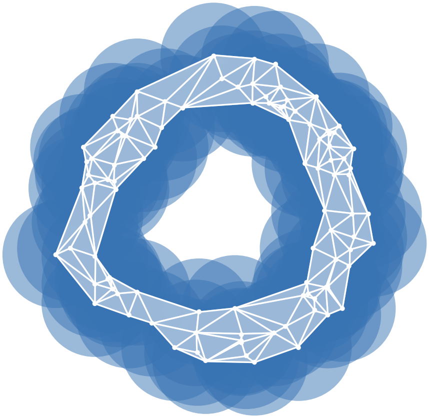
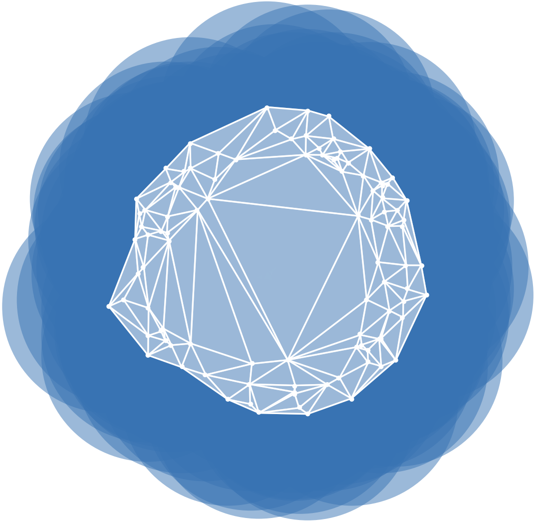


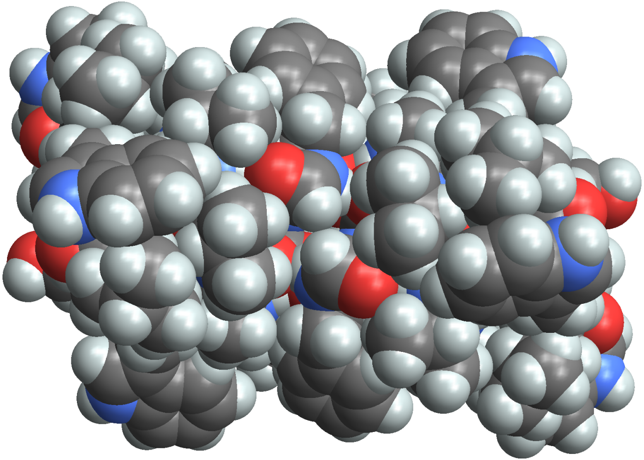








Geometry and topology of biomolecules



Gramicidin (an antibiotic functioning as an ion channel)

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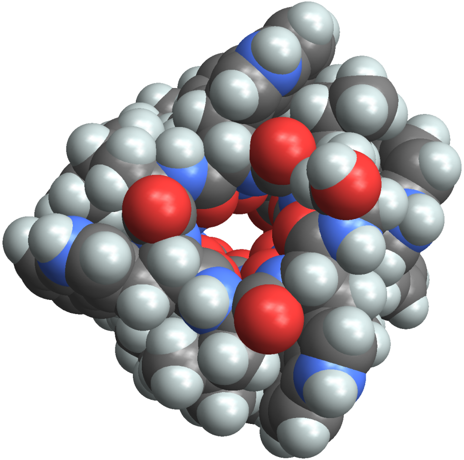

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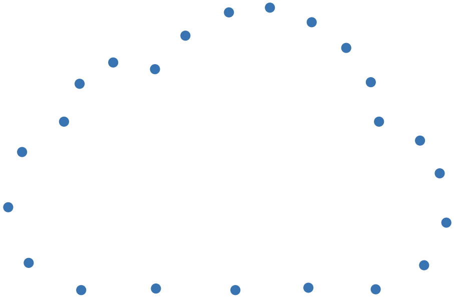

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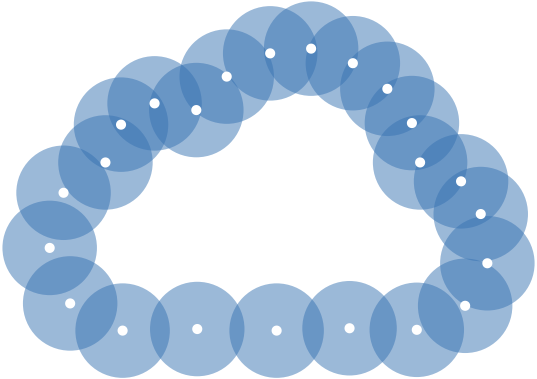

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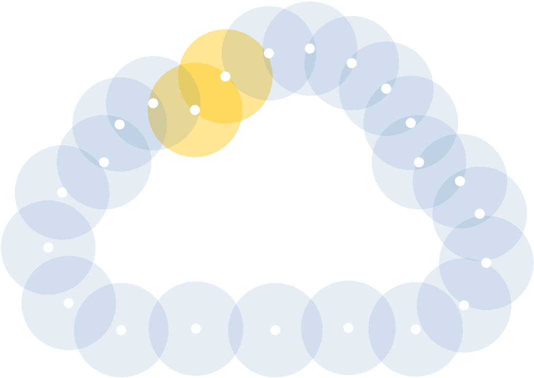

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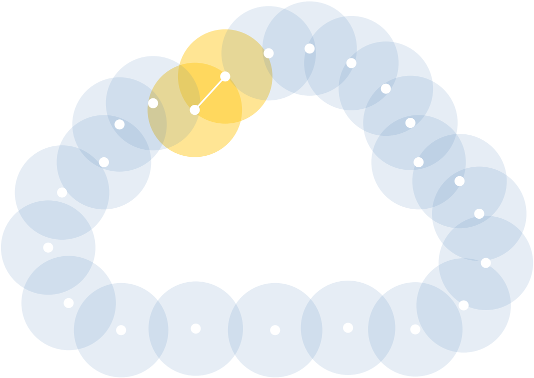

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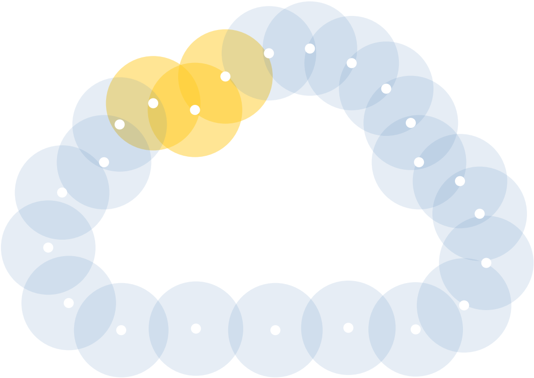

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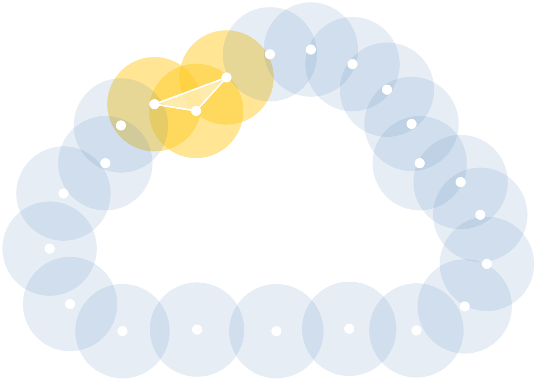

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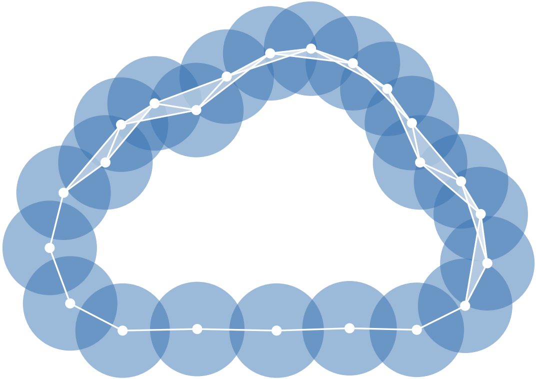

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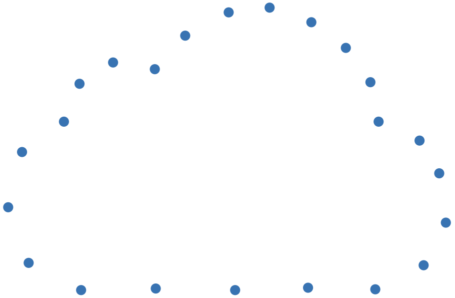

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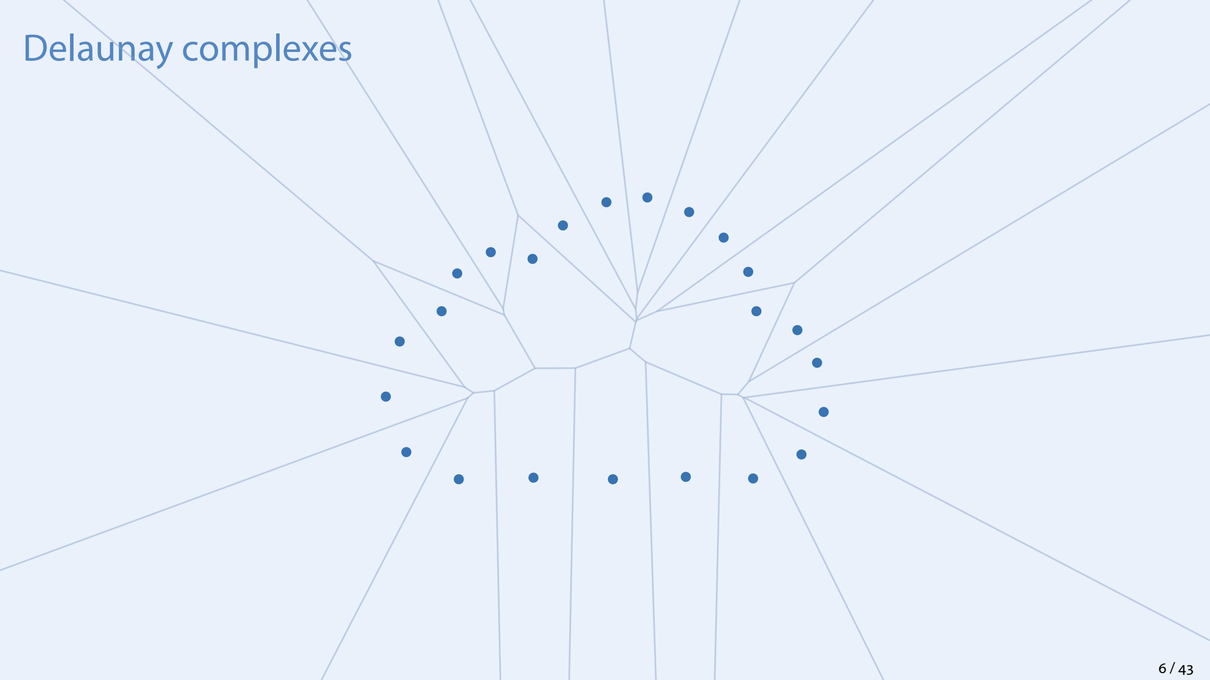

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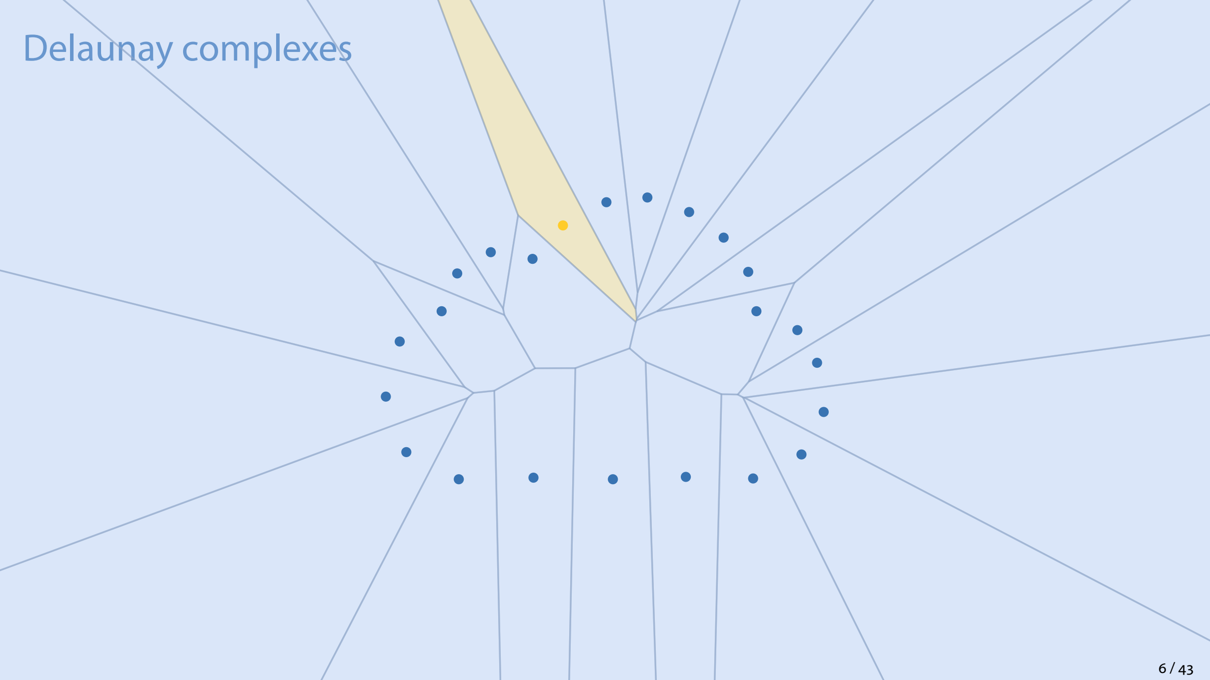

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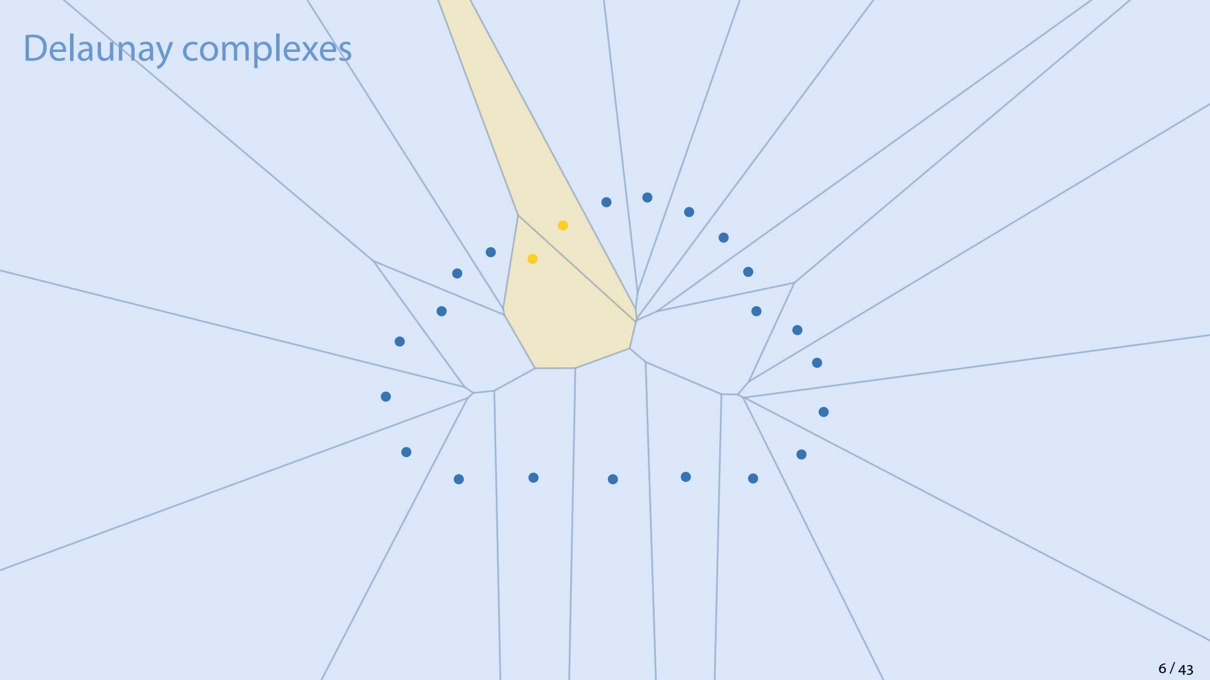

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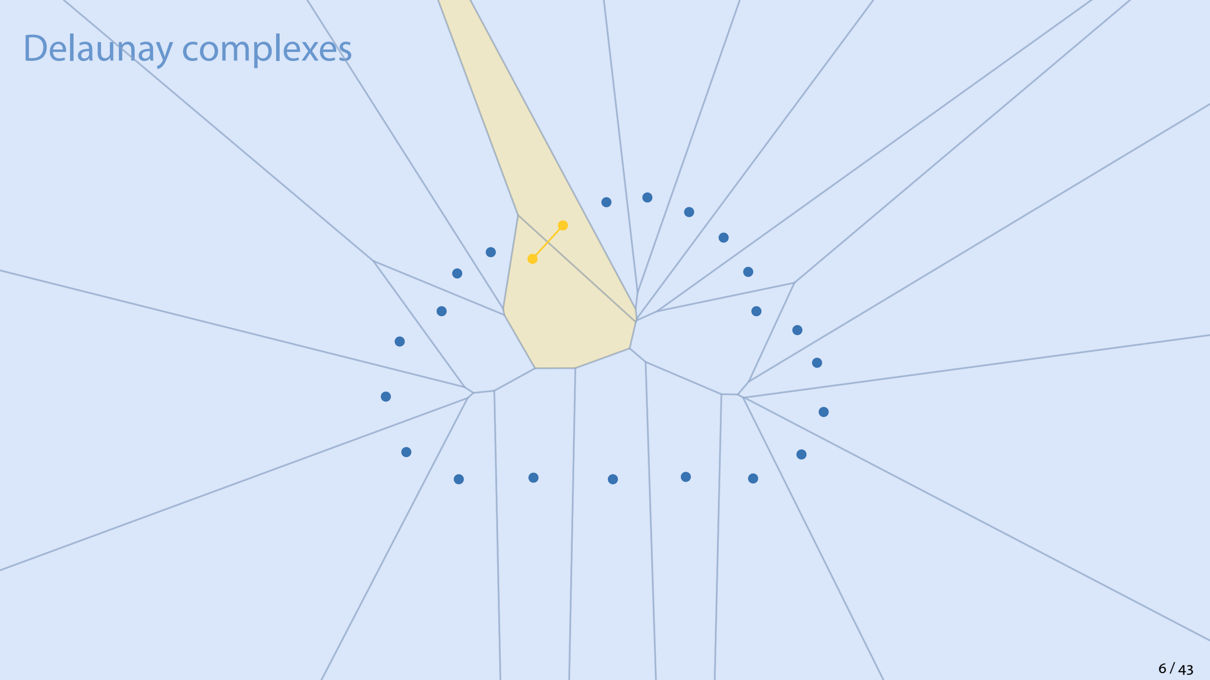

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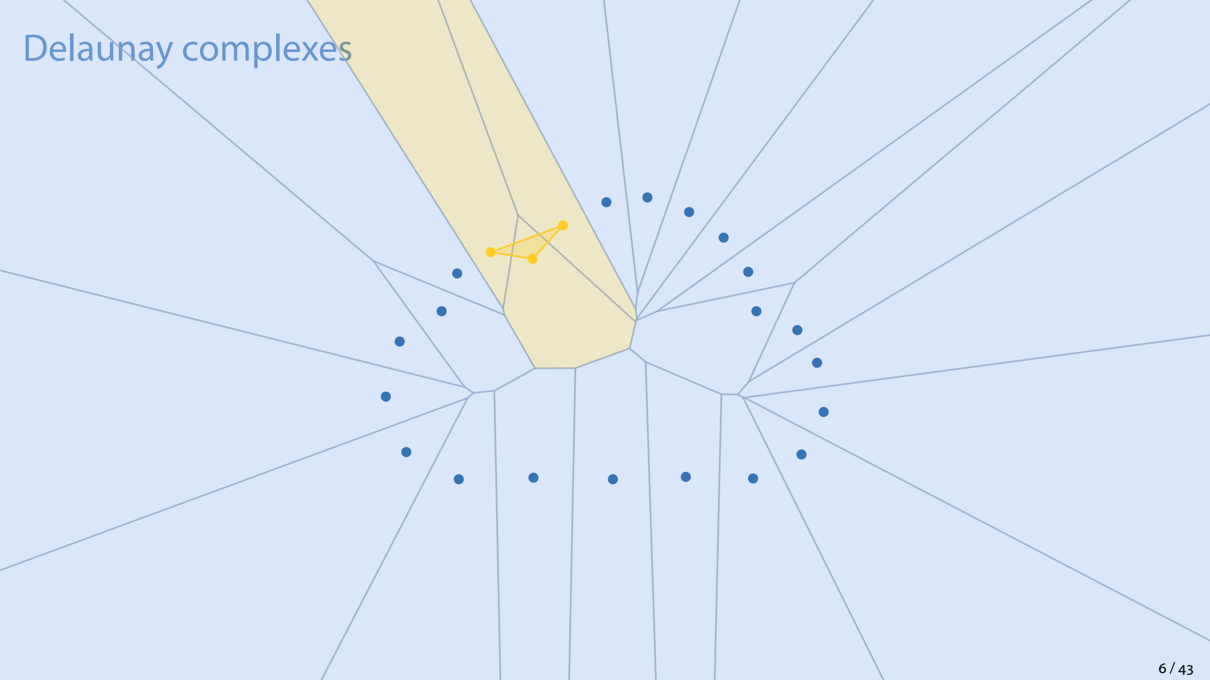

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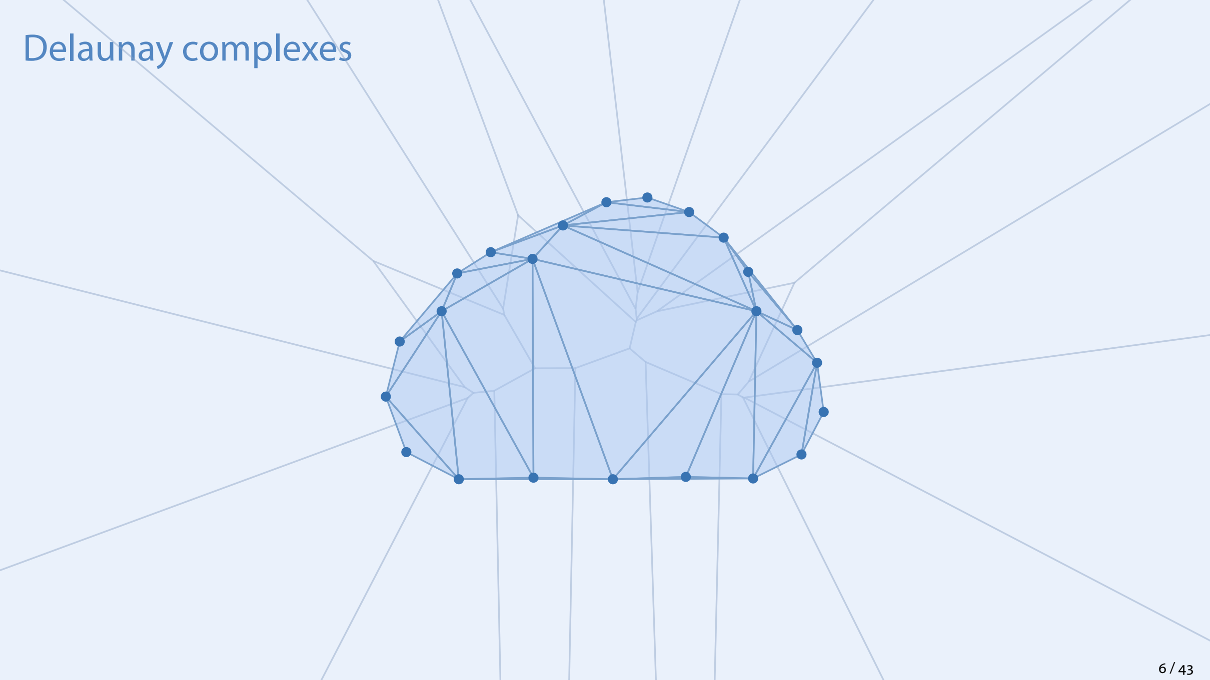

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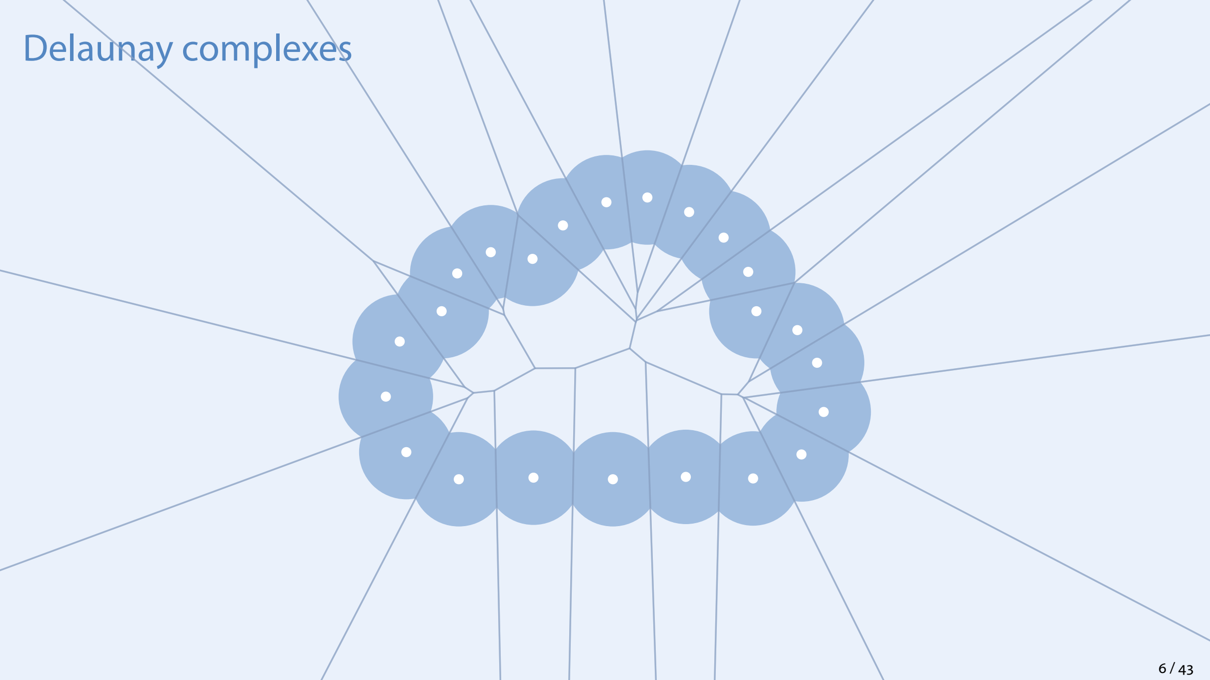

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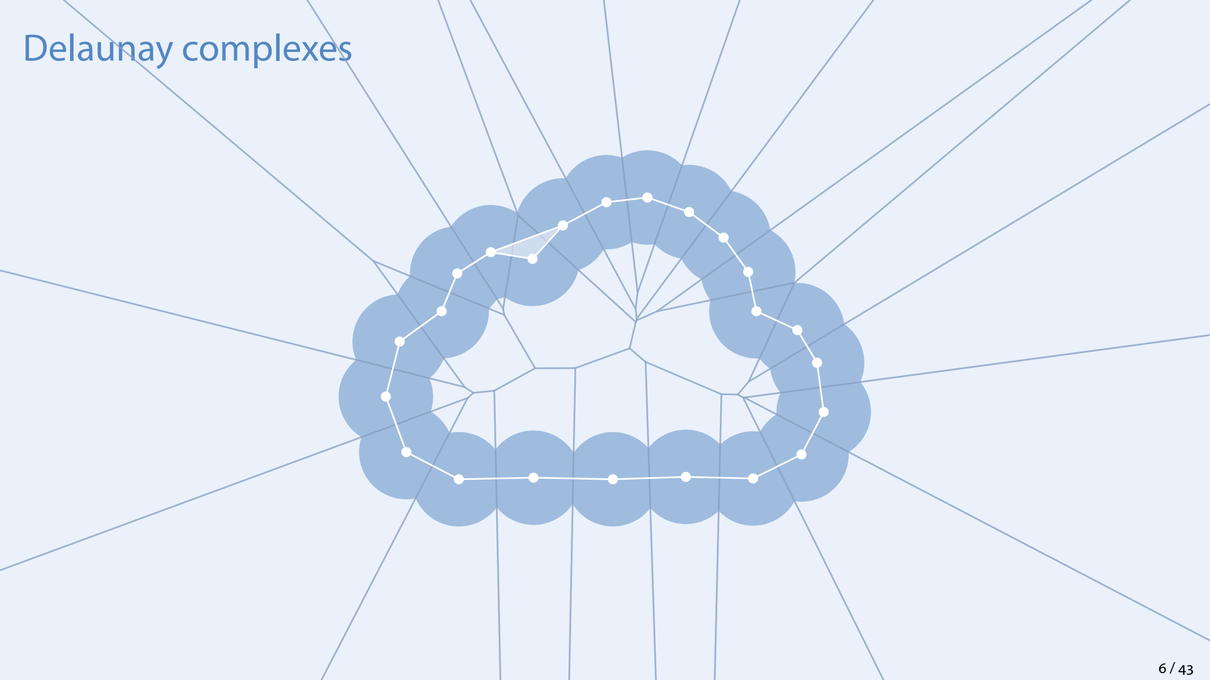

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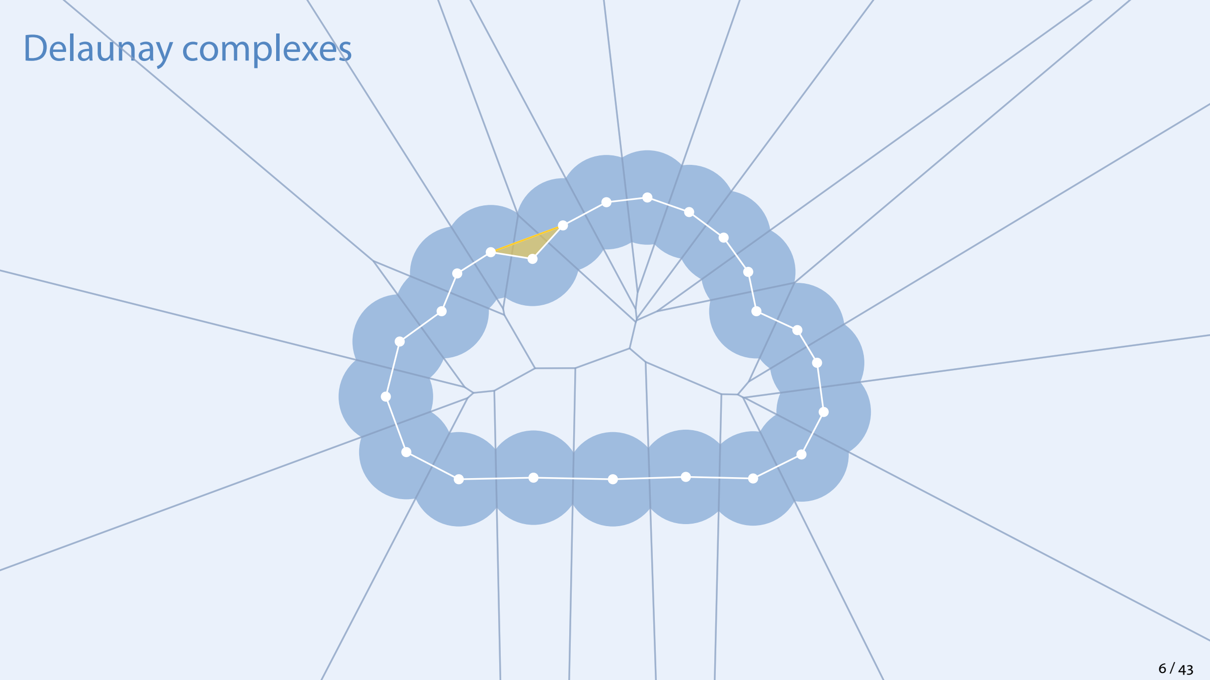

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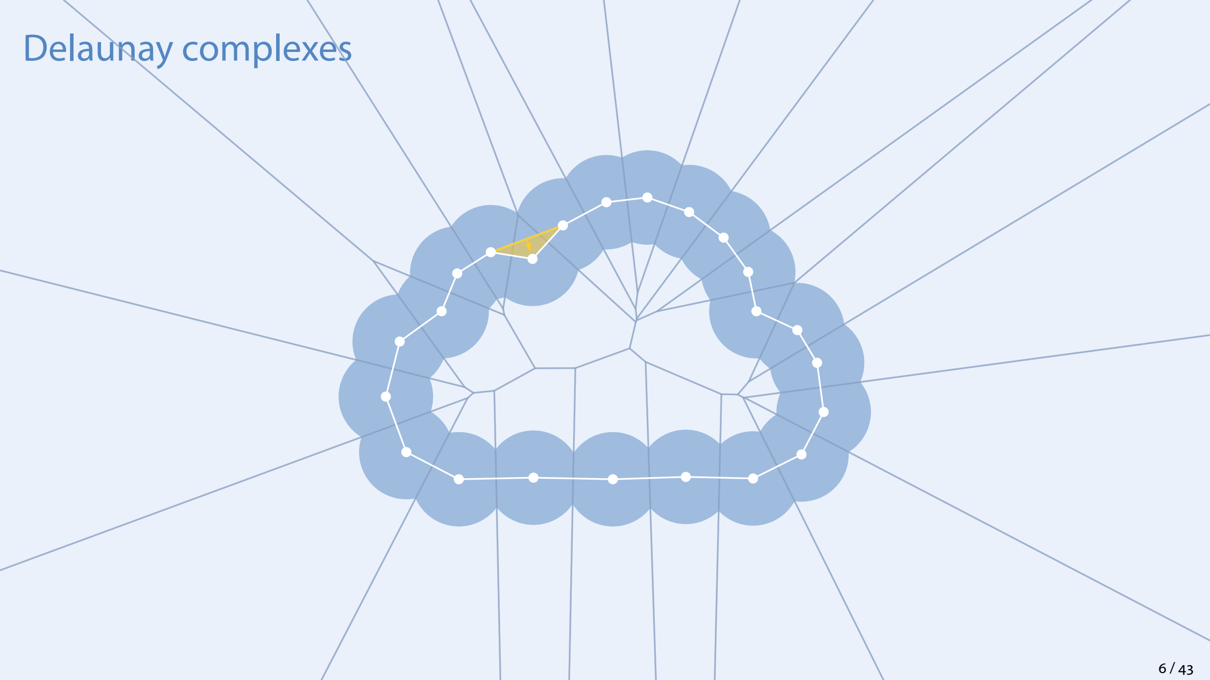

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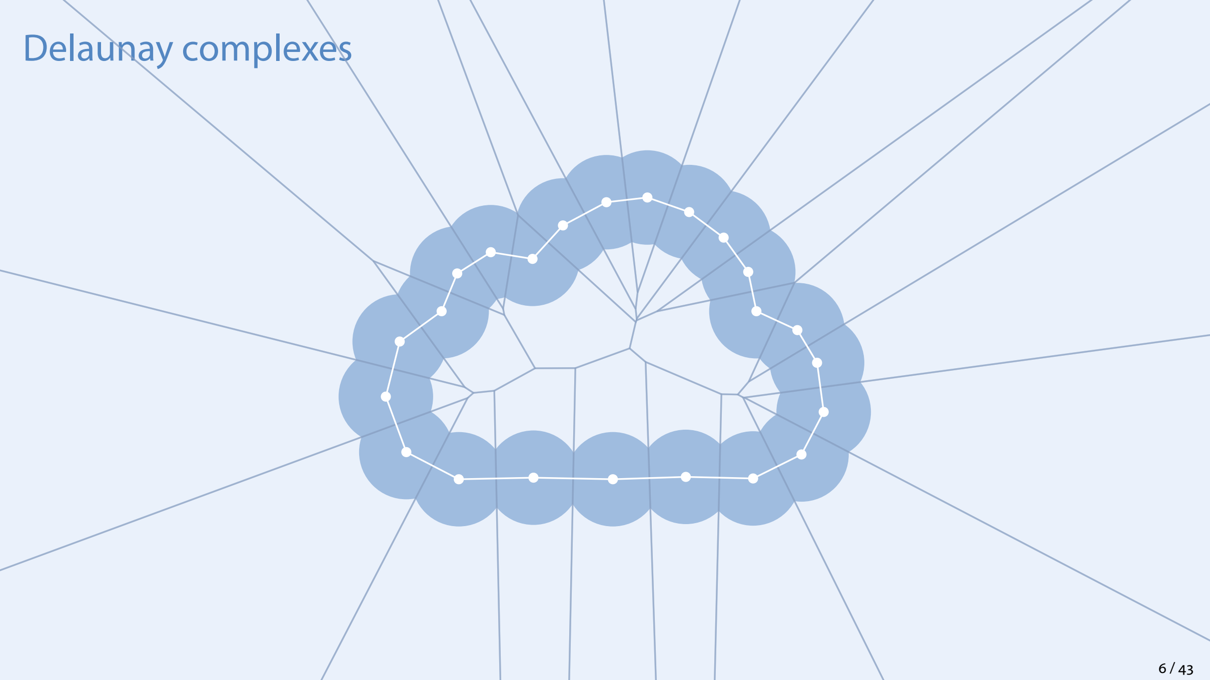
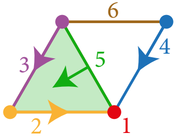


Discrete Morse theory



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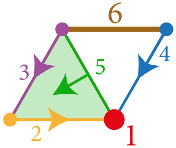
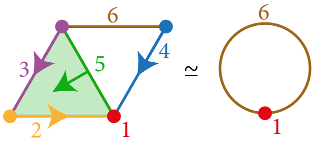


Discrete Morse theory

Theorem (Forman 1998)

A simplicial complex with a discrete Morse function f is homotopy equivalent to a cell complex build from the critical simplices of f.



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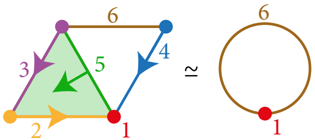
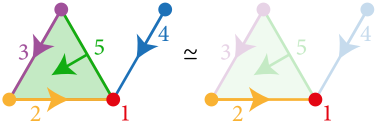


Discrete Morse functions – and their gradients – encode collapses of sublevel sets:



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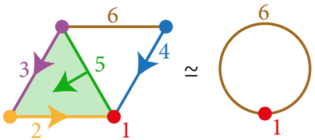

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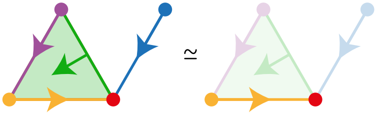

Morse theory for Čech and Delaunay complexes

Proposition

The Čech complexes and the Delaunay complexes (alpha shapes) are sublevel sets of (generalized) discrete Morse functions.

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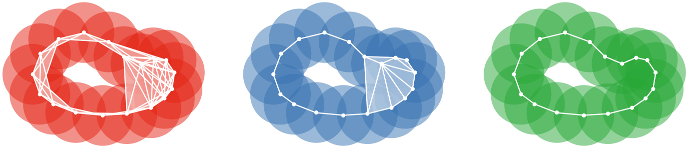
Theorem (B., Edelsbrunner 2017)

Čech, Delaunay, and Wrap complexes are homotopy equivalent through collapses

$$\mathrm{Cech}_r X \searrow \mathrm{Del}_r X \searrow \mathrm{Wrap}_r X,$$

encoded by a single discrete gradient field.



Delaunay and Wrap complexes

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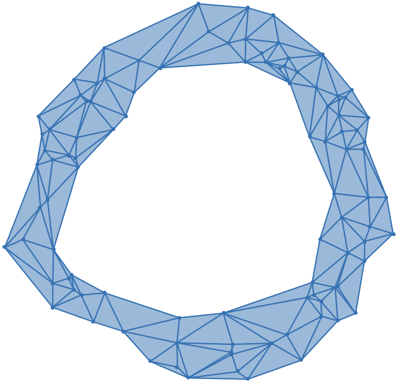

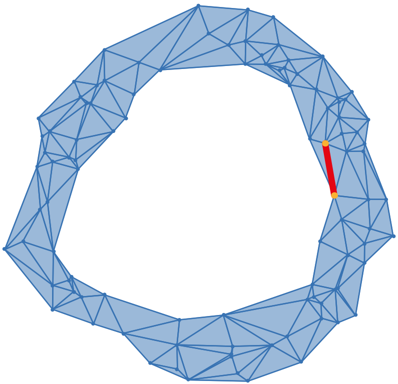

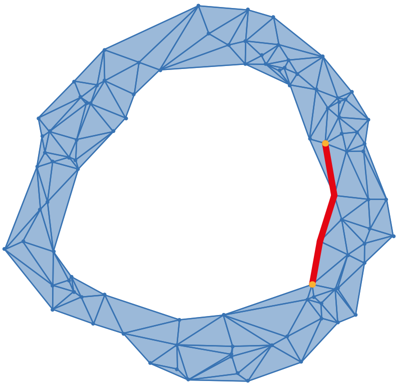

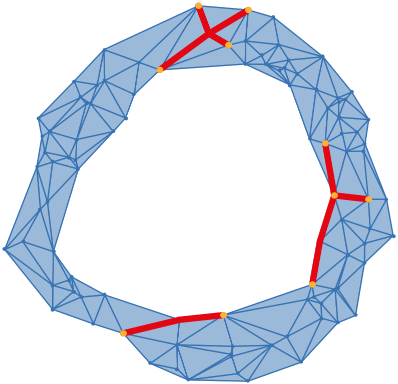

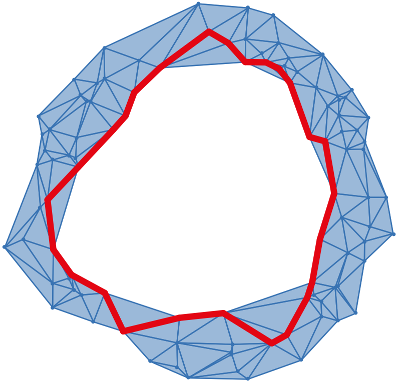

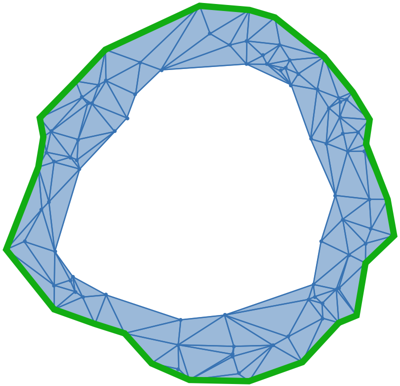

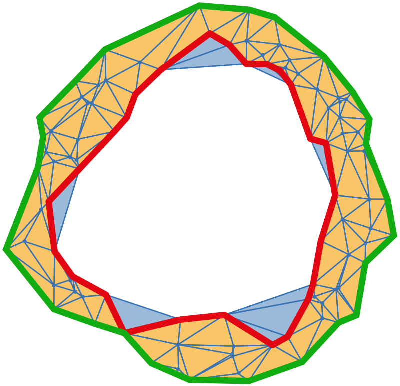

Homology inference

Inferring homology from samples

Given: finite sample $P \subset X$ of unknown shape $X \subset \mathbb{R}^d$

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This can work, but 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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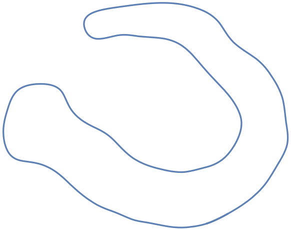

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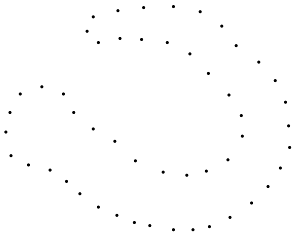

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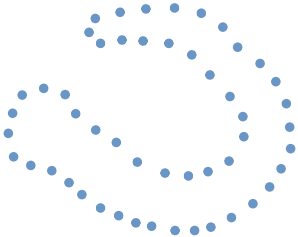

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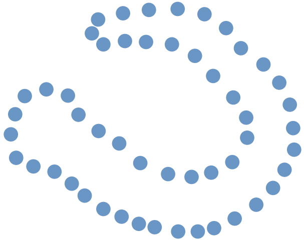

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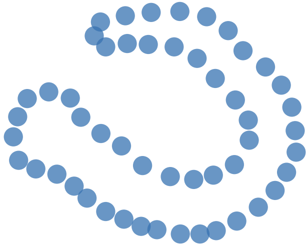

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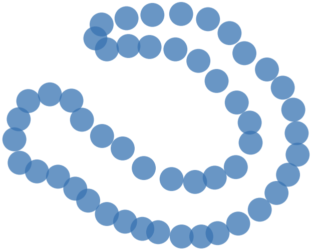

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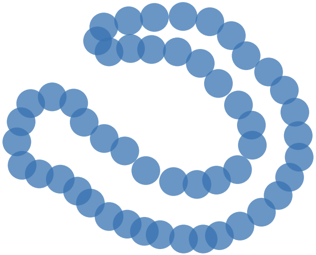

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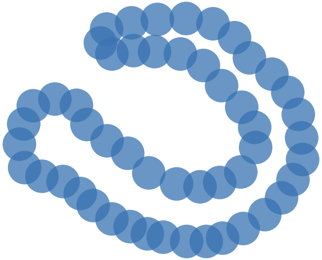

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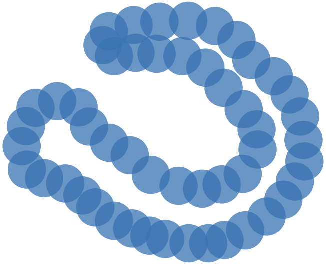

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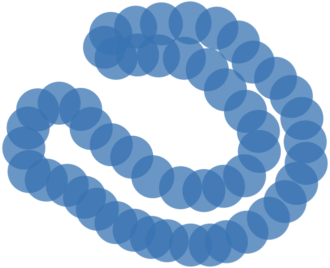

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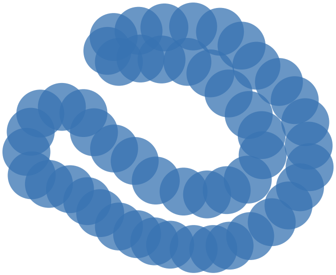

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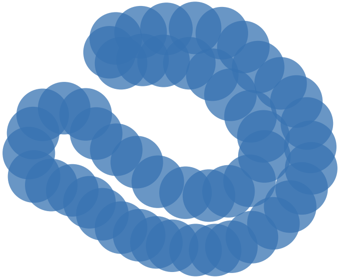

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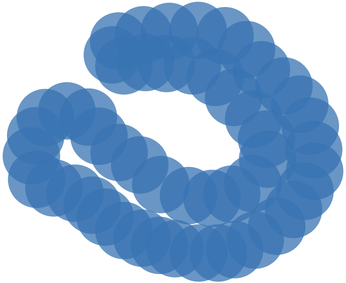

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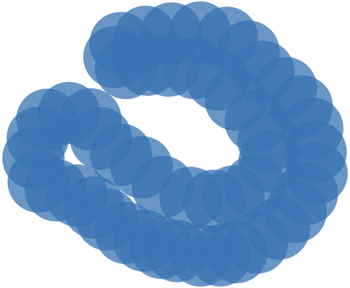

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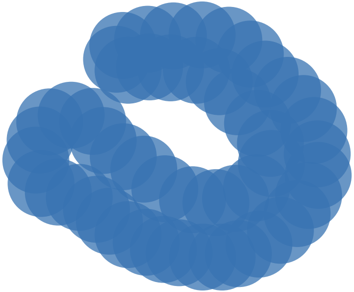

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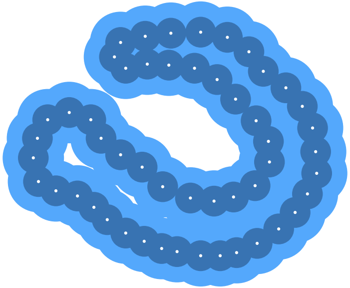

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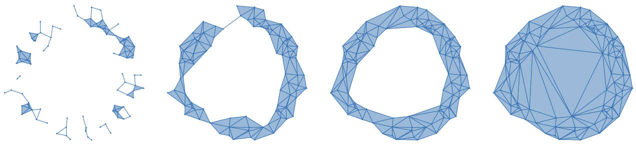

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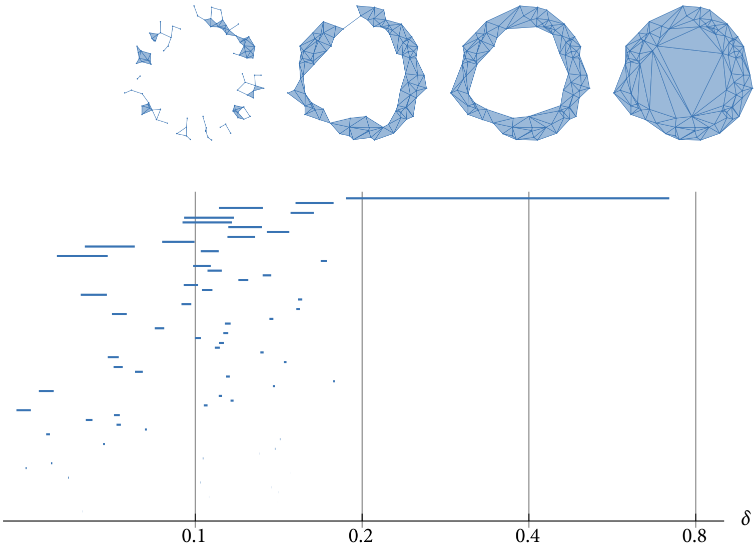

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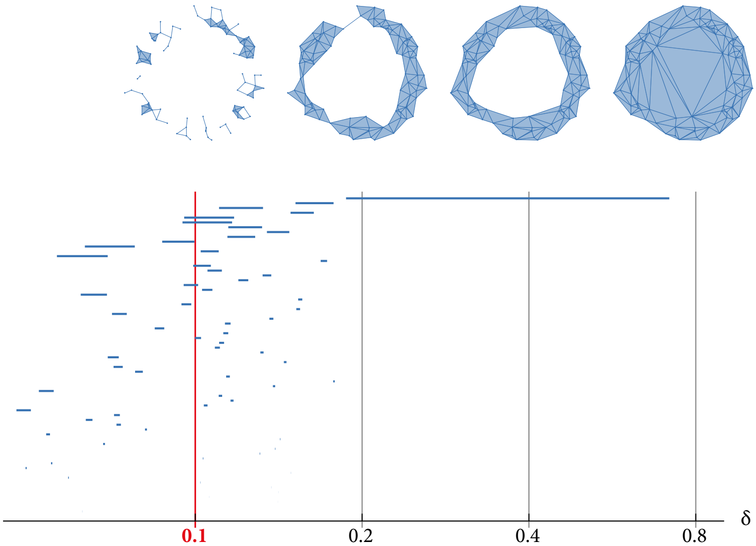

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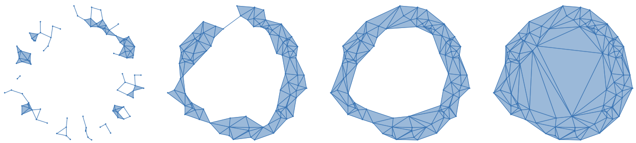

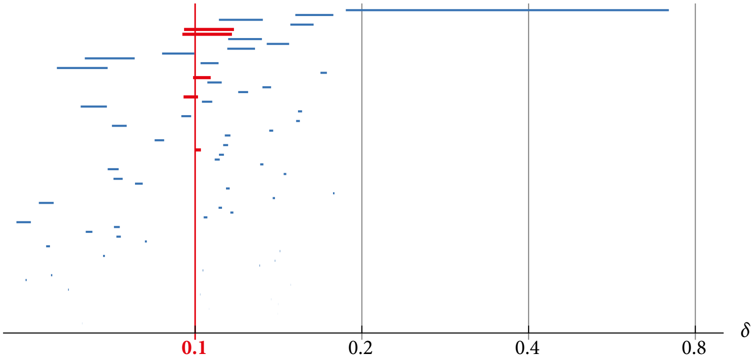

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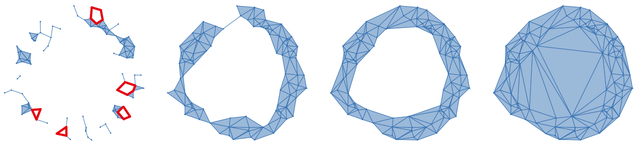

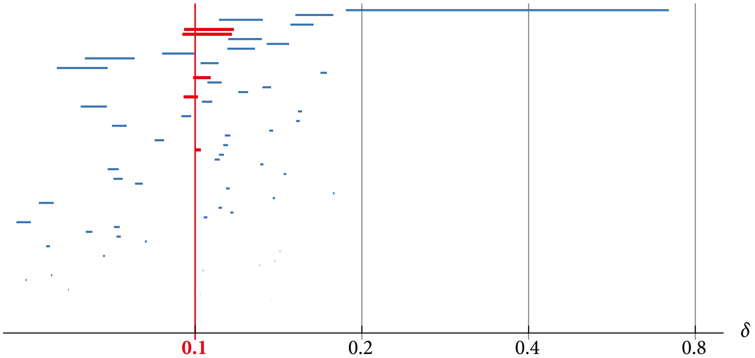

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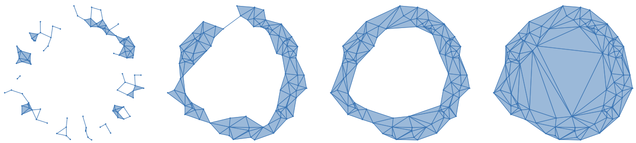

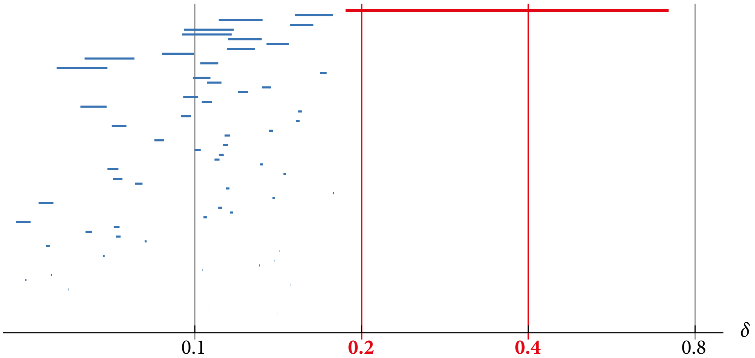

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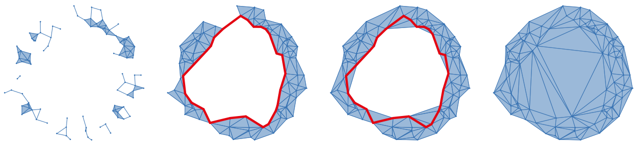

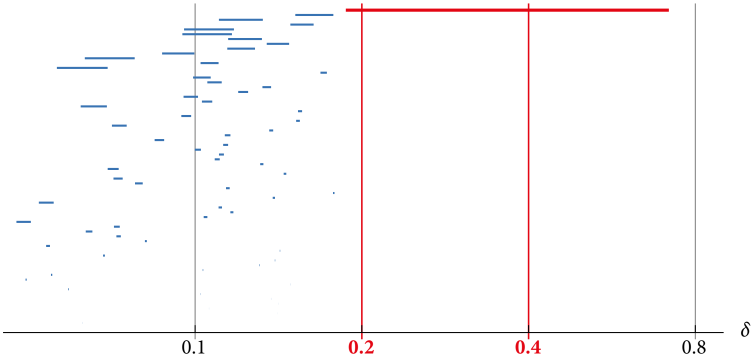

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- A filtration is a certain diagram $K : \mathbf{R} \to \mathbf{Top}$ of topological spaces, indexed over the poset of real numbers $\mathbf{R} := (\mathbb{R}, \leq)$

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

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- Persistent homology is a diagram $M = H_* \circ K : \mathbf{R} \to \mathbf{Vect}$ *(persistence module)*:

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Barcodes: the structure of persistence modules

Theorem (Crawley-Boevey 2015)

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

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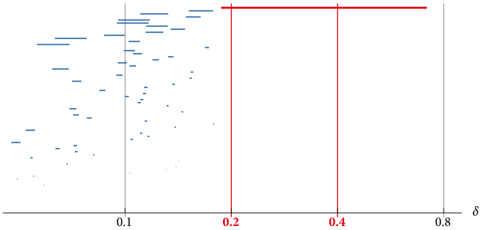
- The supporting intervals form the *persistence barcode*.



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 sublevel set filtrations $f^{-1}(\infty, t]$ and $g^{-1}(\infty, t]$, and*
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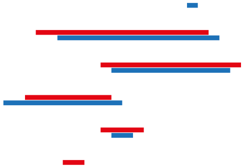
*Then there exists a δ-*matching *between the barcodes, meaning that:*



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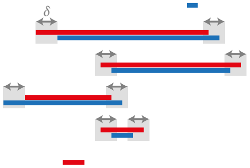

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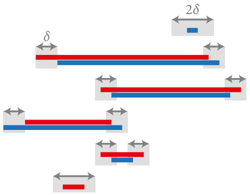

Persistence and stability: the big picture

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

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Applying homology, the persistence modules $H_*(F), H_*(G) : \mathbf{R} \to \mathbf{Vect}$ are *δ-interleaved:*

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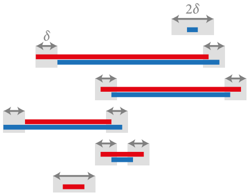
Algebraic stability of persistence barcodes

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.



Structure of persistence sub-/quotient modules

Proposition (B, Lesnick 2015)

Let $M \twoheadrightarrow N$ be an epimorphism of persistence modules.
Then there is an injection of barcodes $B(N) \hookrightarrow B(M)$ such that
if J is mapped to I, then

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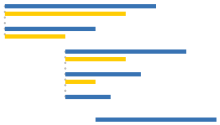

Dually, there is an injection $B(M) \hookrightarrow B(N)$ for monomorphisms $M \hookrightarrow N$.

Induced matchings

For $f : M \to N$ a general morphism of pfd persistence modules, the epi-mono factorization

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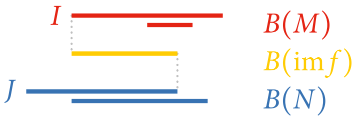
- compose the injections $B(M) \hookleftarrow B(\operatorname{im} f) \hookrightarrow B(N)$ from before to a matching $B(M) \nrightarrow B(N)$



Induced matchings

For $f : M \to N$ a general morphism of pfd persistence modules, the epi-mono factorization

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

gives an *induced matching* between their barcodes:

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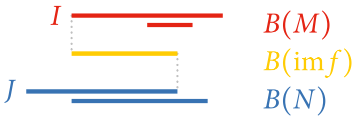


If f is a δ-interleaving morphism, then this induced matching is a δ-matching.

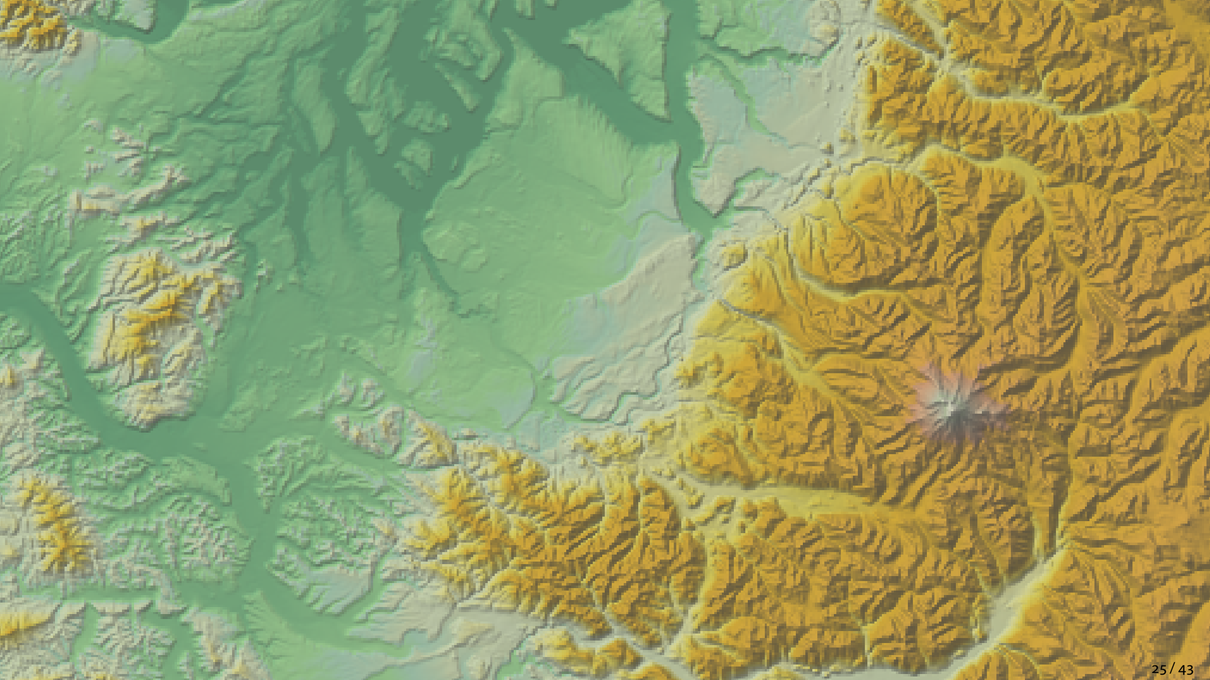
Simplification

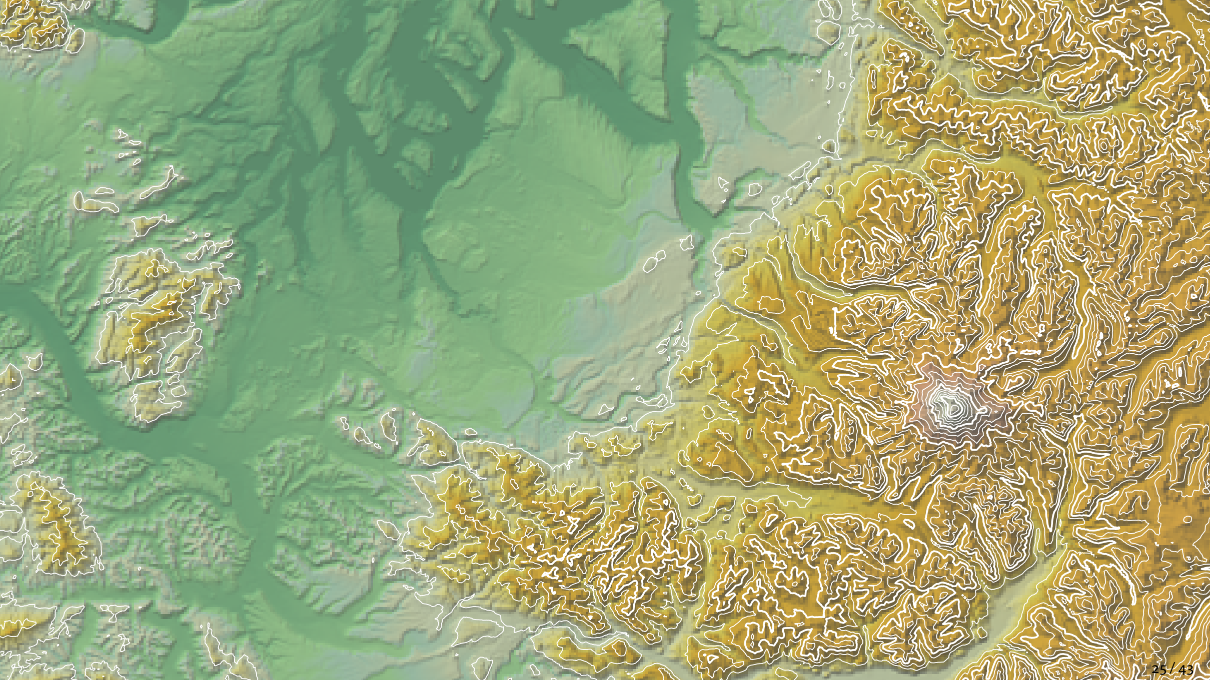
Topological simplification of functions

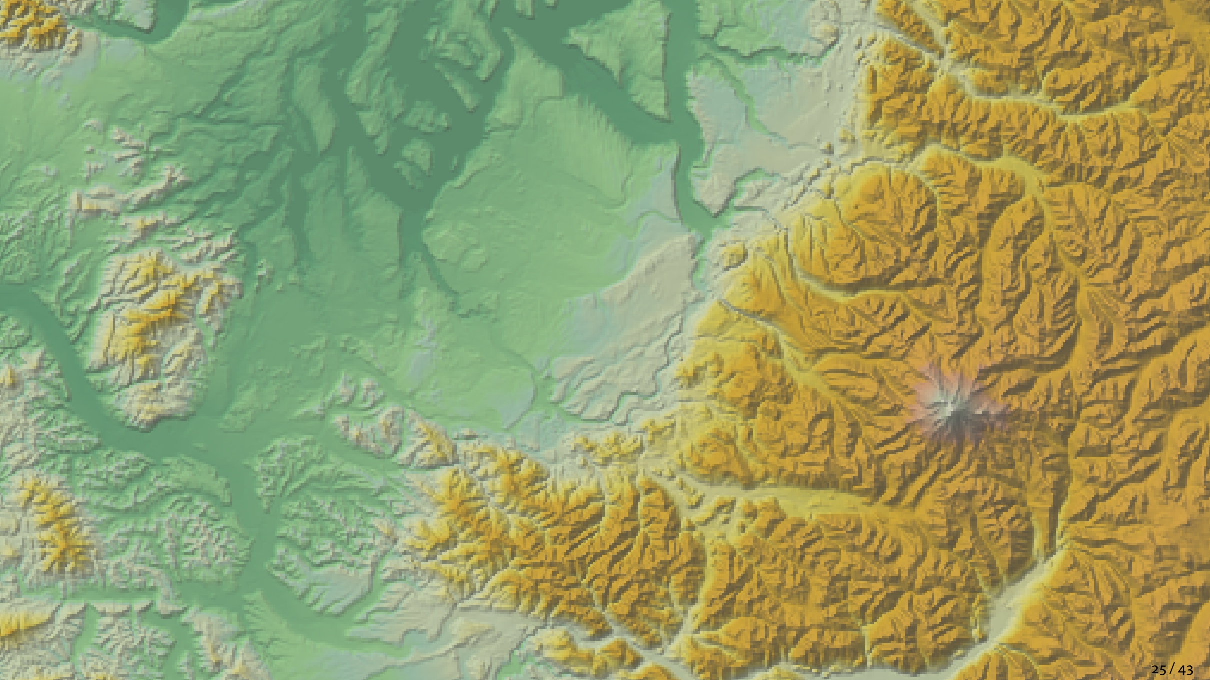
Consider the following problem:

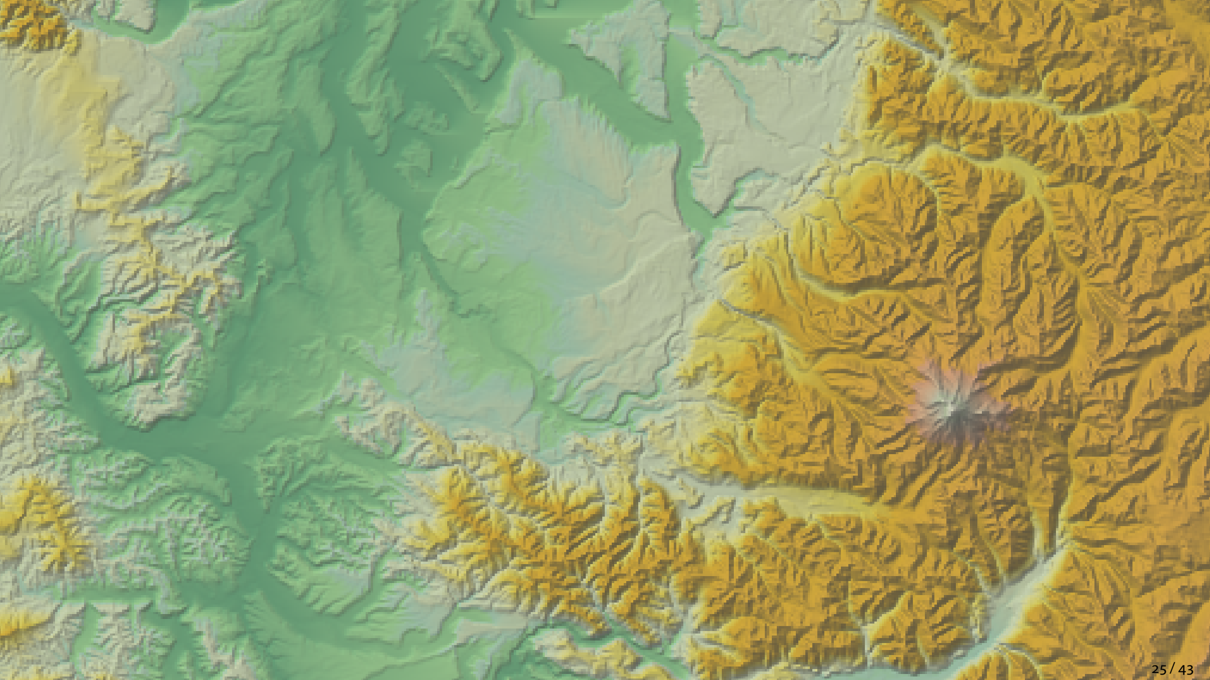
Problem (Topological simplification)

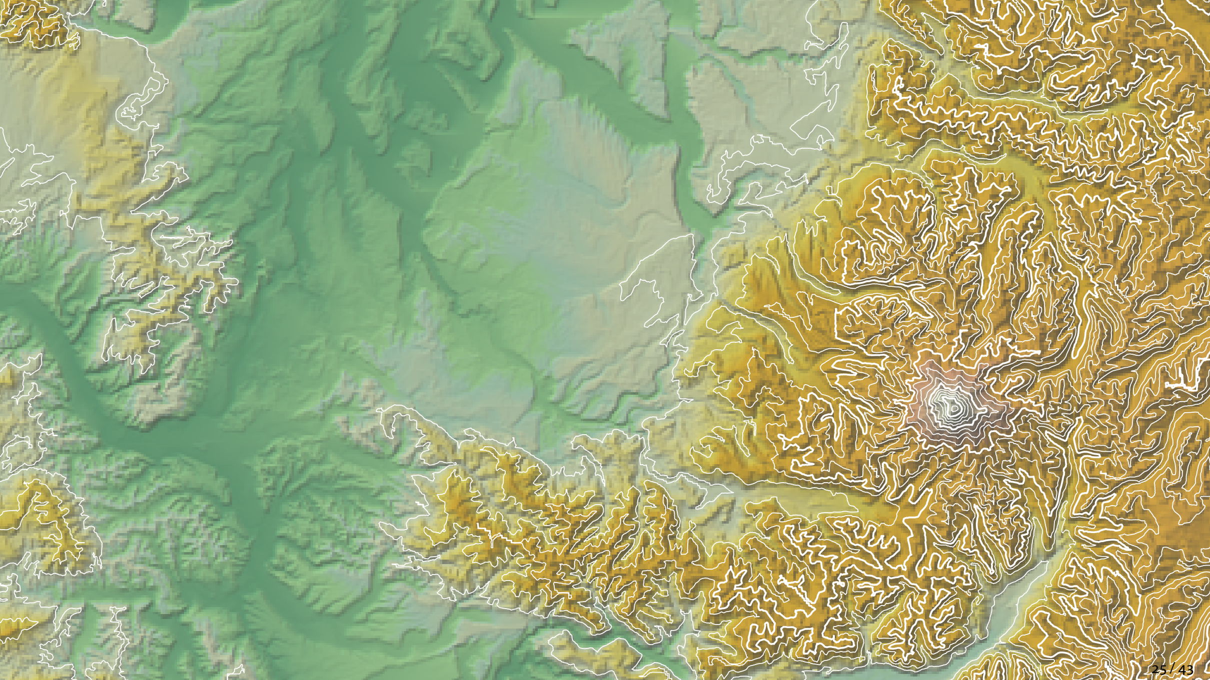
Given a function f and a real number $\delta \geq 0$, find a function f_δ with the minimal number of critical points subject to $\|f_\delta - f\|_\infty \leq \delta$.







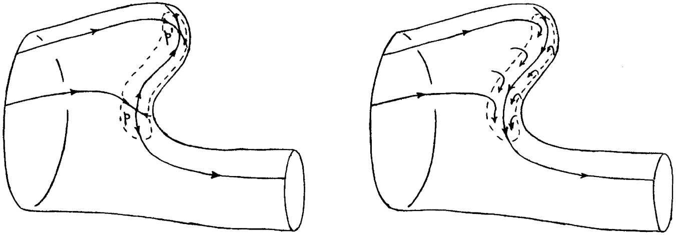




Persistence and Morse theory

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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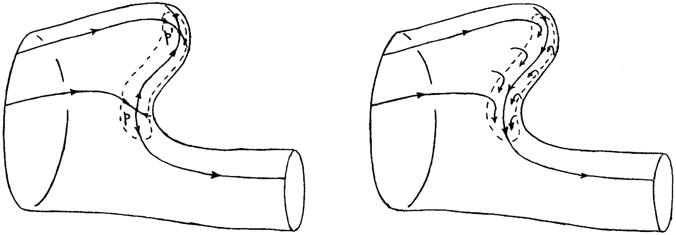

(from Milnor: *Lectures on the h-cobordism theorem*, 1965)

Persistent homology:

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

Combining persistence and Morse theory

For a Morse function:

- critical points correspond to endpoints of barcode intervals

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By stability of persistence barcodes:

Proposition

The critical points 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 $\delta > 0$.
Canceling all pairs with persistence $\leq 2\delta$ yields a function f_δ

- *satisfying $\|f_\delta - f\|_\infty \leq \delta$ and*
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Does not generalize to higher-dimensional manifolds!

Functional topology

When was persistent homology discovered?

H. Edelsbrunner, D. Letscher, and A. Zomorodian
Topological persistence and simplification
Foundations of Computer Science, 2000

V. Robbins
Computational Topology at Multiple Resolutions.
PhD thesis, University of Colorado Boulder, 2000

P. Frosini
A distance for similarity classes of submanifolds of a Euclidean space
Bulletin of the Australian Mathematical Society, 1990.

S. A. Barannikov.
The framed Morse complex and its invariants.
In *Singularities and bifurcations, Adv. Soviet Math. (vol. 21)*, 1994.

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ANNALS OF MATHEMATICS
Vol. 41, No. 2, April, 1940

RANK AND SPAN IN FUNCTIONAL TOPOLOGY

BY MARSTON MORSE

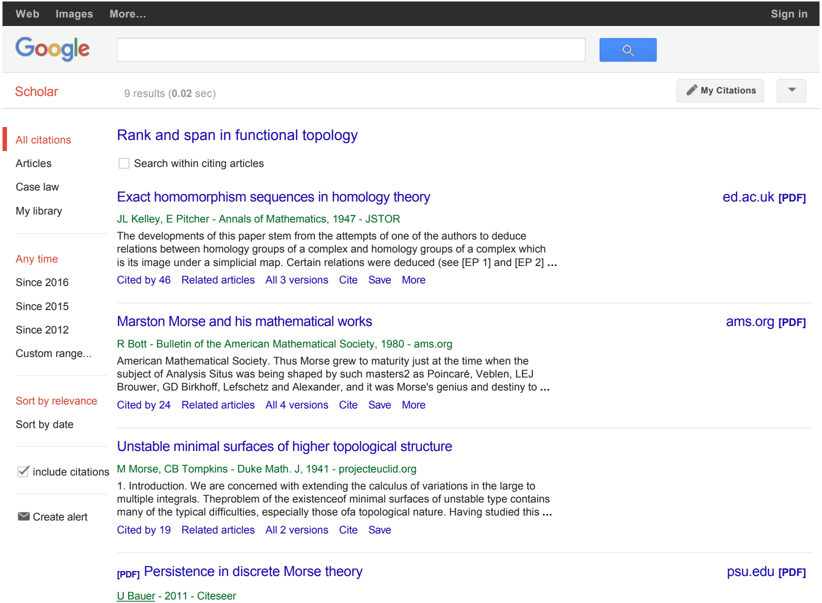
(Received August 9, 1939)

1. Introduction.

The analysis of functions F on metric spaces M of the type which appear in variational theories is made difficult by the fact that the critical limits, such as absolute minima, relative minima, minimax values etc., are in general infinite in number. These limits are associated with relative k-cycles of various dimensions and are classified as 0-limits, 1-limits etc. The number of k-limits suitably counted is called the k^{th} type number m_k of F. The theory seeks to establish relations between the numbers m_k and the connectivities p_k of M. The numbers p_k are finite in the most important applications. It is otherwise with the numbers m_k.

The theory has been able to proceed provided one of the following hypotheses

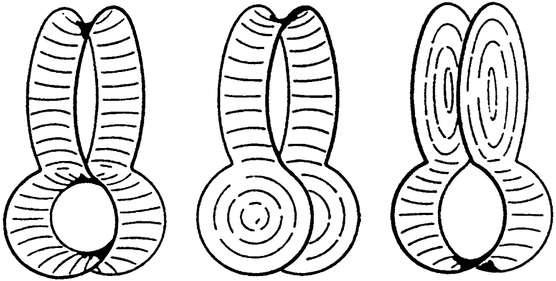
When was persistent homology discovered first?



Motivation and application: minimal surfaces

Problem (Plateau's problem)

Find an immersed disk of least area spanned by a given closed Jordan curve.



(a) (b) (c)

(from Dierkes et al.: *Minimal Surfaces*, 2010)

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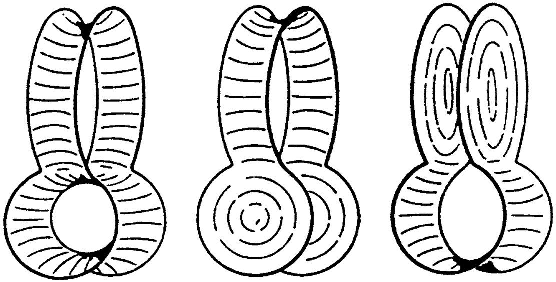

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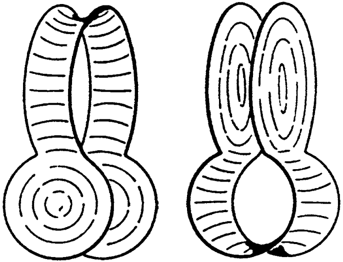
Solution by Douglas (1930):

- identifies minimal surfaces with critical points of the *Douglas functional*

Existence of unstable minimal surfaces

Theorem (Morse, Tompkins 1939; Shiffman 1939)

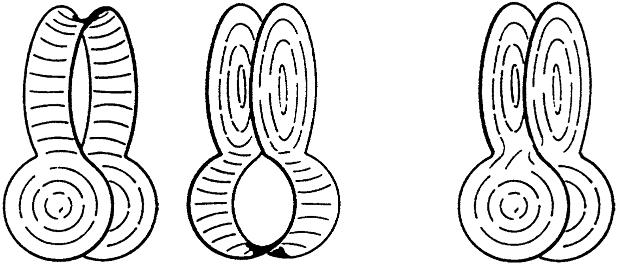
Assume that a given curve bounds two separate stable minimal surfaces.



Existence of unstable minimal surfaces

Theorem (Morse, Tompkins 1939; Shiffman 1939)

Assume that a given curve bounds two separate stable minimal surfaces. Then there also exists an unstable *minimal surface bounding that curve (a critical point that is not a local minimum).*



Q-tame persistence modules

Definition (Chazal et al. 2009)

A persistence module $M : \mathbf{R} \to \mathbf{vect}$ is *q-tame* if for every $s < t$ the structure map $M_s \to M_t$ has finite rank.

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- A q-tame persistence module
  - does not necessarily admit a barcode,
  - but has a submodule at distance 0 that admits a barcode.
- Morse's goal, in modern language:
  - Sufficient conditions for q-tame persistent homology of sublevel sets,
  - which are satisfied by the minimal surface functional

Q-tameness from local connectivity

Theorem (Morse, 1937)

If a function $f\colon X \to \mathbb{R}$ on a metric space X is bounded below and the sublevel set filtration is compact and weakly locally connected, *then it has q-tame persistent Vietoris homology.*

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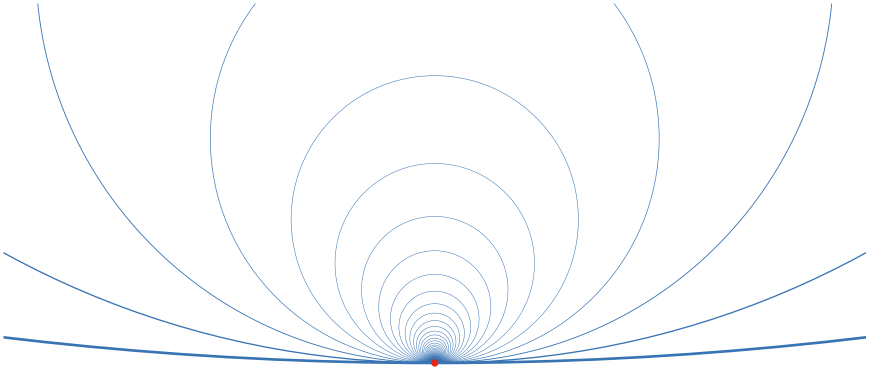

Homologically locally small filtrations

Definition

The sublevel set filtration of a function $f\colon X \to \mathbb{R}$ is *homologically locally connected (HLC)* if

- for any point $x \in X$, any values $f(x) < s < t$, and
- any neighborhood V of x in the sublevel set $f^{-1}(-\infty, t]$,

there is

- a neighborhood $U \subseteq V$ of x in the sublevel set $f^{-1}(-\infty, s]$

such that the inclusion $U \hookrightarrow V$ induces a zero map on homology.

A sufficient condition for q-tame persistence

Theorem (B, Medina-Mardones, Schmahl 2021)

If the sublevel sets of a function $f : X \to \mathbb{R}$ *are compact and HLC, then their persistent homology is q-tame.*

- f is not required to be continuous

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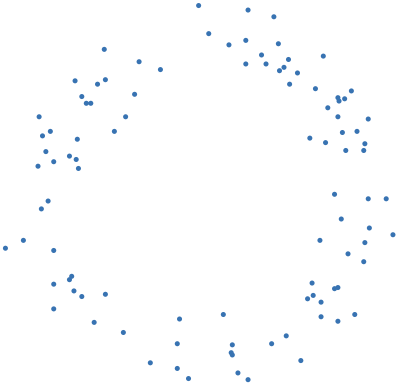
- Conditions are satisfied by the Douglas functional
- Fixes the gap in Morse/Tompkins' proof

Computation

Vietoris–Rips complexes



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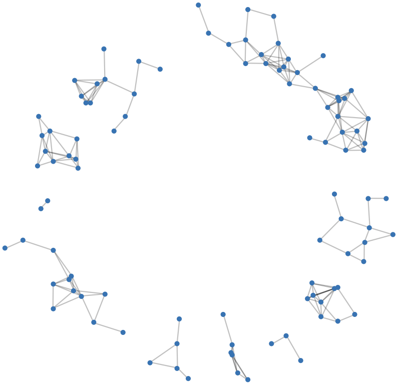

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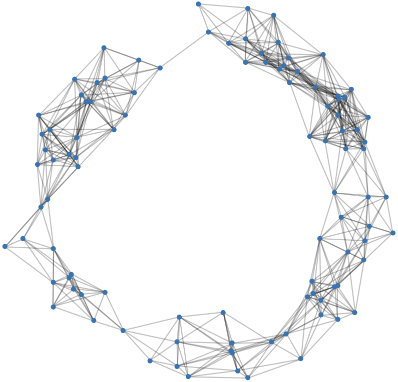

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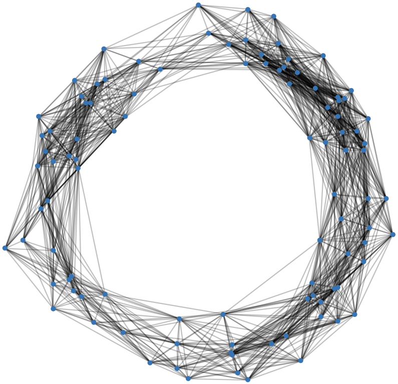

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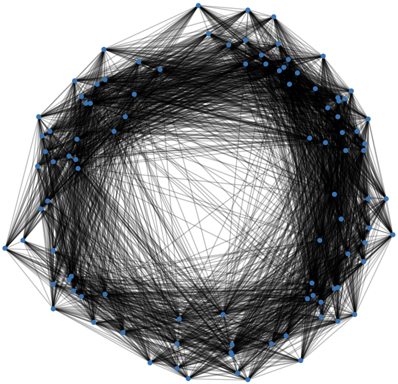

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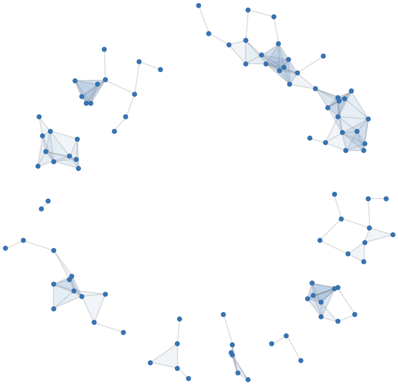

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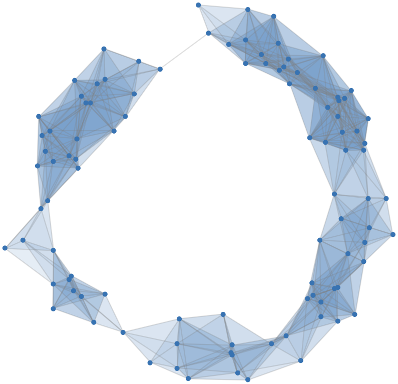

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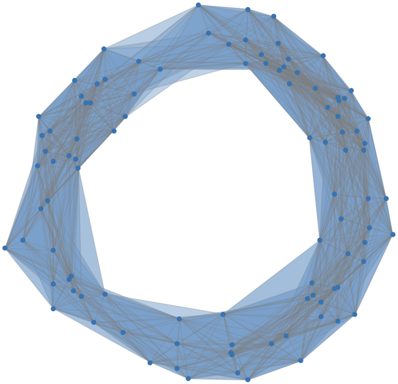

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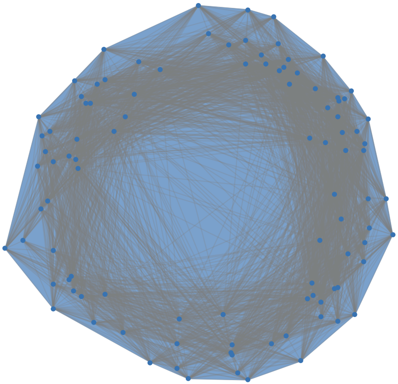

An example computation

Example data set:

- 192 points on $\mathbb{S}^2$
- homology up to dimension 2: over 56 mio. simplices in 3-skeleton

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Some previous software:

- javaplex (Stanford): 3200 seconds, 12 GB
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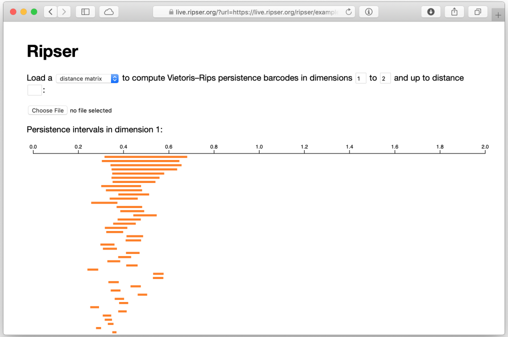
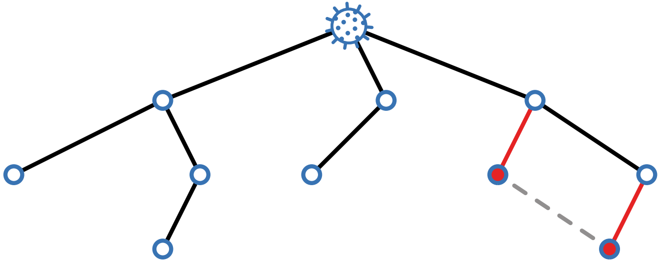


Topology of viral evolution



Joint work with: A. Ott, M. Bleher, L. Hahn (Heidelberg), R. Rabadan, J. Patiño-Galindo (Columbia), M. Carrière (INRIA)

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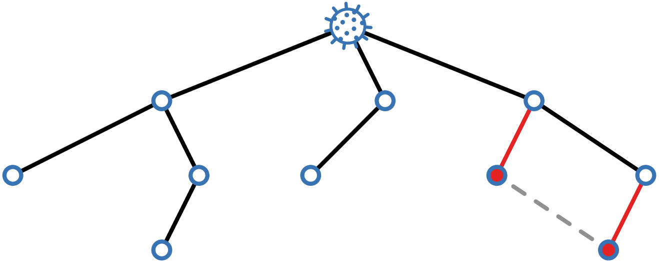

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Observation: Ripser runs unusually fast on genetic distance data

- SARS-CoV2 spike protein: 2 minutes for H_1 of 25556 data points (2.8×10^{12} simplices)

Vietoris–Rips complexes

For a metric space X, the *Vietoris–Rips complex* at scale $t > 0$ is the simplicial complex

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

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Let X be a δ-hyperbolic geodesic space. Then $\mathrm{Rips}_t(X)$ is contractible for all $t \geq 4\delta$.

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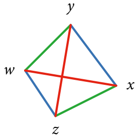
- A metric space X is *δ-hyperbolic* if for all $w, x, y, z \in X$ we have

$$d(w,x) + d(y,z) \leq \max\{d(w,y) + d(x,z), d(w,z) + d(x,y)\} + 2\delta.$$



- 0-hyperbolic spaces are subspaces of trees

Definition

A metric space X is *ν-geodesic* if for all points $x, y \in X$ and all $r, s \geq 0$ with $r + s = d(x, y)$ there exists a point $z \in X$ with $d(x, z) \leq r + \nu$ and $d(y, z) \leq s + \nu$.

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Theorem (B, Roll 2021)

Let X be a finite δ-hyperbolic ν-geodesic space. Then there is a discrete gradient encoding the collapses

$$\mathrm{Rips}_u(X) \searrow \mathrm{Rips}_t(X) \searrow \{*\}$$

for all $u > t \geq 4\delta + 2\nu$.

Apparent pairs

We use the *lexicographic refinement* of the Vietoris–Rips filtration:

- Choose a total order on the vertices
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Proposition

The apparent pairs form a discrete gradient.

Collapsing Vietoris–Rips complexes of trees

Let X be a metric space with the path length metric of a weighted tree $T = (X, E)$.

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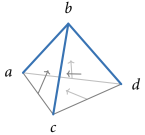
Theorem (B, Roll 2021)

The apparent pairs gradient has critical simplices only on the tree T. It encodes the collapses

$$\mathrm{Rips}_u(X) \searrow \mathrm{Rips}_t(X) \searrow T_t$$

for all $u > t$ such that no tree edge $e \in E$ has length $l(e) \in (t, u]$.



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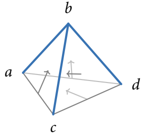
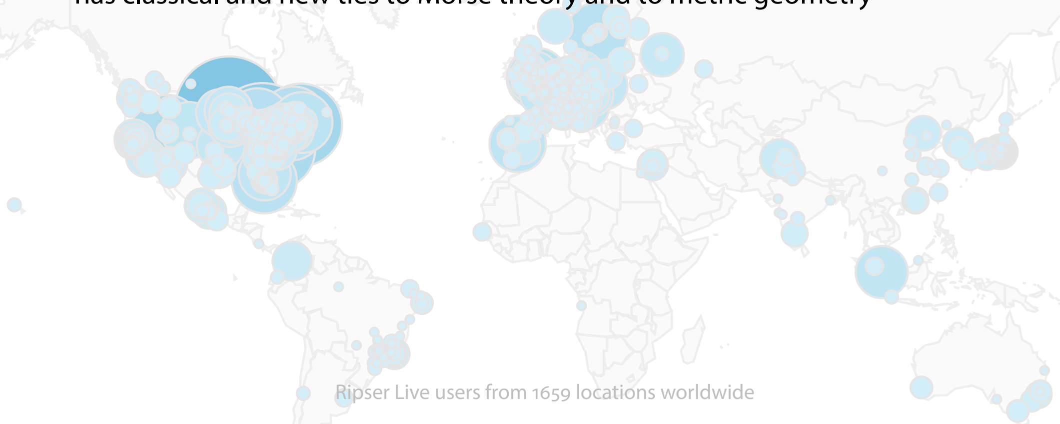


- Explains why Ripser computations are very fast on genetic distances (tree-like)

Conclusion

Persistent homology…

- provides a powerful toolbox for geometric and topological data
- creates new inspiration and challenges for new theory
- has classical and new ties to Morse theory and to metric geometry



Ripser Live users from 1659 locations worldwide