# Gromov-hyperbolicity, geodesic defect, and persistent homology of Vietoris–Rips complexes

Ulrich Bauer

TUM

Jul 28, 2022

Bavarian Geometry & Topology Meeting X

Universität Augsburg

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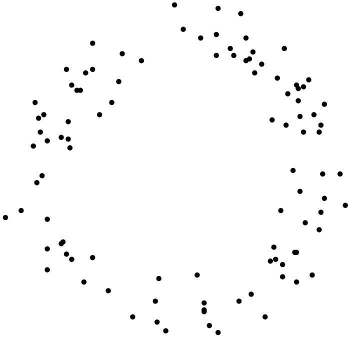
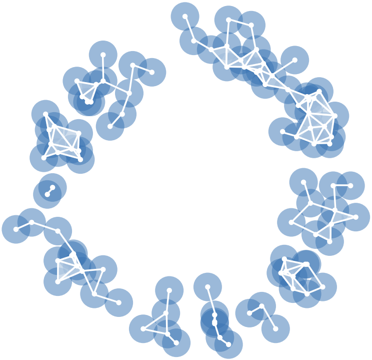
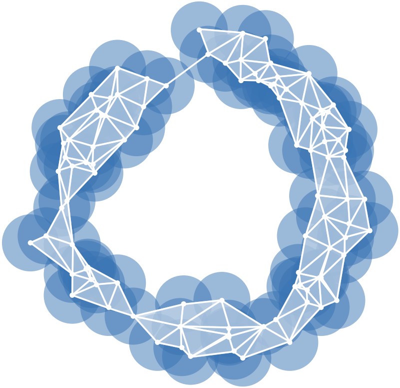
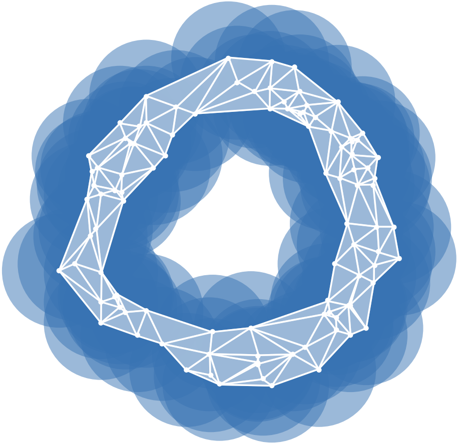
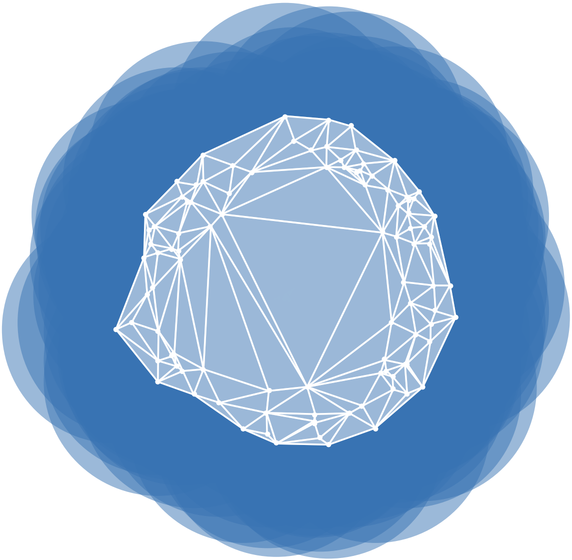


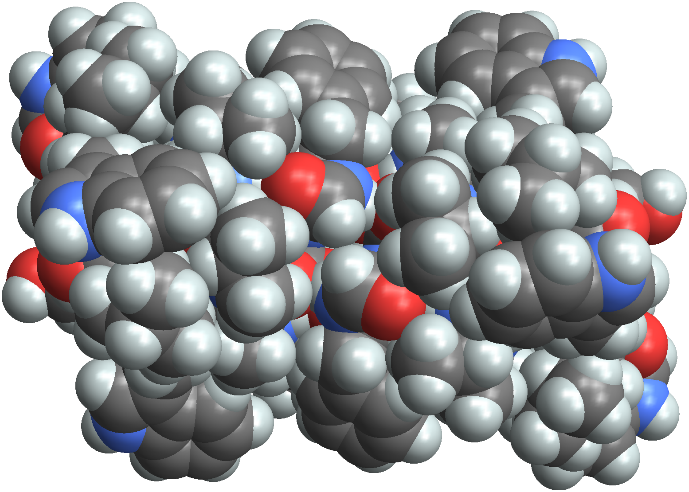








# Geometry and topology of biomolecules



Gramicidin (an antibiotic functioning as an ion channel)

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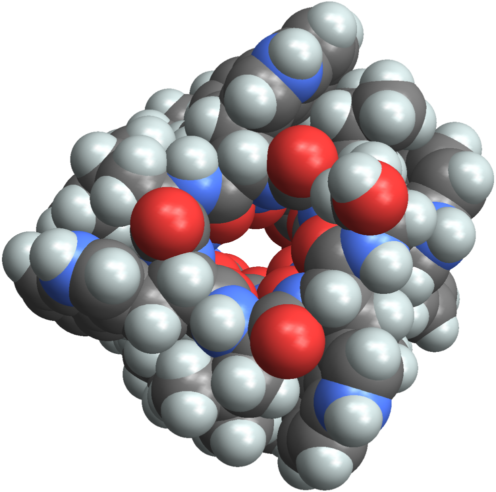

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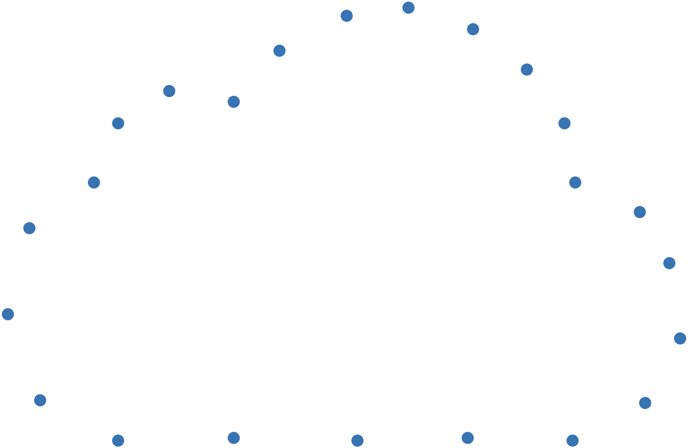
# Čech complexes



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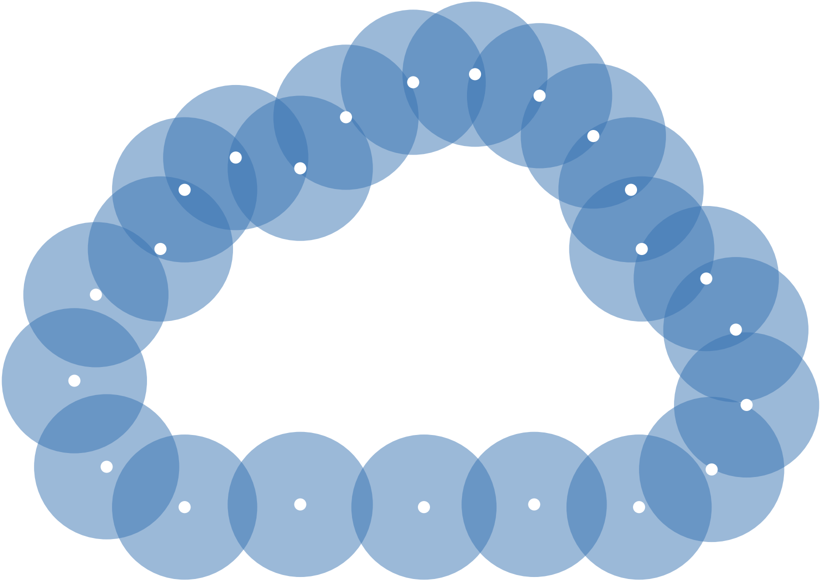

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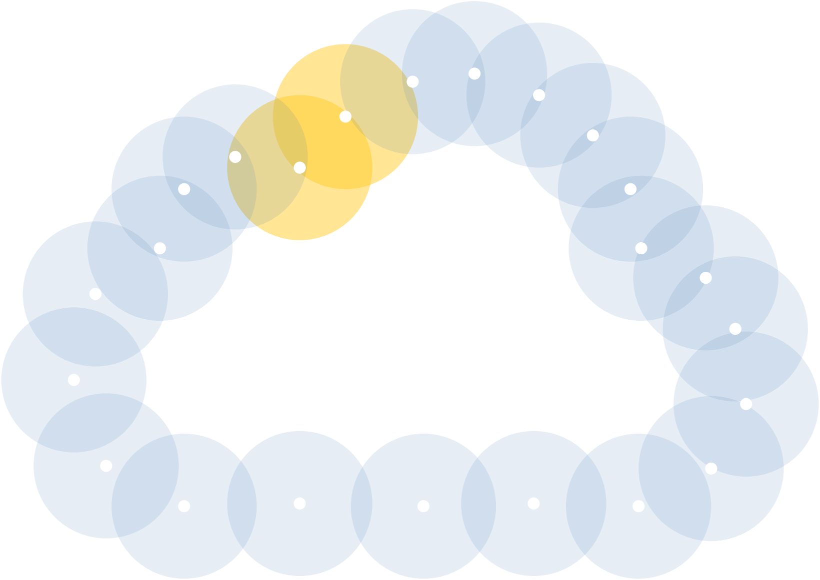

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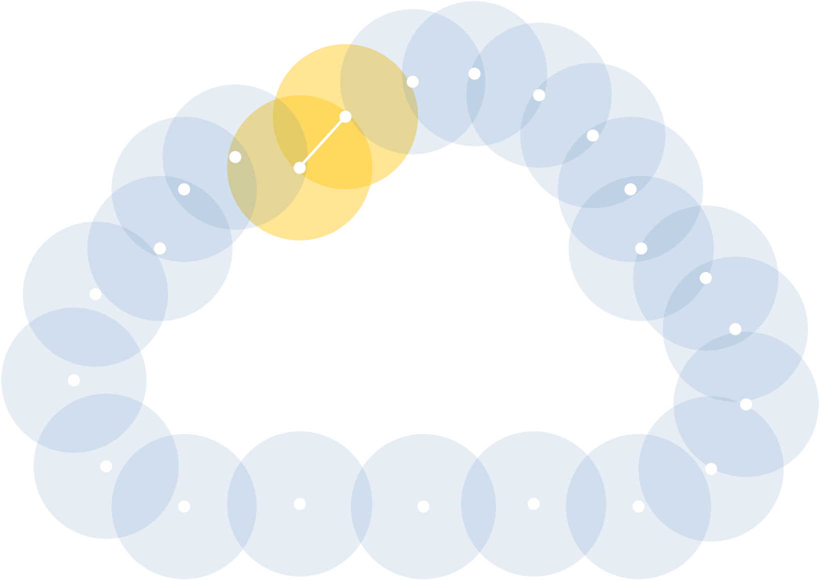

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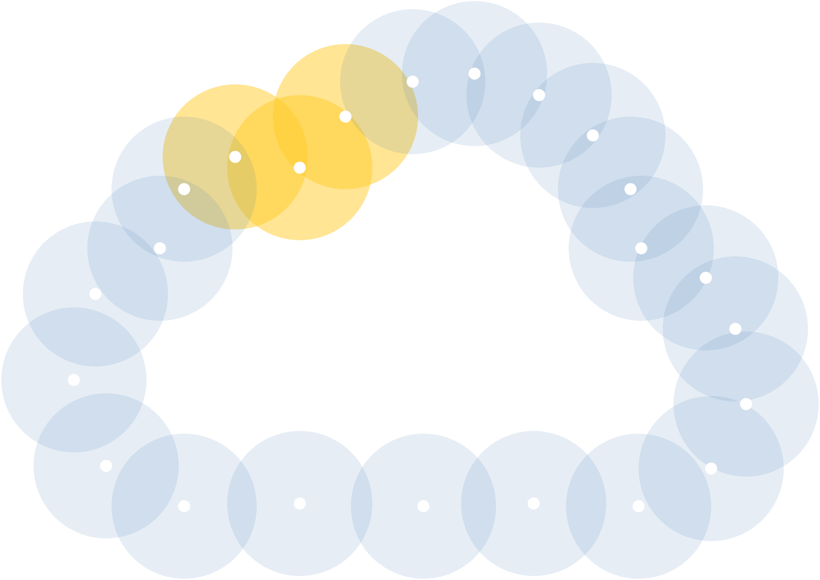

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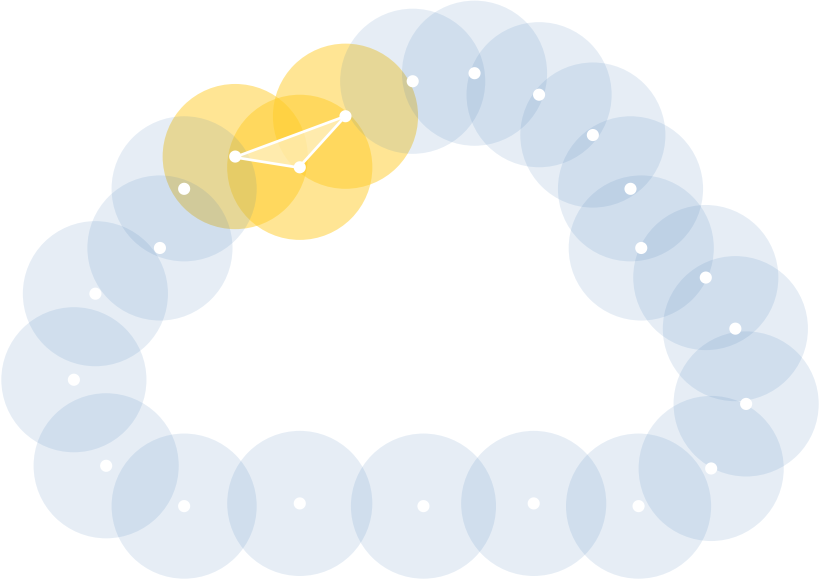

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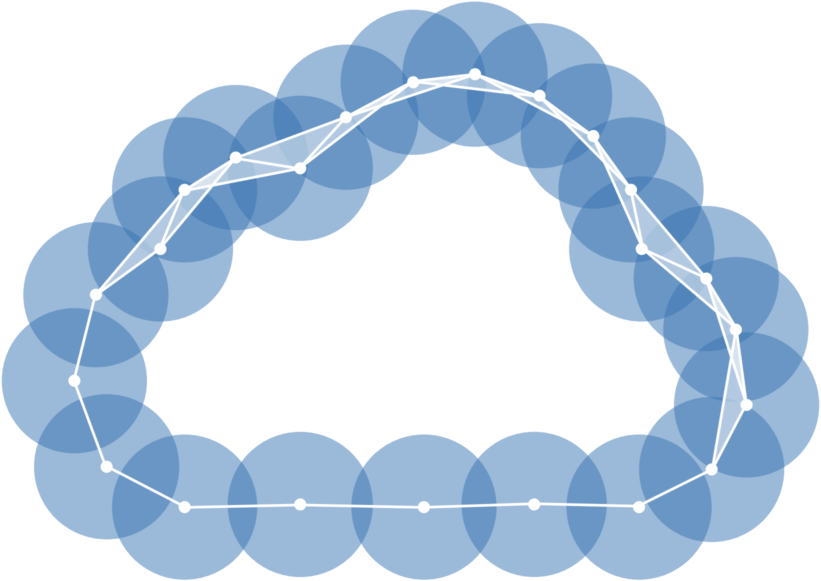

## Definition

Let $X$ be a topological space, and let $\mathcal{U} = (U_i)_{i \in I}$ be a cover of $X$. The *nerve* of $\mathcal{U}$ is the simplicial complex

$$\mathrm{Nrv}(\mathcal{U}) = \left\{ J \subseteq I \;\middle|\; |J| < \infty \text{ and } \bigcap_{i \in J} U_i \neq \varnothing \right\} .$$

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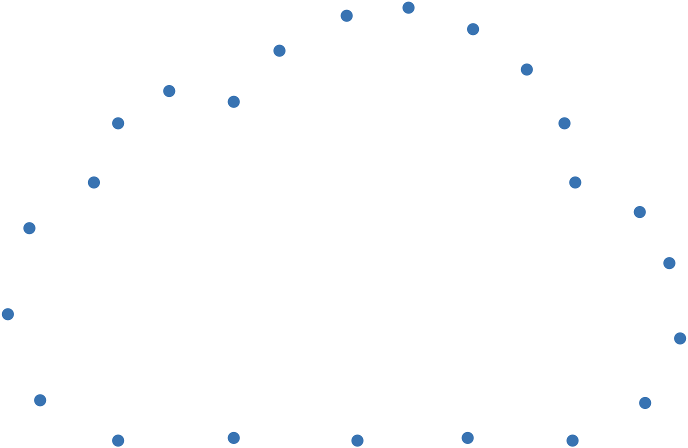
U. Bauer, M. Kerber, F. Roll, and A. Rolle
A Unified View on the Functorial Nerve Theorem and its Variations
Preprint, arXiv:2203.03571, 2022

# Delaunay complexes



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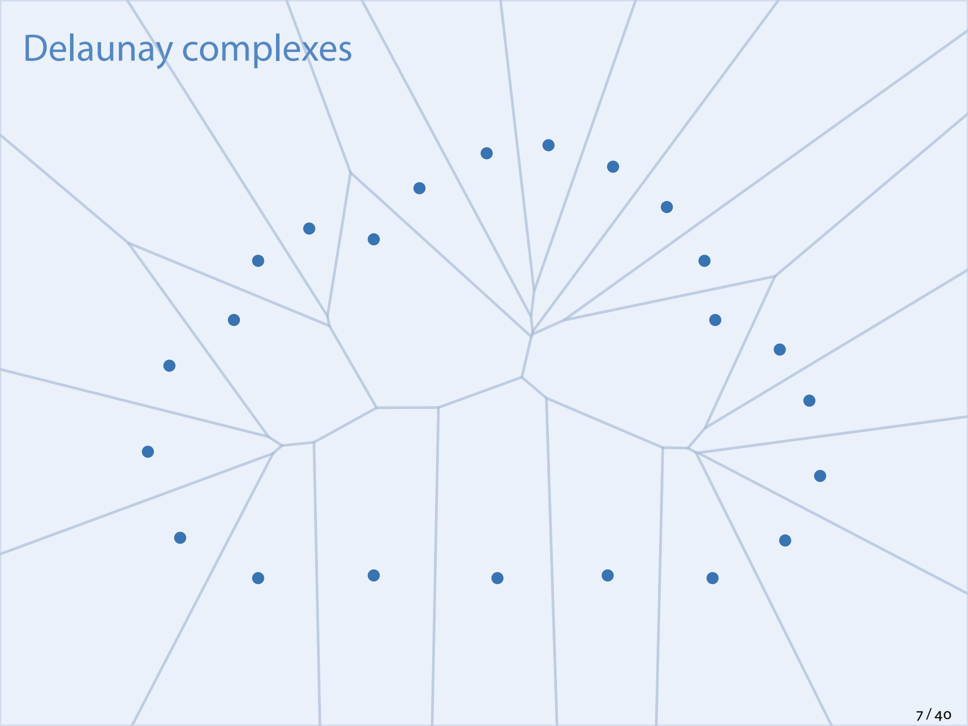

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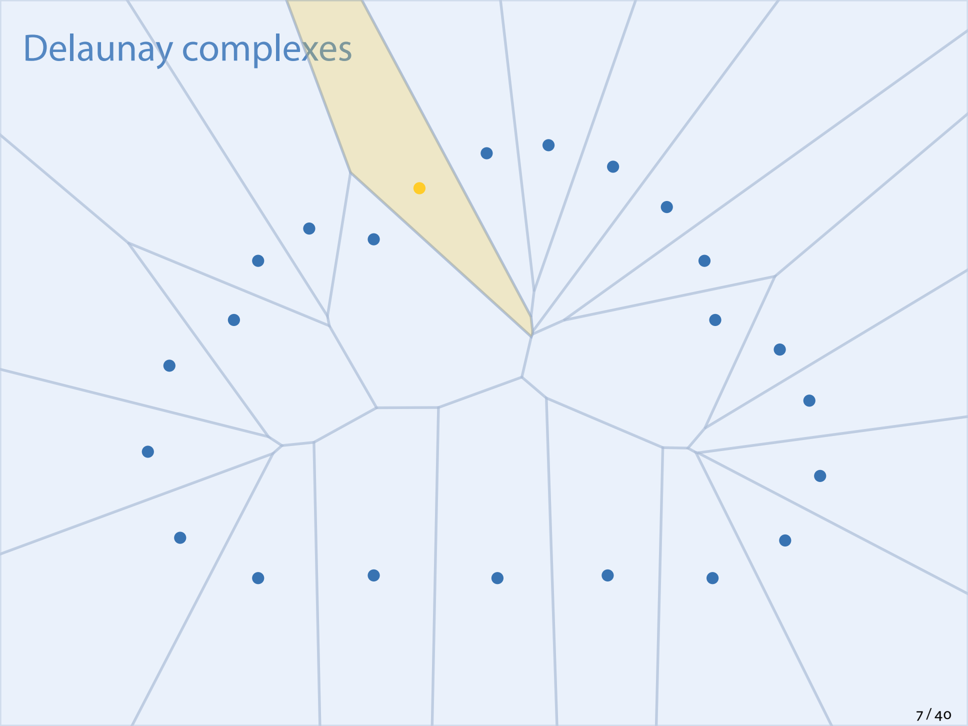

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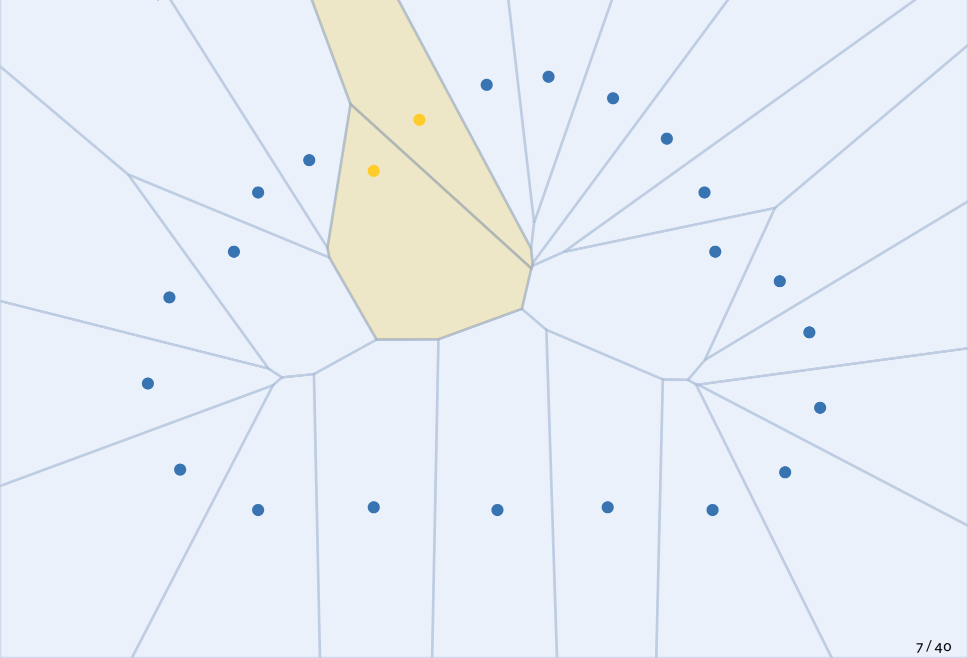

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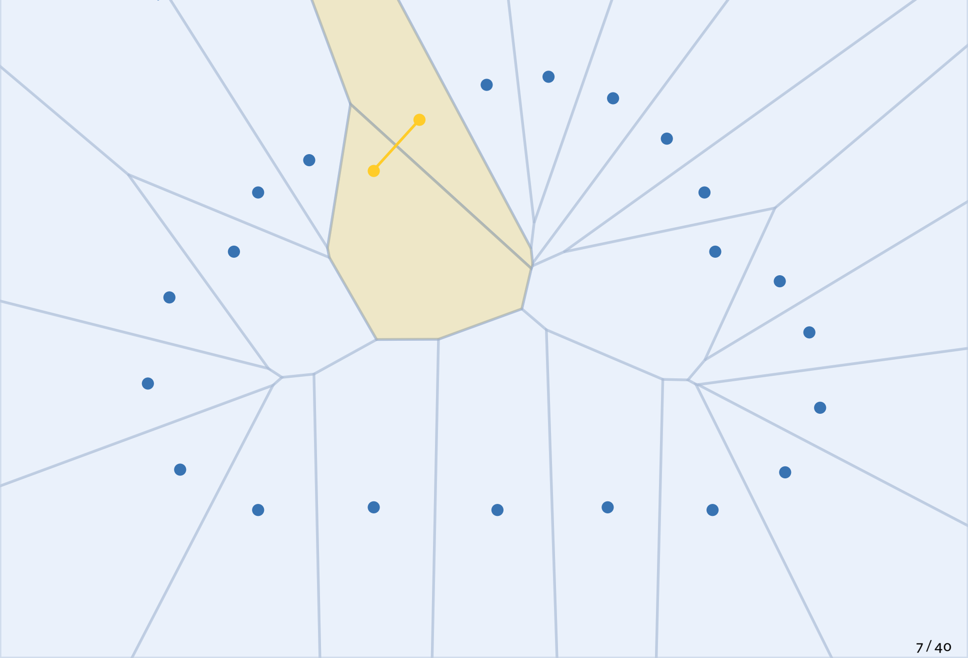

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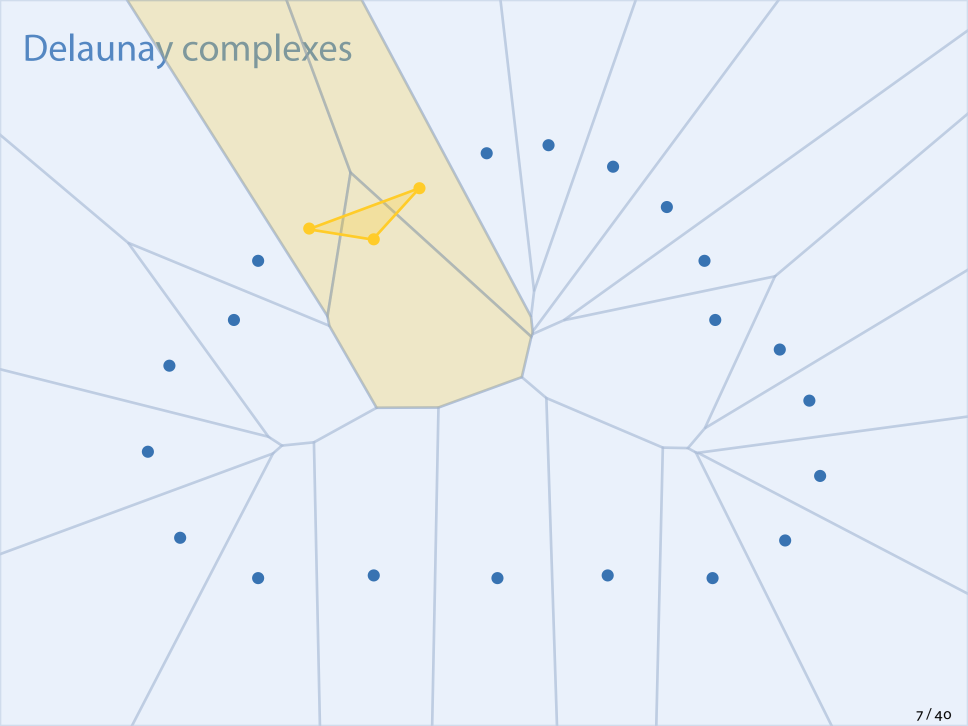

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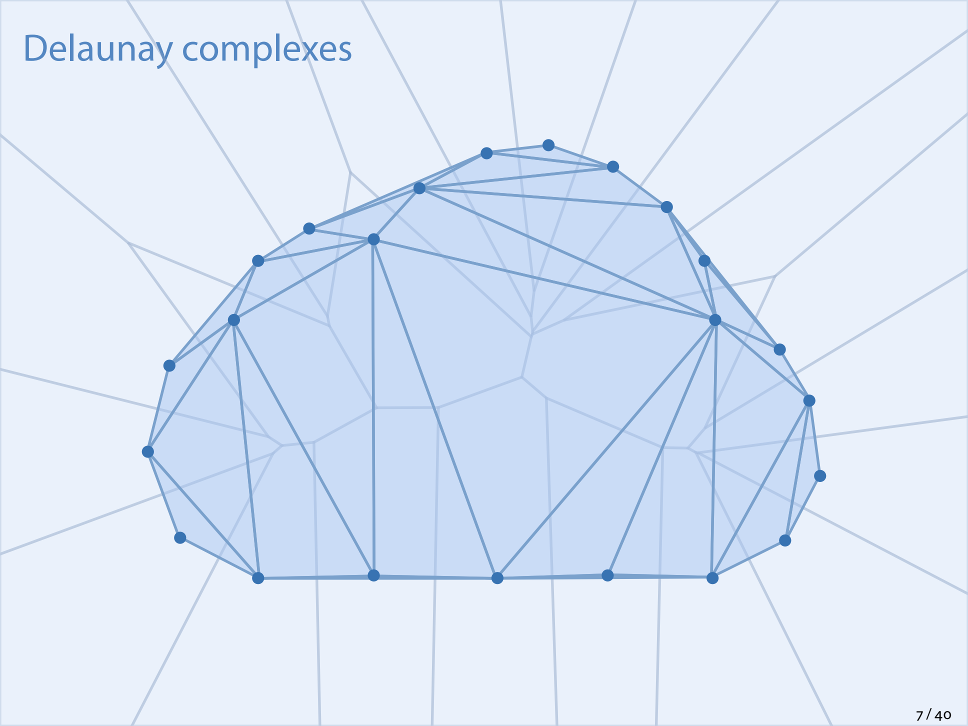

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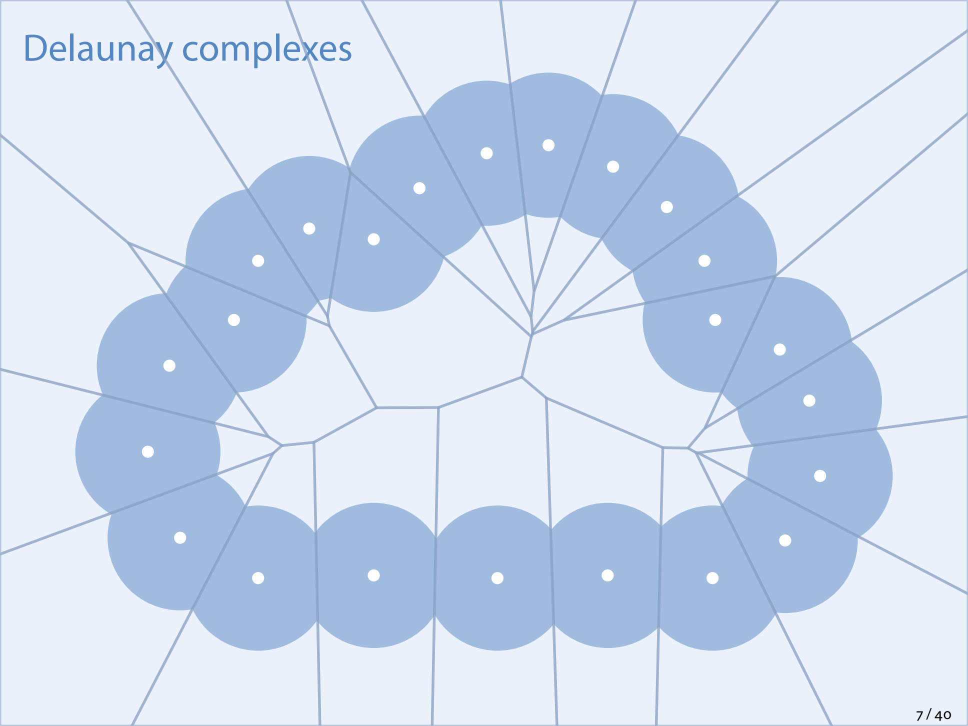

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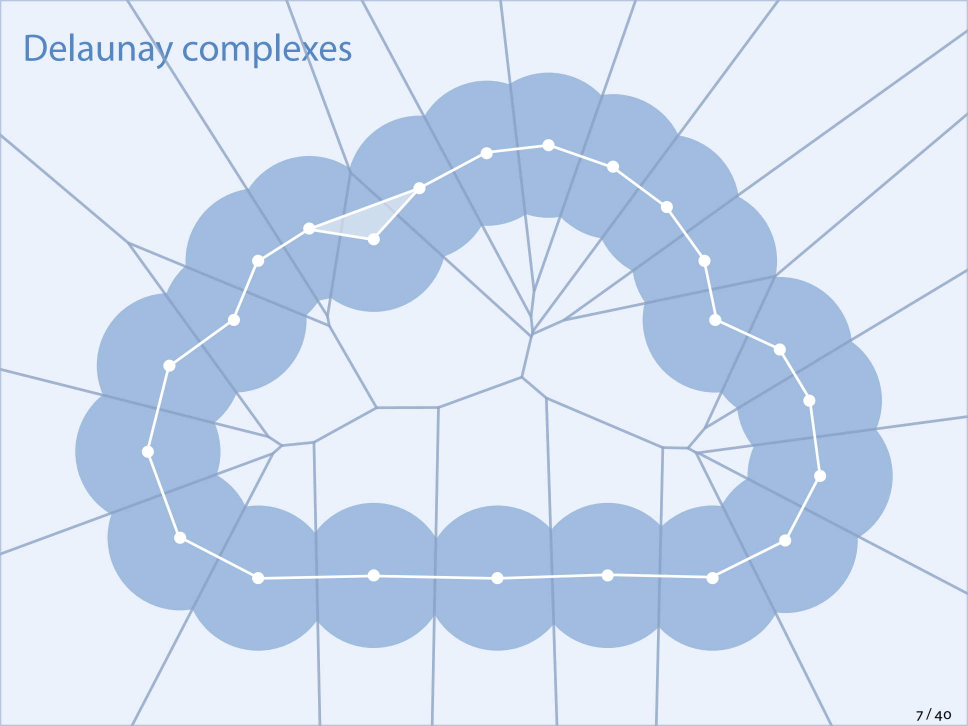

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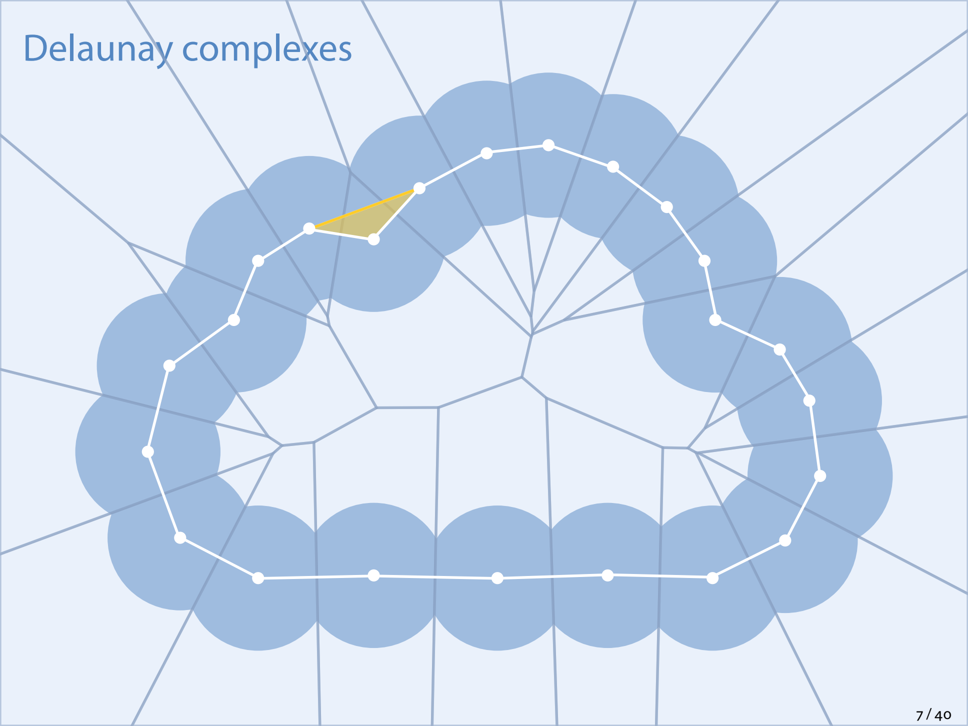

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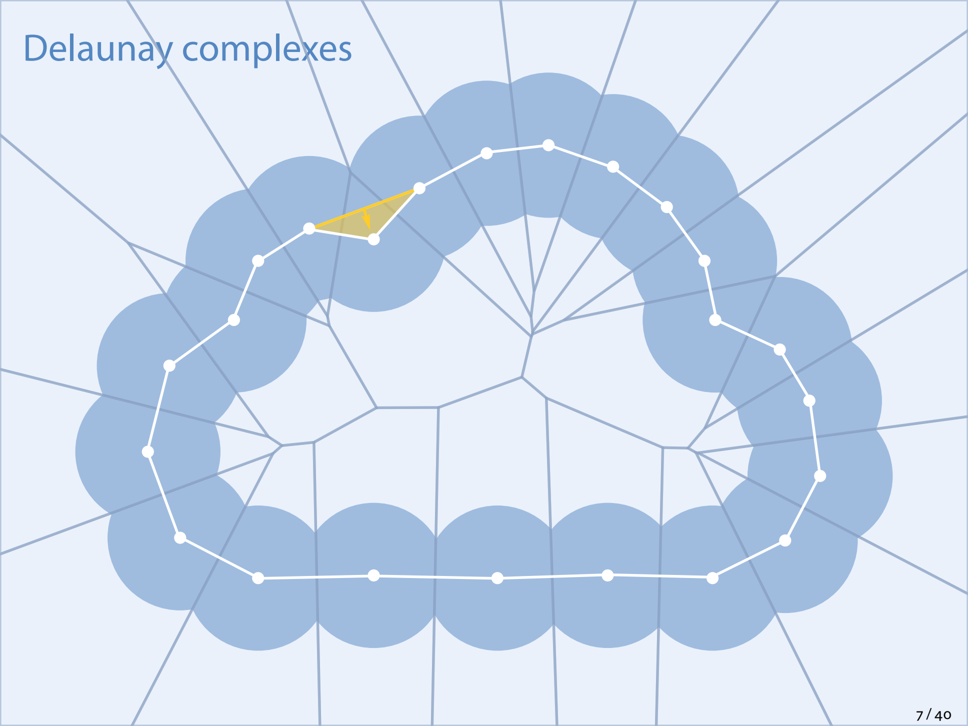

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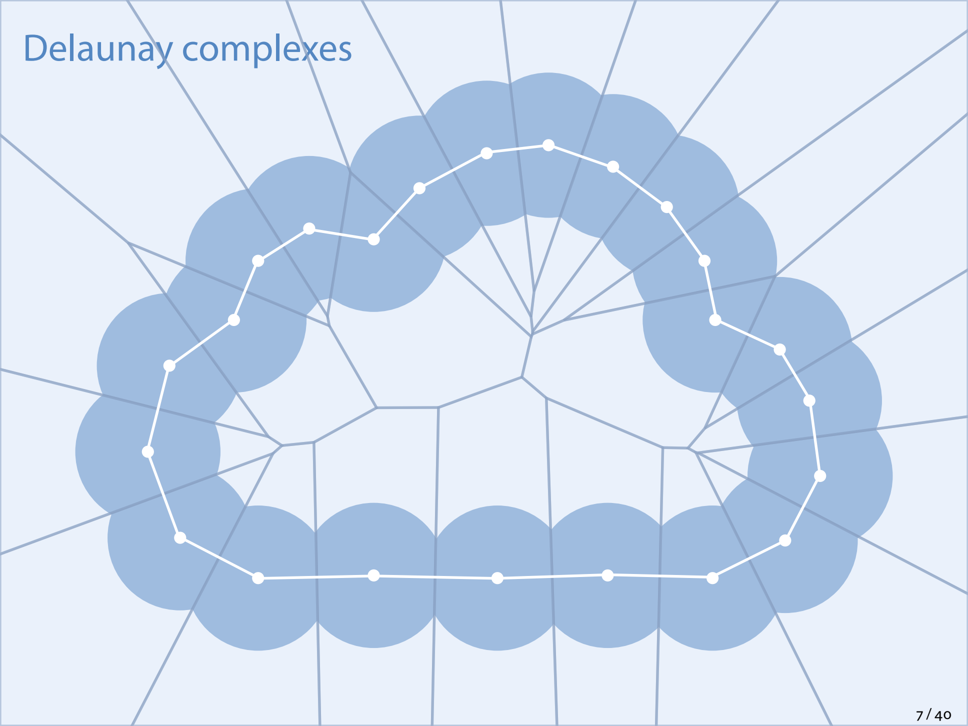
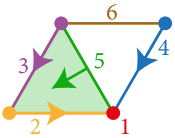


# Discrete Morse theory



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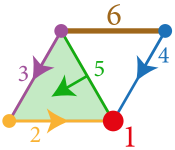

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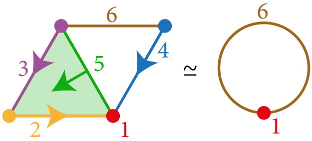
## Theorem (Forman 1998)

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



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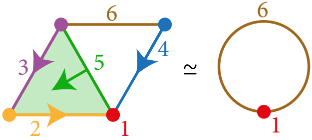
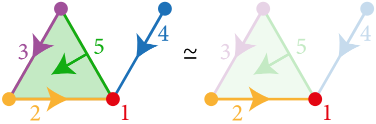



Discrete Morse functions – and their gradients – encode collapses of sublevel sets:



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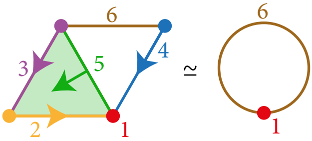


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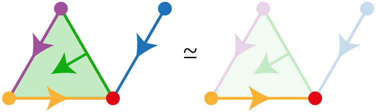
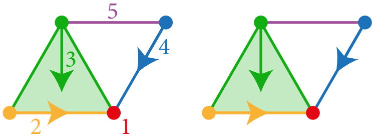


# Generalizing discrete Morse theory

Generalized discrete Morse functions/gradients:



# Morse theory for Čech and Delaunay complexes

### Proposition (B, Edelsbrunner 2014)

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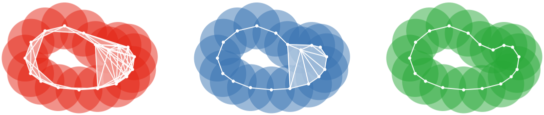
## Theorem (B., Edelsbrunner 2017)

*Čech, Delaunay, and Wrap complexes are related by 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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# 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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*Then $H_*(X) \cong H_*(P_{2\delta})$.*

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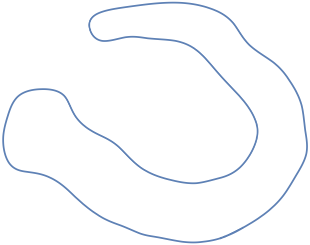

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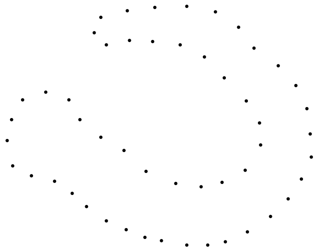

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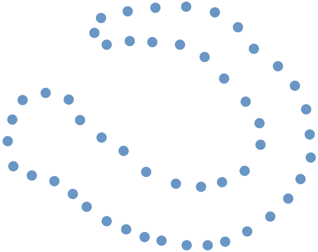

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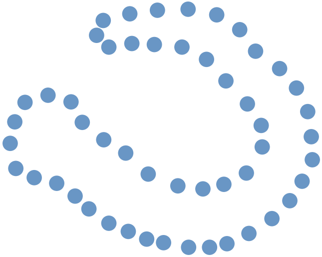

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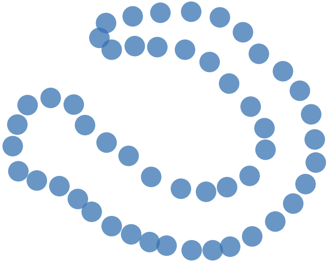

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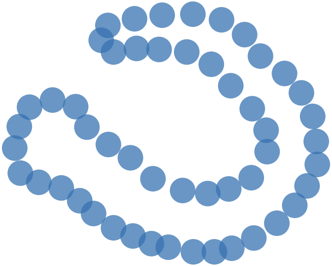

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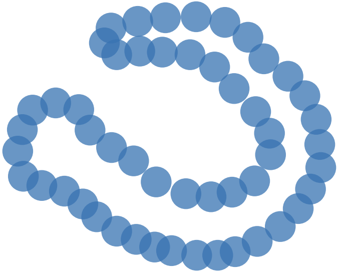

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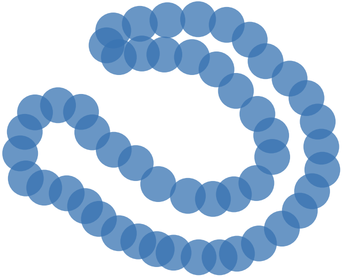

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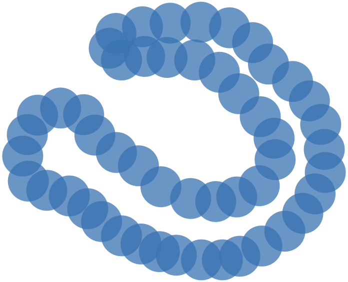

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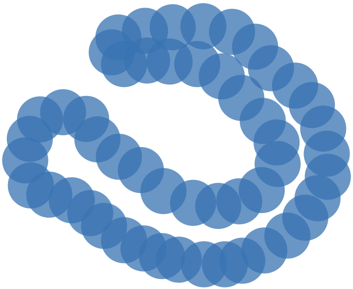

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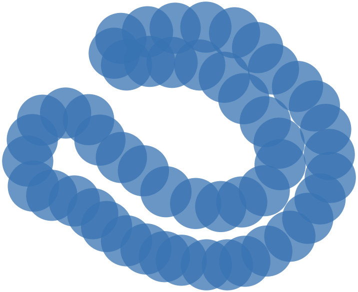

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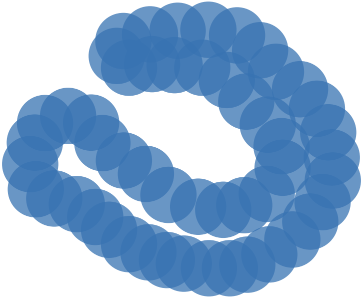

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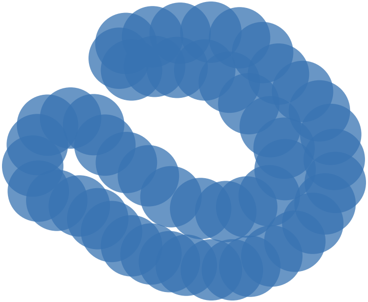

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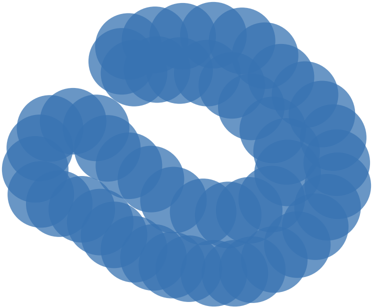

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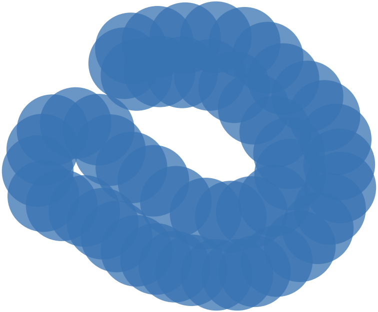

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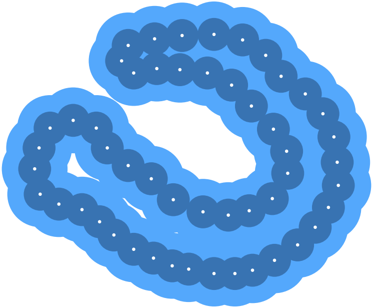

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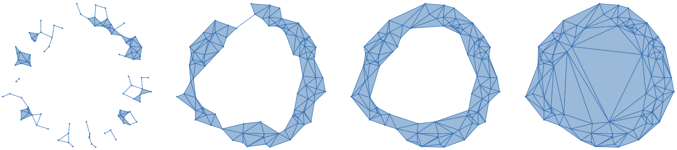

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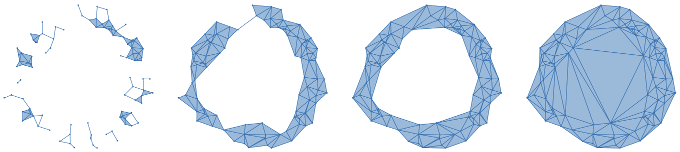

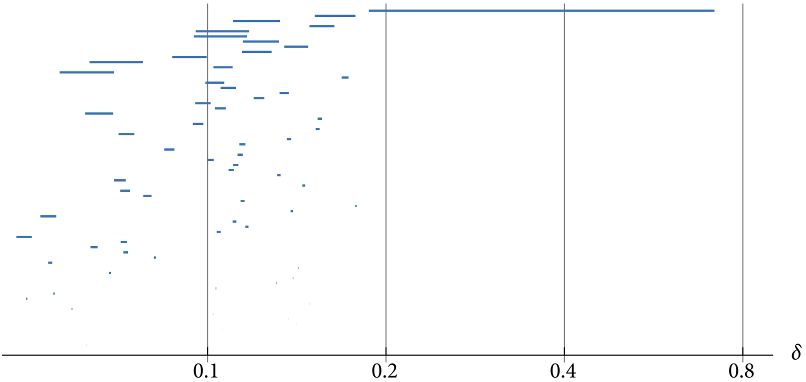

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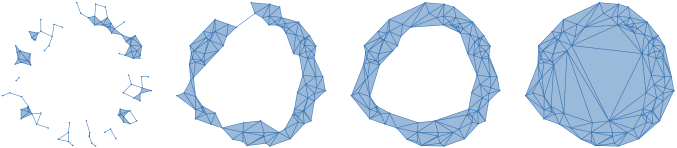

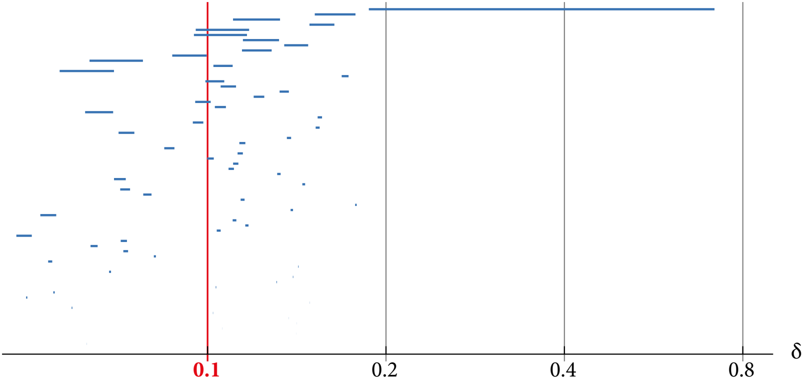

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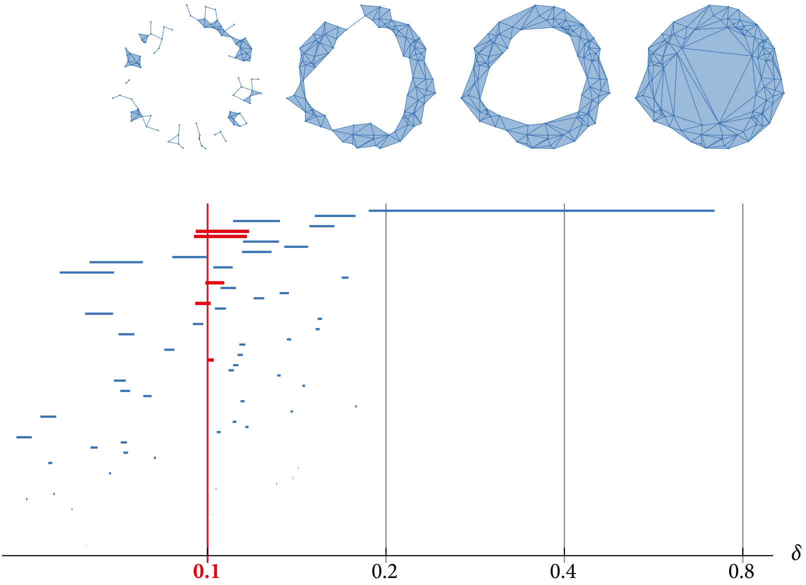

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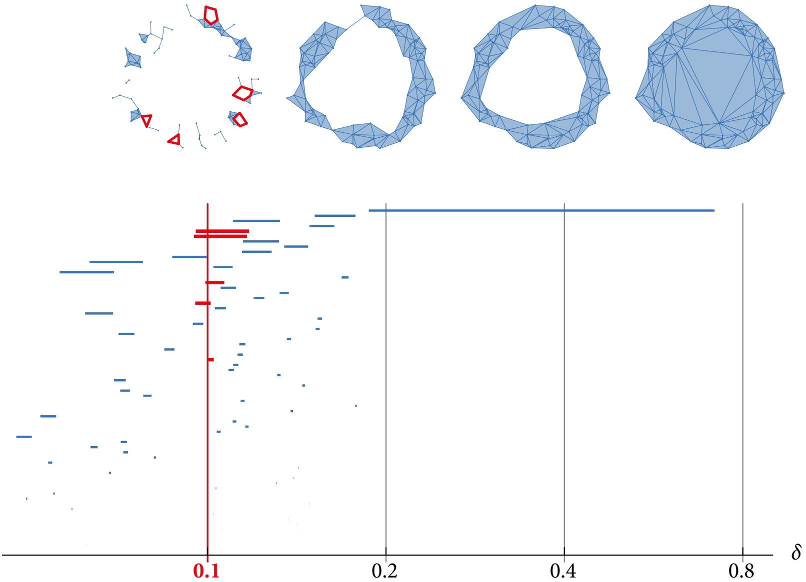

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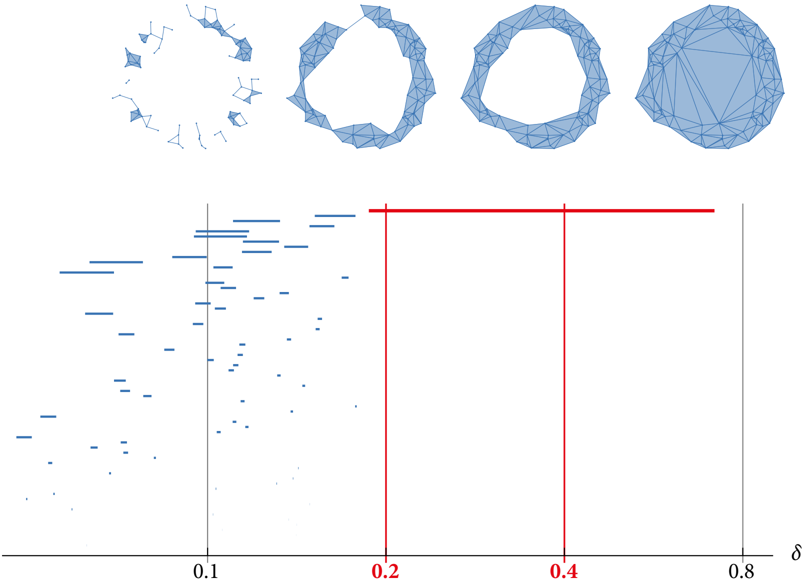

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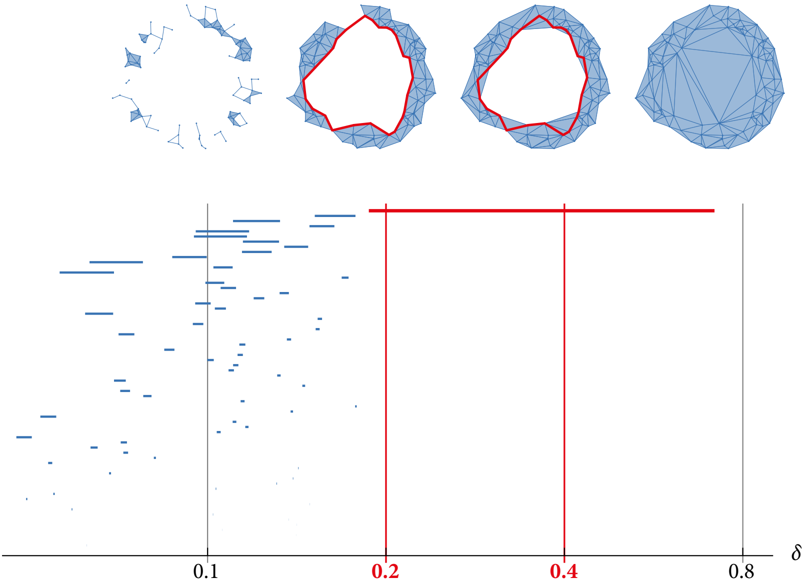

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- Persistent homology is a diagram $M = H_* \circ K : \mathbf{R} \to \mathbf{Vect}$ *(persistence module)*:

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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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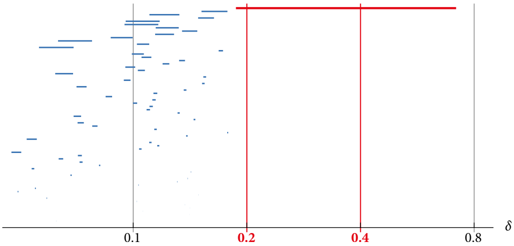
- The supporting intervals form the *persistence barcode*.



# 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).*

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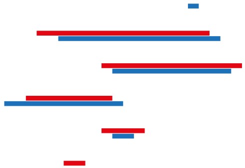

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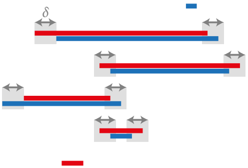

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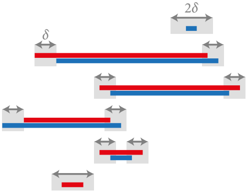

# Persistence and stability: the big picture

| | | |
|---|---|---|
| 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 $\delta$-*interleaved:*

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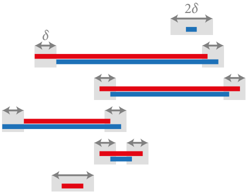
# Algebraic stability of persistence barcodes

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

*If two persistence modules are $\delta$-interleaved, then there exists a $\delta$-matching of their barcodes.*



# Induced matchings

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

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

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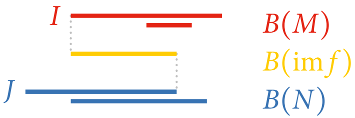

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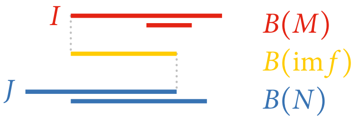
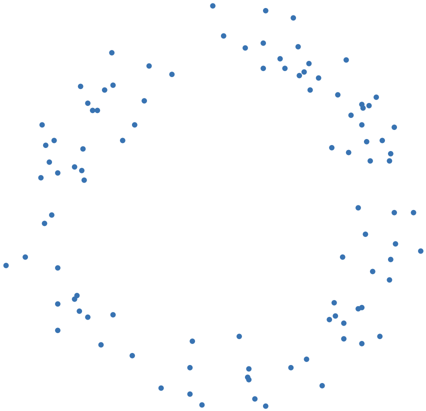



Theorem (Induced Matching theorem; B, Lesnick 2015)

*If $f$ is a $\delta$-interleaving morphism, then this is a $\delta$-matching.*

# Persistence of Vietoris–Rips complexes

# Vietoris–Rips complexes



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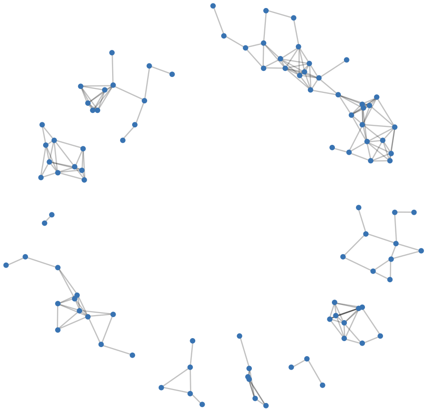

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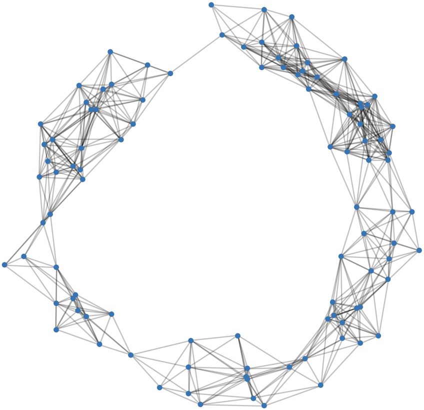

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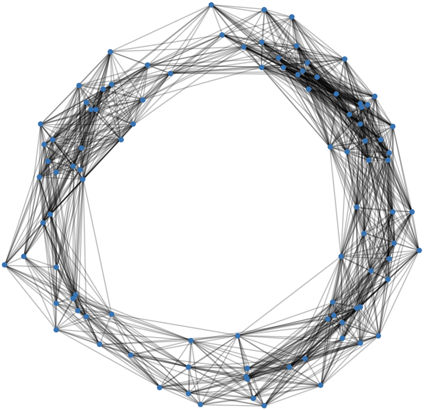

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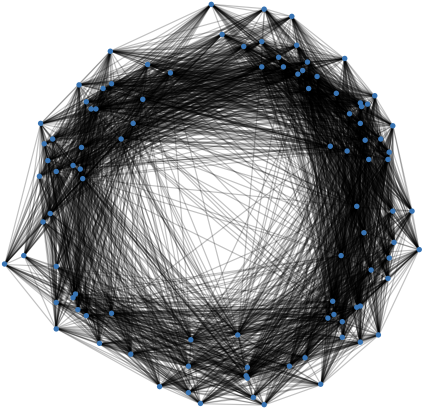

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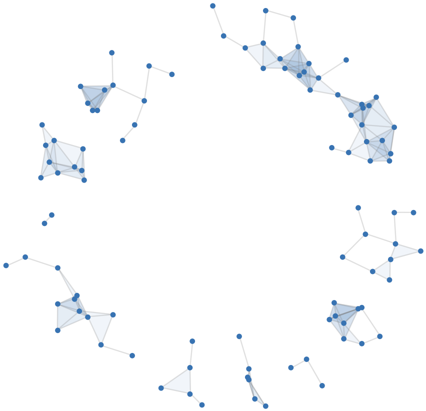

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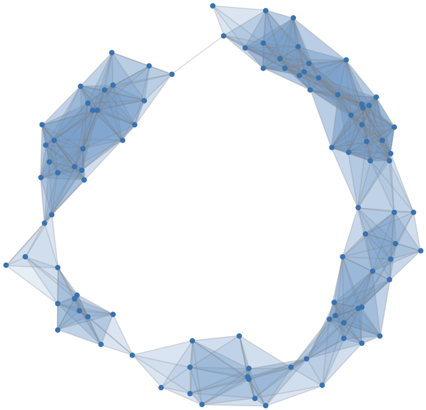

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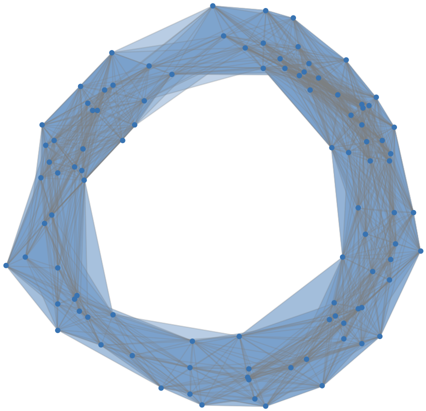

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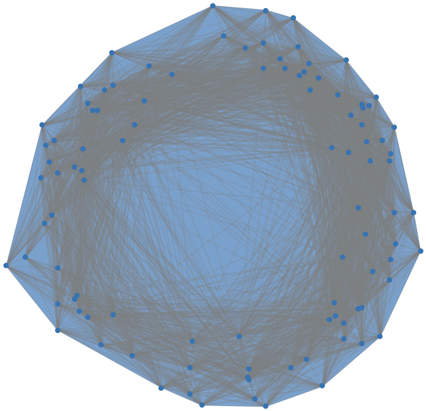

# Vietoris–Rips complexes

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

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

# An example computation

Example data set:

- 192 points on $\mathbb{S}^2$
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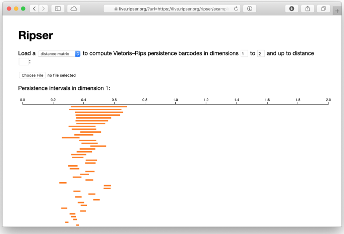

# Apparent pairs:

Ripser uses the following construction for a computational shortcut:

## Definition

In a simplexwise filtration $(K_i = \{\sigma_1, \dots, \sigma_i\})_i$, a pair of simplices $(\sigma, \tau)$ is an *apparent pair* if

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*The apparent pairs form a discrete gradient.*

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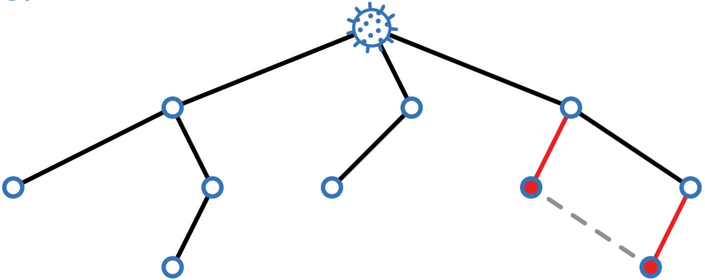
*The apparent pairs form persistence pairs: the cycle $\partial\tau$ gives rise to an interval $[f(\sigma), f(\tau))$ in the persistence barcode.*

# The diameter-lexicographic filtration

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

- Choose a total order on the vertices
- Order simplices by diameter
- Order simplices with same diameter by lexicographic vertex order

# Topology of viral evolution



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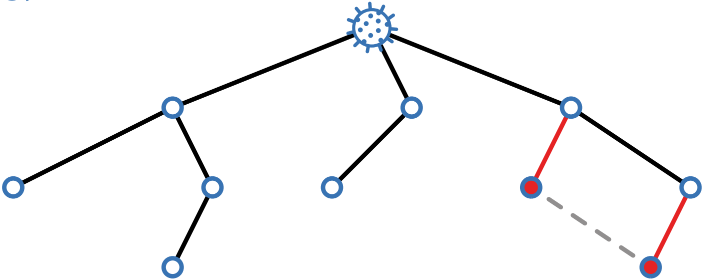

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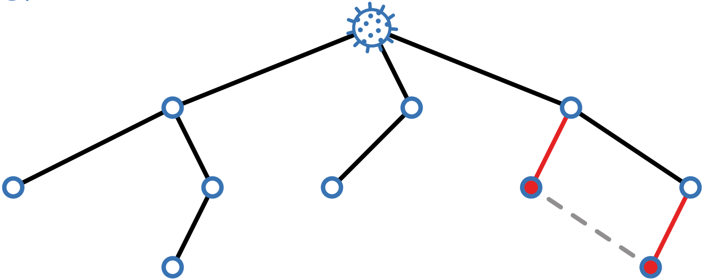

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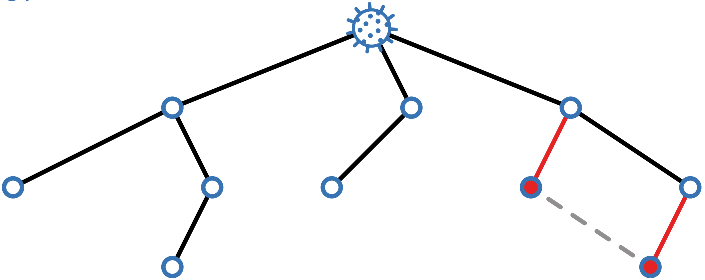

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- $120\,s$ computation time (with data points ordered appropriately)

# The Rips Contractibility Lemma

### Theorem (Rips; Gromov 1988)

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

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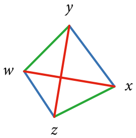
- What about non-geodesic spaces?
- In particular, finite metric spaces?
- Connection to apparent pairs/Ripser?

# Gromov-hyperbolicity

## Definition (Gromov 1988)

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

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



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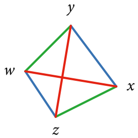


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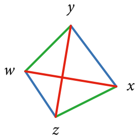



- The hyperbolic plane is $\ln 2$-hyperbolic

- $0$-hyperbolic spaces are subspaces of trees

# Rips contractibility for non-geodesic spaces

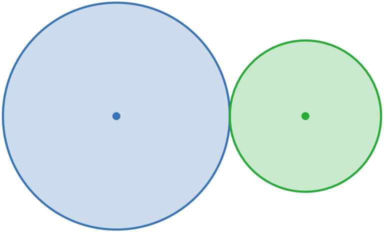
### Theorem (B, Roll 2022)

*Let $X$ be a finite $\delta$-hyperbolic space. Then there is a discrete gradient encoding the collapses*

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

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

# Geodesic defect



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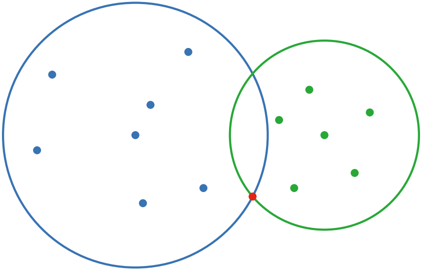

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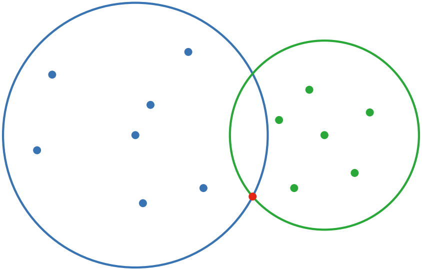

## Definition (Bonk, Schramm 2000)

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

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

The infimum of all such $\nu$ is the *geodesic defect* of $X$.

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$\nu$: geodesic defect of finite $(X, d)$

- lower bound:

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- injective hull (tight span): subspace of $\ell^\infty(X)$

# The tight span of a metric space

Given a metric space $(X, d)$, the *injective hull* is

$$E(X) = \{f\colon X \to \mathbb{R} \mid f(x) + f(y) \geq d(x,y), f(x) = \sup_{y \in X}(d(x,y) - f(y))\},$$

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- contractible [Isbell 1962]

# Density of Kuratowski embedding

## Theorem (Lang 2013 + $\epsilon$)

*Let $X$ be a $\delta$-hyperbolic $\nu$-geodesic metric space. Then the injective hull $E(X)$ is $\delta$-hyperbolic, and every point in $E(X)$ has distance at most $2\delta + \nu$ to $e(X)$.*

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- $E(X) \simeq \{*\}$ (contractibility) □

# Collapsing Vietoris–Rips complexes of generic trees

Consider a *generic* finite metric tree $T = (V, E)$ (distinct distances).

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## Corollary (B, Roll 2022)

*The discrete gradient induces collapses*

$$\operatorname{Rips}_t(X) \searrow T_t \qquad \textit{for all } t \in \mathbb{R}, \textit{ with}$$

$$\operatorname{Rips}_t(X) \searrow T \searrow \{*\} \qquad \textit{for all } t \geq \max l(E), \textit{ and}$$

$$\operatorname{Rips}_u(X) \searrow \operatorname{Rips}_t(X) \qquad \textit{for all } (t, u] \cap l(E) = \varnothing.$$

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

# Arbitrary tree metrics

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- non-generic tree metric
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There is still a compatible gradient:

- independent of choices (*canonical gradient*)
- for generic trees: equals the $\mathrm{diam}$ gradient
- only $V, E$ critical
- induces the same collapses

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Tie breaking for non-distinct pairwise distances:

- Choose total order on vertices
- Order edges lexicographically
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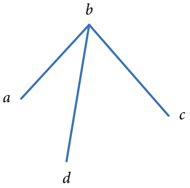

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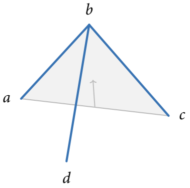

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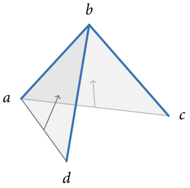

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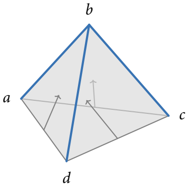

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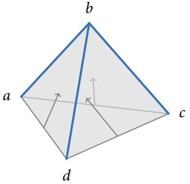


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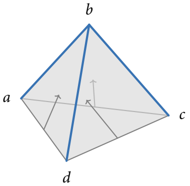


- The canonical gradient (from the previous slide) refines the perturbed gradient (for any choice of total order)
- Hence, the perturbed gradient induces the same collapses

# Collapsing Rips complexes of trees with apparent pairs

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

- Choose a root and extend the tree order to a total order.

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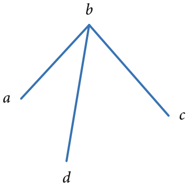
### Theorem (B, Roll 2022)

*The apparent pairs gradient for the resulting filtration order has critical simplices only on the tree $T$. It induces 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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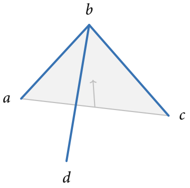

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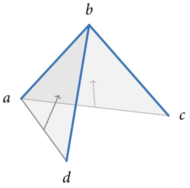

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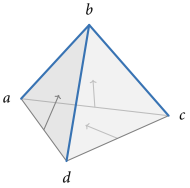

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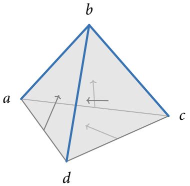

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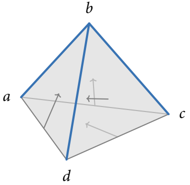

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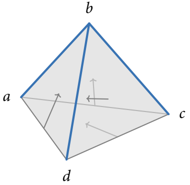


- Explains why Ripser is very fast on genetic distances (tree-like)

U. Bauer, M. Kerber, F. Roll, and A. Rolle

A Unified View on the Functorial Nerve Theorem and its Variations

Preprint, arXiv:2203.03571, 2022

U. Bauer, H. Edelsbrunner

The Morse Theory of Čech and Delaunay Complexes

*Transactions of the AMS*, 2017.

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Induced matchings and the algebraic stability of persistence barcodes

*Journal of Computational Geometry*, 2015.

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Gromov hyperbolicity, geodesic defect, and apparent pairs in Vietoris-Rips filtrations

*Symposium on Computational Geometry*, 2022.

U. Bauer

Ripser: efficient computation of Vietoris–Rips persistence barcodes

*Jounal of Applied and Computational Topology*, 2021