Connect the dots

From data through complexes to persistent homology

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Technical University of Munich (TUM)

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DFG Deutsche Forschungsgemeinschaft German Research Foundation

SFB TRR 109 Discretization in Geometry and Dynamics

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MDSI

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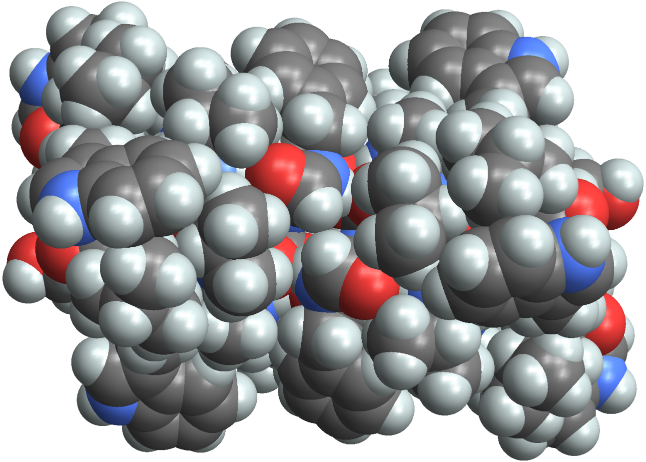
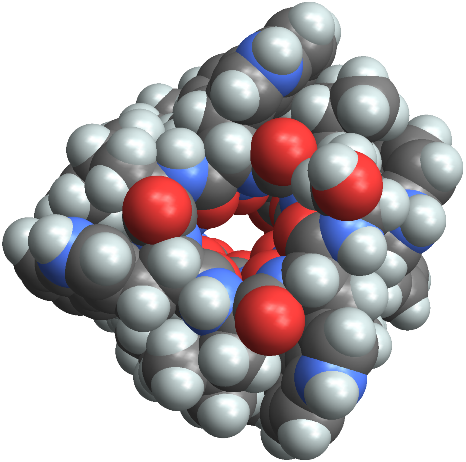
Geometry and topology of biomolecules



Gramicidin (an antibiotic functioning as an ion channel)

Geometry and topology of biomolecules



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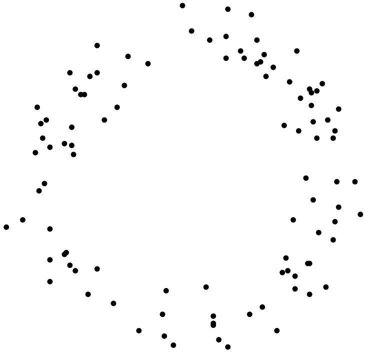

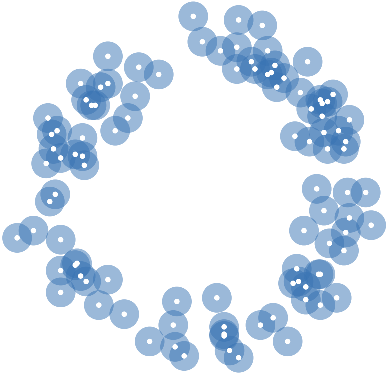

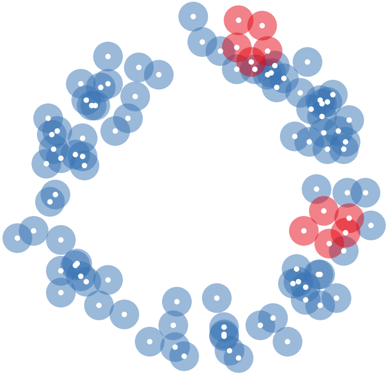

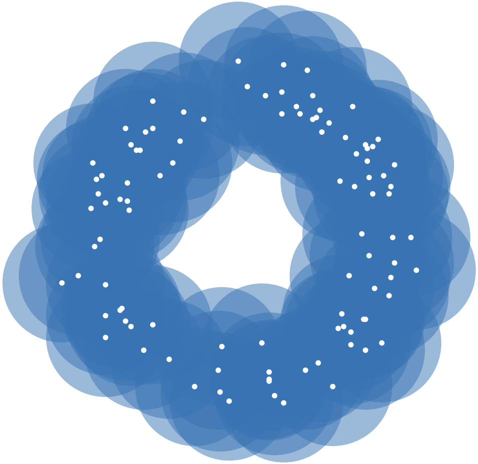

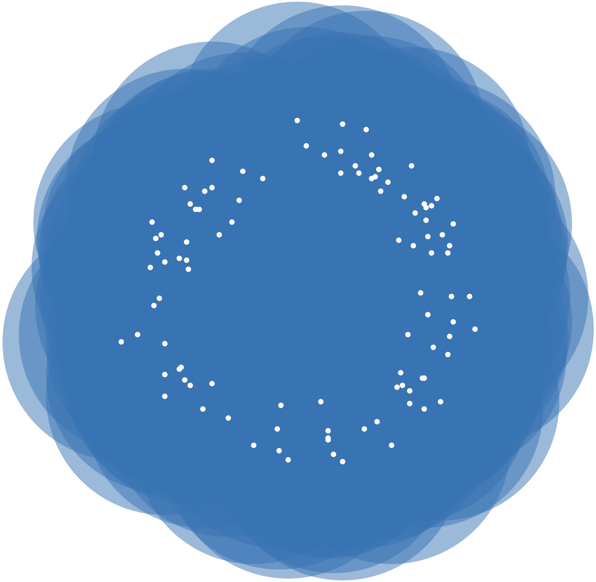

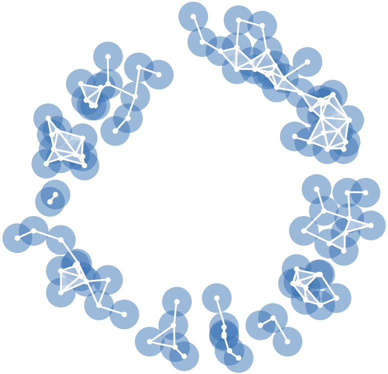

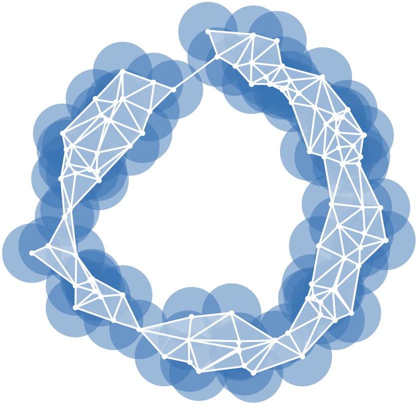

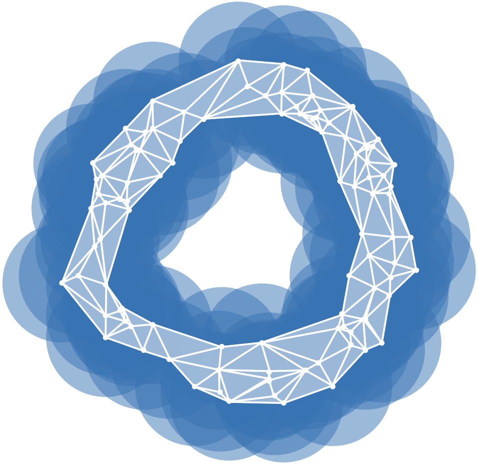

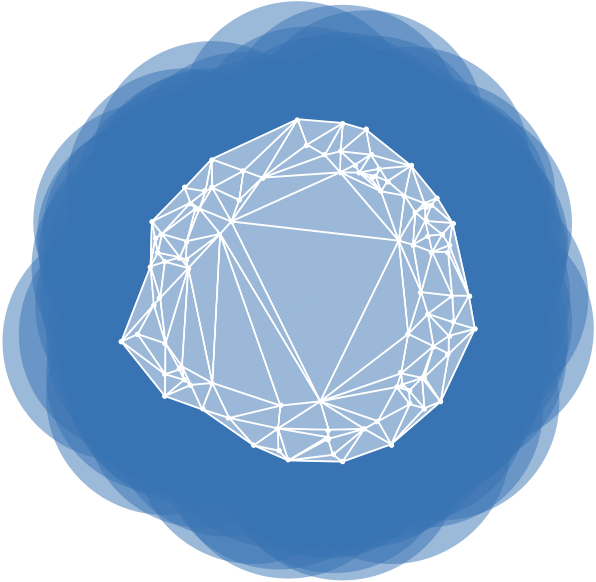

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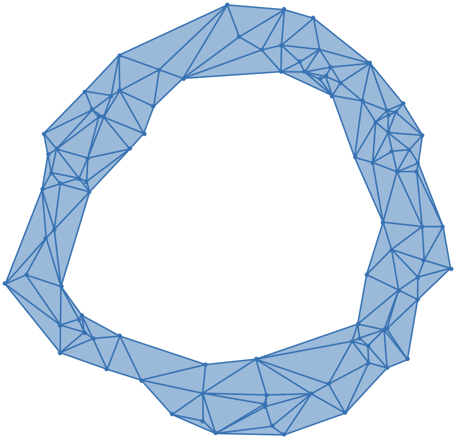

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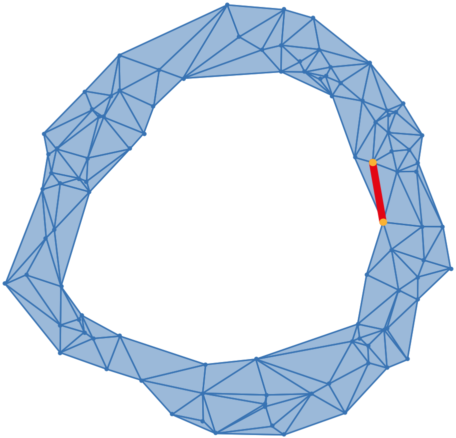

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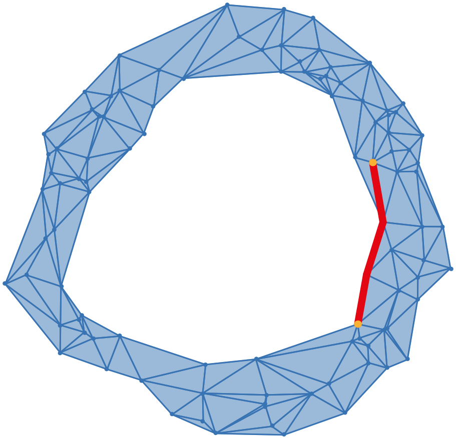

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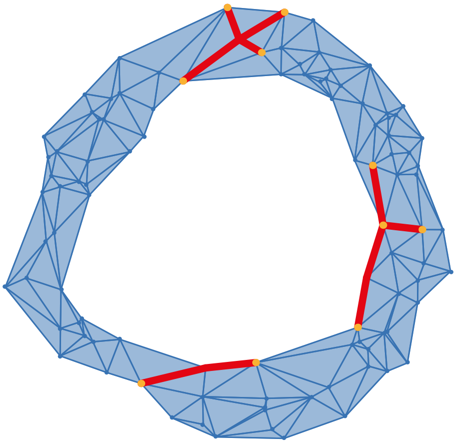

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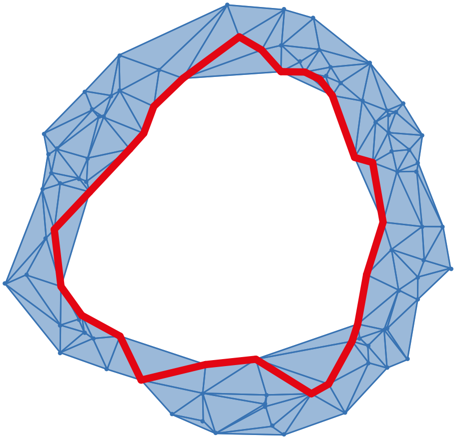

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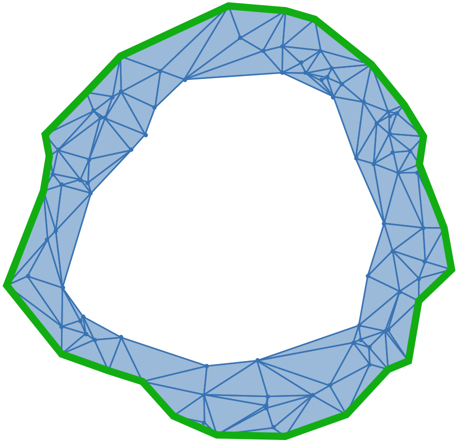

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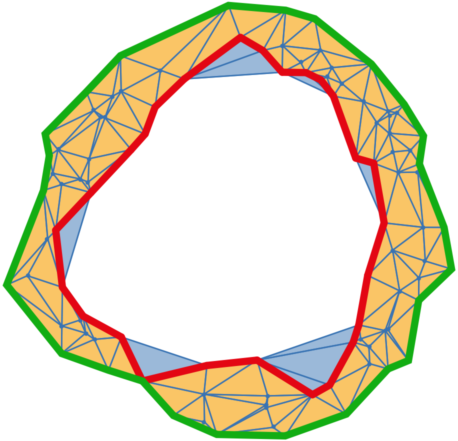
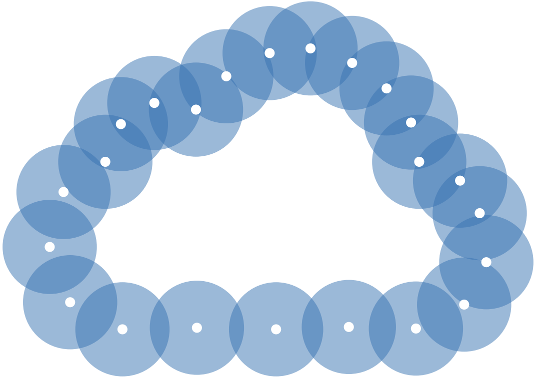


Geometric complexes

Čech complexes



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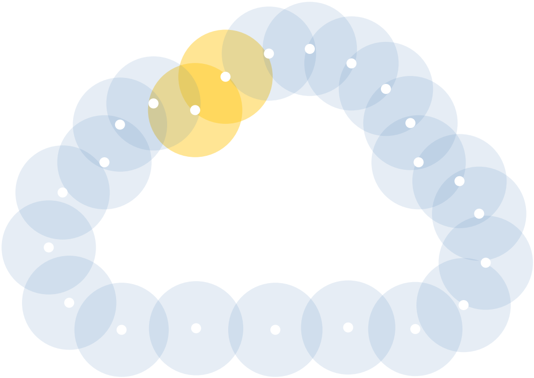

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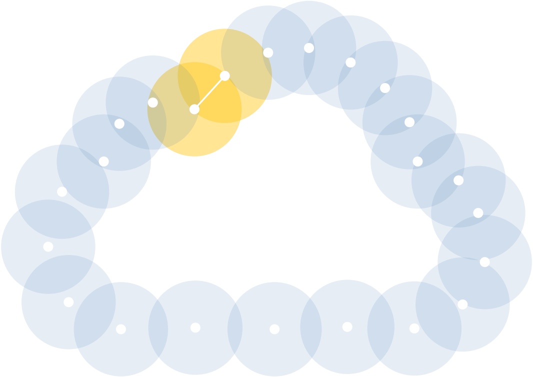

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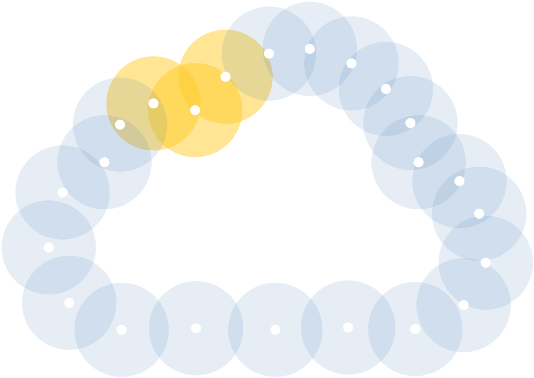

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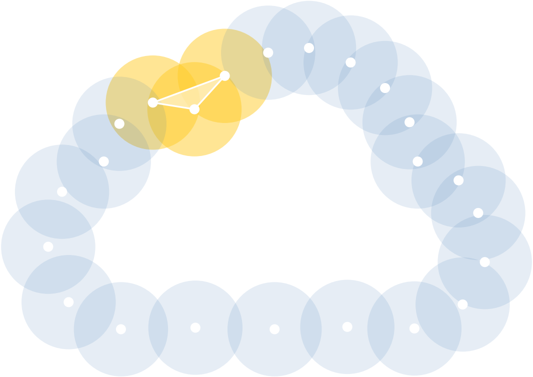

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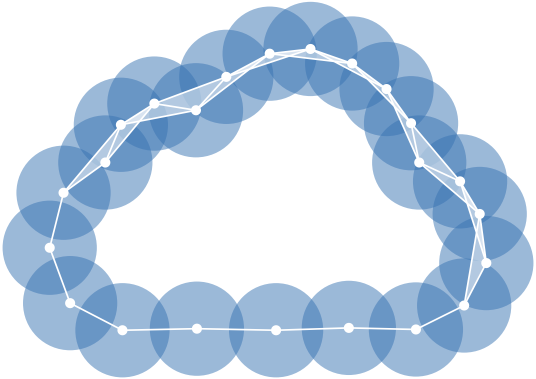
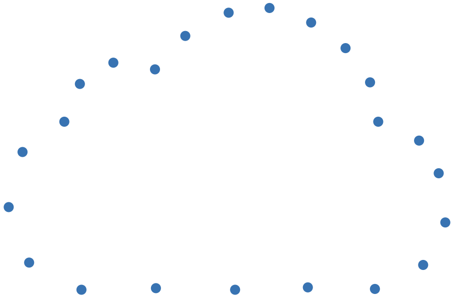


Delaunay complexes



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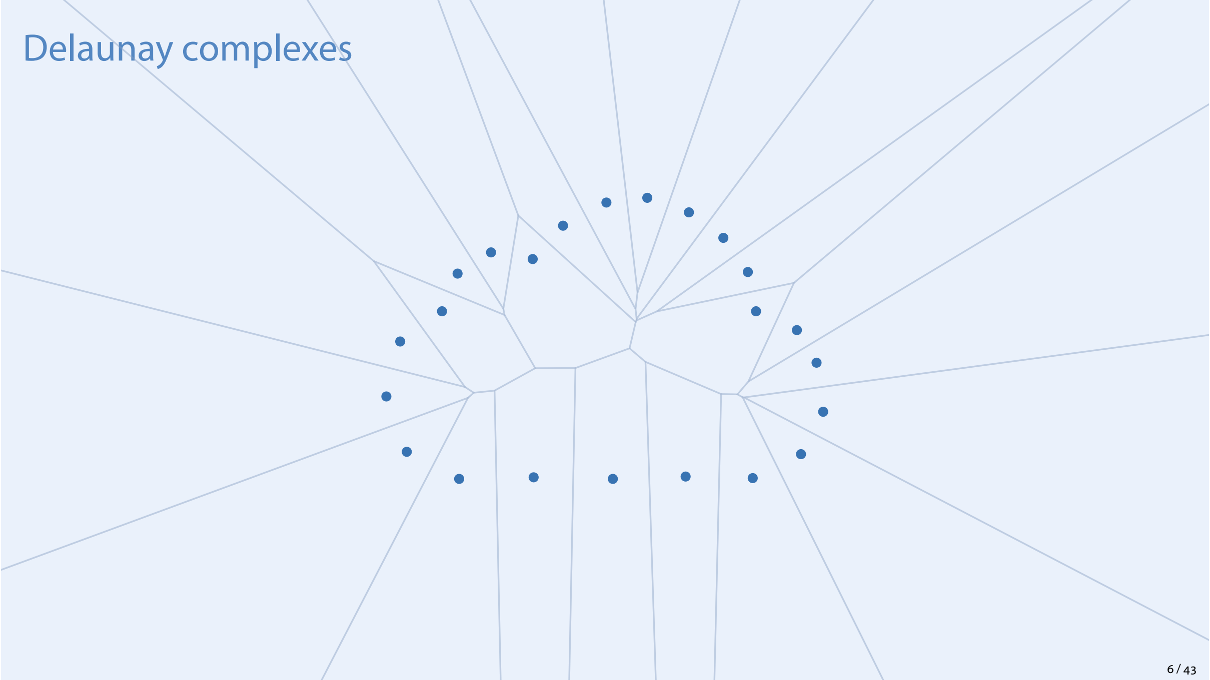

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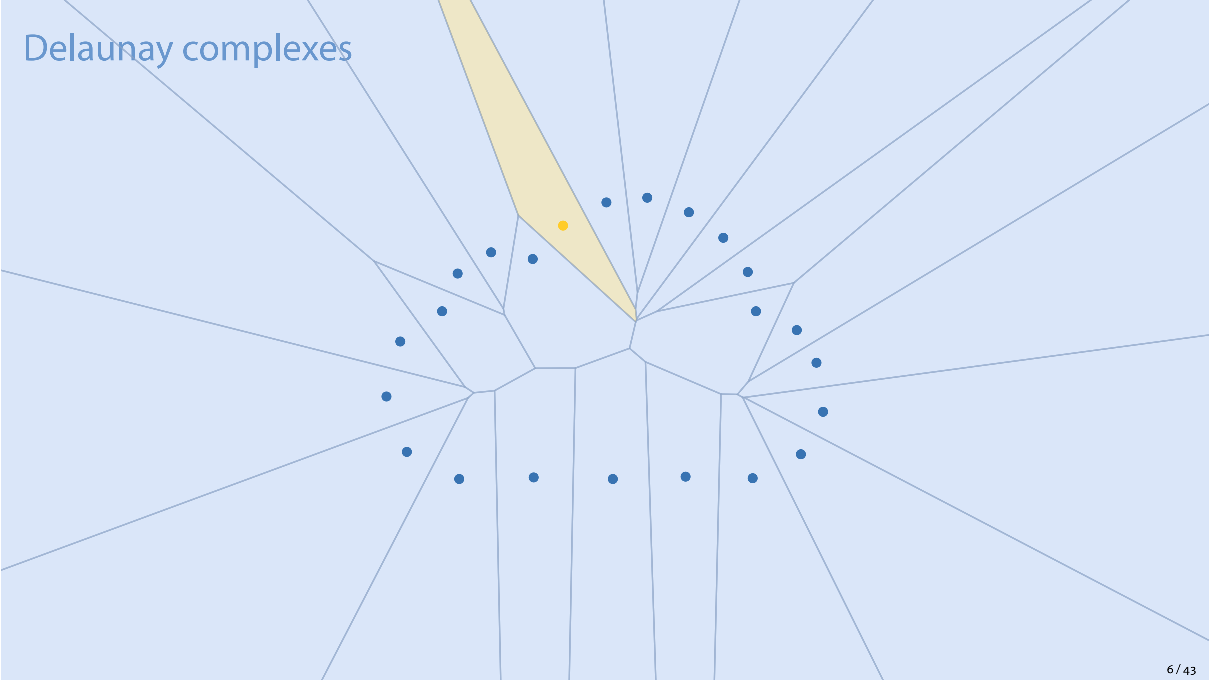

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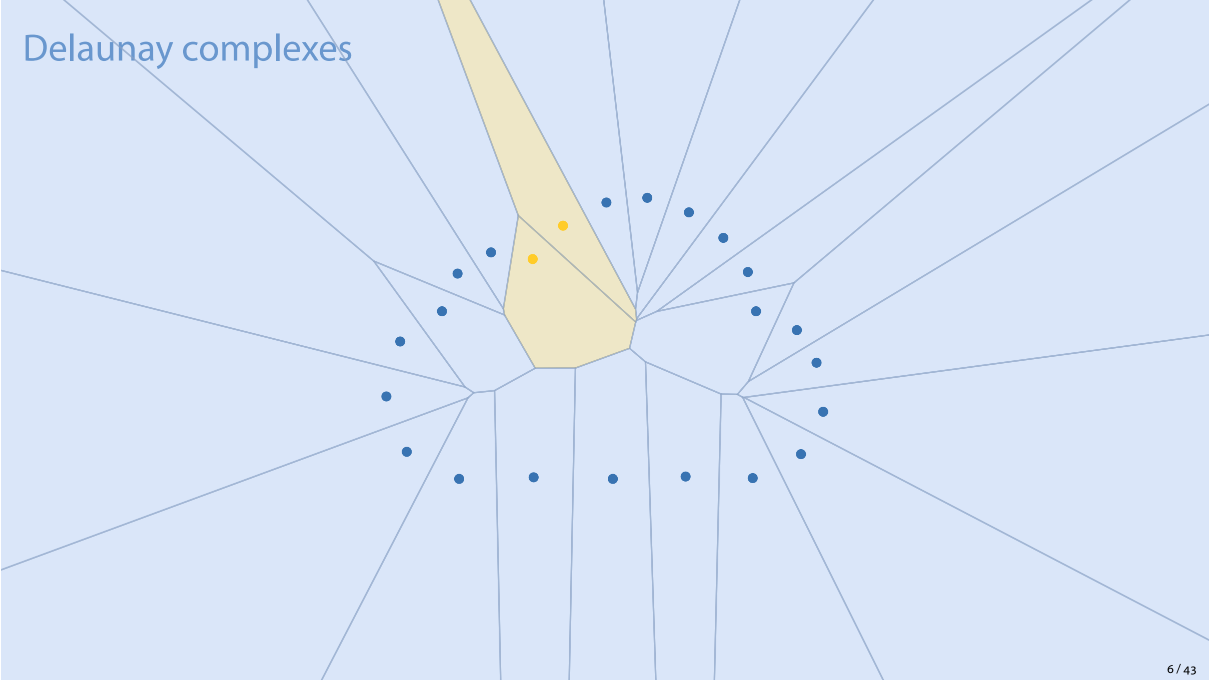

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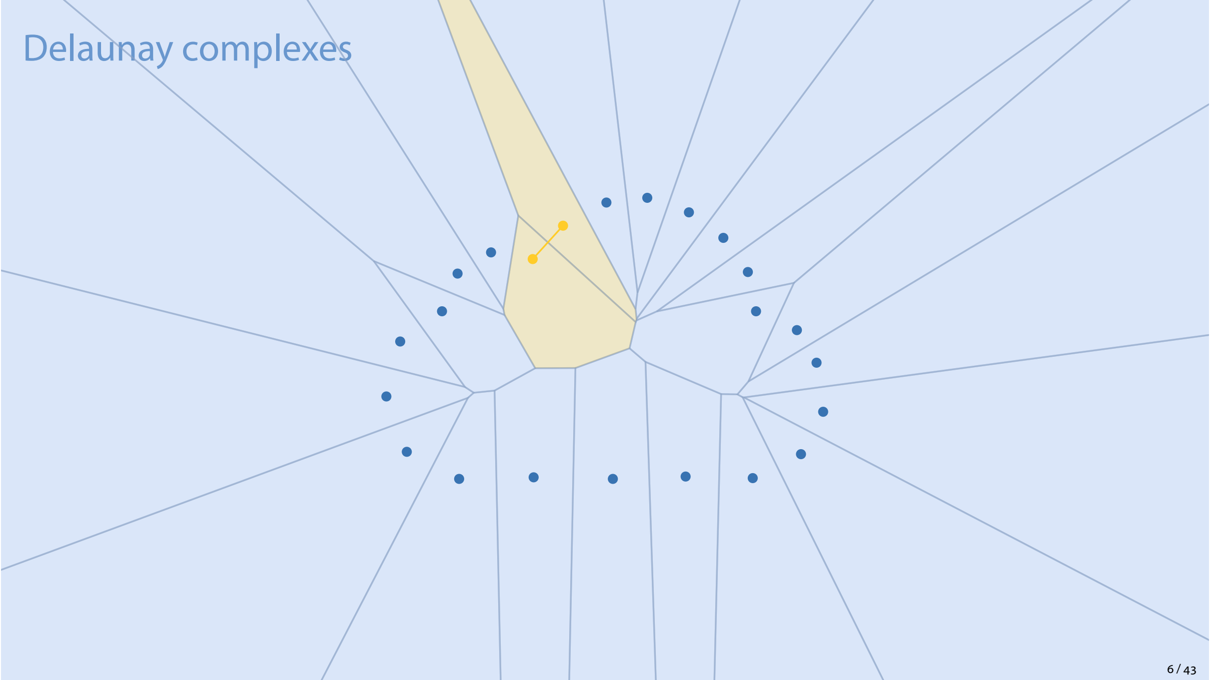

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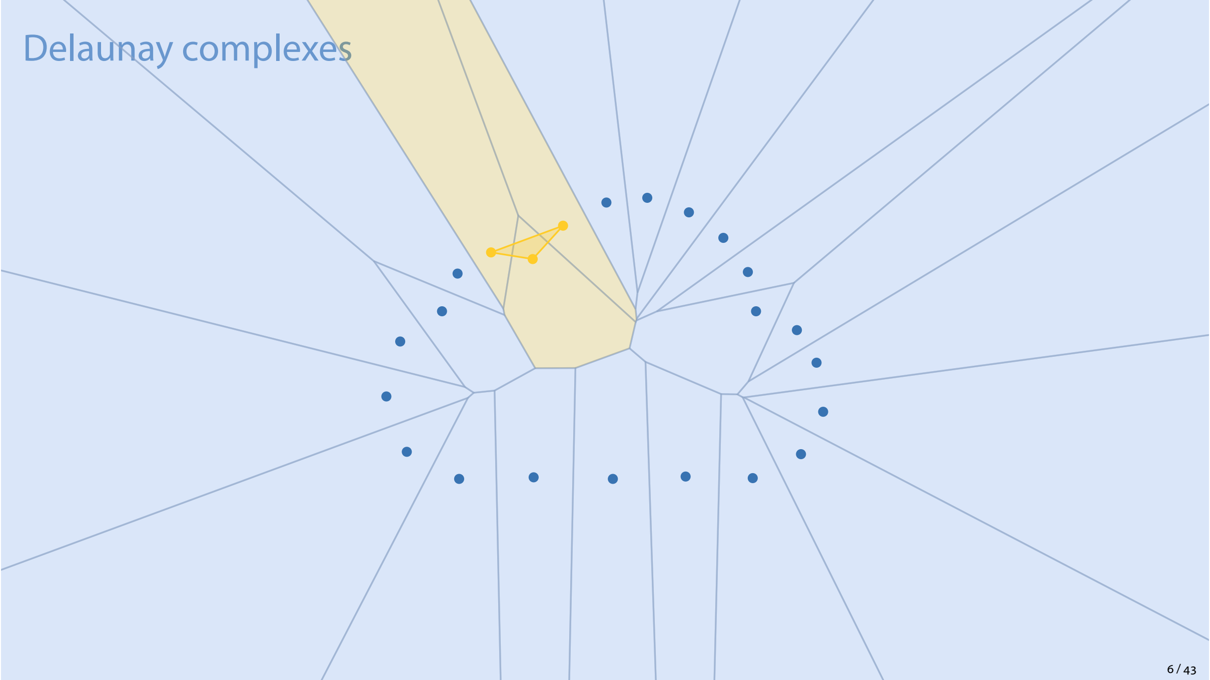

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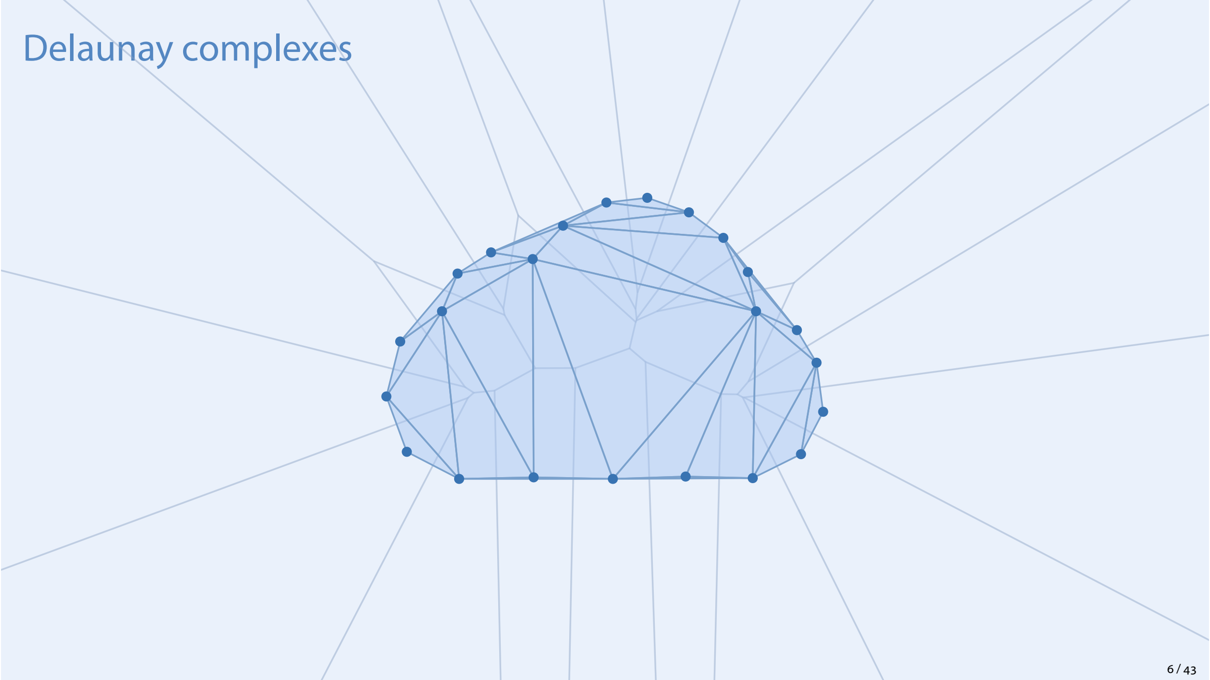

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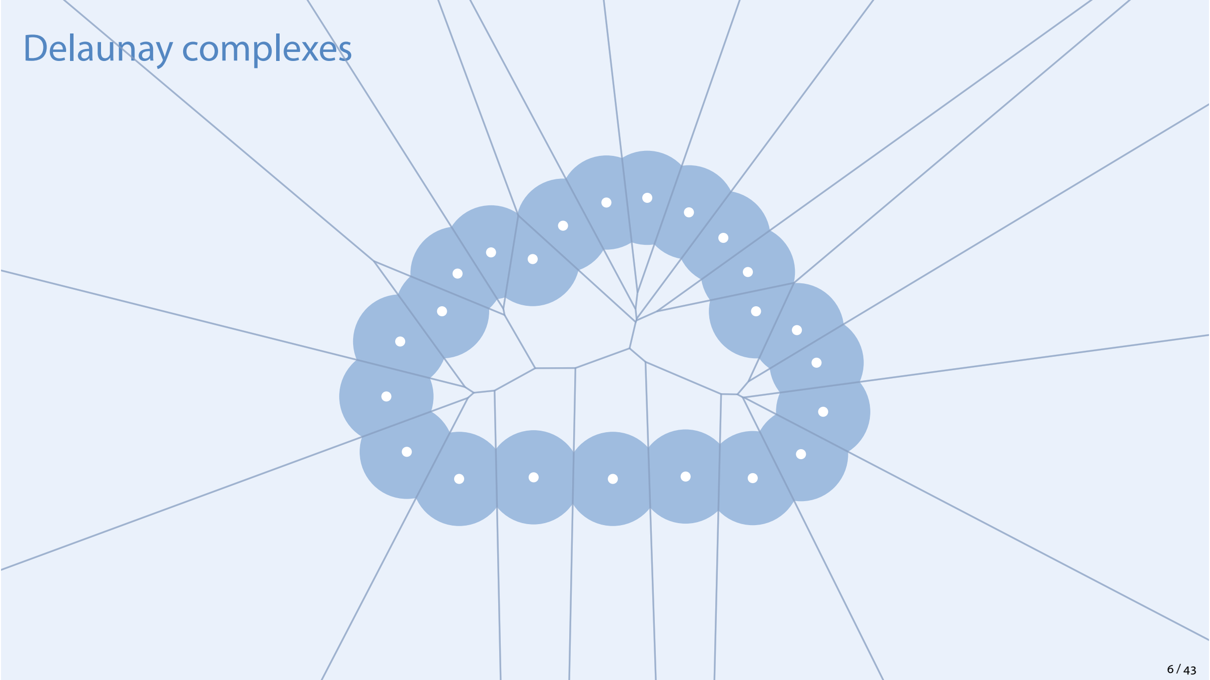

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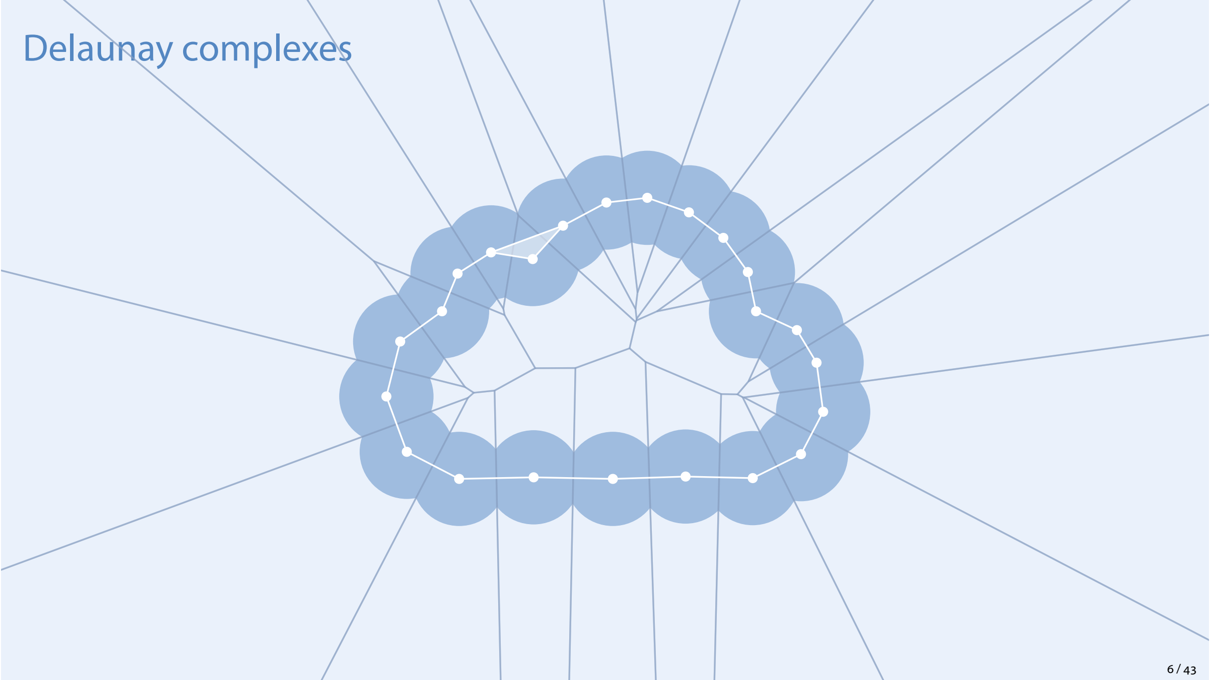

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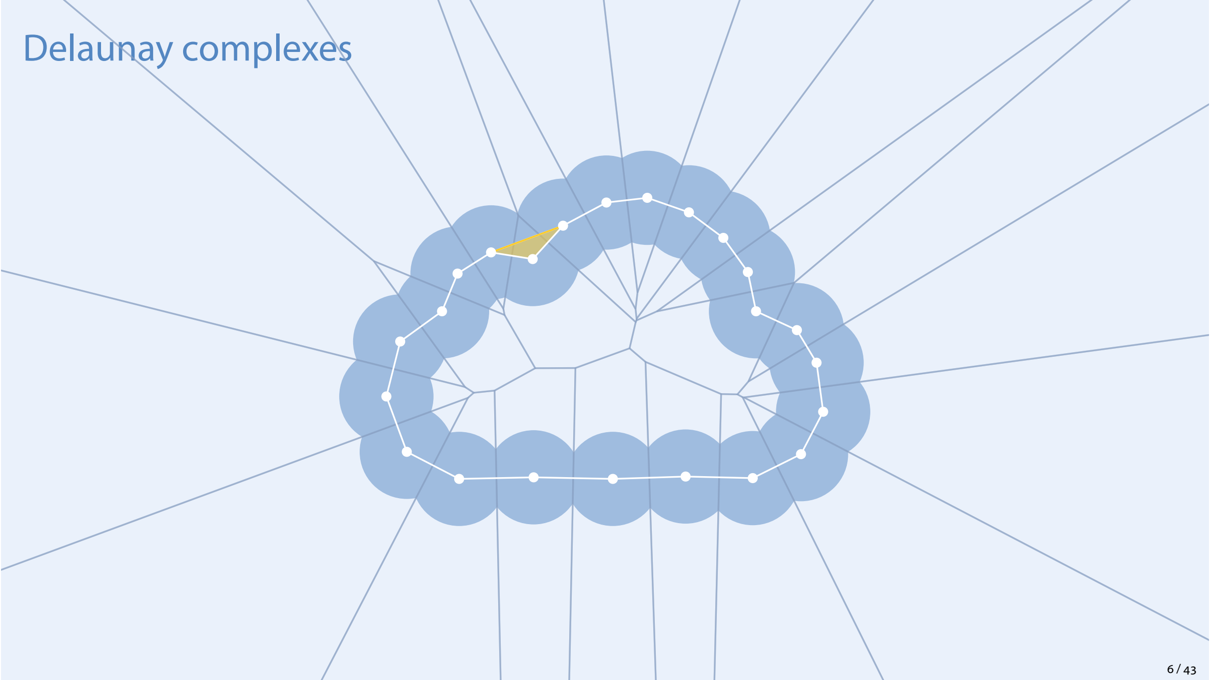

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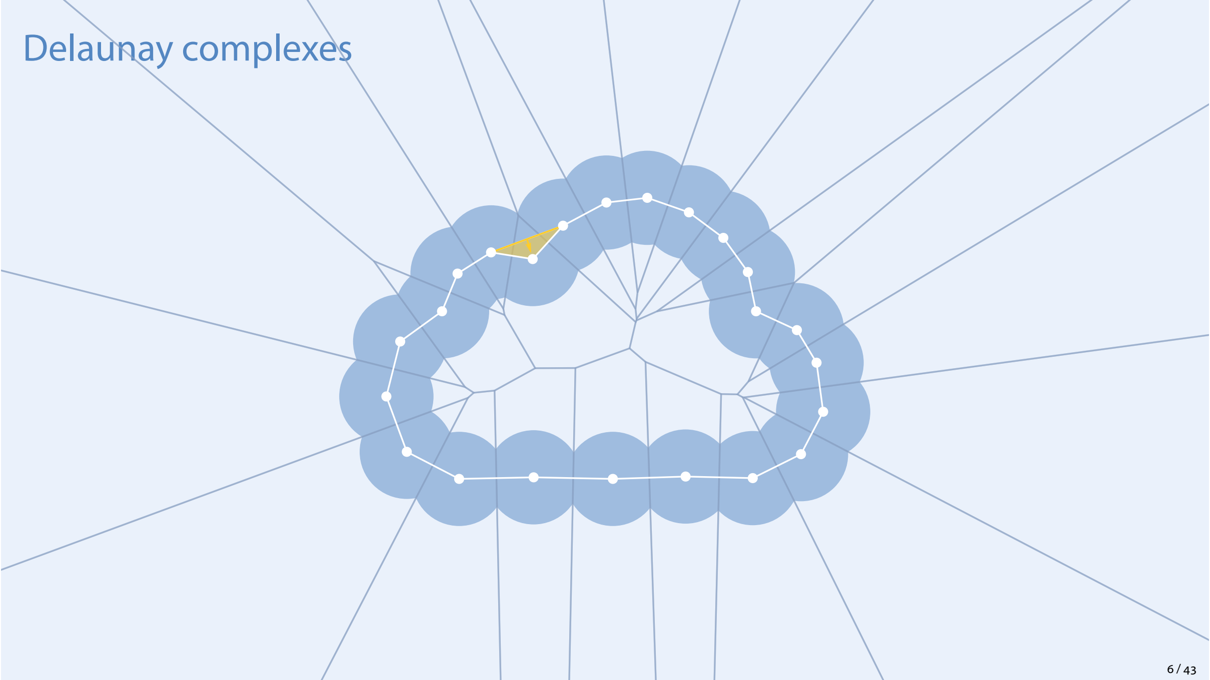

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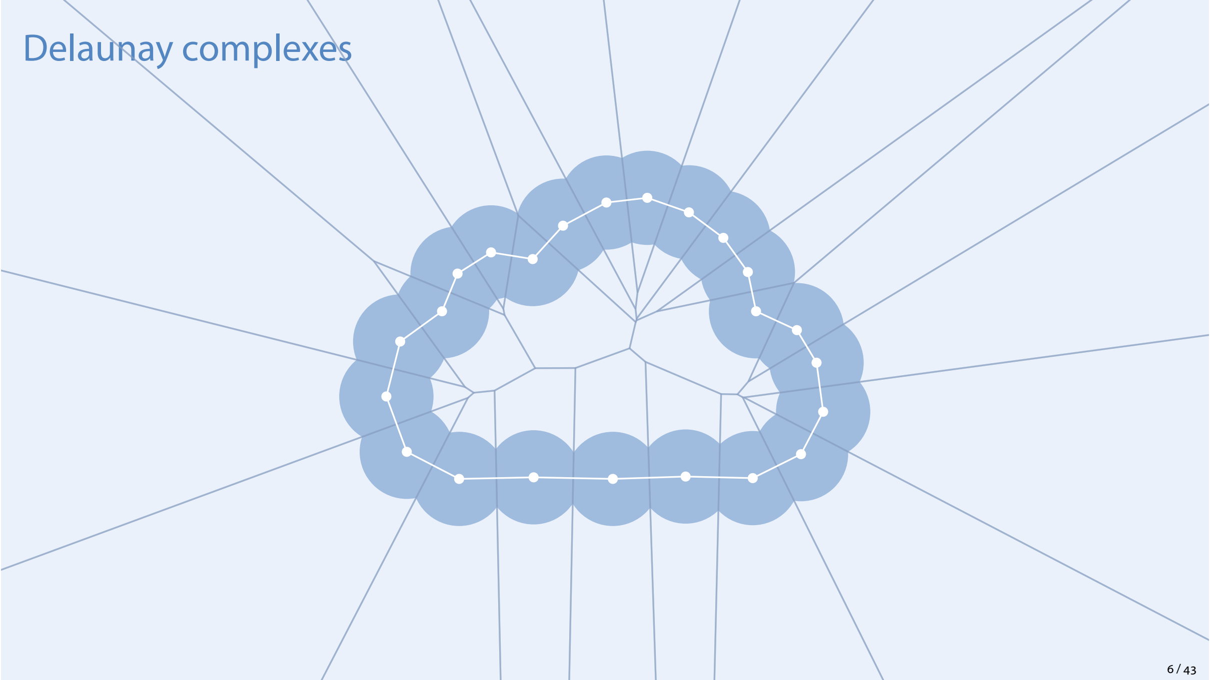
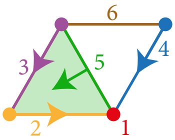


Discrete Morse theory



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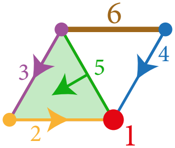
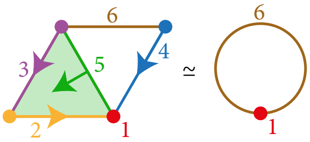


Discrete Morse theory

Theorem (Forman 1998)

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



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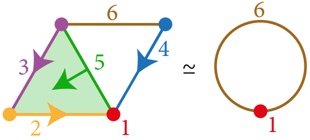
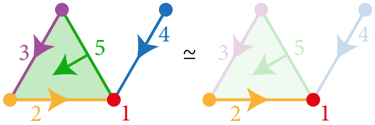


Discrete Morse functions – and their gradients – encode *collapses* of sublevel sets:



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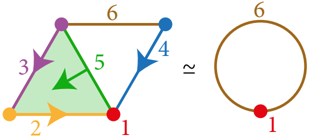

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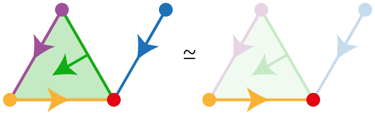
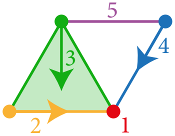
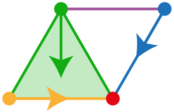


Generalizing discrete Morse theory

Generalized gradients are a partition into intervals in the face poset (instead of just facet pairs):





Morse theory for Čech and Delaunay complexes

Proposition (B, Edelsbrunner 2014)

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

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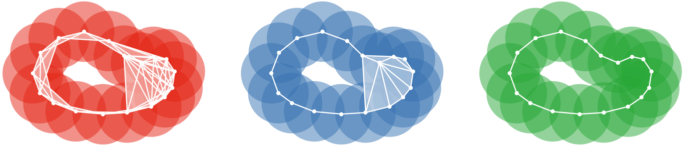
Theorem (B., Edelsbrunner 2017)

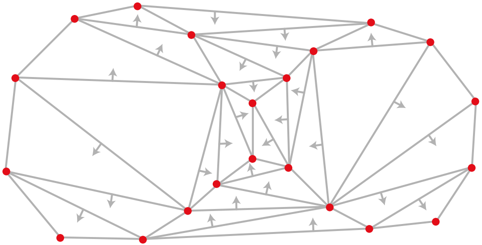
Čech, Delaunay, and Wrap complexes (at any scale r) are related by collapses encoded by a single discrete gradient field:

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



Wrap complexes

Consider the gradient V of the Delaunay radius function $\mathrm{Del}(X) \to \mathbb{R}$.



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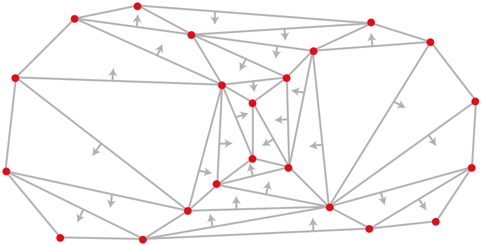

Definition (Edelsbrunner 1995; B, Edelsbrunner 2017)

$\mathrm{Wrap}_r(X)$ is the *descending complex* of V on $\mathrm{Del}_r X$: the smallest subcomplex of $\mathrm{Del}_r X$ that

- contains all critical simplices
- is compatible with V (a union of intervals of V).

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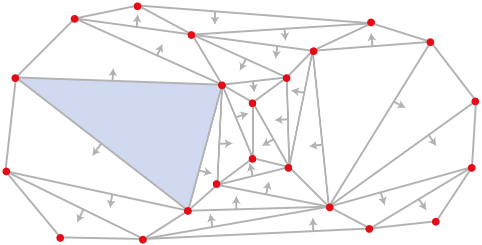

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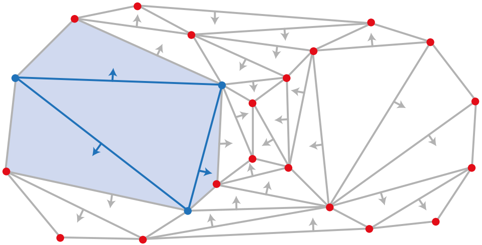

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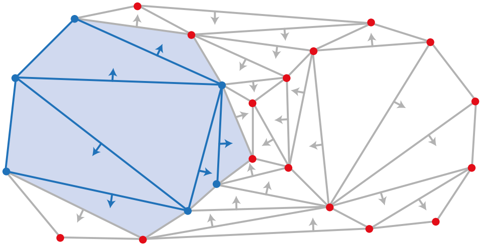

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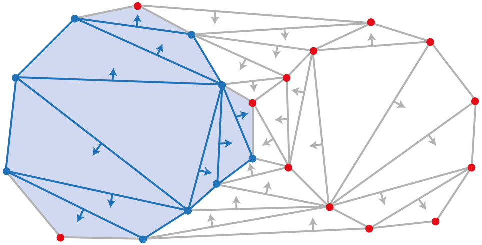

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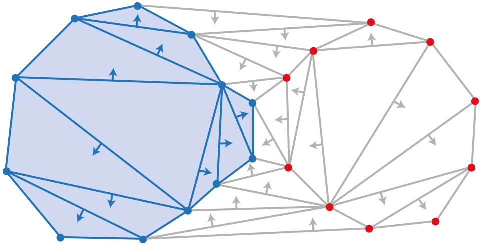

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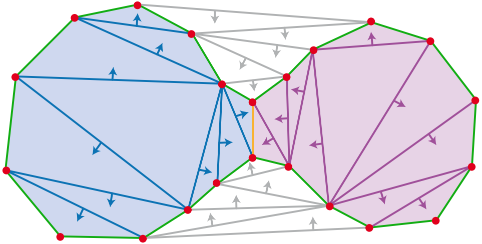

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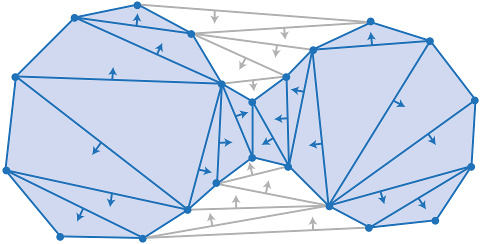

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Delaunay and Wrap complexes

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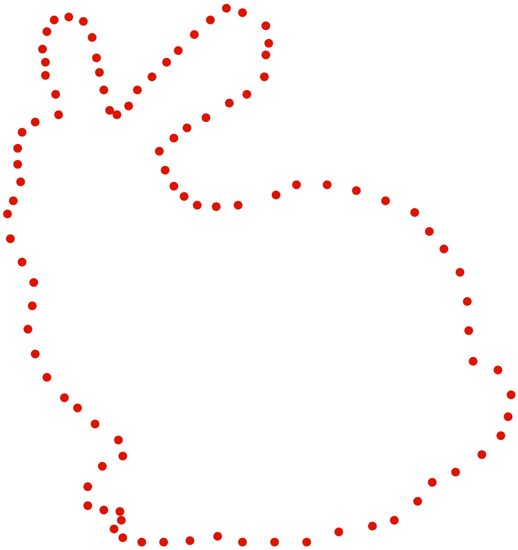
Wrap complexes and lexicographically minimal cycles



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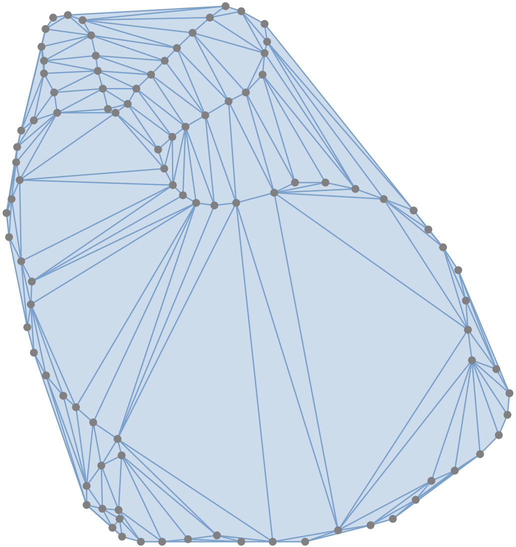

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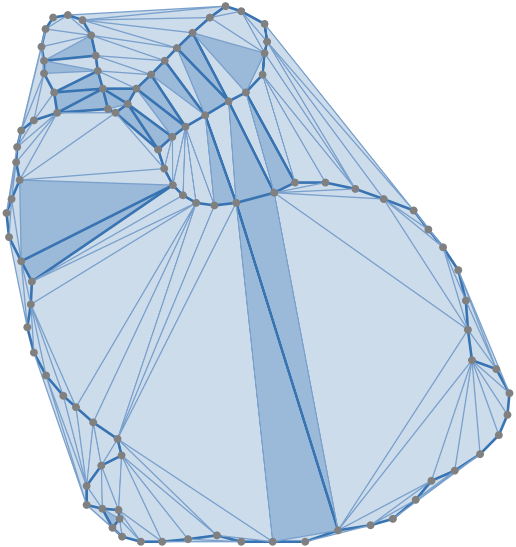

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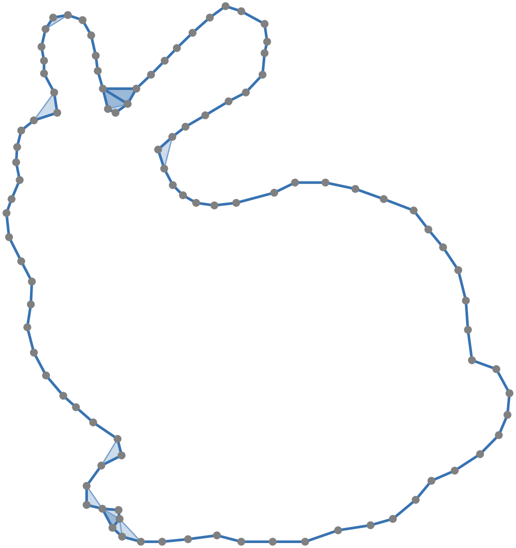

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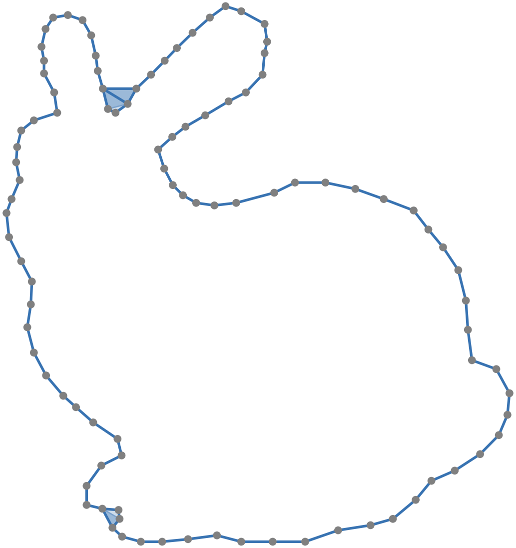

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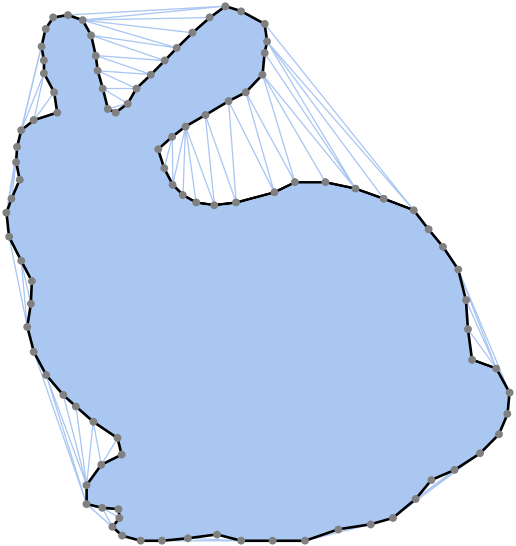

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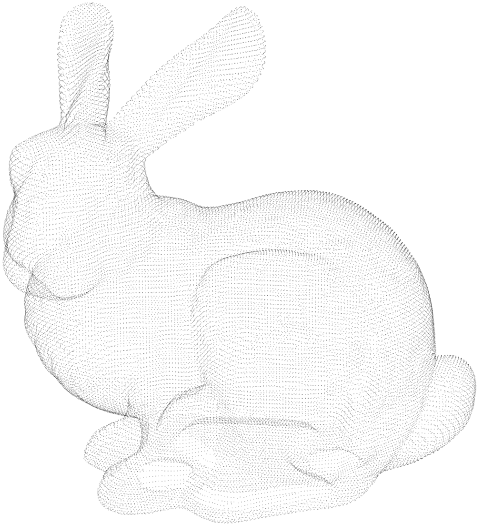

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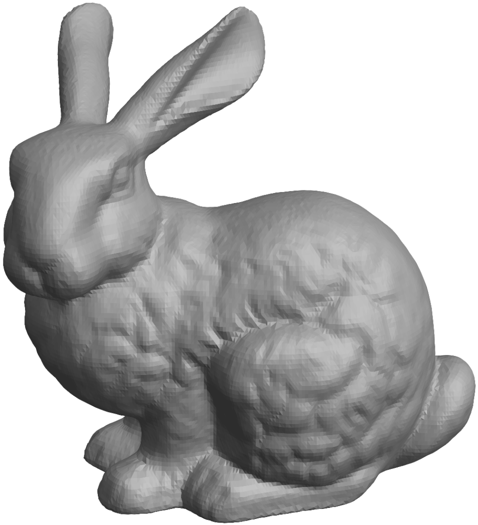
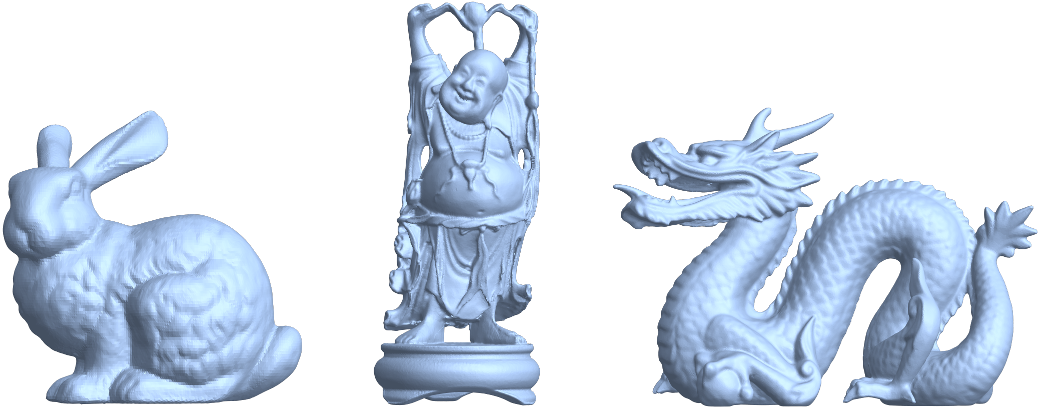


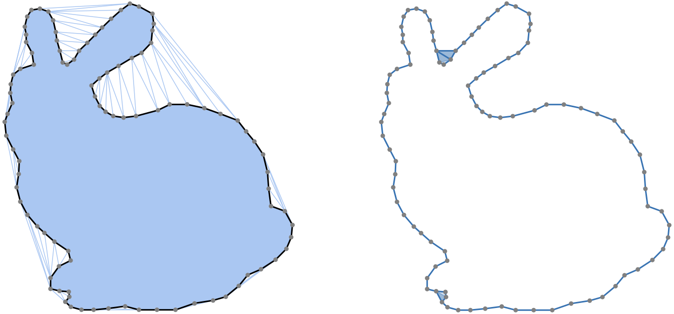
Point cloud reconstruction with minimal cycles



Minimal cycles within Wrap complexes

Theorem (B, Roll 2022)

Let $X \subset \mathbb{R}$ be a finite subset in general position and let $r \in \mathbb{R}$. Then the lexicographically minimal cycles of $\mathrm{Del}_r(X)$ are supported on $\mathrm{Wrap}_r(X)$.



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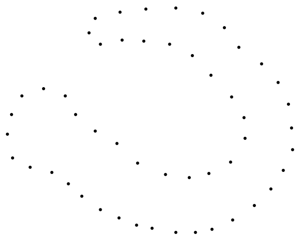

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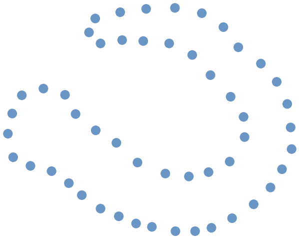

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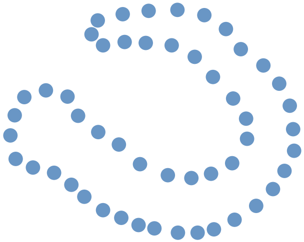

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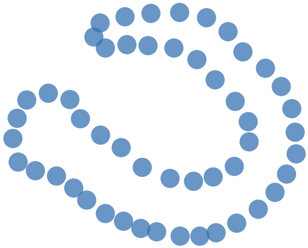

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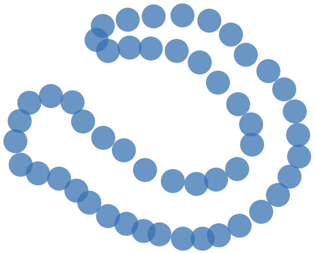

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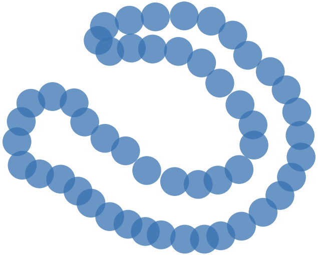

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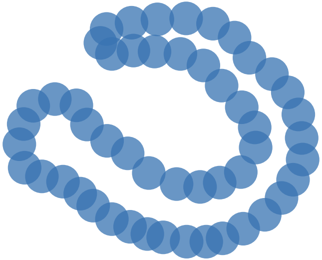

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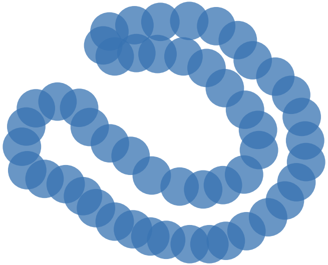

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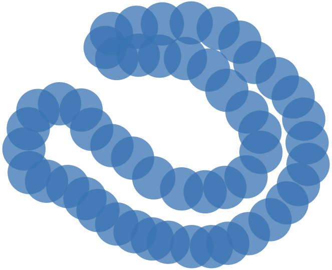

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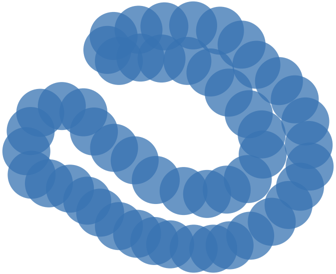

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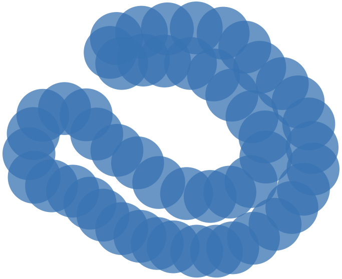

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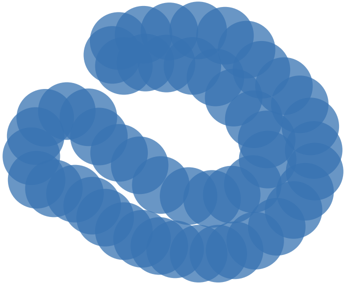

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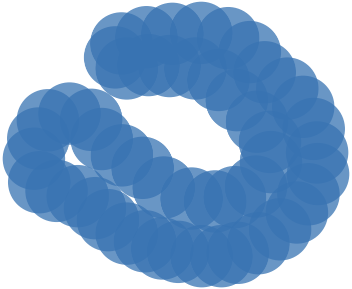

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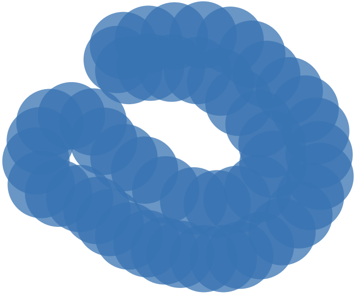

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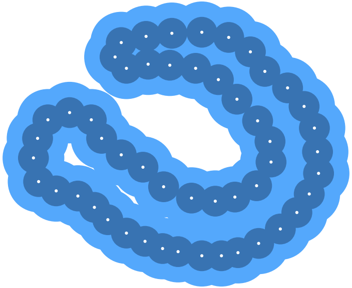

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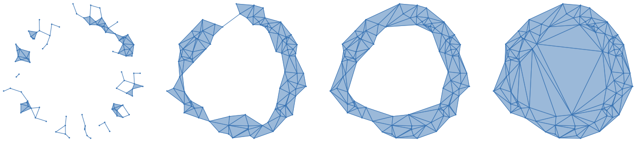
& H_*(P_\delta) \arrow[ur, two heads] \arrow[dr, two heads] & & H_*(P_{2\delta}) \arrow[ur] & \\
& & \operatorname{im} H_*(P_\delta \hookrightarrow P_{2\delta}) \arrow[ur, hook] & &
\end{tikzcd}$$

$\square$

Persistent homology

What is persistent homology?



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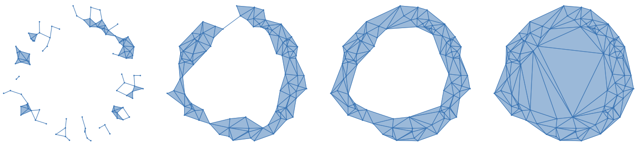

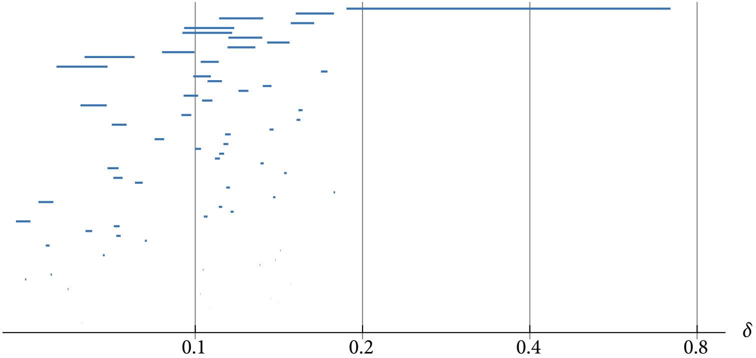

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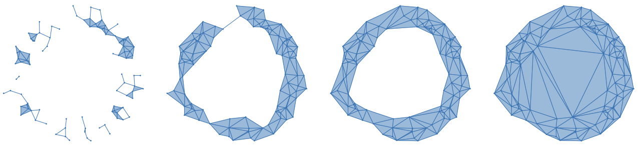

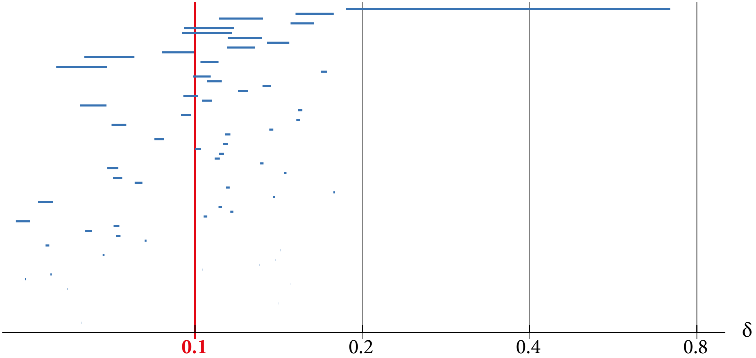

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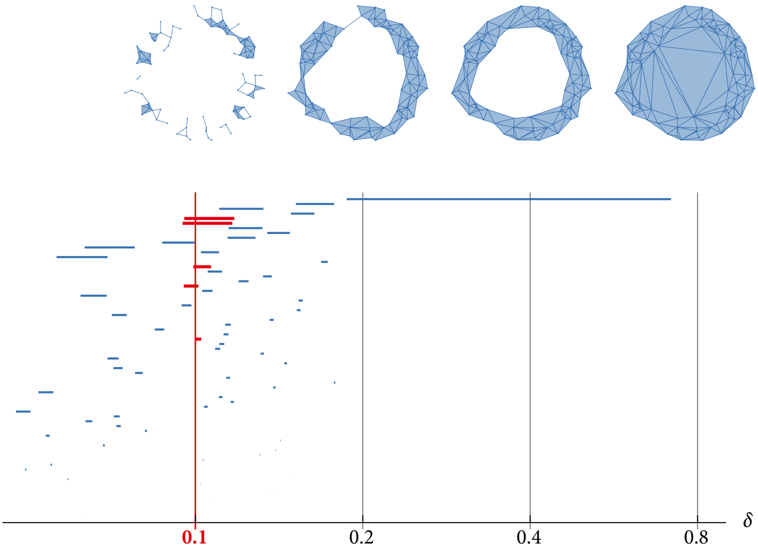

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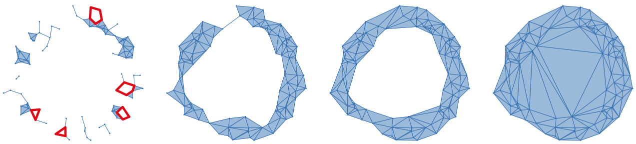

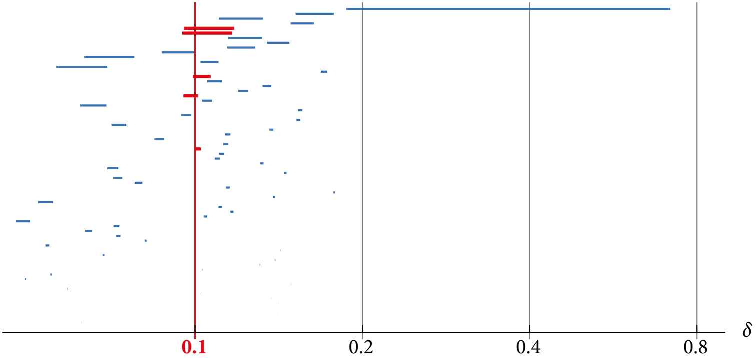

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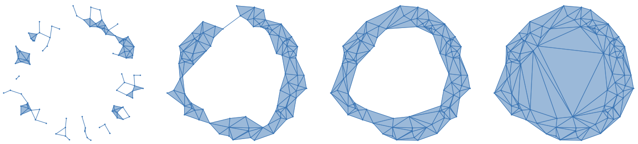

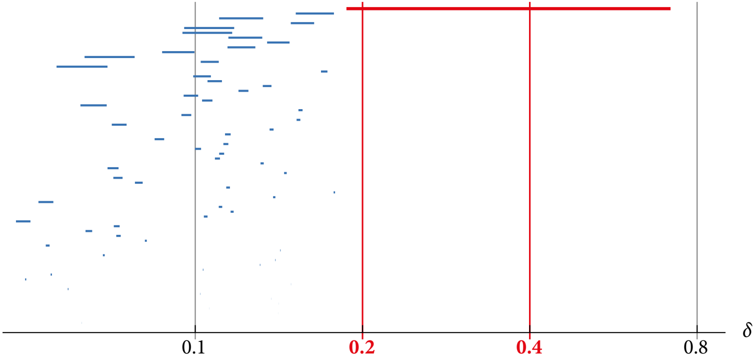

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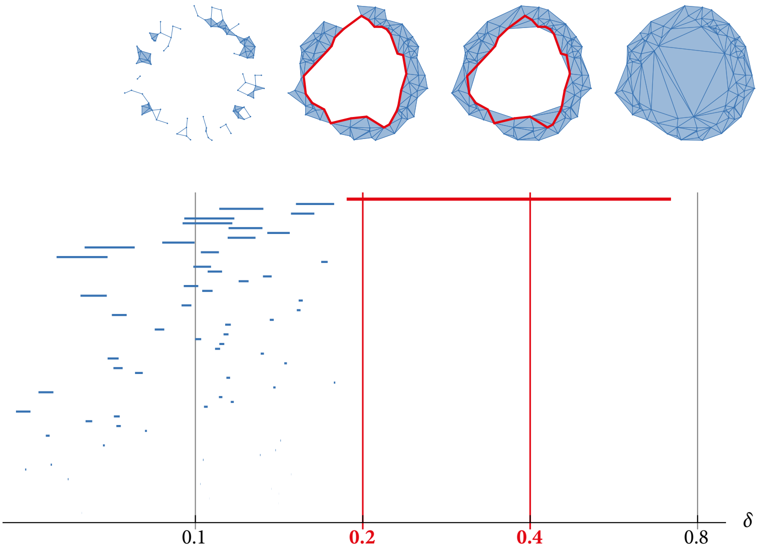

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- A filtration is a certain diagram $K : \mathbf{R} \to \mathbf{Top}$ of topological spaces, indexed over the poset of real numbers $\mathbf{R} := (\mathbb{R}, \leq)$

$$\cdots\cdots\rightarrow K_s \hookrightarrow K_t \cdots\cdots\rightarrow$$

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

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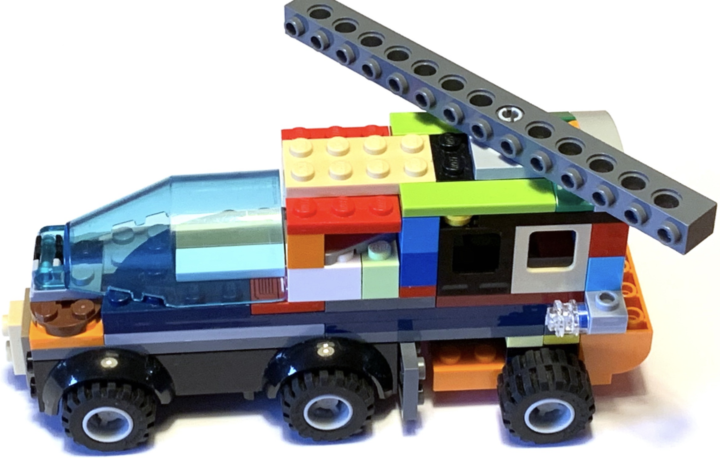

Barcodes: the structure of persistence modules

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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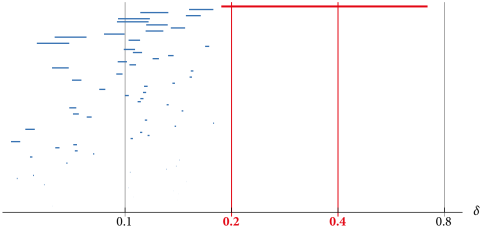
- The supporting intervals form the *persistence barcode.*



Stability

Persistence and stability: the big picture

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

Persistence and stability: the big picture

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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, 2016; B, Lesnick 2015)

If two persistence modules are δ-interleaved,
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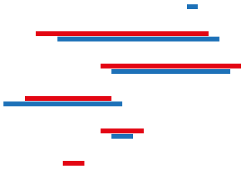

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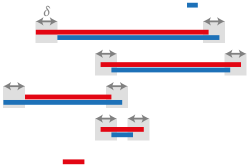

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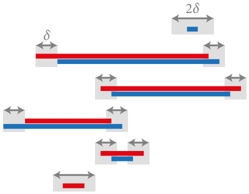

Structure of persistence sub-/quotient modules

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*
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This construction is functorial (compatible with composition).

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Dually, for a monomorphism $N \hookrightarrow O$ there is an injection $B(N) \hookrightarrow B(O)$.

Induced matchings

Any morphism of pfd persistence modules $f : M \to N$ factors through its image as an epimorphism followed by a monomorphism:

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

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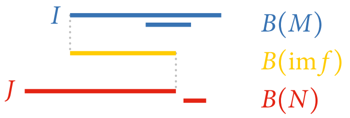

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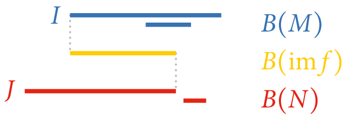


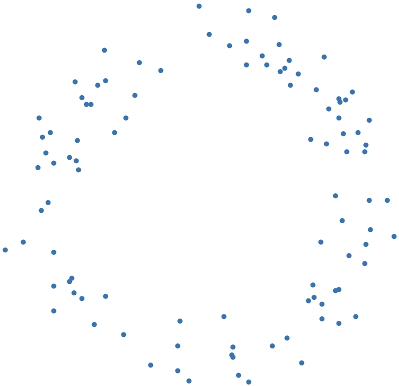
If f is a δ-interleaving morphism, then this induced matching is a δ-matching.

Persistence of Vietoris–Rips complexes

Vietoris–Rips complexes

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

$$\mathrm{Rips}_t(X) = \{S \subseteq X \mid S \neq \varnothing \text{ finite}, \operatorname{diam} S \leq t\}.$$



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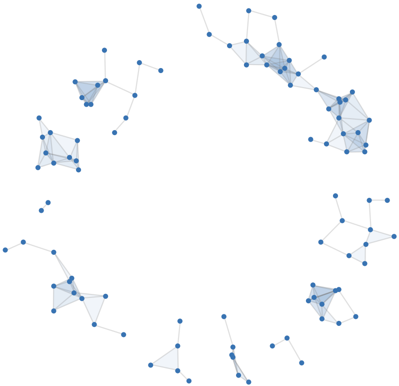

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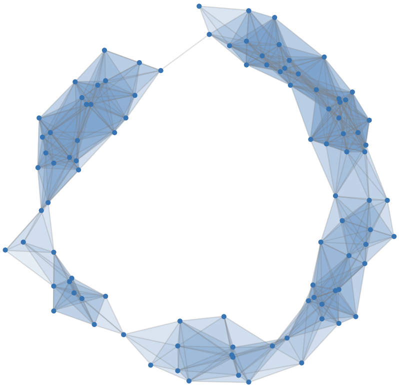

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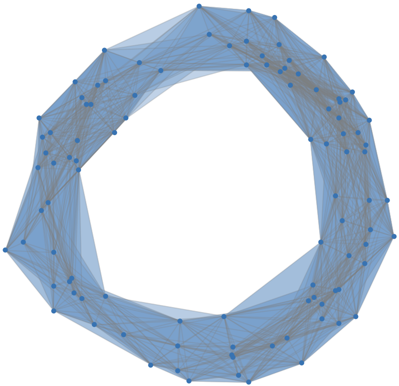

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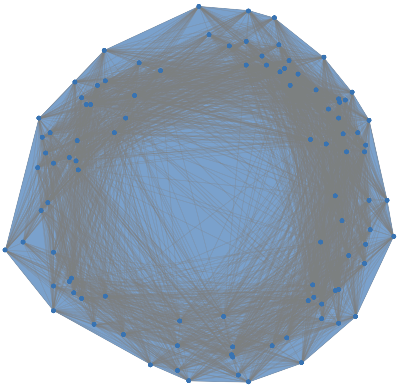
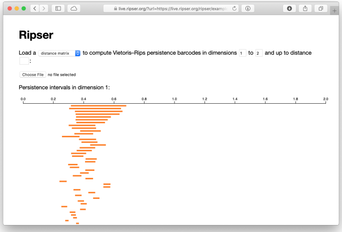
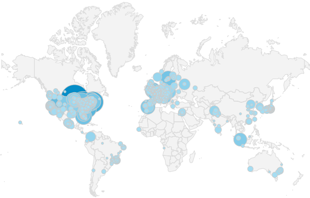


Ripser: software for computing Vietoris–Rips persistence barcodes

Open source software (`ripser.org`)

- significantly faster / more memory efficient than previous codes
- de facto standard for topological data analysis applications
- most popular GitHub project on persistent homology





Ripser users from 935 different locations

Computational improvements based on

- *implicit matrix representations*
- *apparent pairs*, connecting persistence to discrete Morse theory

Apparent pairs

Ripser uses the following pairing of simplices (for the filtration, we break ties lexicographically):

Definition (B 2016, 2021)

In a simplexwise filtration $(K_i = \{\sigma_1, \ldots, \sigma_i\})_i$, two simplices (σ_i, σ_j) form an *apparent pair* if

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Special cases and equivalent definitions have been (re)discovered independently multiple times

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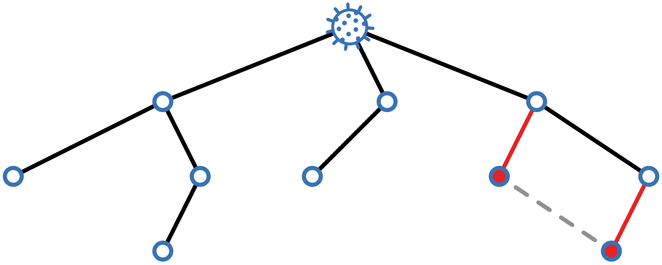
Proposition (B, Roll 2022)

Any generalized discrete Morse function is refined by apparent pairs.

Topology of viral evolution



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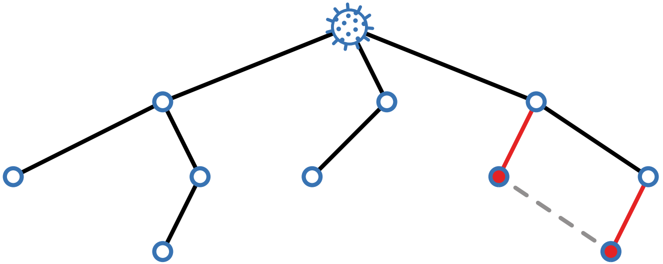

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Observation: Ripser runs unusually fast on genetic distance data

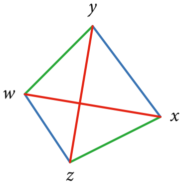
- SARS-CoV2 RNA sequences (spike protein)
- 25556 data points (2.8×10^{12} simplices in 2-skeleton)
- $120\,s$ computation time (with data points ordered appropriately)

Gromov-hyperbolicity

Definition (Gromov 1988)

A metric space X is δ-*hyperbolic* (for $\delta \geq 0$) if for all $w, x, y, z \in X$ we have

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



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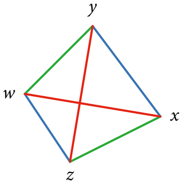

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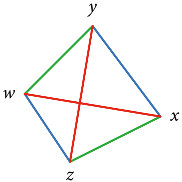
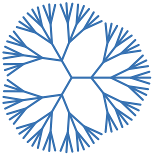


- The hyperbolic plane is $(\ln 2)$-hyperbolic.

- The 0-hyperbolic spaces are precisely the metric trees and their subspaces.



Rips Contractibility

Theorem (Rips; Gromov 1988)

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

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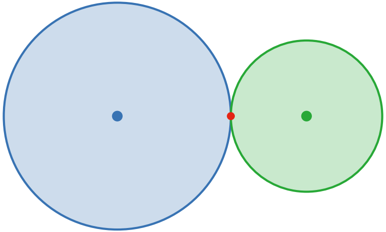
Theorem (B, Roll 2022)

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

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

for all $u > t \geq 4\delta + 2\nu$, where ν is the geodesic defect *of X.*

Geodesic defect



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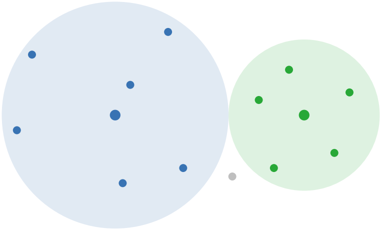

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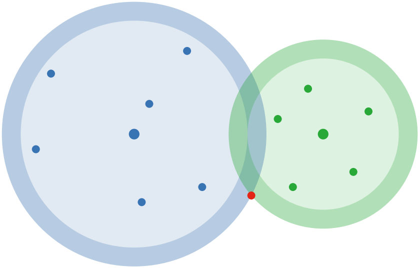

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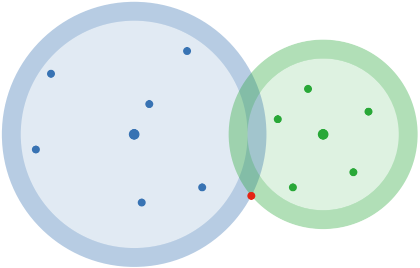

Definition (Bonk, Schramm 2000)

A metric space X is *ν-geodesic* if for all points $x, y \in X$ and all $r, s \geq 0$ with $r + s = d(x, y)$ we have

$$B_{r+\nu}(x) \cap B_{s+\nu}(y) \neq \varnothing.$$

The infimum of all such ν is the *geodesic defect* of X.

The diameter function of generic trees

Proposition (B, Roll 2022)

Consider a finite weighted tree (V, E) *with a* generic *path length metric (distinct pairwise distances). Then the diameter function* $\operatorname{diam}\colon \Delta(V) \to \mathbb{R}$ *is a generalized discrete Morse function.*

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- *The apparent pairs refine this gradient.*

Theorem (B, Roll 2022)

The apparent pairs of the diameter function for a generic tree metric space X *induces the collapses*

$$
\begin{aligned}
&\operatorname{Rips}_t(X) \searrow T_t && \text{for all } t \in \mathbb{R}, \text{ with}\\
&\operatorname{Rips}_t(X) \searrow T \searrow \{*\} && \text{for } t \geq \max l(E), \text{ and}\\
&\operatorname{Rips}_u(X) \searrow \operatorname{Rips}_t(X) && \text{whenever } l(e) \notin (t,u] \text{ for all } e \in E.
\end{aligned}
$$

In particular, the persistent homology is trivial in degrees > 0.

Tree metrics beyond the generic case

Why is Ripser particularly fast on genetic distances (tree-like)?

- Consider a weighted finite tree $T = (V, E)$, viewed as a metric space X.
- Choose an arbitrary root and extend the rooted tree partial order to a total order.

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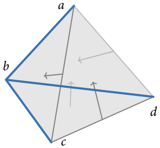

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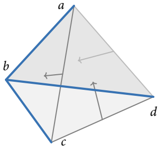

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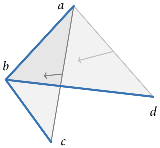

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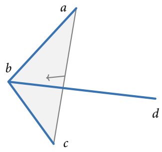

Origins

When was persistent homology discovered first?

When was persistent homology discovered first?

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?

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Rank and span in functional topology

Search within citing articles

Exact homomorphism sequences in homology theory
ed.ac.uk [PDF]

JL Kelley, E Pitcher - Annals of Mathematics, 1947 - JSTOR

The developments of this paper stem from the attempts of one of the authors to deduce relations between homology groups of a complex and homology groups of a complex which is its image under a simplicial map. Certain relations were deduced (see [EP 1] and [EP 2] ...

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Marston Morse and his mathematical works
ams.org [PDF]

R Bott - Bulletin of the American Mathematical Society, 1980 - ams.org

American Mathematical Society. Thus Morse grew to maturity just at the time when the subject of Analysis Situs was being shaped by such masters2 as Poincaré, Veblen, LEJ Brouwer, GD Birkhoff, Lefschetz and Alexander, and it was Morse's genius and destiny to ...

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Unstable minimal surfaces of higher topological structure

M Morse, CB Tompkins - Duke Math. J, 1941 - projecteuclid.org

1. Introduction. We are concerned with extending the calculus of variations in the large to multiple integrals. Theproblem of the existenceof minimal surfaces of unstable type contains many of the typical difficulties, especially those ofa topological nature. Having studied this ...

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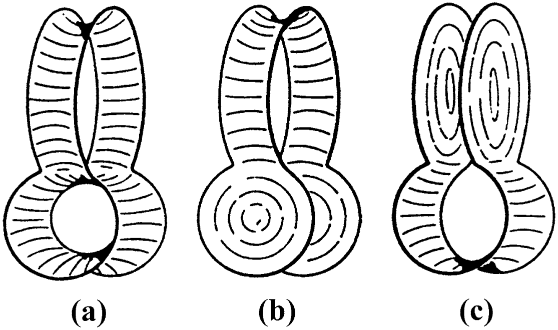
U Bauer - 2011 - Citeseer

Motivation and application: minimal surfaces

Problem (Plateau's problem)

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



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

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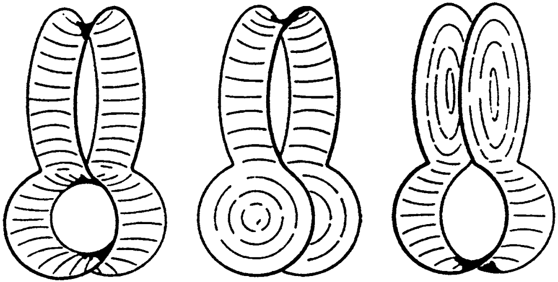


(a) (b) (c)

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

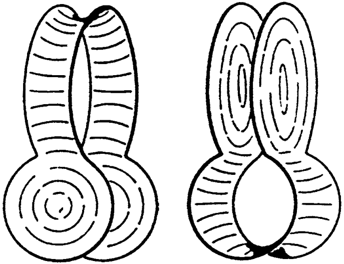
Solution by Douglas (1930):

- 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.



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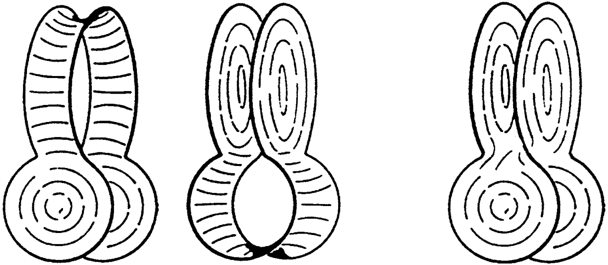
Theorem (Morse, Tompkins 1939; Shiffman 1939)

Assume that a given curve bounds two separate stable minimal surfaces.
Then that curve also bounds an unstable *minimal surface (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 all structure maps $M_s \to M_t$ $(s < t)$ have finite rank.

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Morse's main technical result, in modern language:

- The minimal surface functional has q-tame persistent homology.

Q-tameness from local connectivity

Theorem (Morse, 1937)

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

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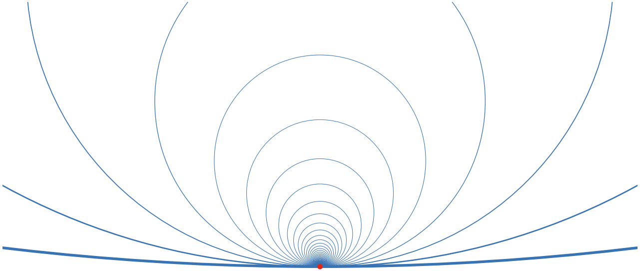

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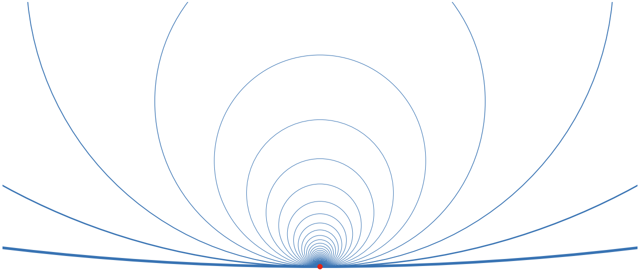


Theorem (B, Medina-Mardones, Schmahl 2021)

If the sublevel set filtration of $f: X \to \mathbb{R}$ is compact and homologically locally connected, *then it has q-tame persistent homology.*

Simplification

Topological simplification of functions

Consider the following problem:

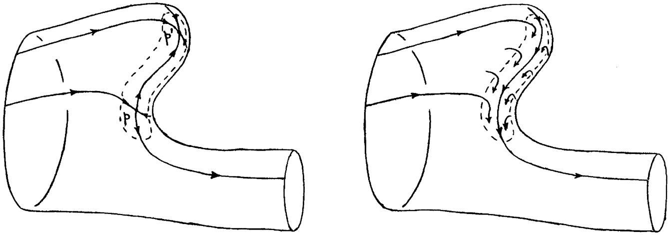
Problem (Topological simplification)

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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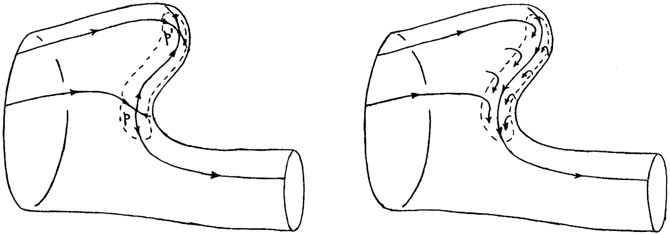

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For a Morse function:

- critical points correspond to endpoints of barcode intervals

Combining persistence and Morse theory

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*
- *achieving the lower bound on the number of critical points.*

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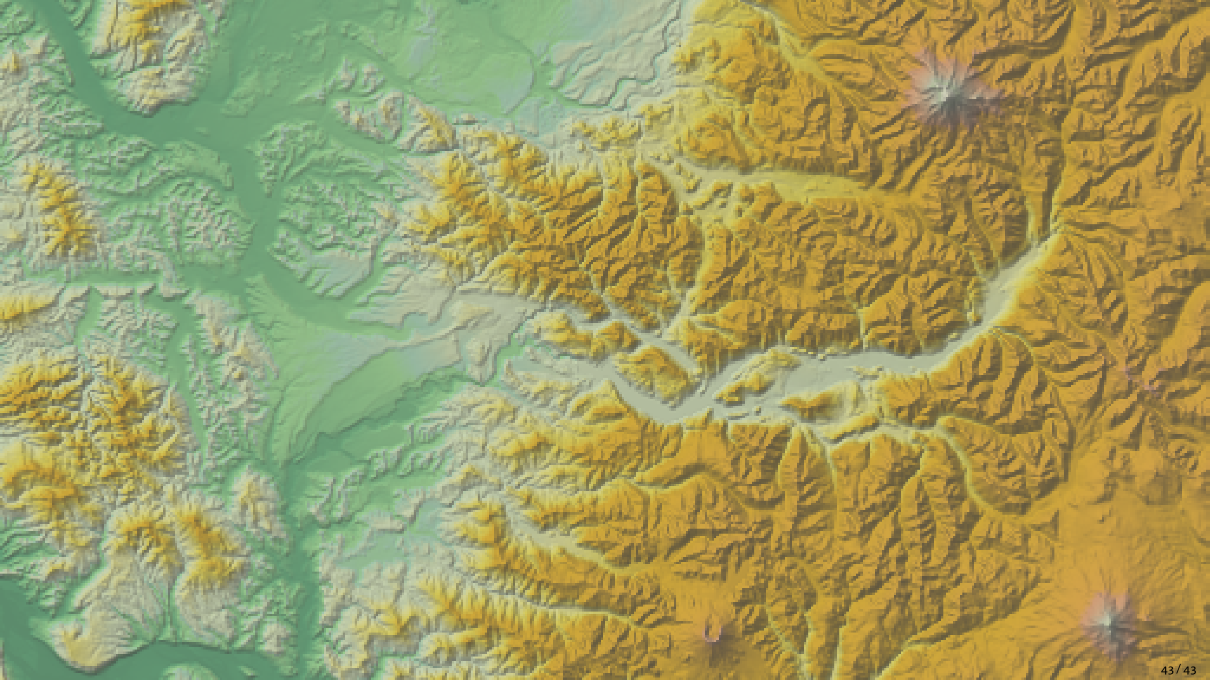
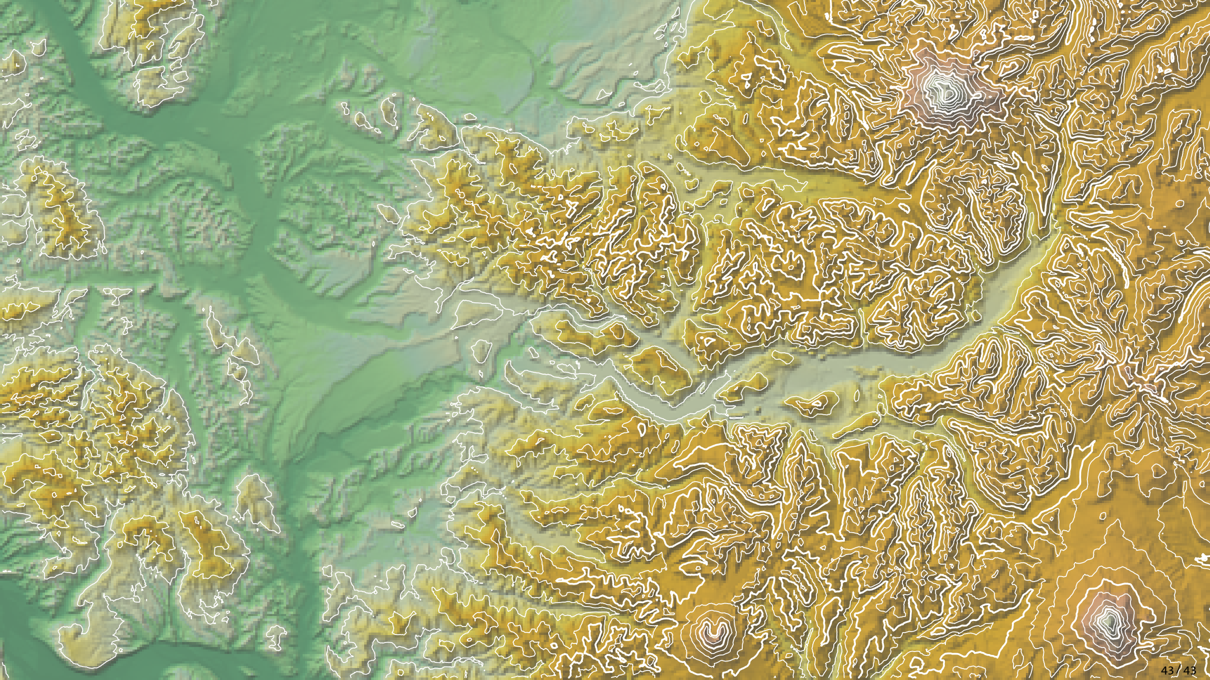
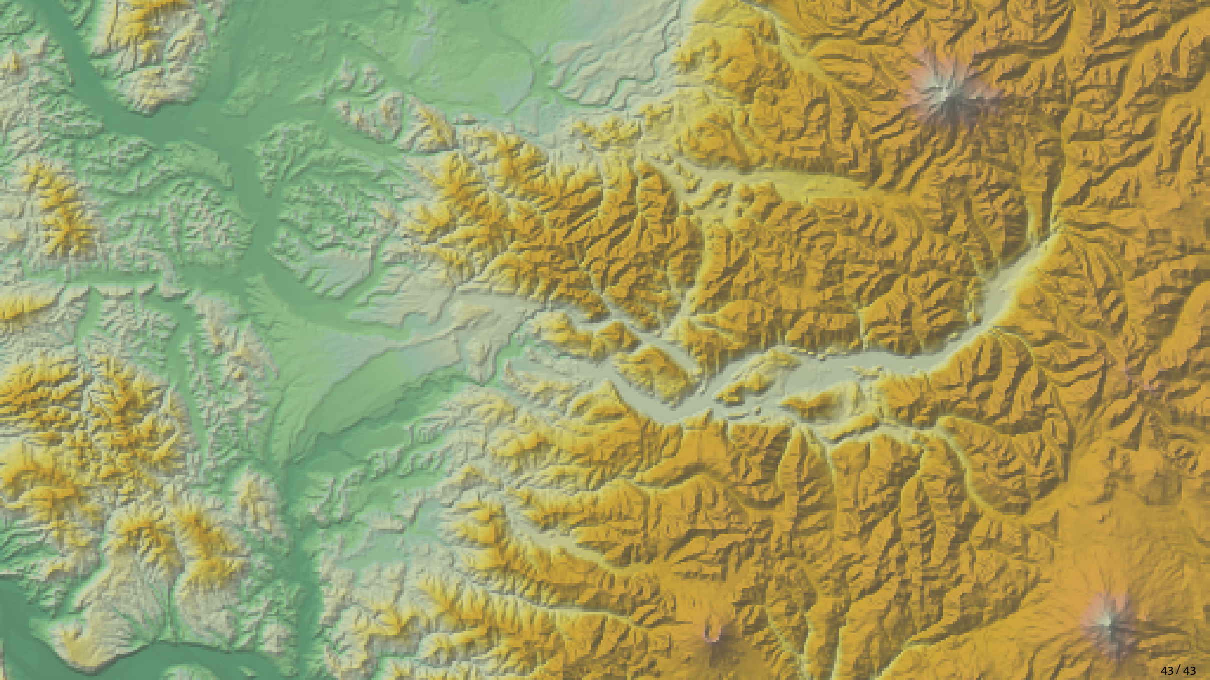
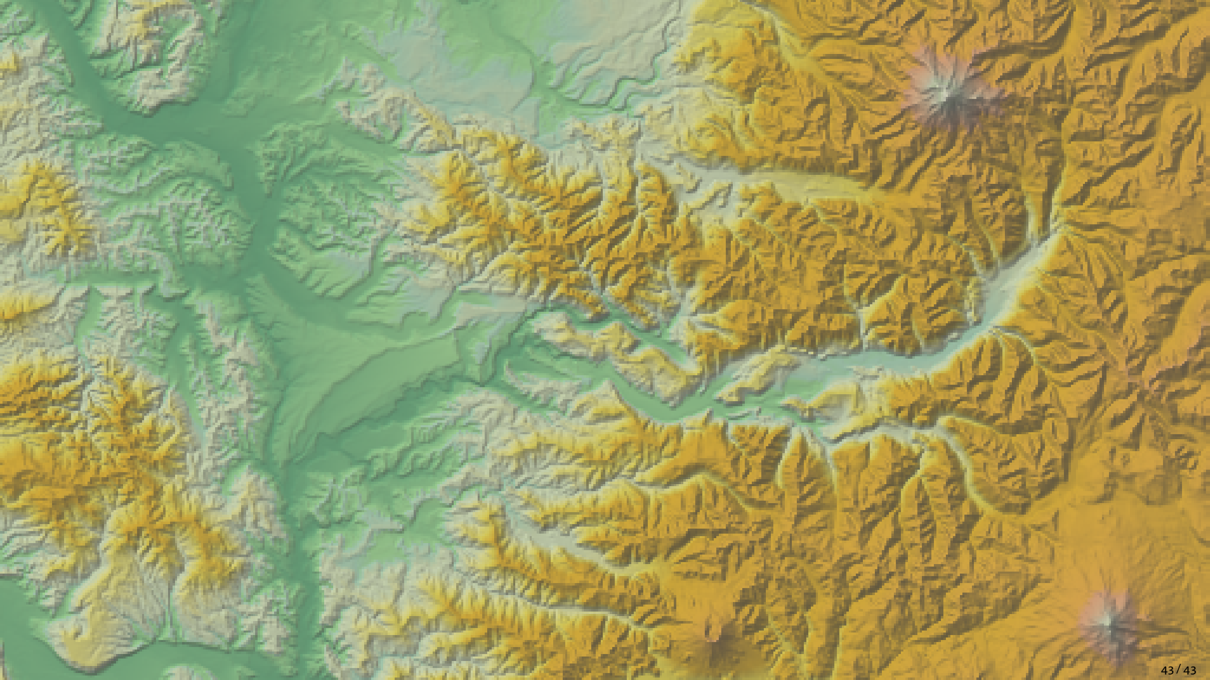
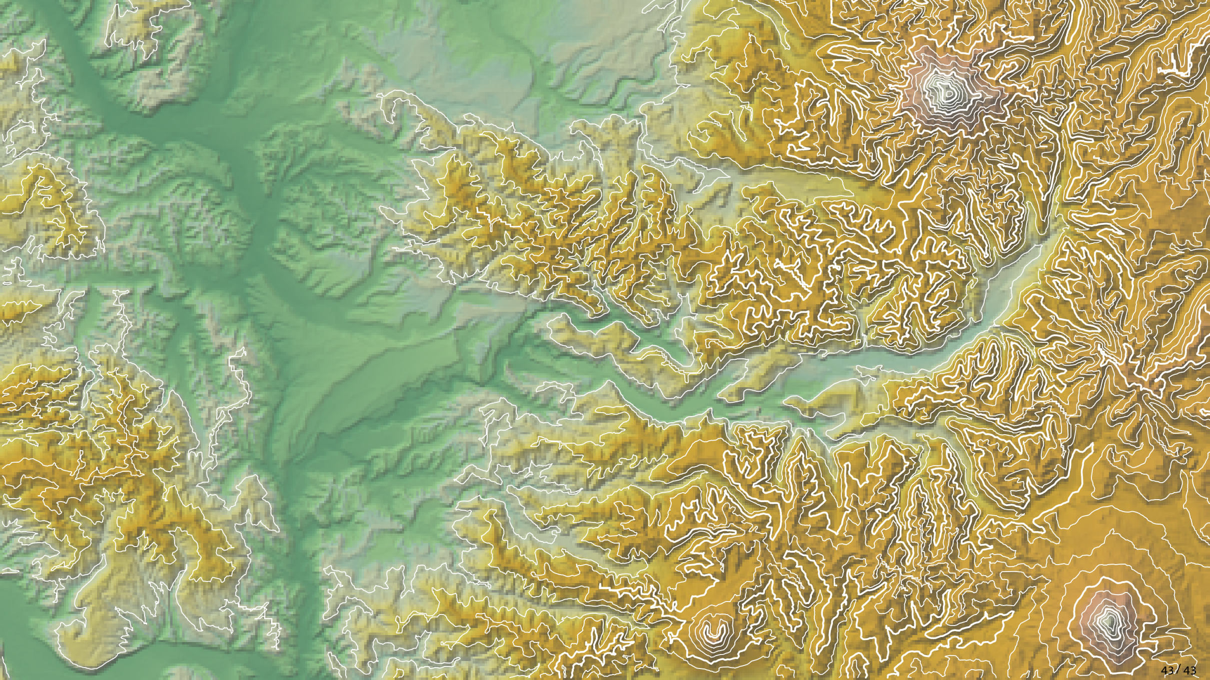
Does not generalize to higher-dimensional manifolds!











Thanks for your attention!