Discrete Morse theory and persistence of geometric complexes

Elements of computational geometry & topology

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Technical University of Munich (TUM)

February 26, 2024

Dagstuhl-Seminar 24092 *Applied and Combinatorial Topology*

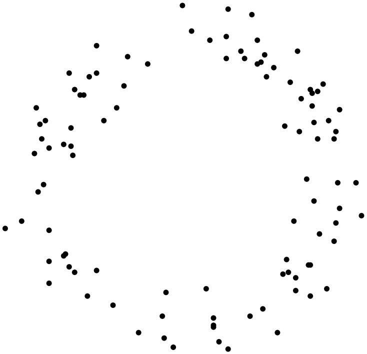
Funded by

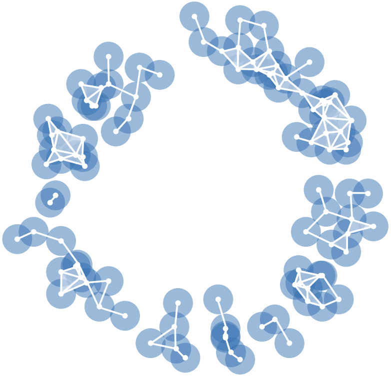
Deutsche Forschungsgemeinschaft
German Research Foundation

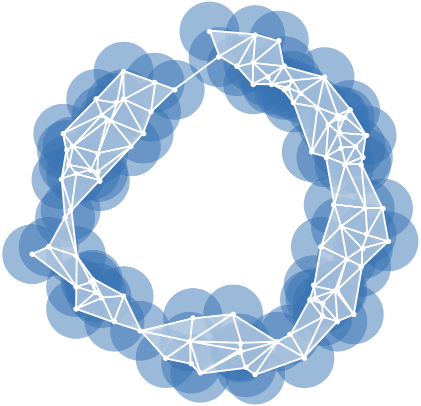
SFB TRR 109 Discretization in Geometry and Dynamics

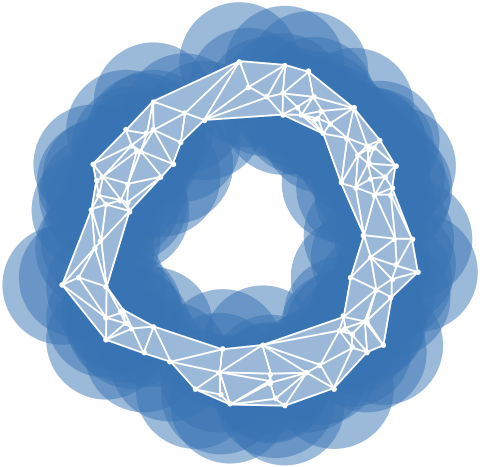
Technical University of Munich

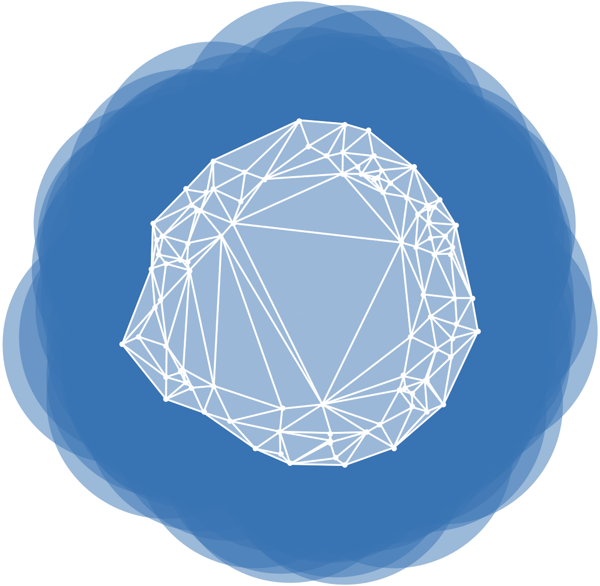
Munich Center for Machine Learning





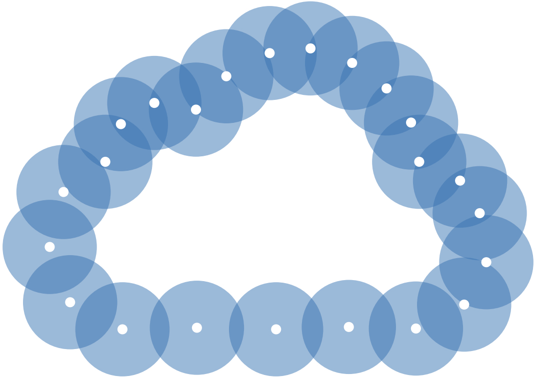






Geometric complexes

Čech complexes



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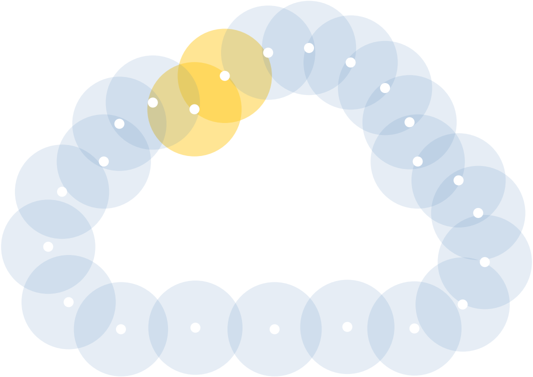

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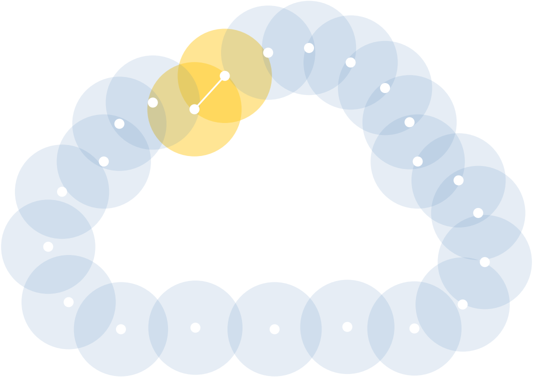

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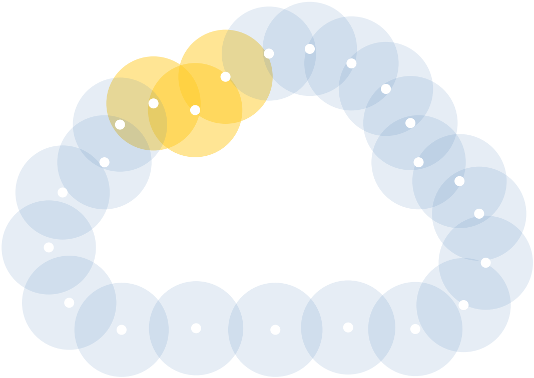

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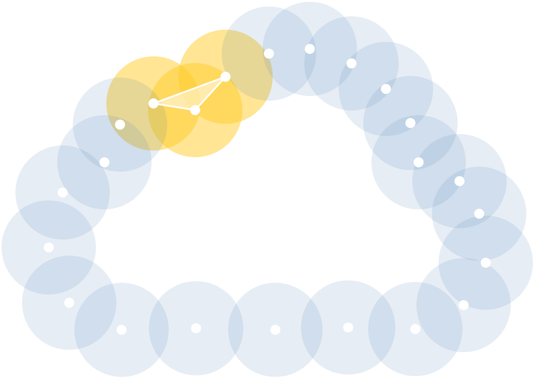

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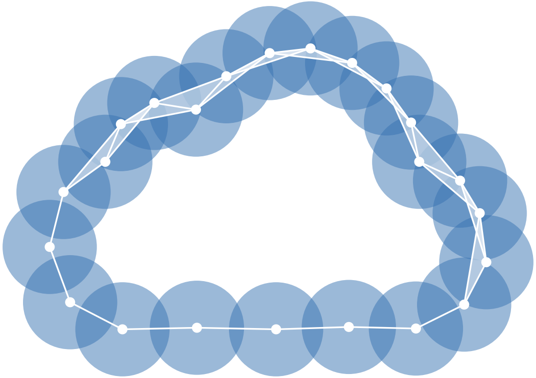

Nerves

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

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

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

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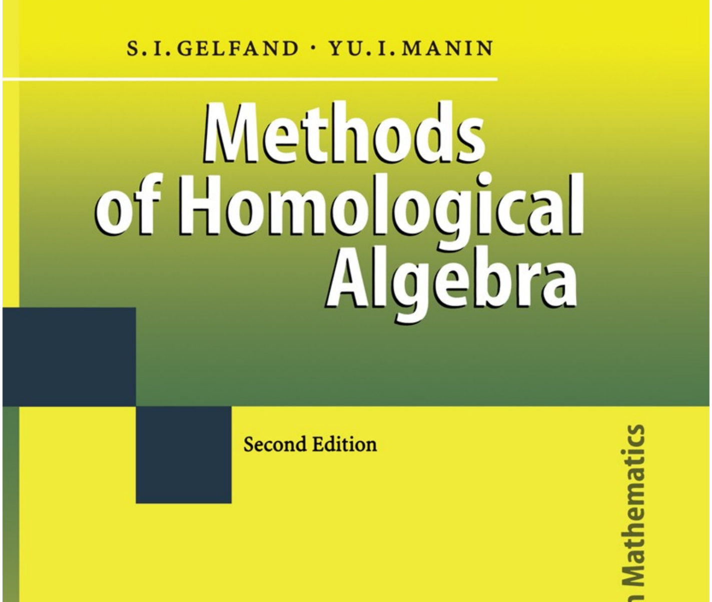


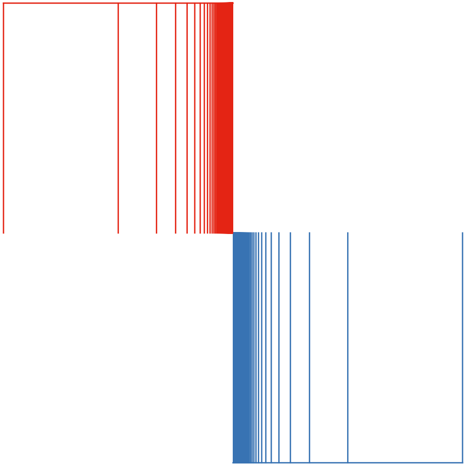
3. Nerve of a Covering

Let Y be a topological space, $U = (U_\alpha)$ be its covering (either by open or by closed sets), α running over some set A. Let

$$X_n = \{(\alpha_0, \ldots, \alpha_n) \,|U_{\alpha_0} \cap \ldots \cap U_{\alpha_n} \neq \emptyset\},$$
$$X(f)\,(\alpha_0, \ldots, \alpha_n) = \left(\alpha_{f(0)}, \ldots, \alpha_{f(m)}\right) \quad \text{for} \quad f : [m] \to [n].$$

This simplicial set reflects the combinatorial structure of a covering. One can show that if the covering U is locally finite and all nonempty finite intersections $U_{\alpha_0} \cap \ldots \cap U_{\alpha_n}$ are contractible, then the geometric realization $|X|$ of X is homotopically equivalent to Y, so that the topology can be efficiently encoded into combinatorical data.

Nerve theorems, almost true



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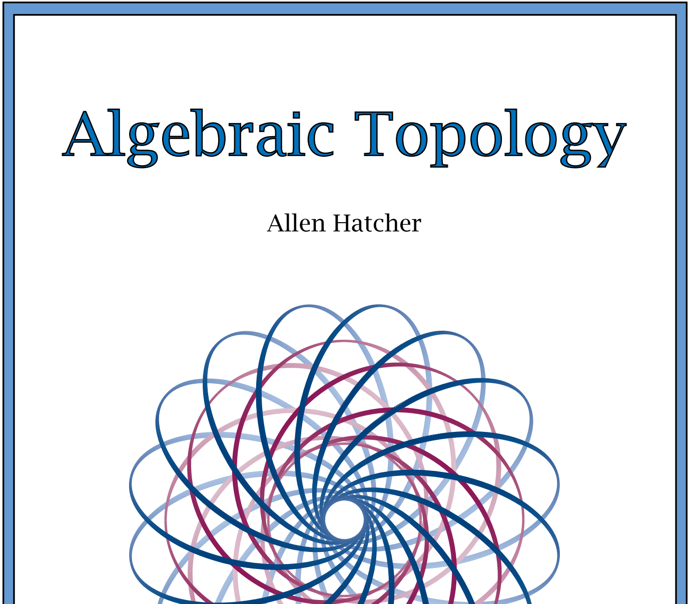
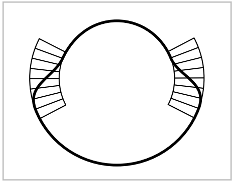


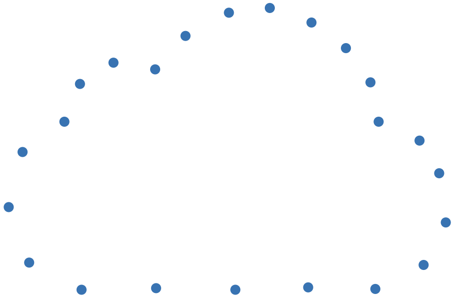
Nerve theorems, almost true

Since X is paracompact there is a partition of unity subordinate to the cover $\mathcal{U}$. This is a family of maps $\varphi_\alpha : X \to [0,1]$ satisfying three conditions: The support of each φ_α is contained in some $X_{i(\alpha)}$, only finitely many φ_α's are nonzero near each point of X, and $\sum_\alpha \varphi_\alpha = 1$. Define a section $s : X \to \Delta X_{\mathcal{U}}$ of p by setting $s(x) = \sum_\alpha \varphi_\alpha(x) x_{i(\alpha)}$. The figure shows the case $X = S^1$ with a cover by two arcs, the heavy line indicating the image of s. In the general case the section s embeds X as a retract of $\Delta X_{\mathcal{U}}$, and it is a deformation retract since points in fibers $p^{-1}(x)$ can move linearly along line segments to $s(x)$. $\square$



Corollary 4G.3. *If $\mathcal{U}$ is an open cover of a paracompact space X such that every nonempty intersection of finitely many sets in $\mathcal{U}$ is contractible, then X is homotopy equivalent to the nerve $N\mathcal{U}$.*

Delaunay complexes



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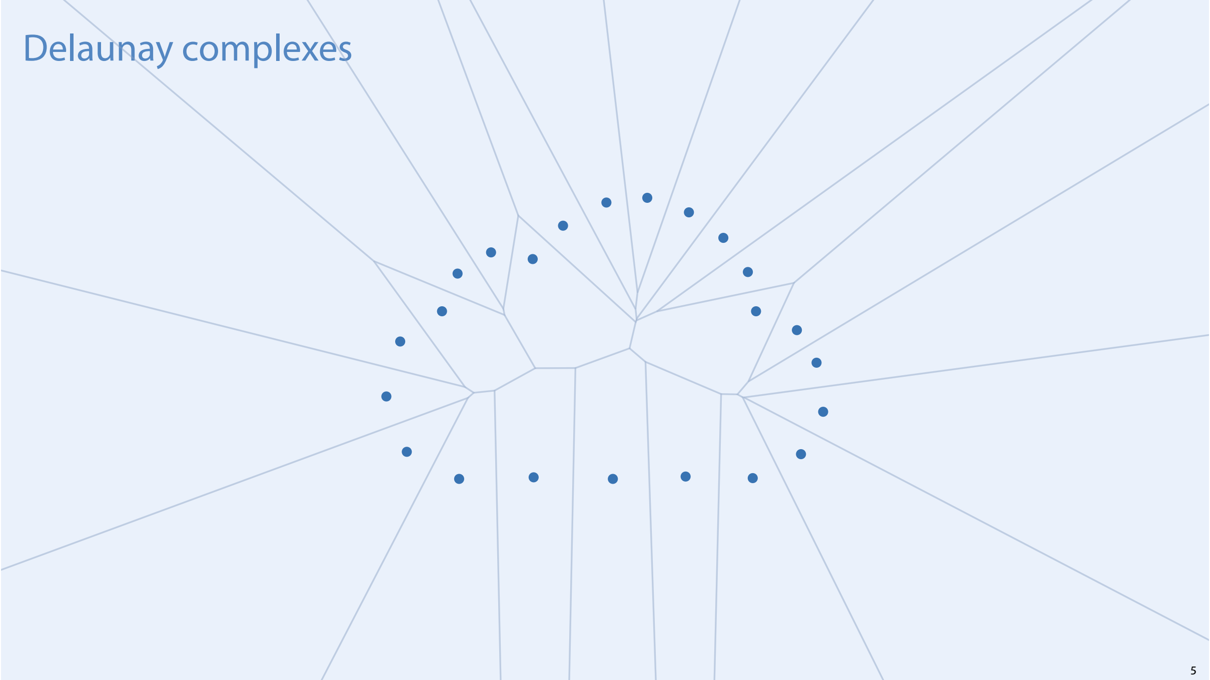

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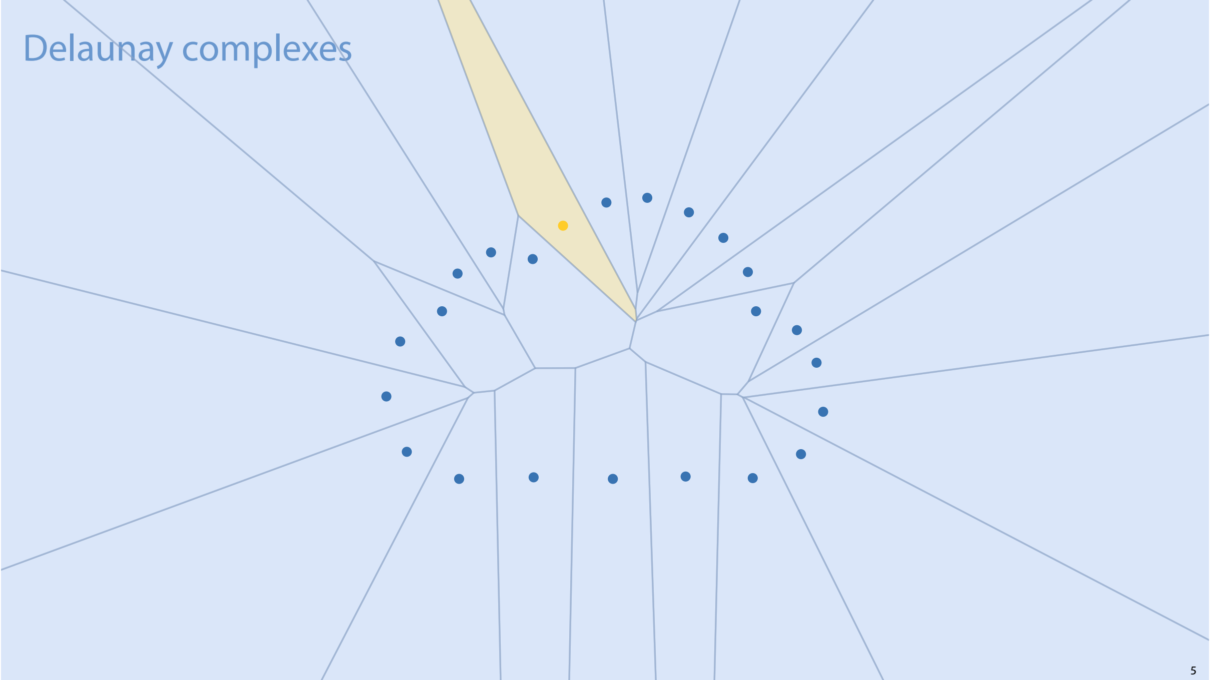

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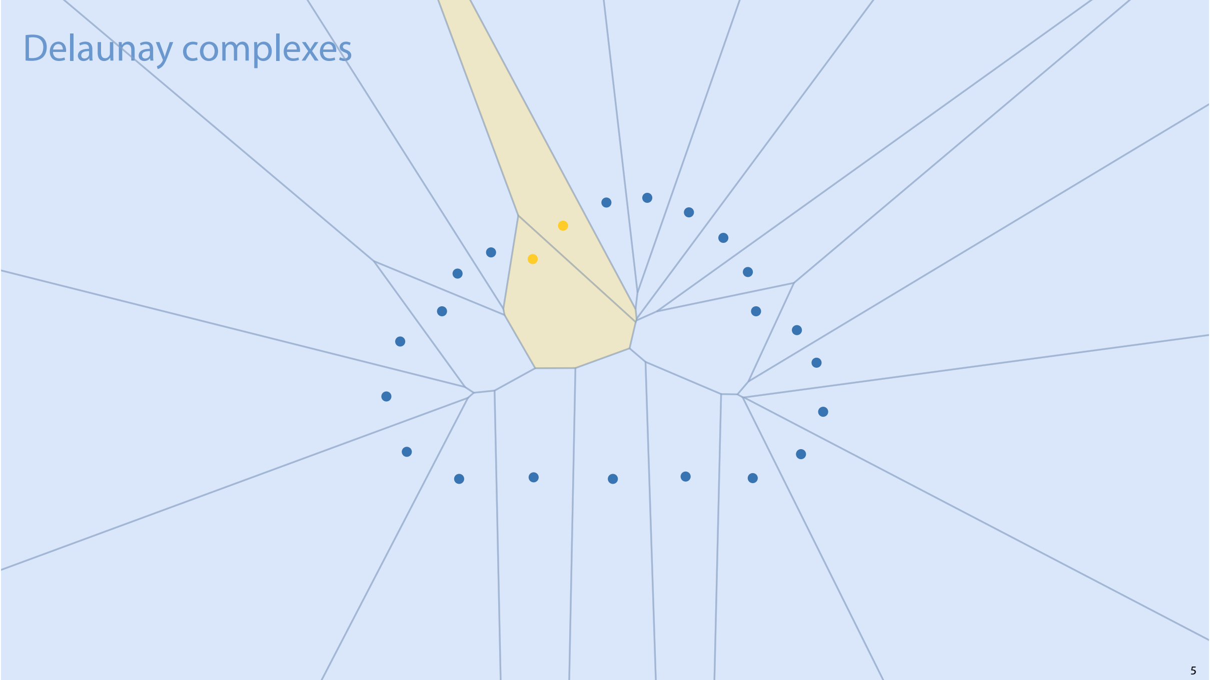

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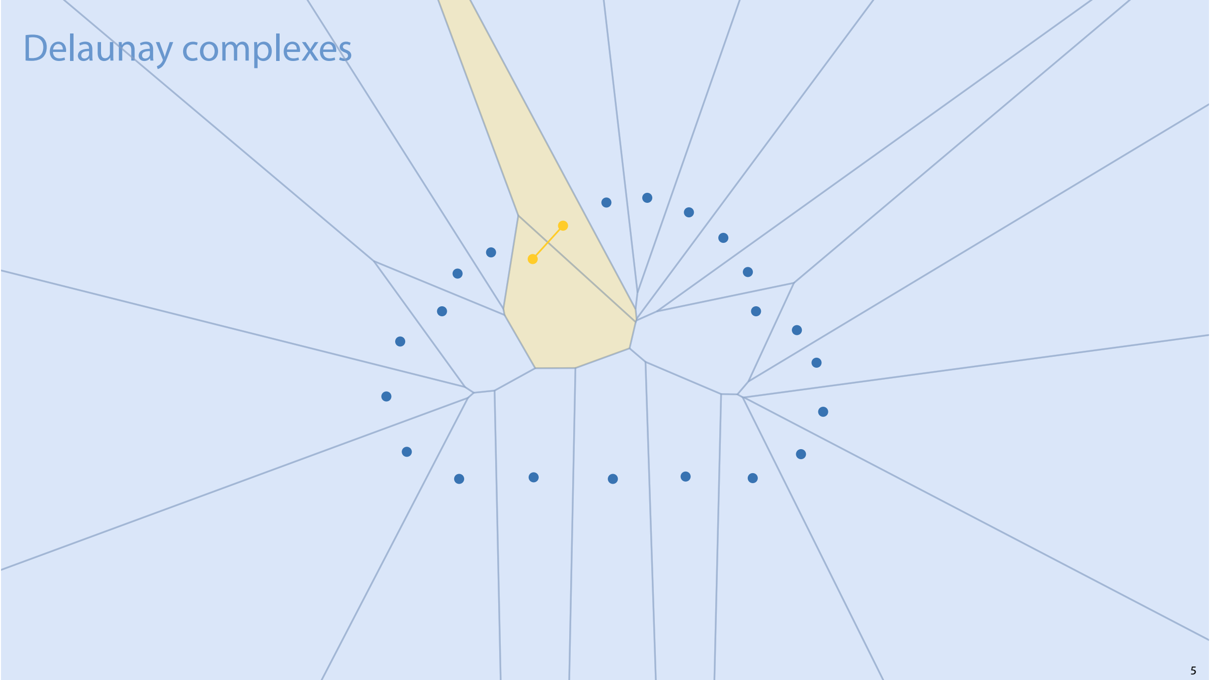

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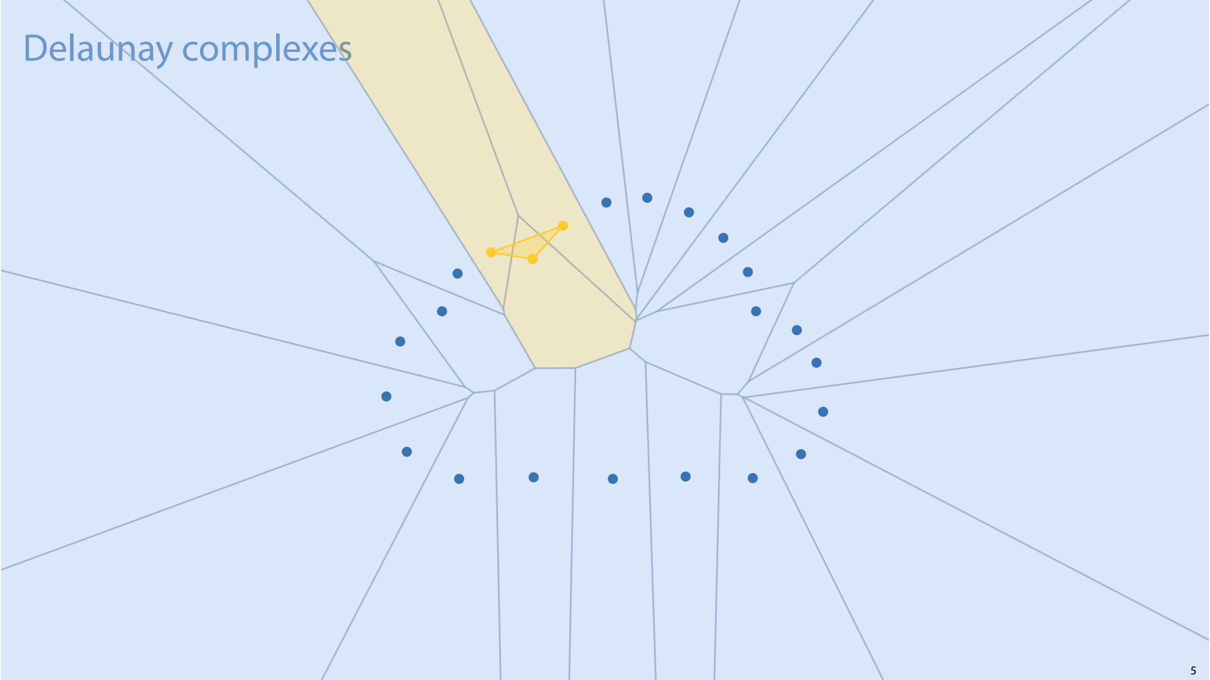

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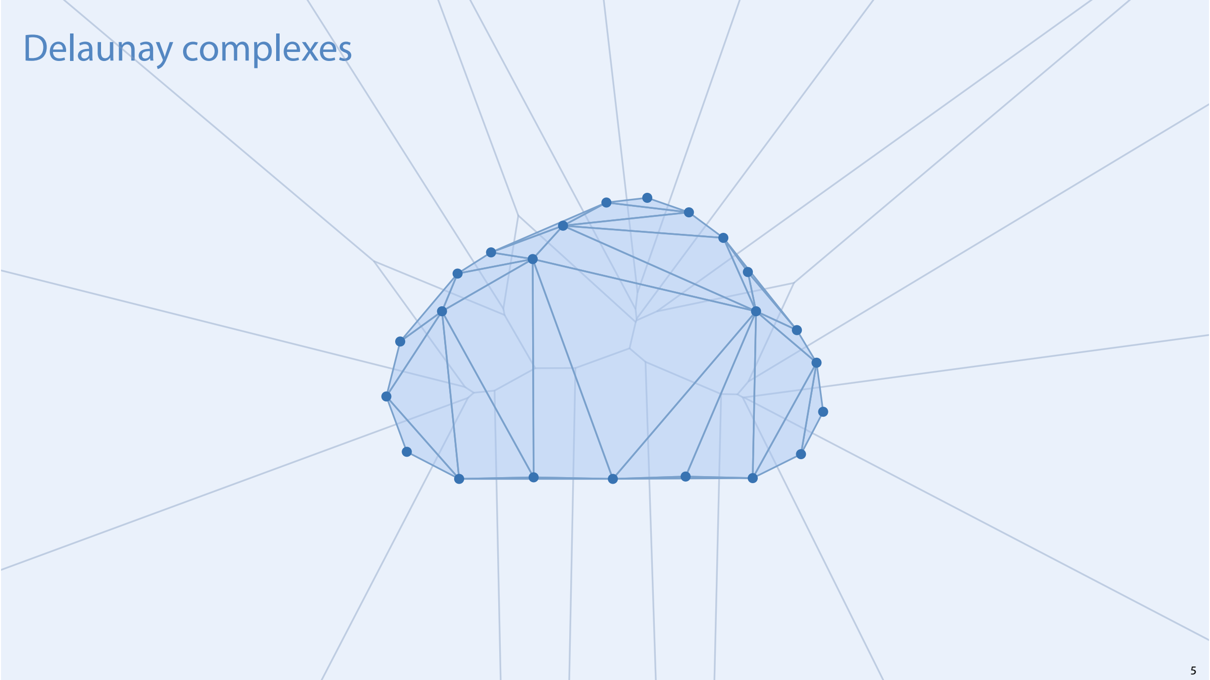

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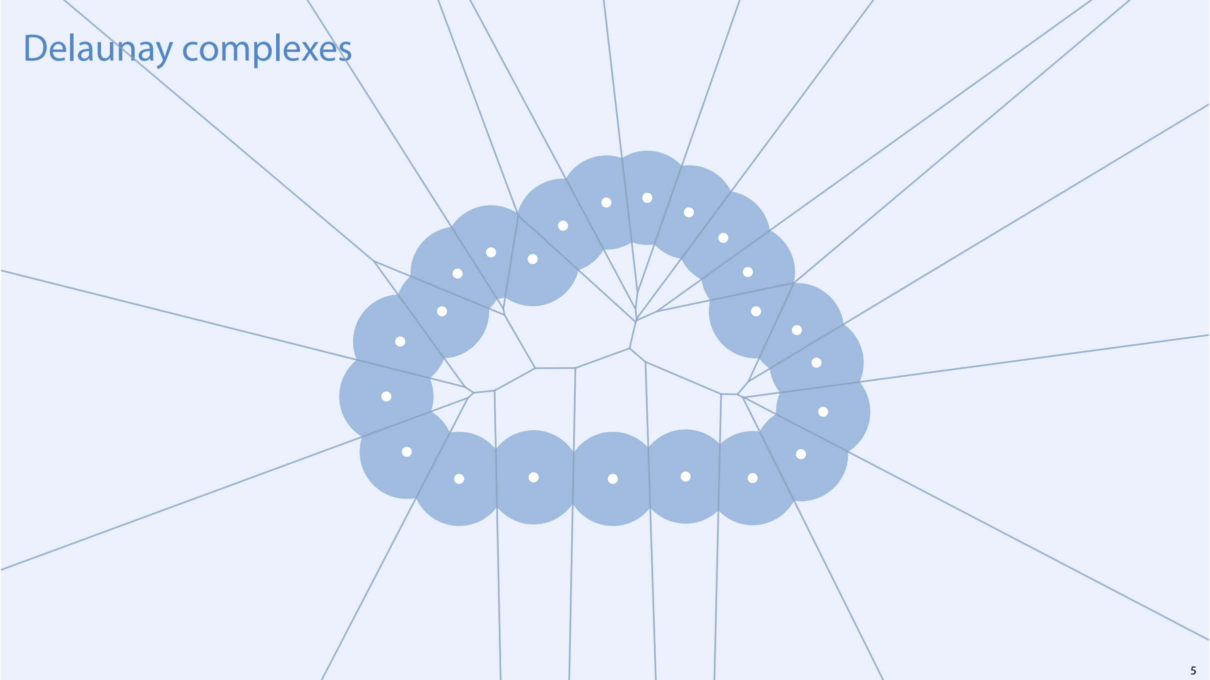

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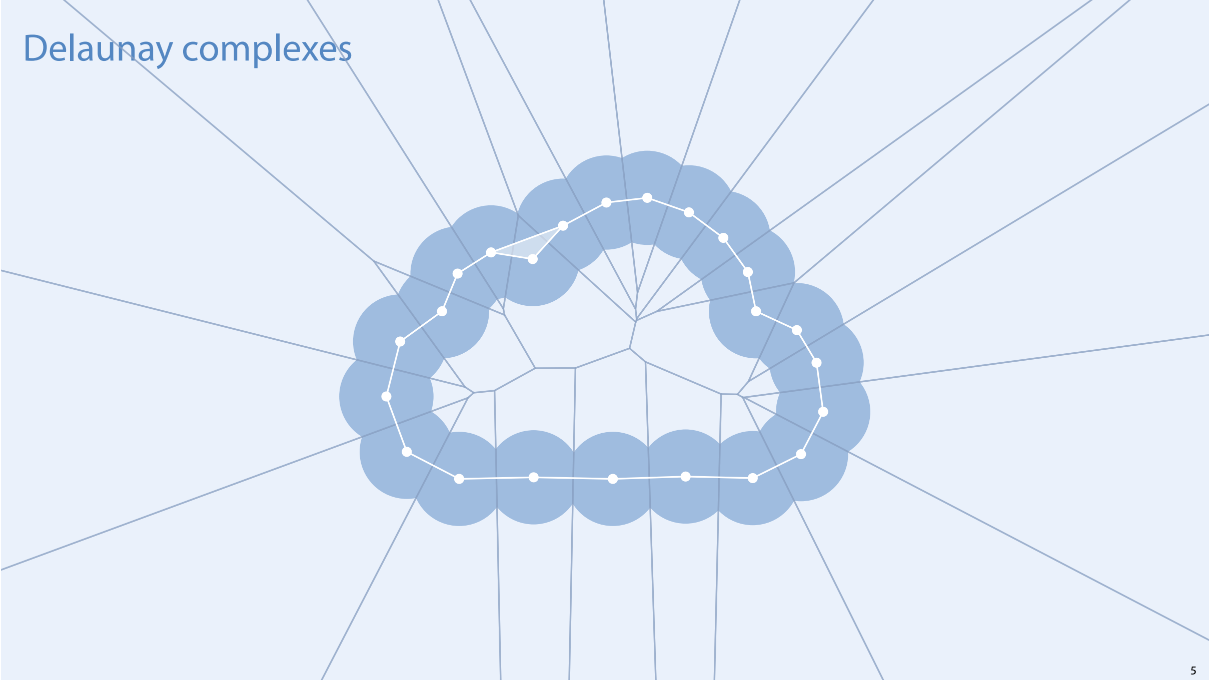

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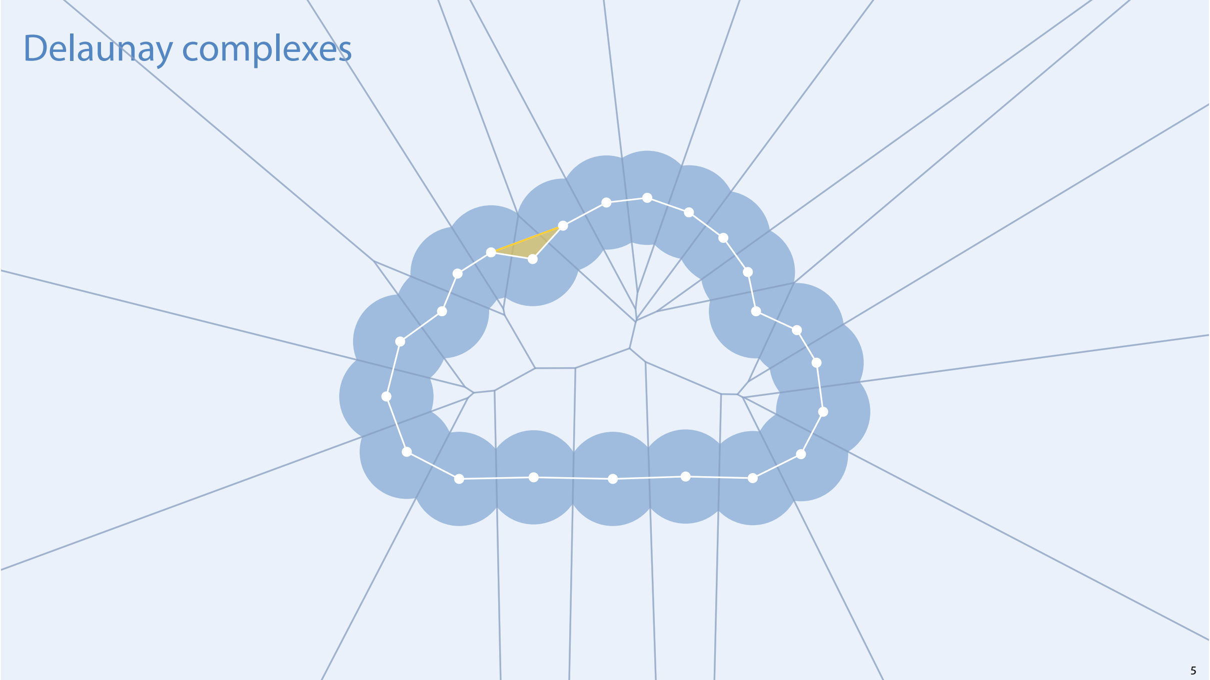

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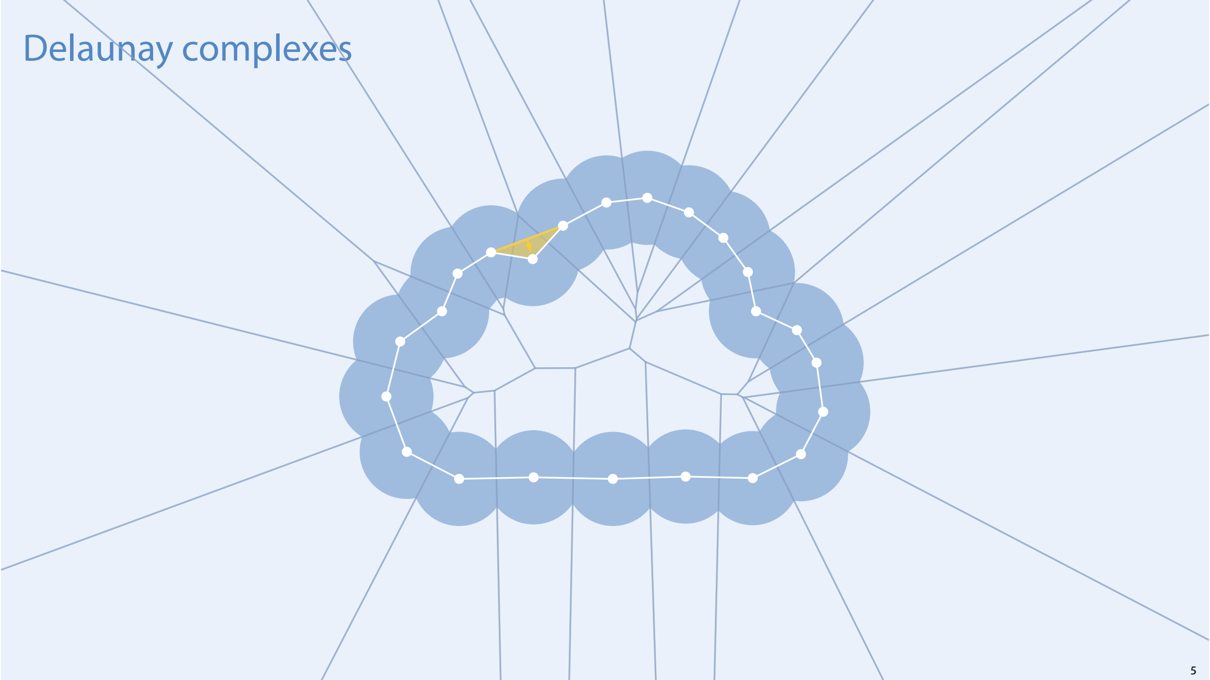

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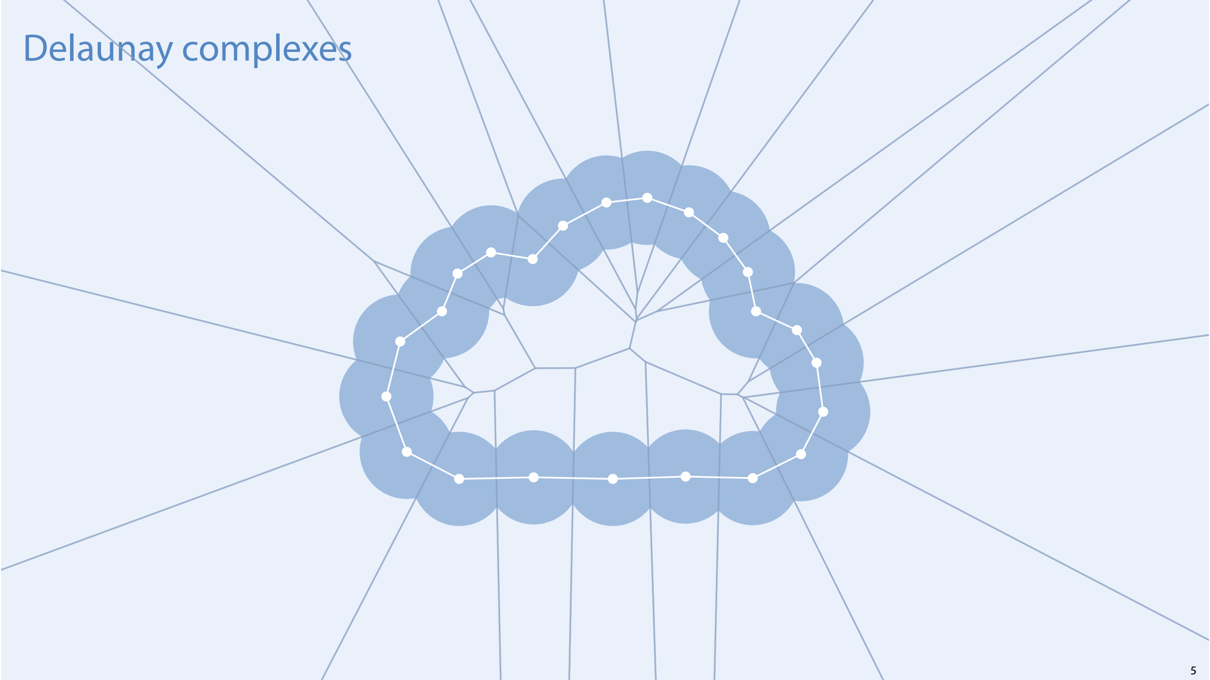
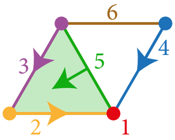


Discrete Morse theory



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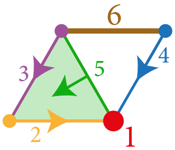

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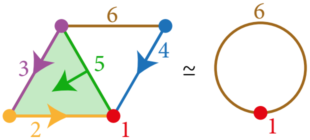
Theorem (Forman 1998)

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



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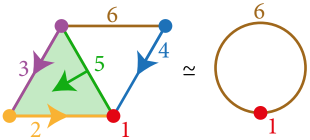
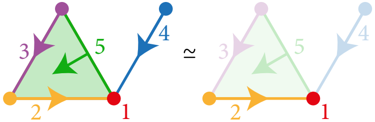


Discrete Morse functions – and their gradients – encode *collapses* of sublevel sets:



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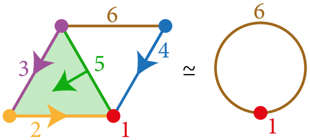

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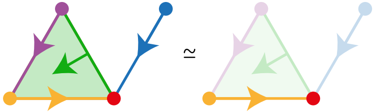
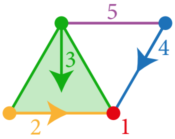
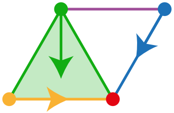


Generalizing discrete Morse theory

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



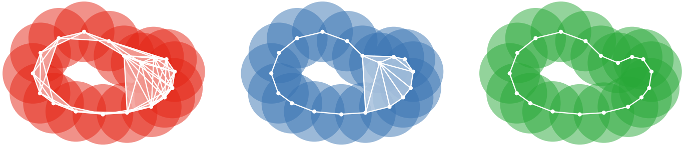


Morse theory for Čech and Delaunay complexes

Theorem (B, Edelsbrunner 2017)

Čech, Delaunay, and Wrap complexes (at any scale r) of a point set $X \subset \mathbb{R}^d$ in general position are related by collapses encoded by a single discrete gradient field:

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



Morse theory of Čech and Delaunay complexes

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The Čech function and the Delaunay function of a point set $X \subset \mathbb{R}^d$ *in general position are generalized discrete Morse functions.*

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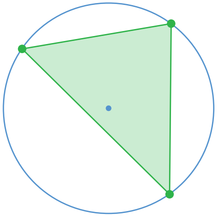
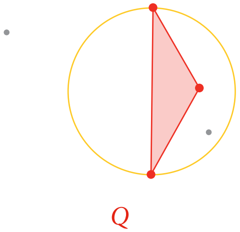
- $f_D(Q) = f_C(Q)$
- *Q is a critical simplex of f_C*
- *Q is a critical simplex of f_D*
- *Q is a* centered *Delaunay simplex*
  (containing the circumcenter in the interior)



Čech intervals

Lemma

Let $Q \subseteq X$ be a simplex with smallest enclosing sphere S.
Then $Q' \subseteq X$ has the same smallest enclosing sphere S iff



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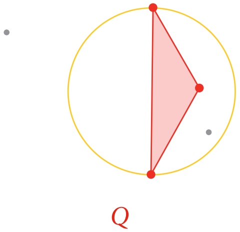

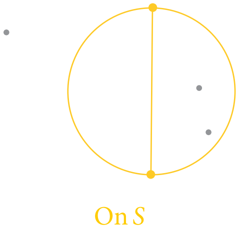

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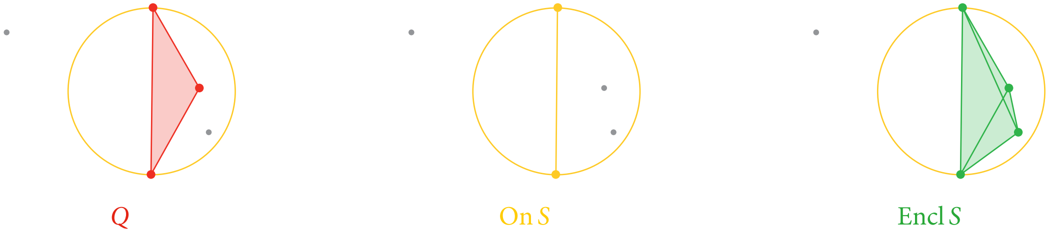

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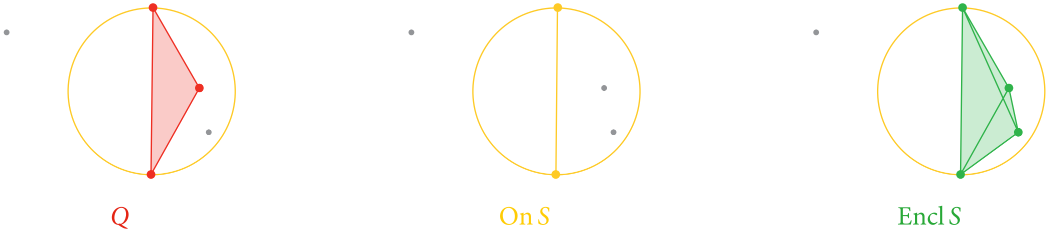

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$$\mathrm{Front}\, S = \{x \in \mathrm{On}\, S \mid \mu_x > 0\},$$

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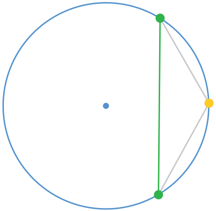

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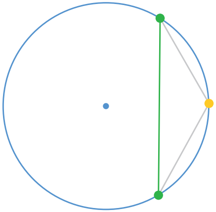

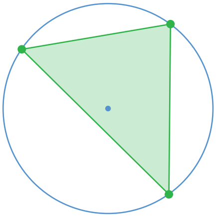

Delaunay intervals

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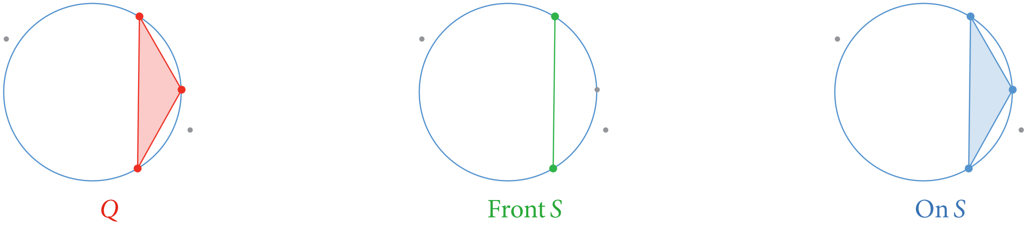

Čech and Delaunay intervals from Karush–Kuhn–Tucker conditions

Proposition

A sphere S is the smallest sphere enclosing Q and excluding E iff

- *S is the smallest circumsphere of some simplex $P \subseteq X$,*
- $Q \in [\operatorname{Front} S, \operatorname{Encl} S]$*, and*
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Čech and Delaunay intervals from Karush–Kuhn–Tucker conditions

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A sphere S is the smallest sphere enclosing Q and excluding E iff

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Corollary

The Čech gradient is given by the intervals of the form $[\mathrm{On}\, S, \mathrm{Encl}\, S]$.

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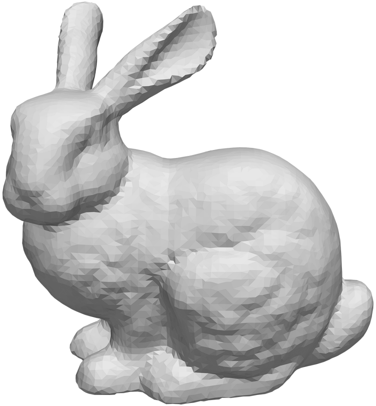
The Čech gradient is given by the intervals of the form $[\mathrm{On}\, S, \mathrm{Encl}\, S]$.
The Delaunay intervals is given by the intervals of the form $[\mathrm{Front}\, S, \mathrm{On}\, S]$.

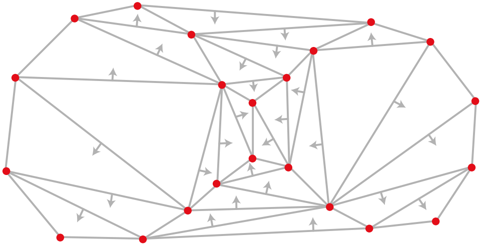
Wrap complexes

Foundation of the surface reconstruction software *Wrap* (Edelsbrunner 1995, Geomagic)



Wrap complexes

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



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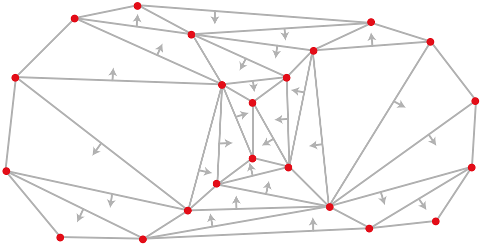

Definition (Edelsbrunner 1995; B, Edelsbrunner 2017)

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

- the smallest subcomplex of $\mathrm{Del}_r\, X$ that
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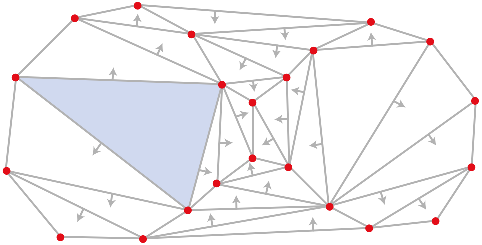

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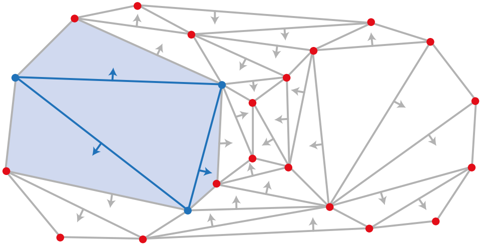

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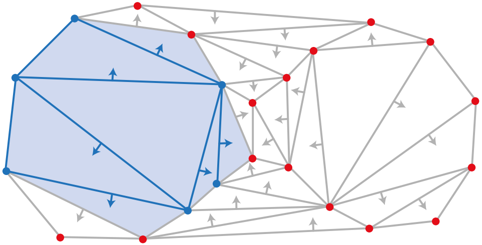

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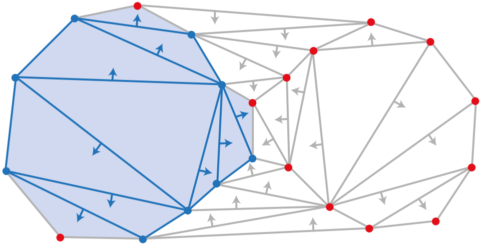

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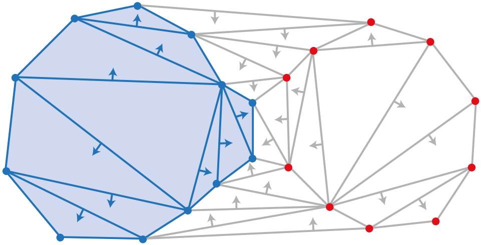

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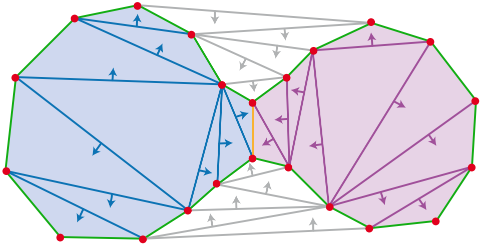

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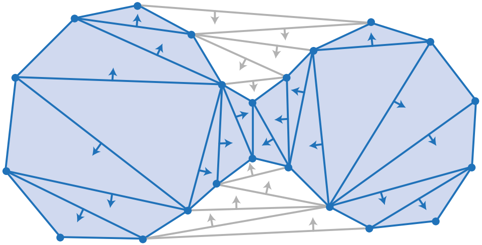

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Delaunay and Wrap complexes

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Persistence of Delaunay filtrations

Algorithm (matrix reduction)

Require: D: $m \times n$ matrix

Ensure: $R = D \cdot V$ is reduced, V is full rank upper triangular

    function Reduce(D)

        $R = D$, $V = I(n)$

        while there exist $i < j$ such that $\mathrm{pivot}\, R_i = \mathrm{pivot}\, R_j$ **do**

            add column R_i to column R_j

            add column V_i to column V_j

        return R, V

Algorithm (exhaustive matrix reduction)

Require: D: $m \times n$ matrix
Ensure: $R = D \cdot V$ is reduced, V is full rank upper triangular

function Reduce(D)
  $R = D$, $V = I(n)$
  while there exist $i < j$ such that R_j has a nonzero entry in row pivot R_i **do**
    add column R_i to column R_j
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    return R, V

Proposition

The resulting columns R_j are minimal (in a lexicographic order) within their homology class (in K_{j-1}).

Standard reduction and exhaustive reduction

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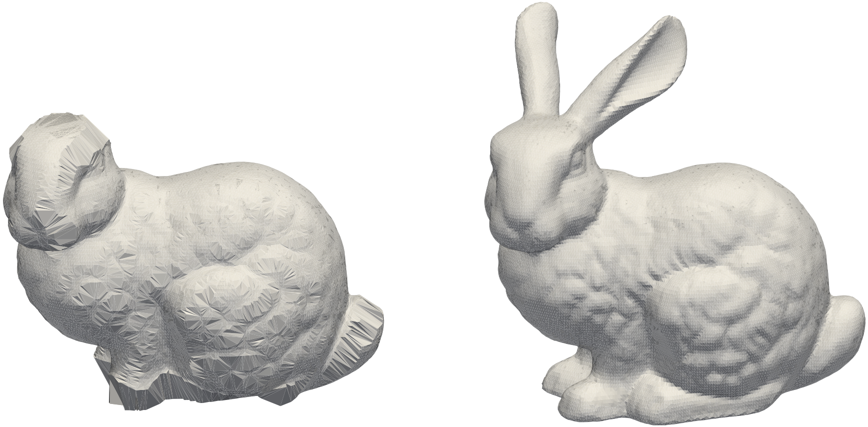
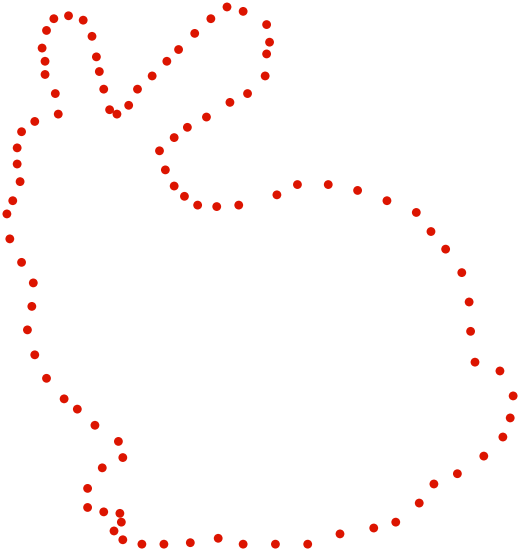


Wrap complexes and lexicographically minimal cycles



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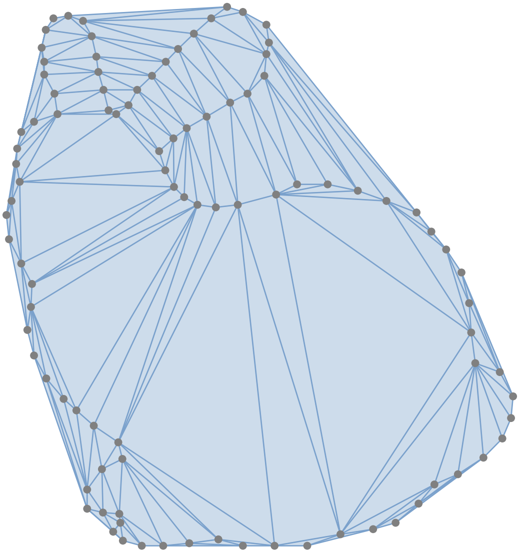

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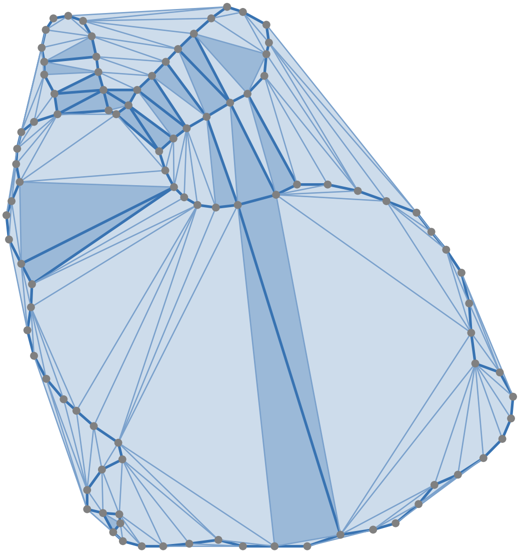

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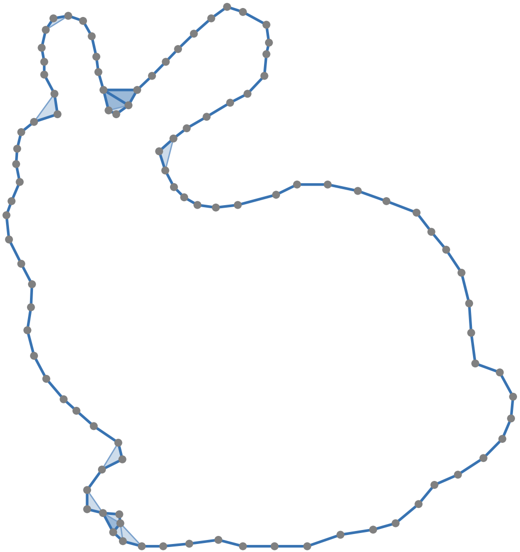

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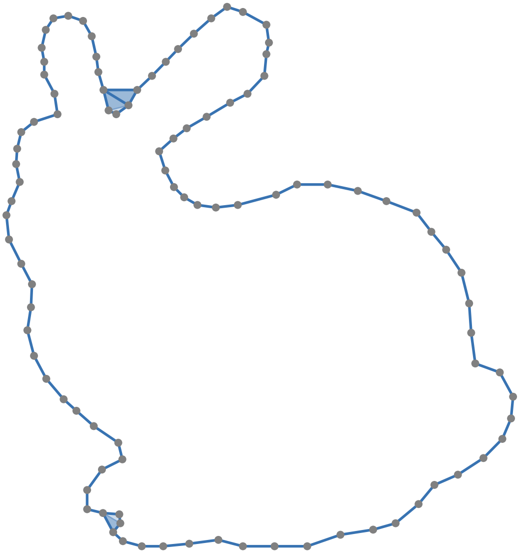

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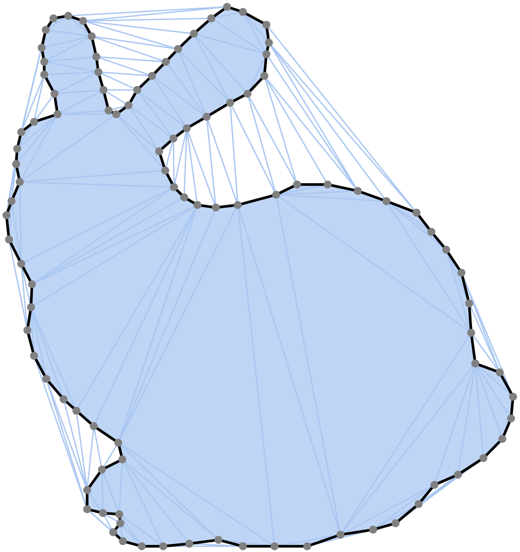

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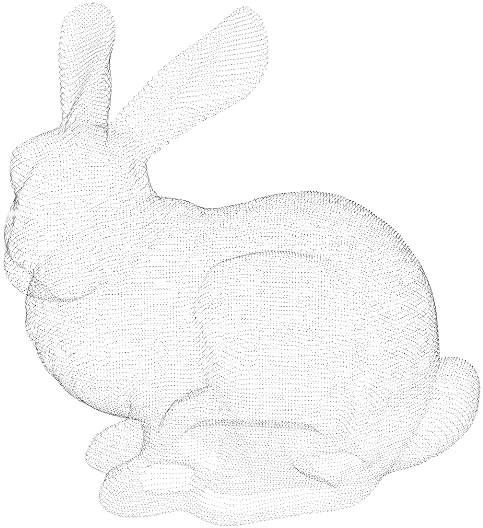

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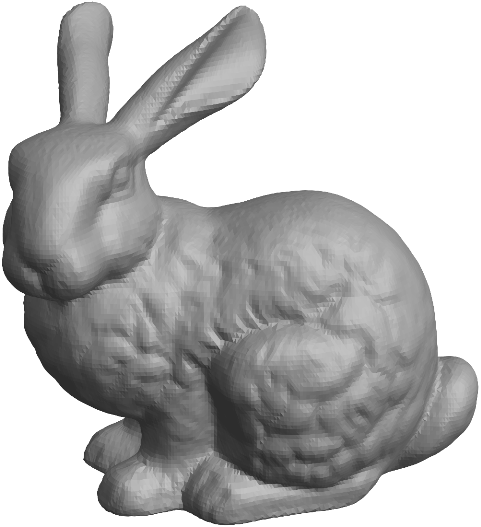
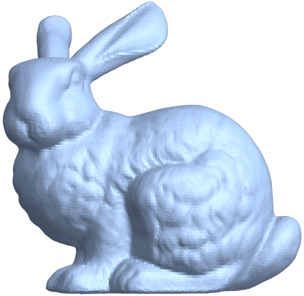
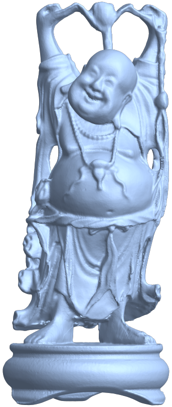
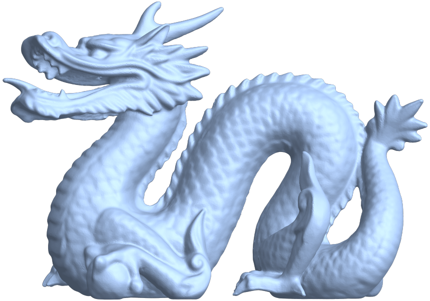


Point cloud reconstruction with minimal cycles





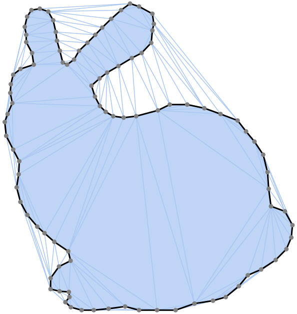


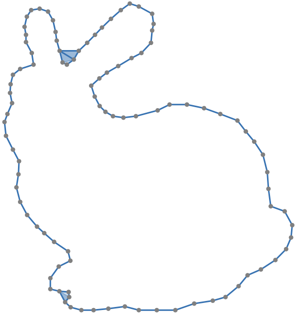
Wrap complexes support minimal cycles

Theorem (B, Roll 2022)

Let $X \subset \mathbb{R}$ be a finite subset in general position and let $r \in \mathbb{R}$.

- *Exhaustive matrix reduction computes the minimal cycles homologous to a simplex boundary.*
- *Any lexicographically minimal cycle of $\mathrm{Del}_r(X)$ is supported on $\mathrm{Wrap}_r(X)$.*



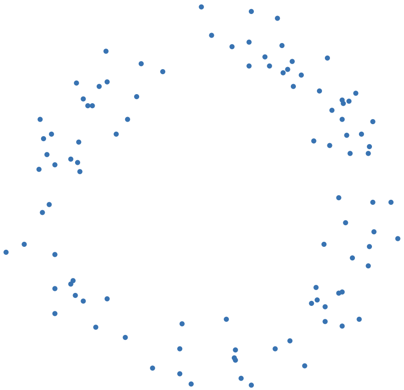


Vietoris–Rips persistence

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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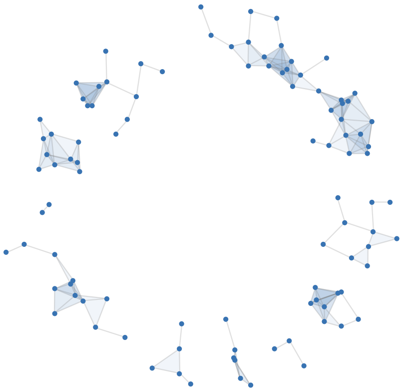

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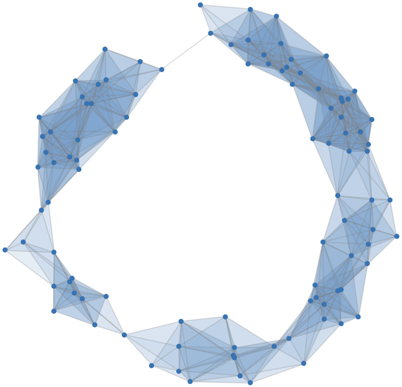

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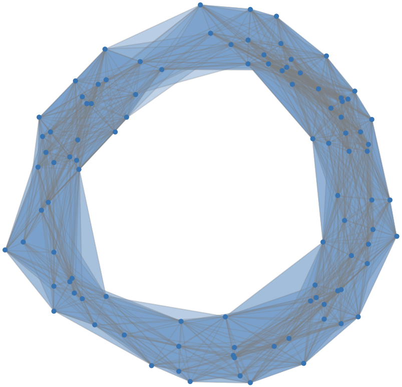

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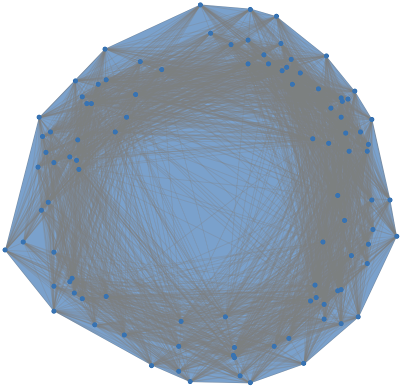
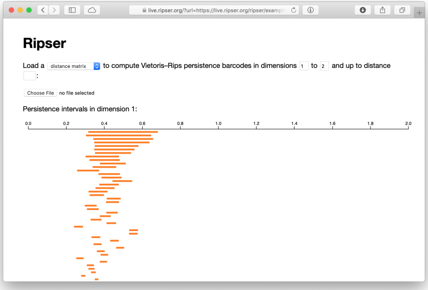
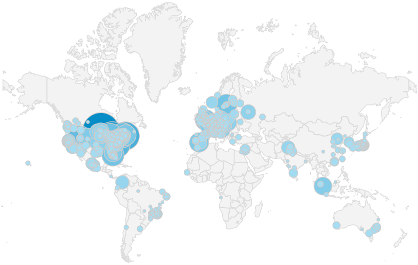


Ripser: software for computing Vietoris–Rips persistence barcodes

Open source software (`ripser.org`)





Ripser users across the globe

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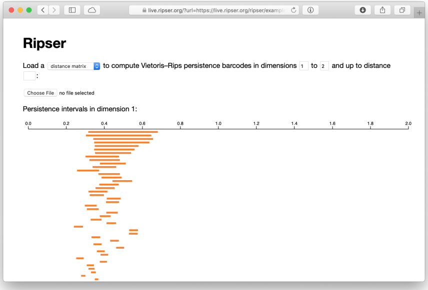

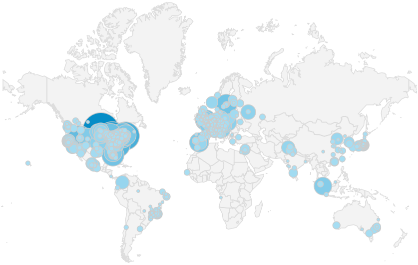

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Computational improvements based on

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

Apparent pairs

Ripser uses the following pairing of simplices (breaking ties in the filtration 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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Special cases and equivalent definitions have been (re)discovered independently multiple times

- Kahle 2011, Robbins 2015, Henselmann-Petrusek 2017, Lampret 2020, Feichtner-Kozlov 2020, …

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Proposition (B 2021)

The apparent pairs are both

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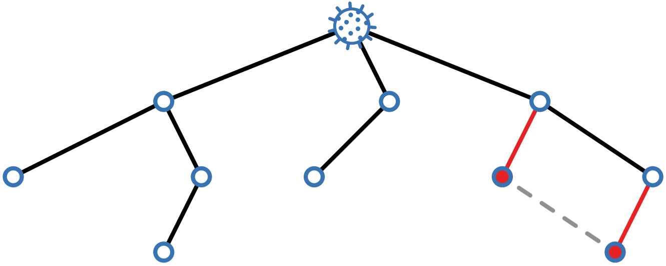
Proposition (B, Roll 2022)

Any generalized discrete Morse function is refined by apparent pairs.

Topology of viral evolution



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

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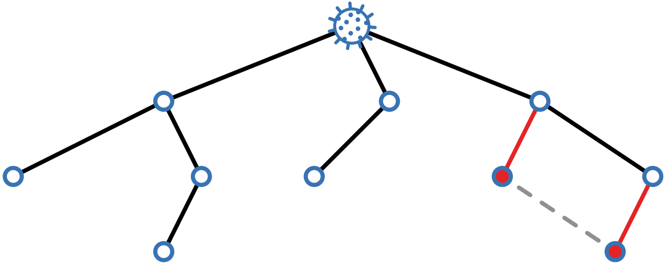

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Observation: Ripser runs unusually fast on genetic distance data

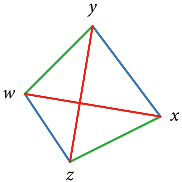
- SARS-CoV2 RNA sequences (spike protein)
- 25556 data points (2.8×10^{12} simplices in 2-skeleton)
- $120\,s$ computation time (with data points ordered appropriately)

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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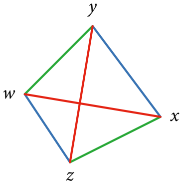

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- The hyperbolic plane is $(\ln 2)$-hyperbolic.

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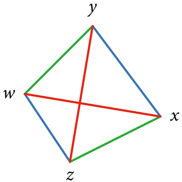
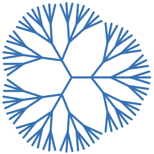


- The hyperbolic plane is $(\ln 2)$-hyperbolic.

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



Rips Contractibility

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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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What about

- non-geodesic spaces? In particular, finite metric spaces?

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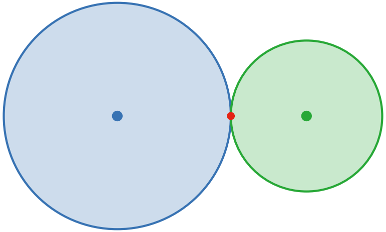
Theorem (B, Roll 2022)

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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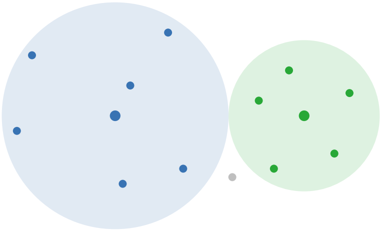

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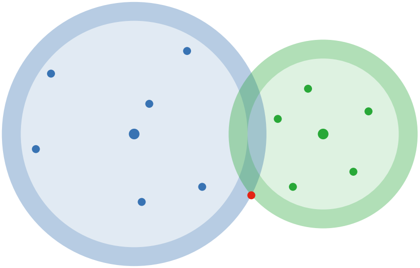

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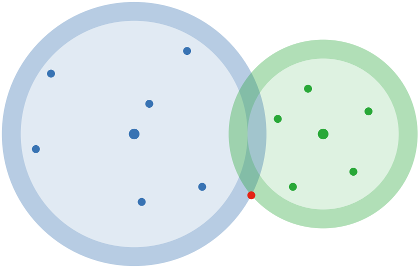

Definition (Bonk, Schramm 2000)

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

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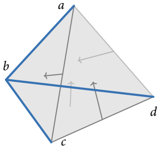

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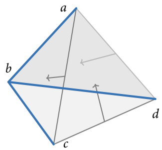

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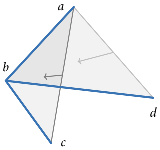

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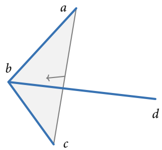

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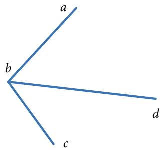

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Gromov hyperbolicity, geodesic defect, and apparent pairs in Vietoris-Rips filtrations

Symposium on Computational Geometry, 2022. doi:10.4230/LIPIcs.SoCG.2022.15

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