Bridging Morse theory and persistent homology of geometric complexes

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TUM

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DFG Deutsche Forschungsgemeinschaft German Research Foundation

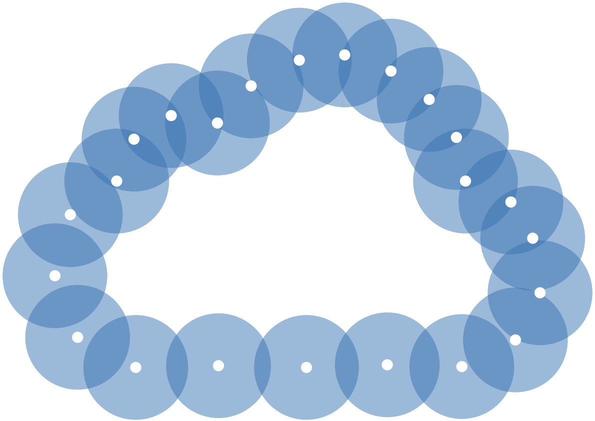
SFB TRR 109 Discretization in Geometry and Dynamics

Technische Universität München

MDSI

Munich Center for Machine Learning

Čech complexes



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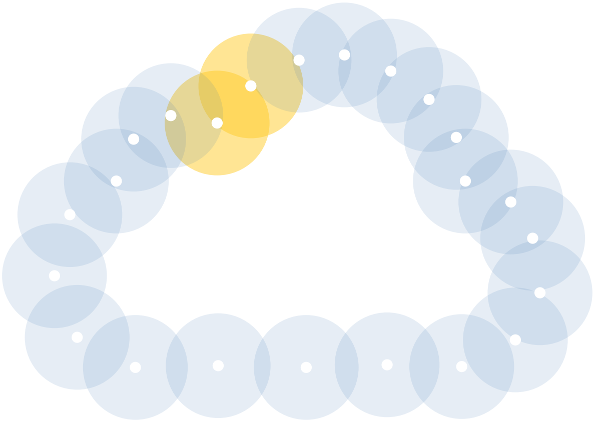

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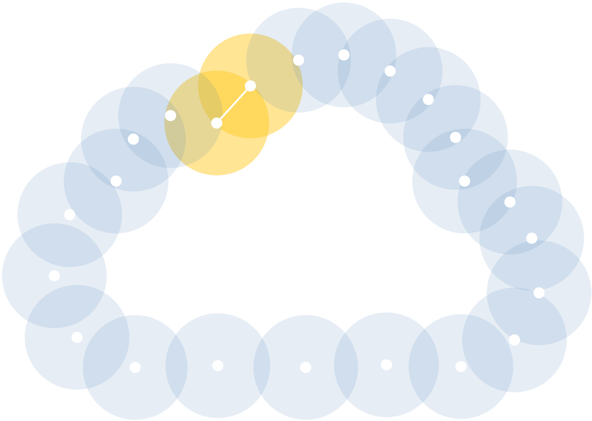

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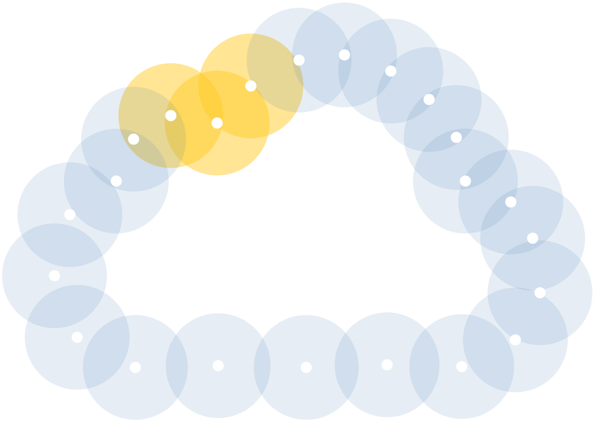

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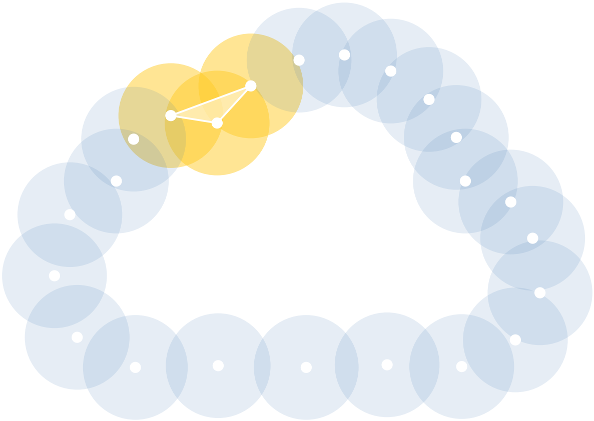

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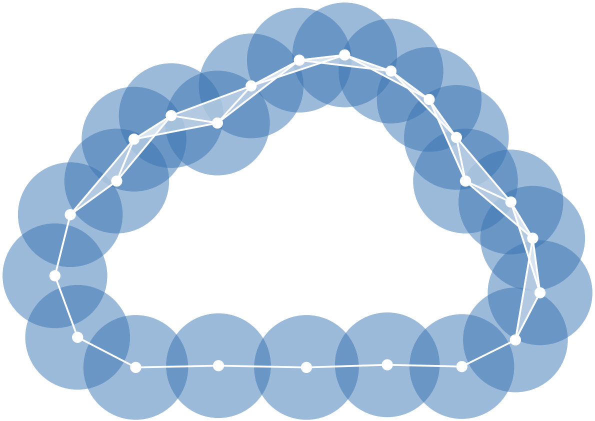

Nerves

Definition (Alexandrov 1928)

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

$$\mathrm{Nrv}(\mathcal{U}) = \{J \subseteq I \mid 0 < |J| < \infty \text{ and } \bigcap_{i \in J} U_i \neq \varnothing\}$$

recording the nonempty intersections of cover elements.

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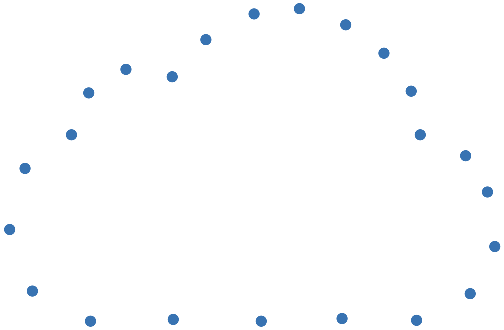
U. Bauer, M. Kerber, F. Roll, and A. Rolle
A Unified View on the Functorial Nerve Theorem and its Variations
Expositiones Mathematicae, 2023. doi:10.1016/j.exmath.2023.04.005

Delaunay complexes



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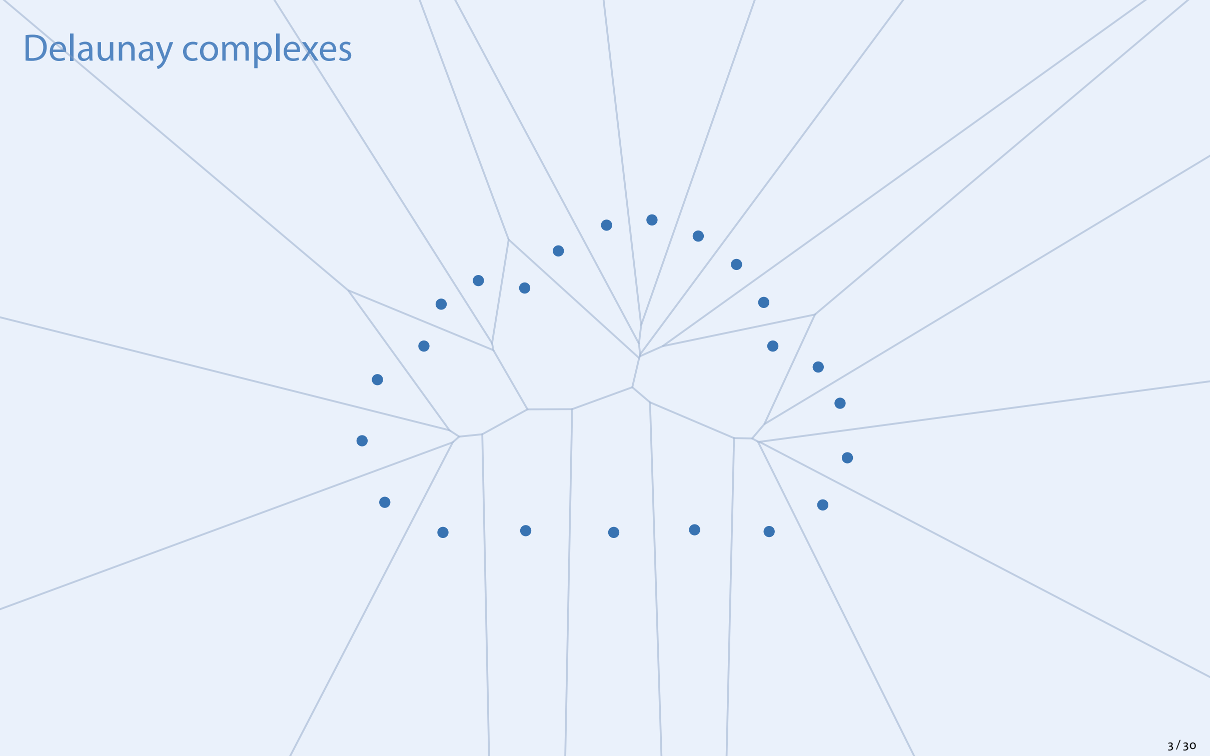

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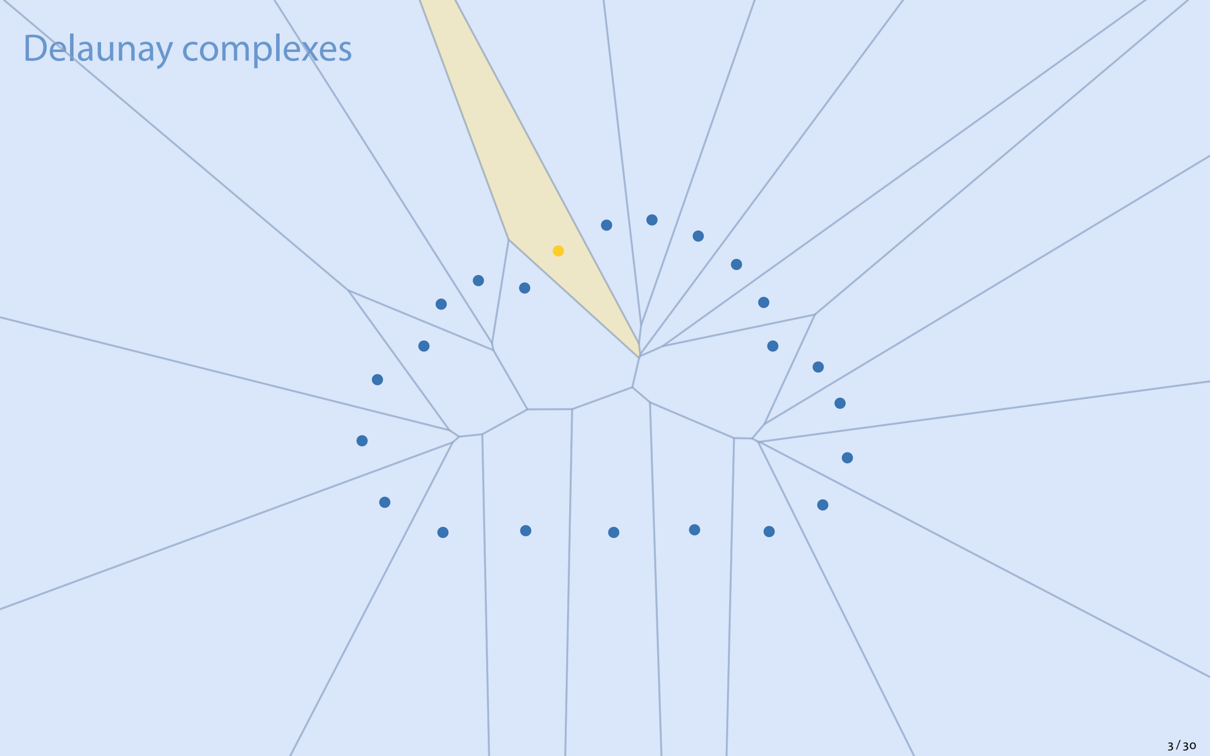

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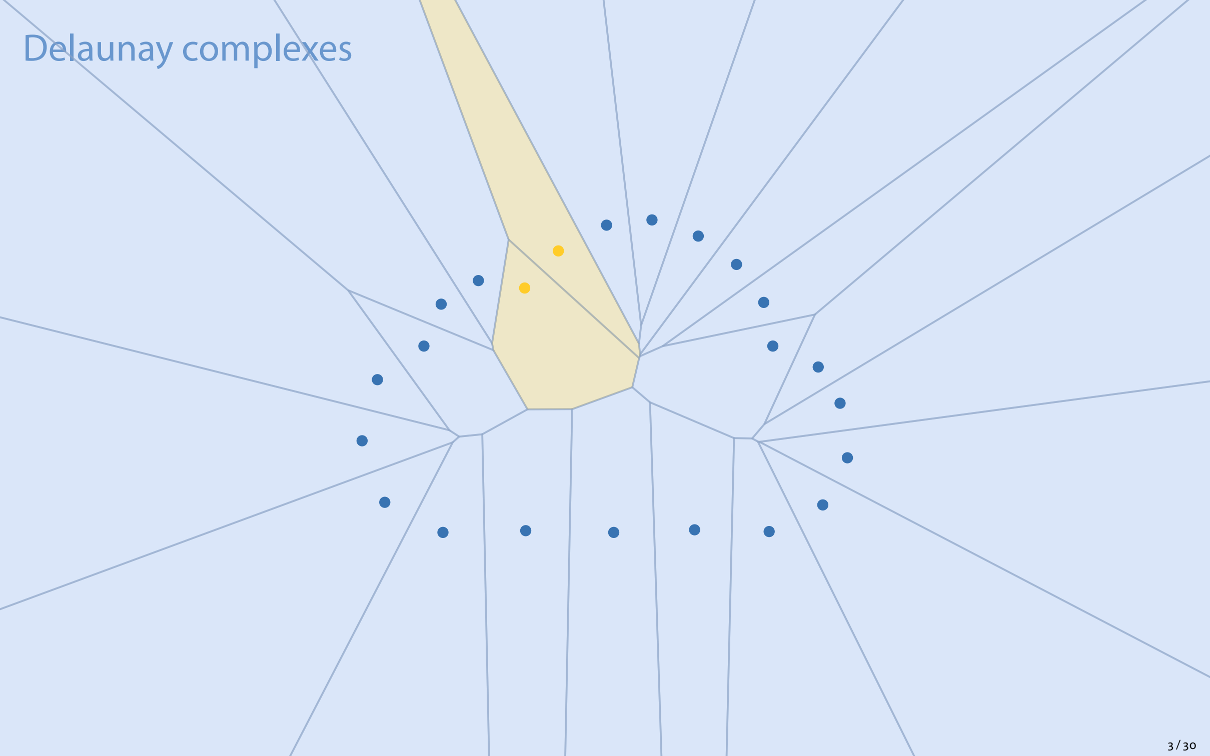

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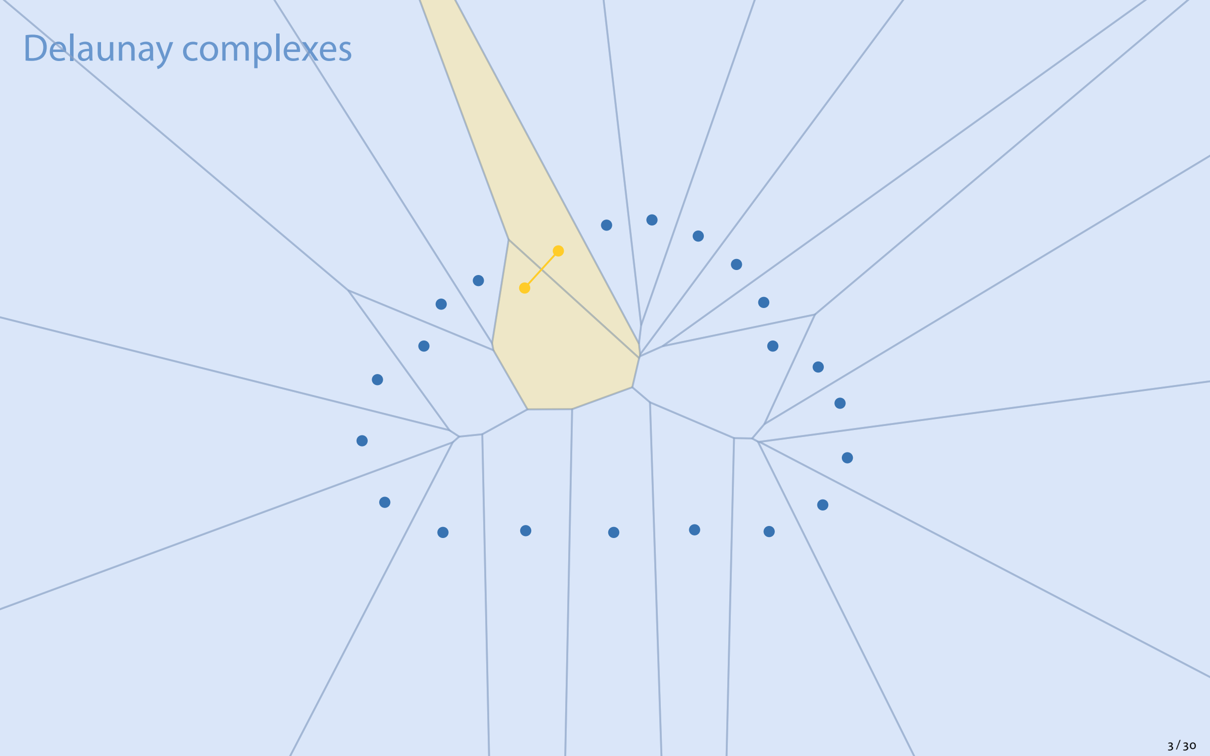

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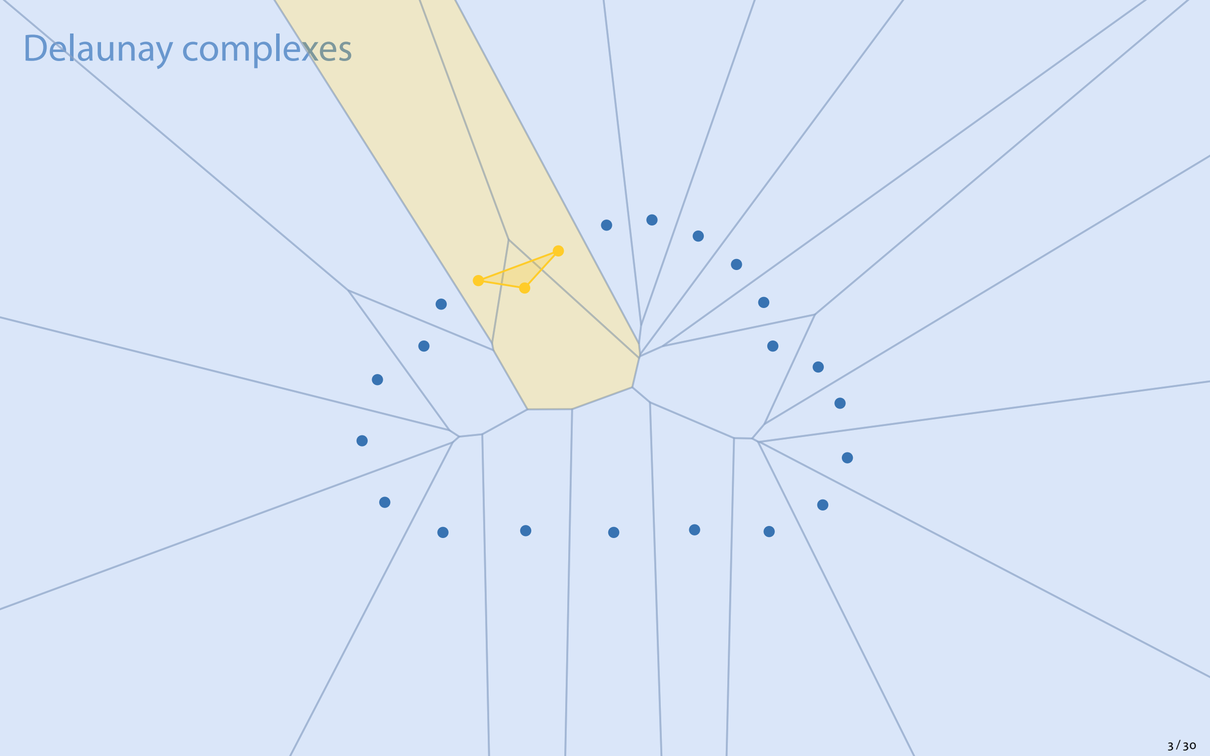

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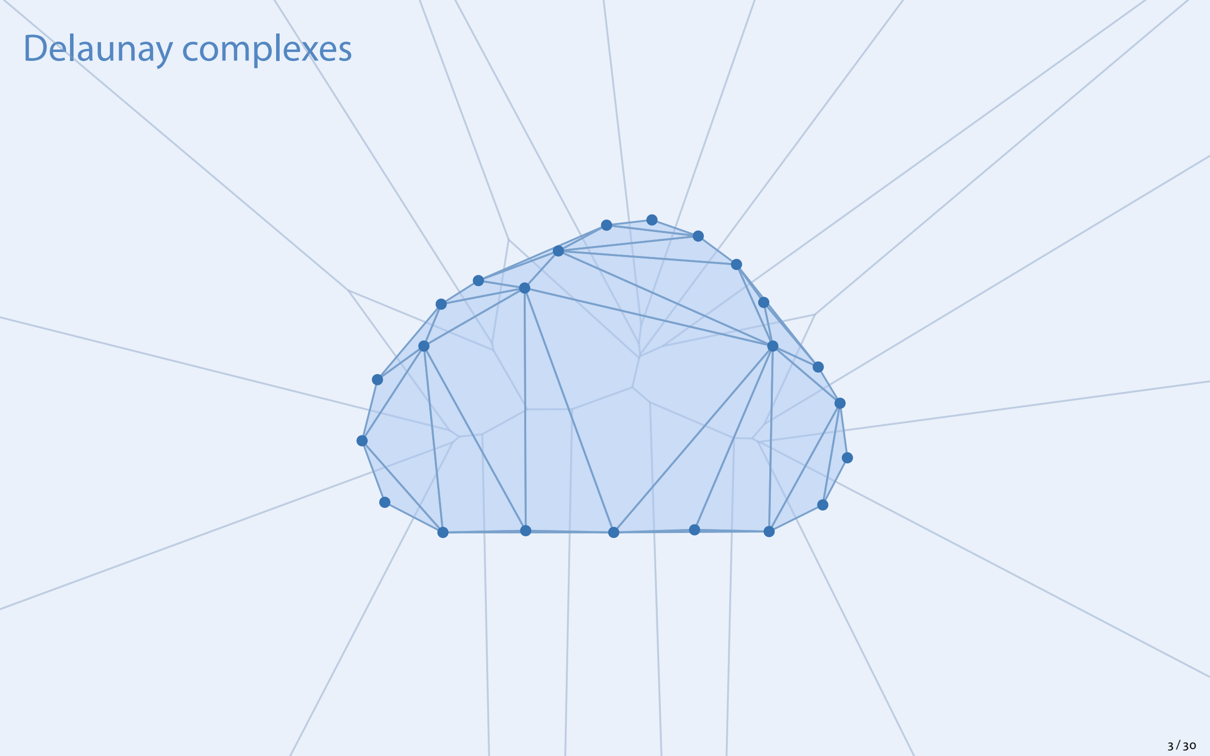

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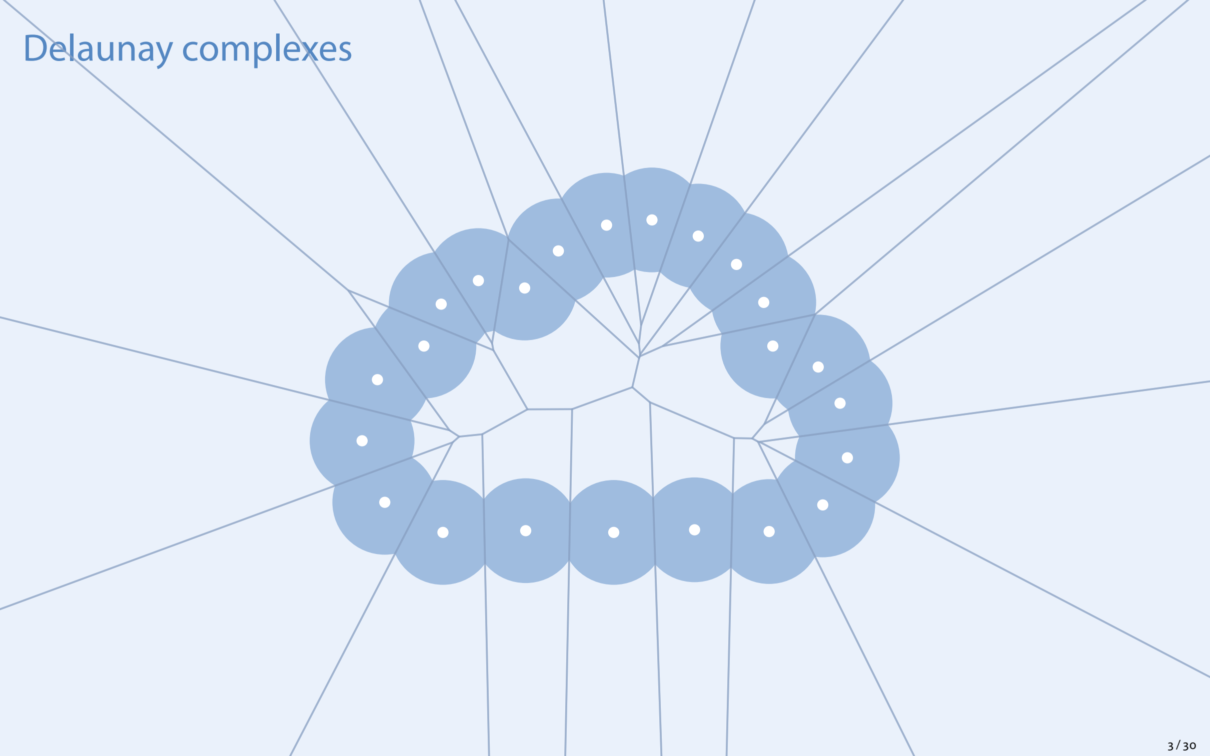

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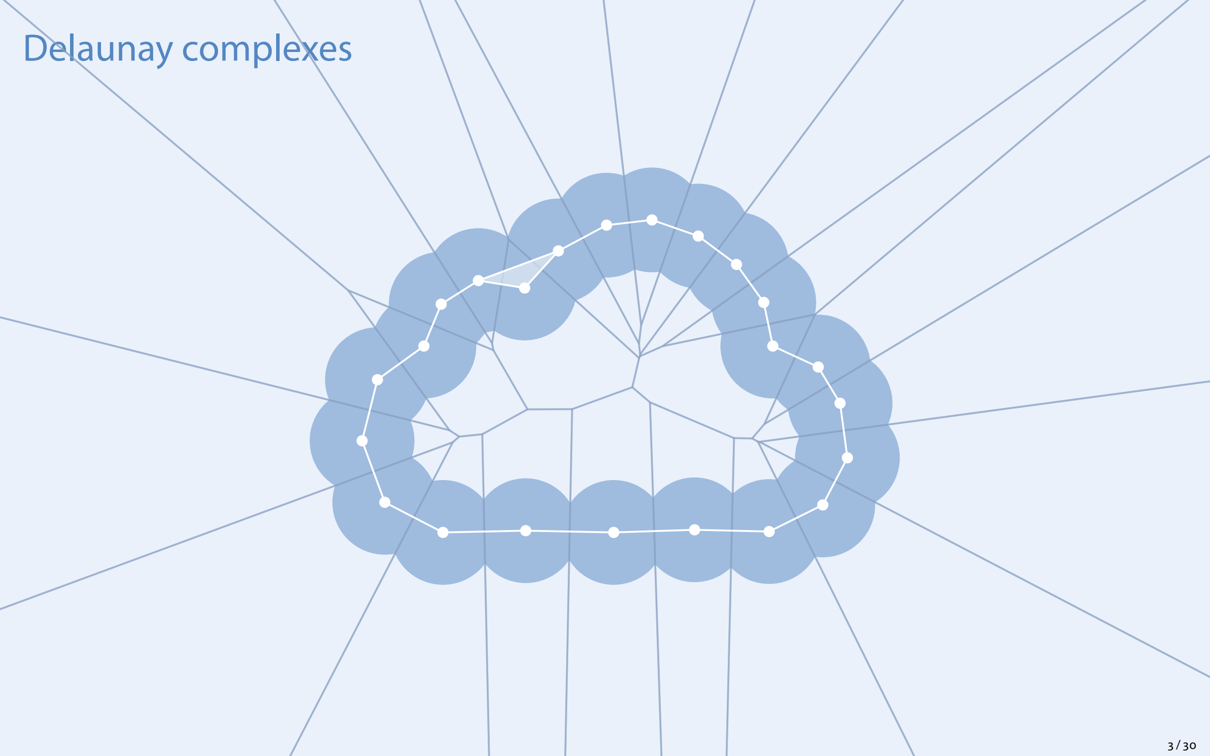
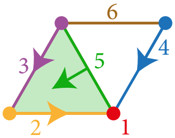


Discrete Morse theory



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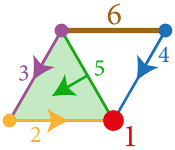

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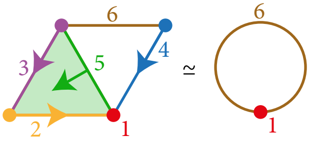
Theorem (Forman 1998)

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



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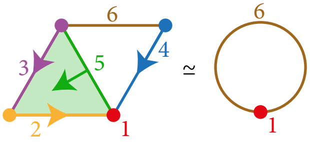
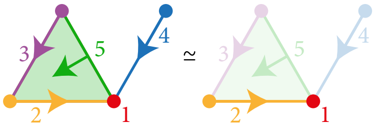


Discrete Morse functions – and their gradients – encode collapses of sublevel sets:



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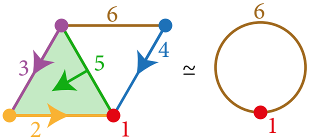

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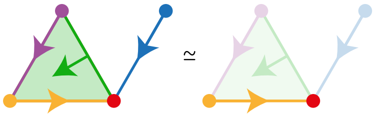
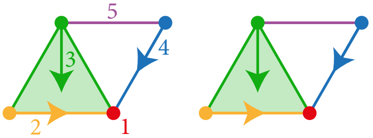


Generalizing discrete Morse theory

Generalized gradients consist of 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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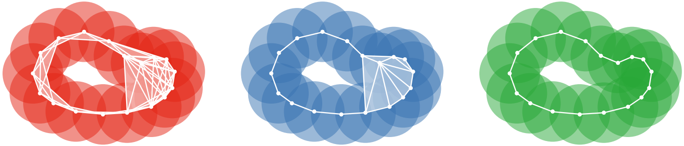
Theorem (B., Edelsbrunner 2017)

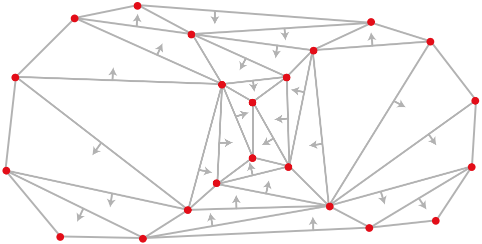
Čech, Delaunay, and Wrap complexes (at any scale r) are related by collapses encoded by a single discrete gradient field:

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



Wrap complexes

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



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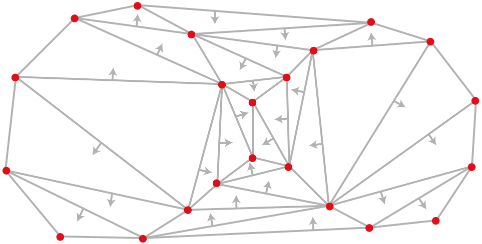

Definition (Edelsbrunner 1995; B, Edelsbrunner 2017)

$\mathrm{Wrap}_r(X)$ 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 a union of intervals of V.

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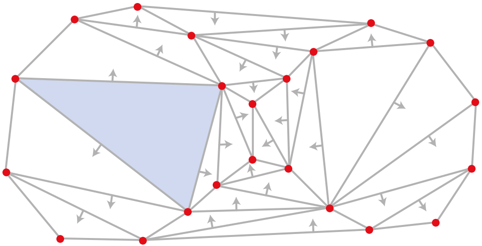

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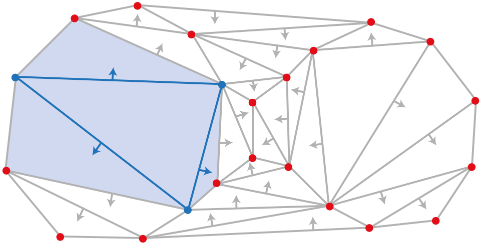

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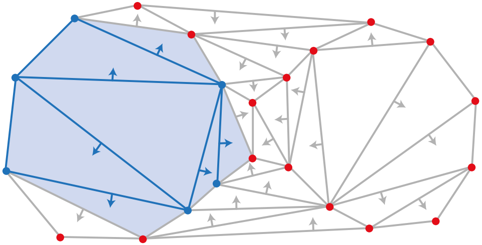

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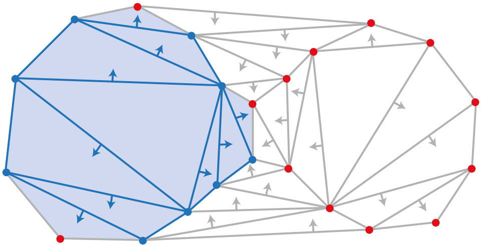

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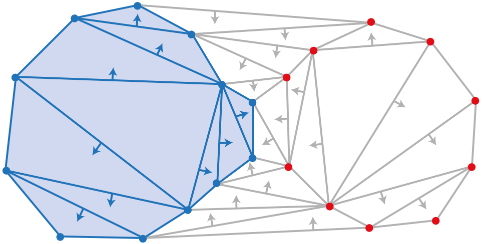

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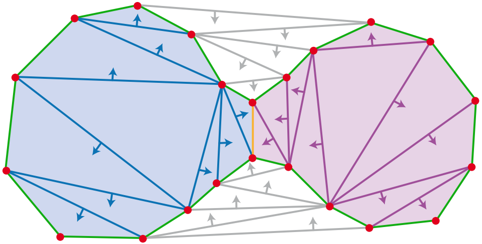

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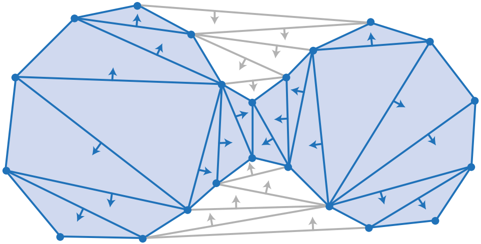

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Delaunay and Wrap complexes

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Vietoris–Rips complexes

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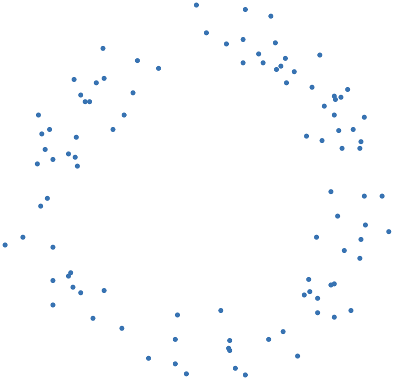
$$\mathrm{Rips}_t(X) = \{S \subseteq X \mid S \neq \varnothing \text{ finite}, \operatorname{diam} S \leq t\}.$$



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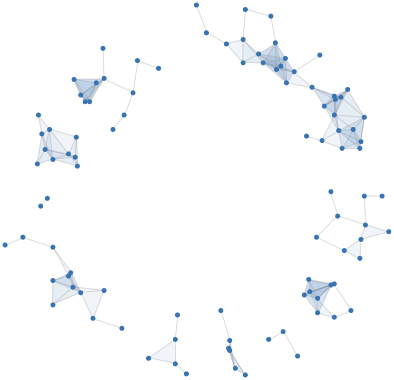

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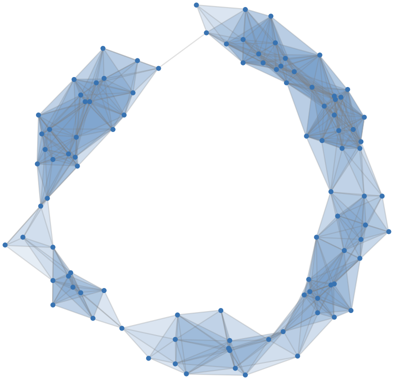

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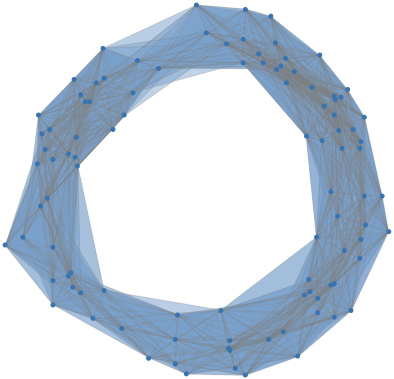

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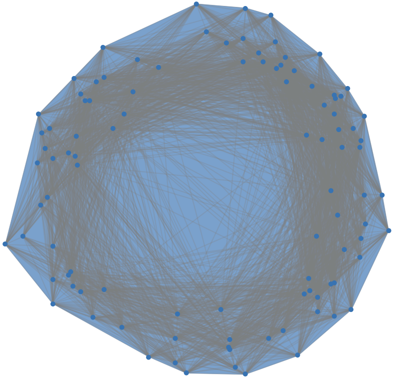
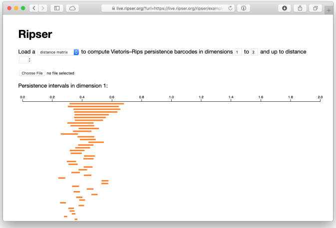
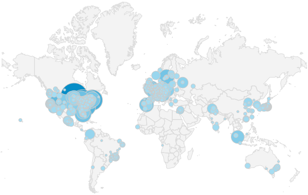


Ripser: software for computing Vietoris–Rips persistence barcodes

Open source software (`ripser.org`)

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





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 $(K_i = \{\sigma_1, \dots, \sigma_i\})_i$, two simplices (σ_i, σ_j) form an *apparent pair* if

- σ_i is the latest proper face of σ_j, and
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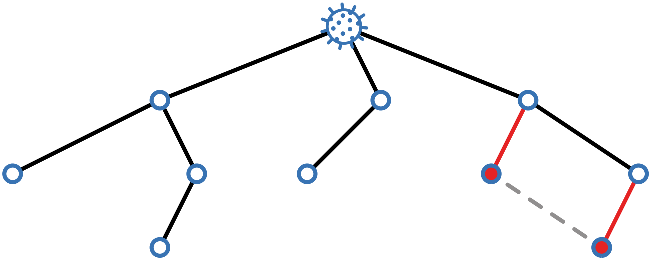
Proposition (B 2021)

The apparent pairs are both gradient pairs and persistence pairs.

Proposition (B, Roll 2022)

Consider a generalized discrete Morse function f, and the simplexwise filtration from lexicographic refinement. Then the zero-persistence apparent pairs form a gradient that refines the gradient of f.

Topology of viral evolution



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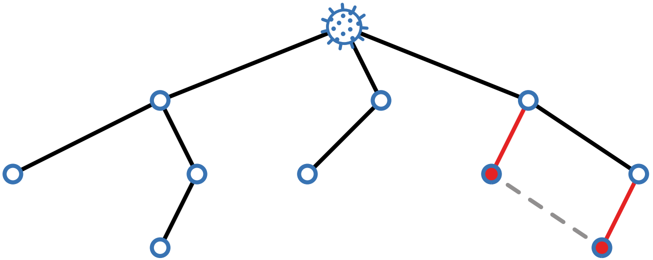

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Observation: Ripser runs unusually fast on genetic distance data

- 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)

The Rips Contractibility Lemma

Theorem (Rips; Gromov 1988)

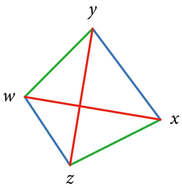
Let X be a δ-hyperbolic geodesic metric space. Then $\mathrm{Rips}_t(X)$ is contractible for all $t \geq 4\delta$.

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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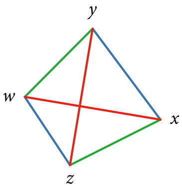

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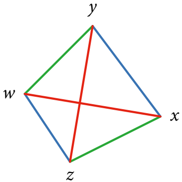
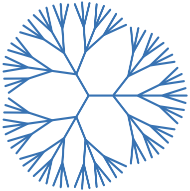


- The hyperbolic plane is $(\ln 2)$-hyperbolic.

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



Rips contractibility for non-geodesic spaces

- What about non-geodesic spaces? In particular, finite metric spaces?
- What about collapsiblility?
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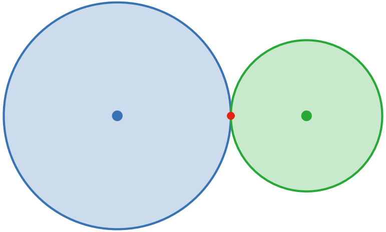
Theorem (B, Roll 2022)

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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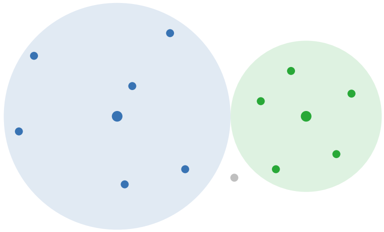

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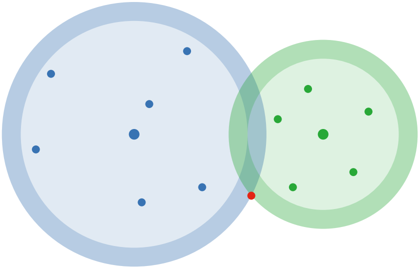

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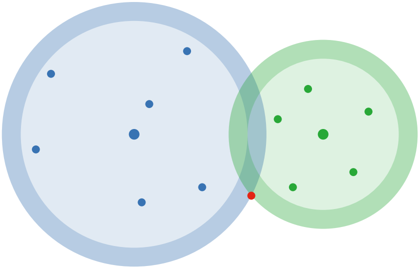

Definition (Bonk, Schramm 2000)

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.*

Collapsing Vietoris–Rips complexes of generic trees

Theorem (B, Roll 2022)

The discrete gradient of the diameter function for a generic tree metric space X induces the collapses

$$\begin{aligned} \mathrm{Rips}_t(X) &\searrow T_t && \textit{for all } t \in \mathbb{R}, \textit{ with} \\ \mathrm{Rips}_t(X) &\searrow T \searrow \{*\} && \textit{for } t \geq \max l(E), \textit{ and} \\ \mathrm{Rips}_u(X) &\searrow \mathrm{Rips}_t(X) && \textit{whenever } (t,u] \cap l(E) = \varnothing. \end{aligned}$$

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

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Example: phylogenetic trees

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- The apparent gradient in turn refines the perturbed gradient (for a suitable vertex ordering).

Collapsing Rips complexes of trees with apparent pairs

Consider the metric space X given by the path length metric on a weighted finite tree $T = (V, E)$.

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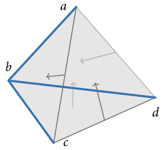

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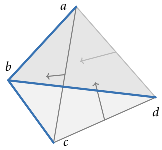

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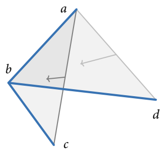

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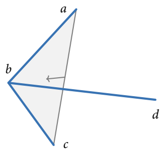

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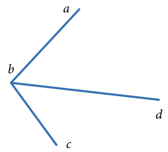

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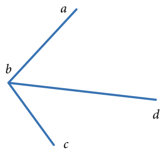
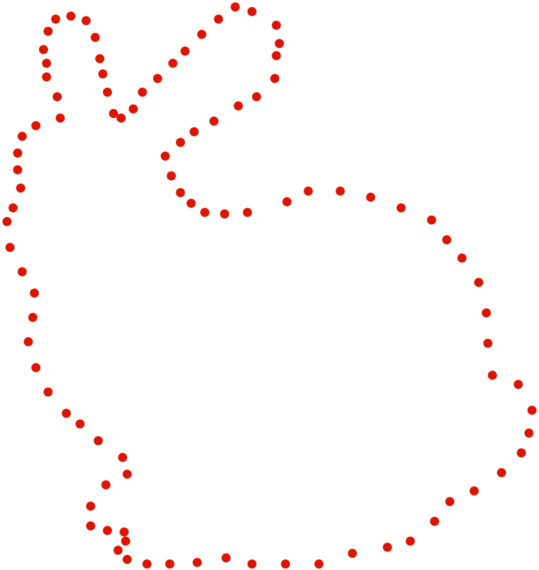


- Explains why Ripser is extraordinarily fast on genetic distances (tree-like)

Wrap complexes and lexicographically minimal cycles



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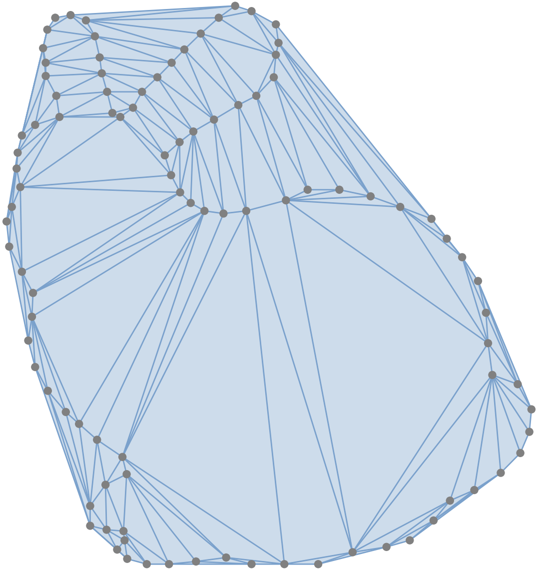

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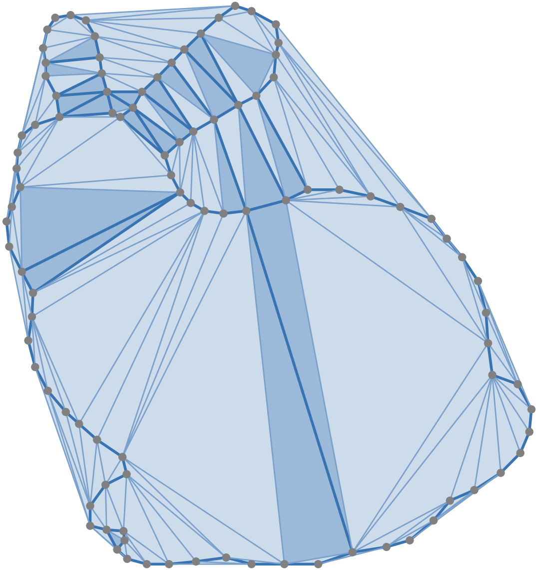

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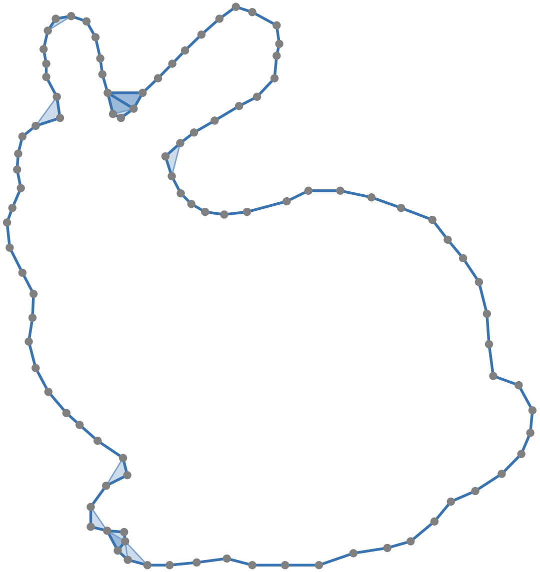

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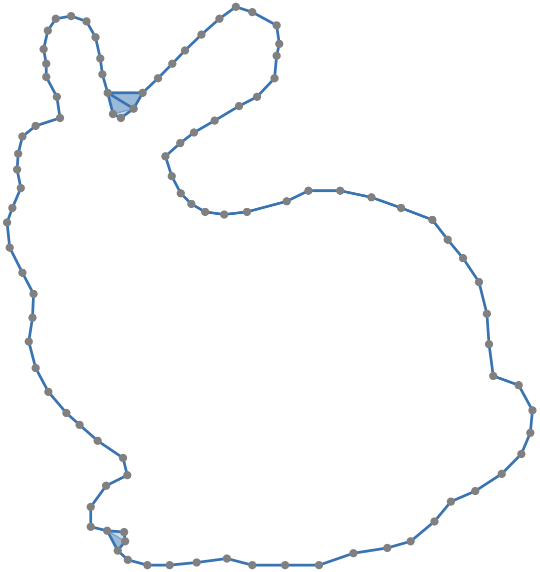

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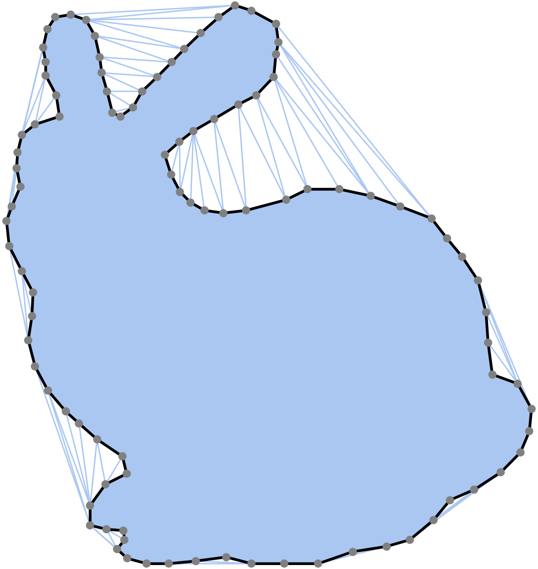

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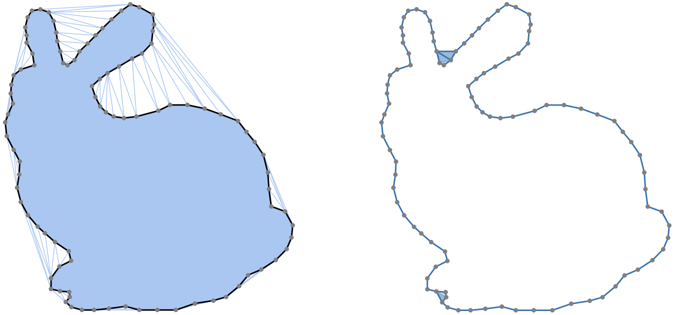
- The resulting representative cycles are lexicographically minimal

Minimal cycles and 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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Definition

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- All further definitions of discrete Morse theory apply verbatim

Algebraic gradients from persistent homology

Let $R = D \cdot V$ be the result of exhaustive reduction of the boundary matrix D (for the Delaunay filtration, breaking ties lexicographically).

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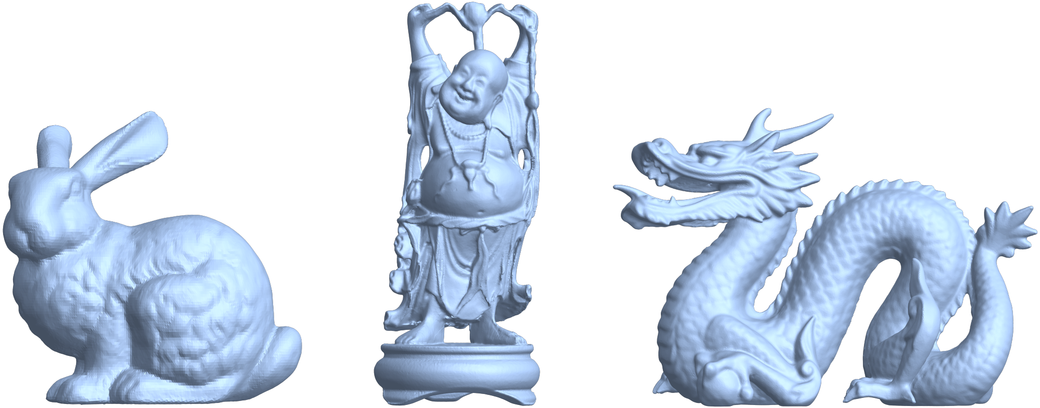
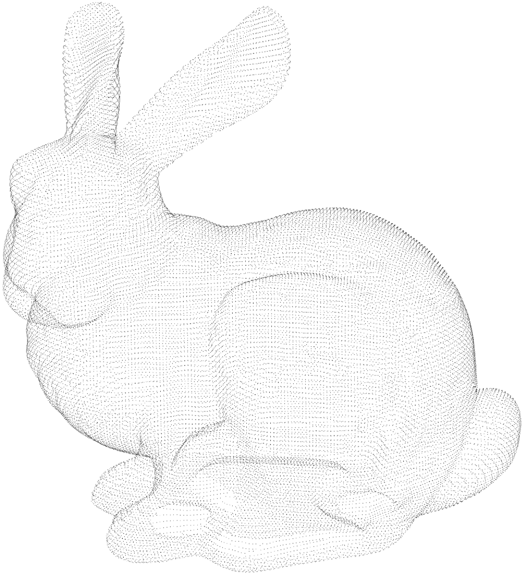
  - Thus, the minimal cycles are also supported on the Wrap complex.

Point cloud reconstruction with lexicographically minimal cycles



Computing minimal cycles with exhaustive reduction



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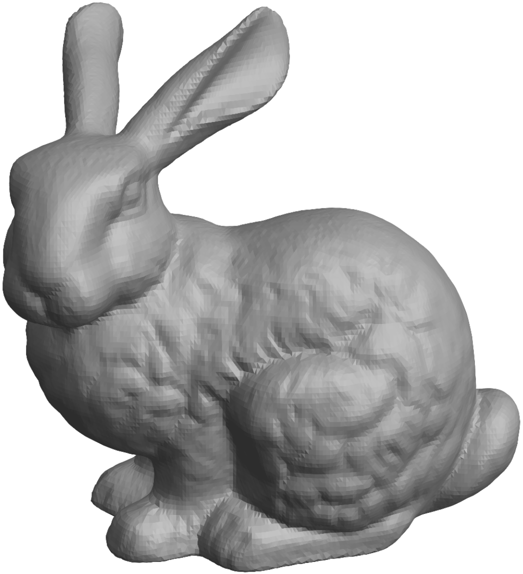
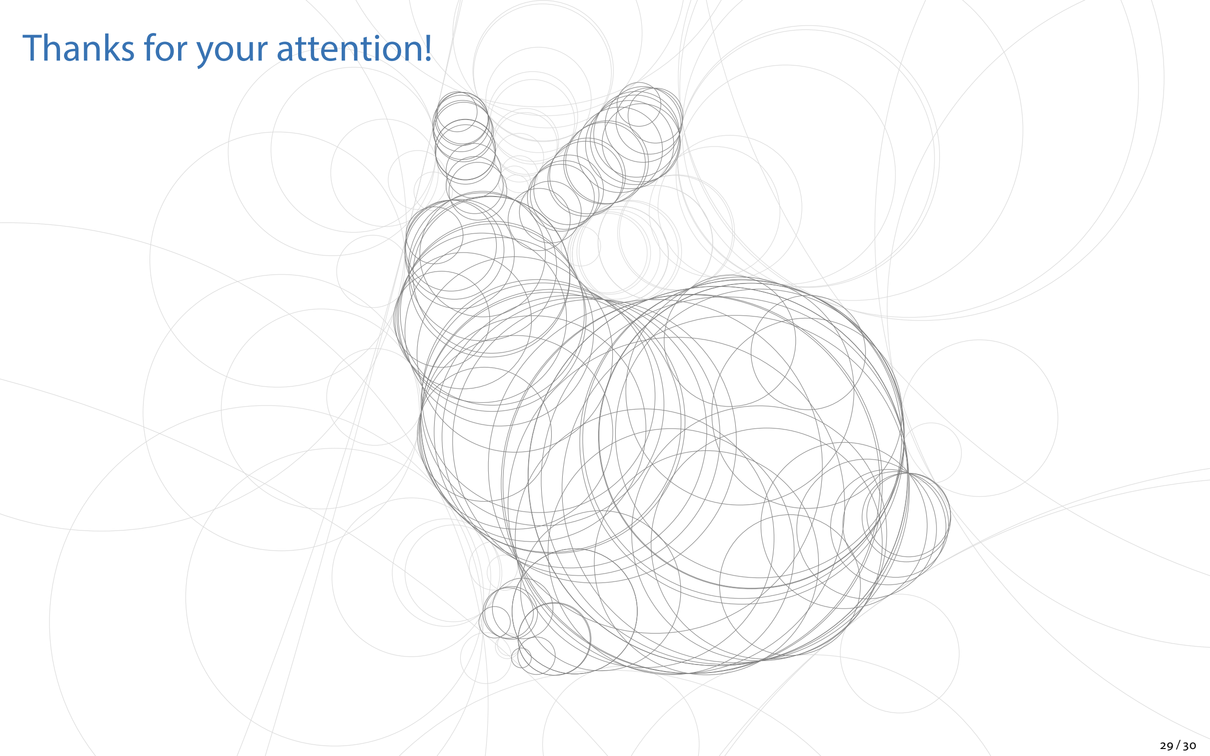


Thanks for your attention!



Further reading

U. Bauer, F. Roll
Gromov hyperbolicity, geodesic defect, and apparent pairs in Vietoris-Rips filtrations
Symposium on Computational Geometry, 2022. doi:10.4230/LIPIcs.SoCG.2022.15

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Connecting Discrete Morse Theory and Persistence: Wrap Complexes and Lexicographic Optimal Cycles
Preprint, 2022. arXiv:2212.02345

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A Unified View on the Functorial Nerve Theorem and its Variations
Expositiones Mathematicae, 2023. doi:10.1016/j.exmath.2023.04.005

U. Bauer, H. Edelsbrunner
The Morse Theory of Čech and Delaunay Complexes
Transactions of the AMS, 2017. doi:10.1090/tran/6991