

Apparent pairs in geometry & topology

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Technical University of Munich (TUM)

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SFB
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109

Discretization
In Geometry
and DynamIcs

Technical
University
of Munich

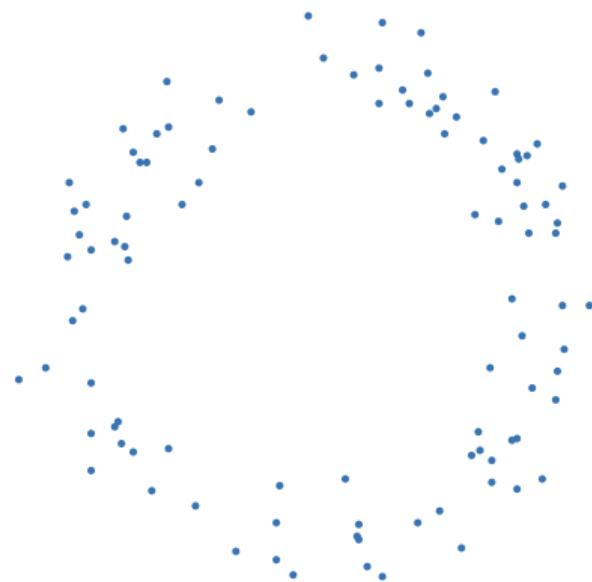


MCMCL
Munich Center for Machine Learning

Vietoris–Rips complexes

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

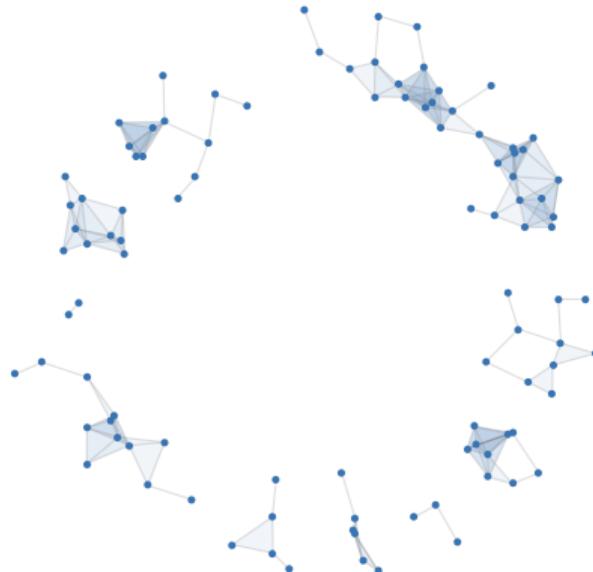
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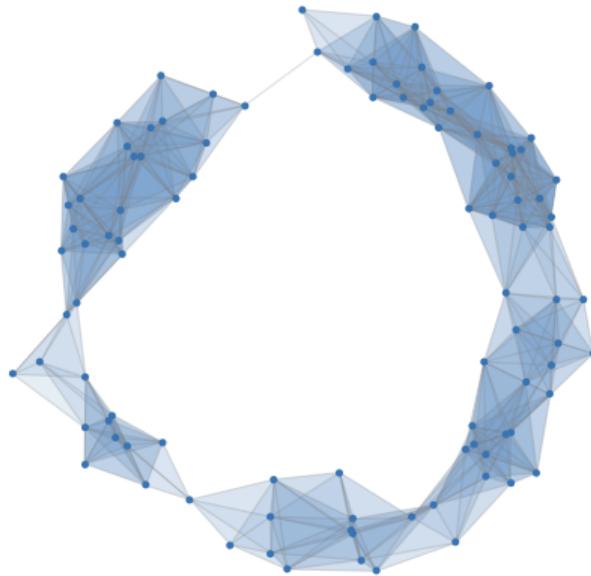
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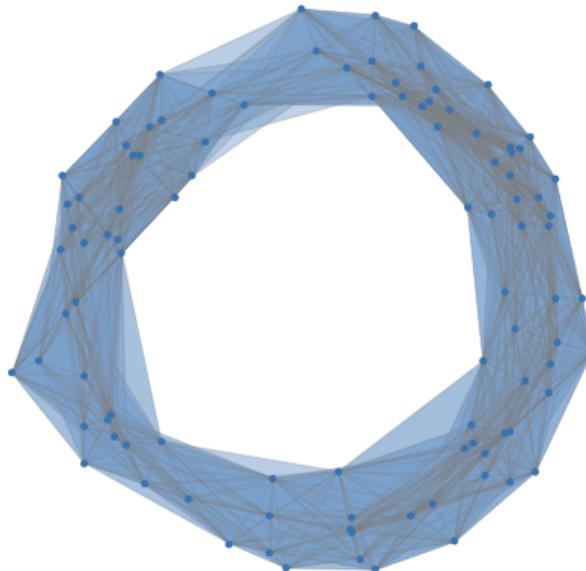
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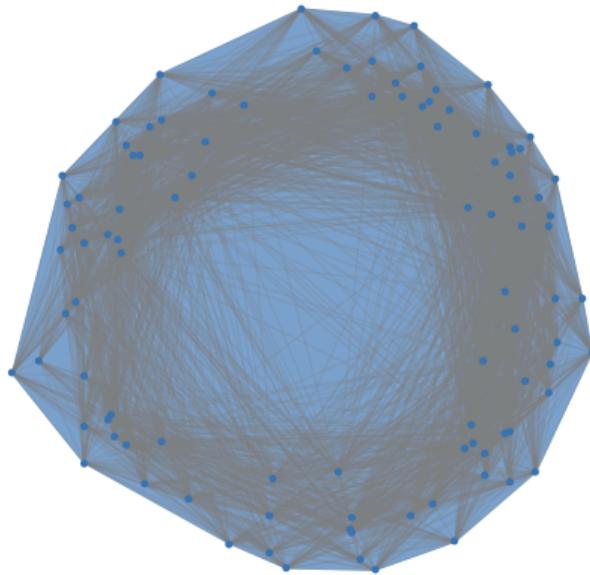
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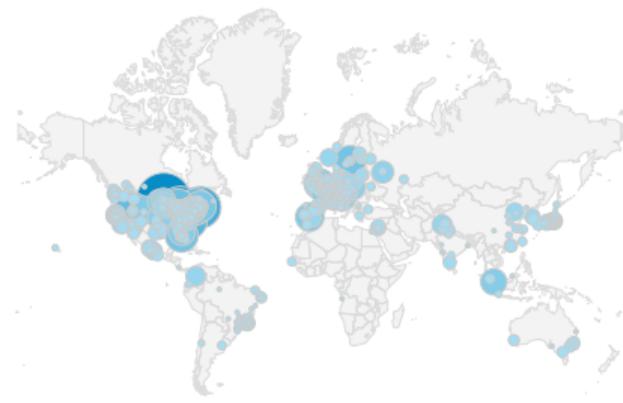
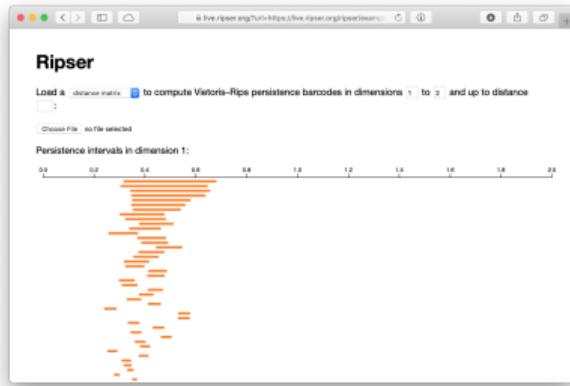
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Ripser: software for computing Vietoris–Rips persistence barcodes

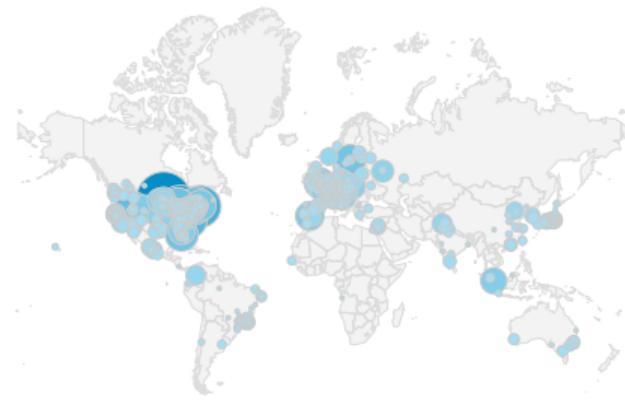
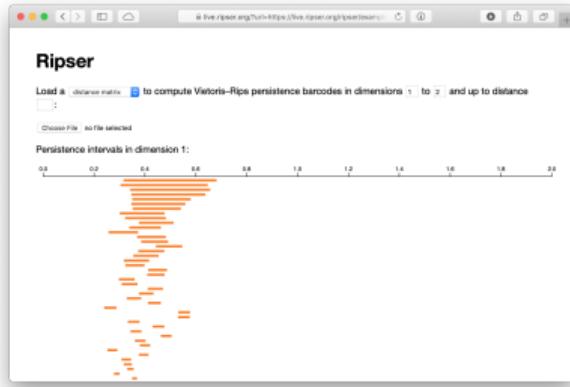
Open source software (ripser.org)



Ripser users worldwide

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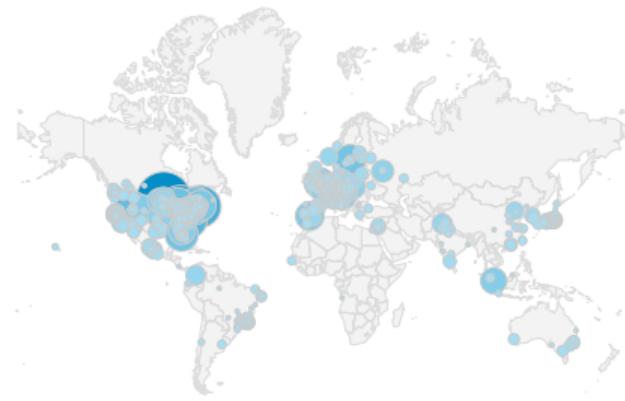
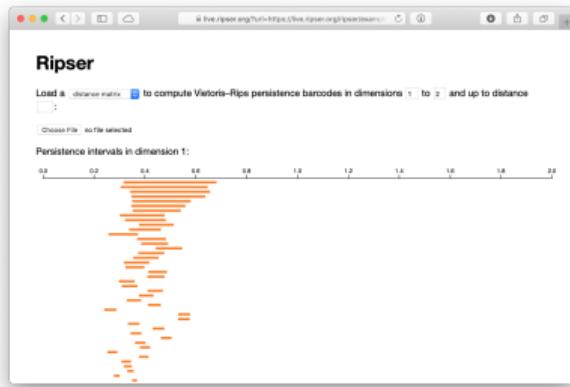
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Efficient matrix algorithm based on

- *clearing*: avoiding unnecessary column operations
- computing persistent *cohomology*

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Efficient matrix algorithm based on

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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
- σ_j is the earliest proper coface of σ_i .

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

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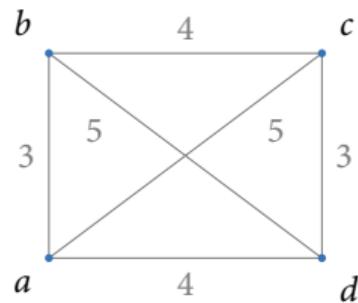
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Proposition (B 2021)

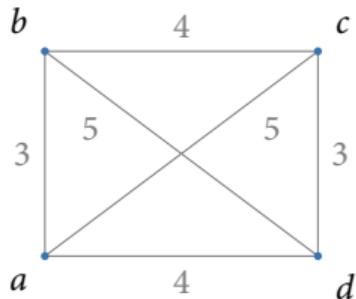
The apparent pairs are both

- *persistence pairs (creating/destroying a feature in homology) and*
- *gradient pairs (in the sense of discrete Morse theory).*

Apparent pairs of the diameter-lexicographic filtration

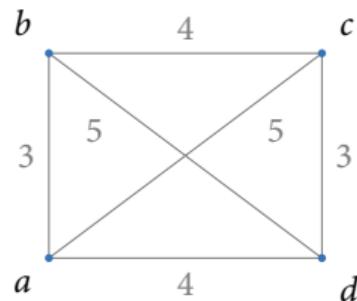


Apparent pairs of the diameter-lexicographic filtration



$$\partial_1 = \begin{pmatrix} (a,b):3 & & & & \\ & (c,d):3 & & & \\ & & (a,d):4 & & \\ & & & (b,c):4 & \\ & & & & (a,c):5 \\ 1 & & 1 & & 1 \\ \textcolor{blue}{1} & & & & 1 \\ & 1 & & 1 & \\ & & 1 & 1 & \\ & & & & 1 \end{pmatrix} \begin{matrix} (a) \\ (b) \\ (c) \\ (d) \end{matrix}$$

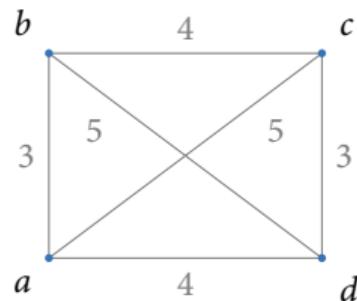
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A shortcut for finding pivots

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Shortcut for finding the pivot (latest) facet of a simplex τ :

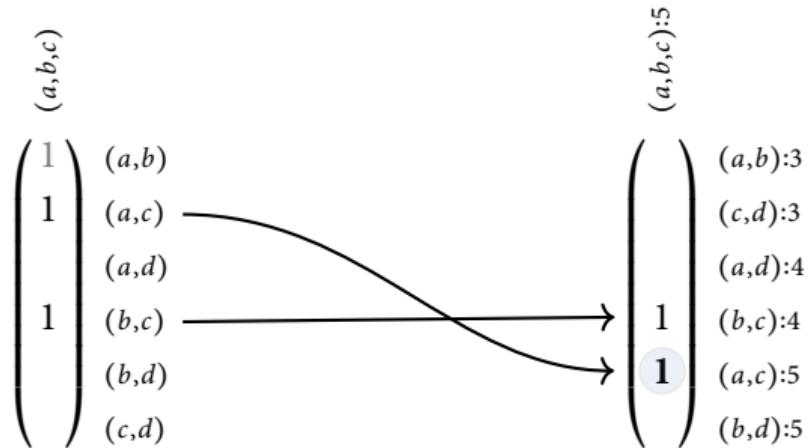
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- Enumerate facets σ of τ in (reverse) lexicographic order

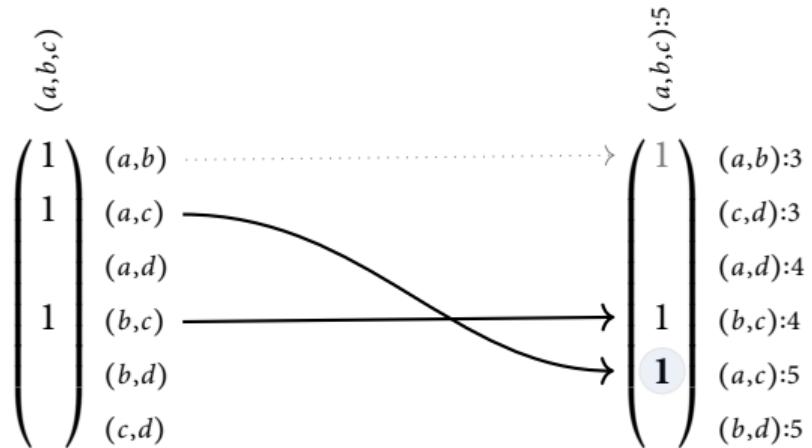
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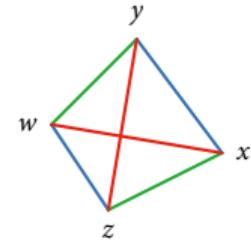
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Gromov-hyperbolicity

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

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



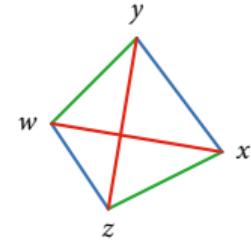
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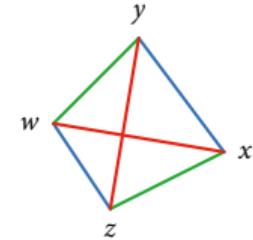
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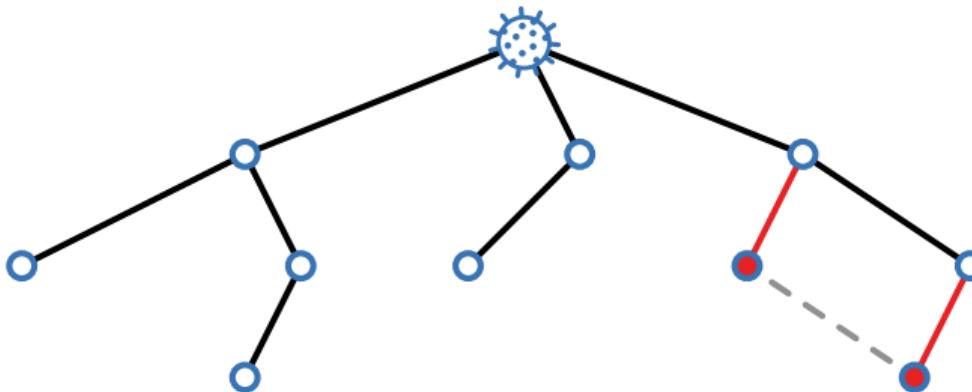
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- Metric trees and their subspaces are precisely the 0-hyperbolic spaces.

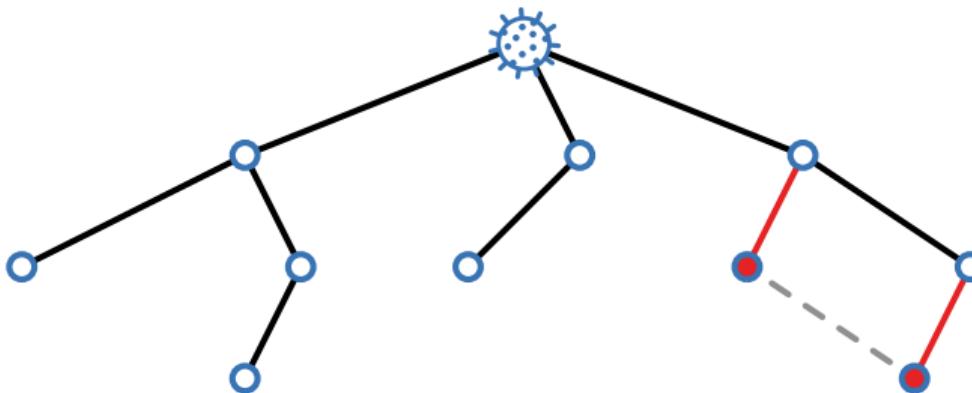


Topology of viral evolution



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

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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)

Rips complexes of hyperbolic spaces

Theorem (Rips; Gromov 1988)

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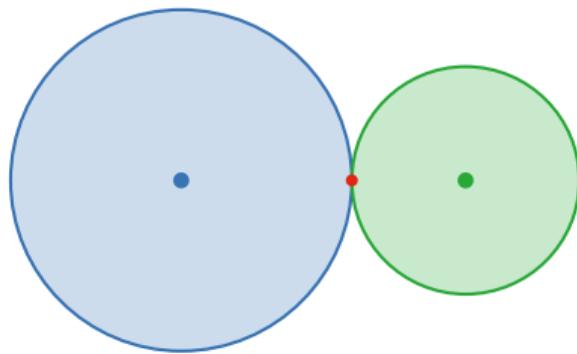
Theorem (B, Roll 2022)

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

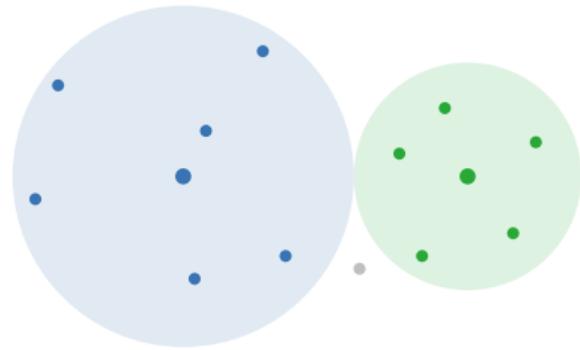
$$\text{Rips}_u(X) \searrow \text{Rips}_t(X) \searrow \{\ast\}$$

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

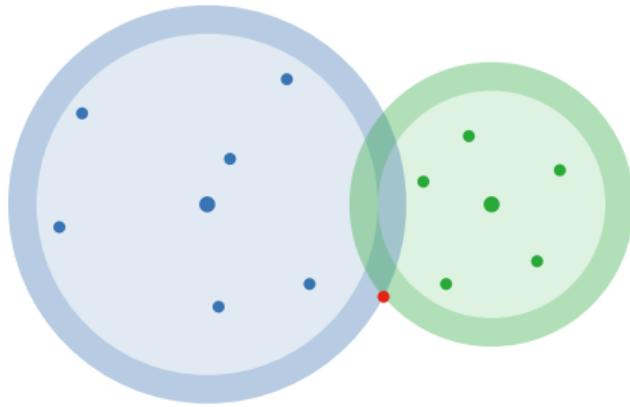
Geodesic defect



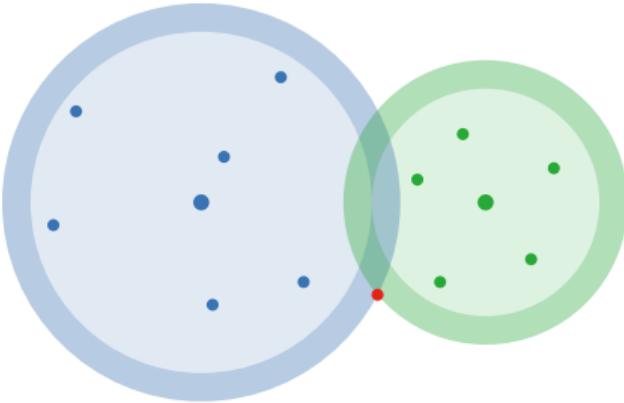
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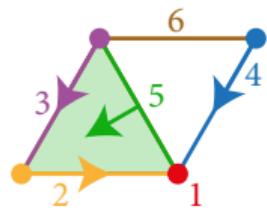
Definition (Bonk, Schramm 2000)

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

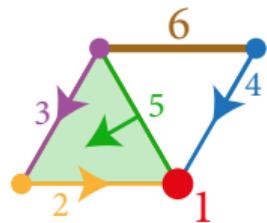
$$B_{r+\nu}(x) \cap B_{s+\nu}(y) \neq \emptyset.$$

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

Discrete Morse theory



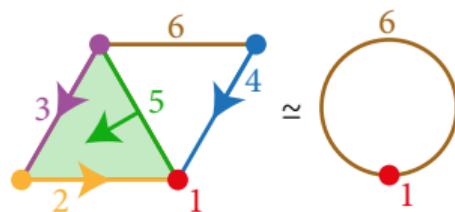
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Theorem (Forman 1998)

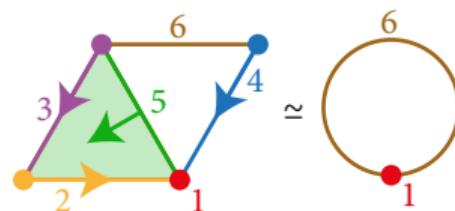
A simplicial complex with a discrete Morse function f is homotopy equivalent to a space (a CW complex) built from the critical simplices off.



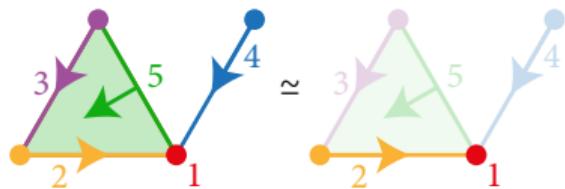
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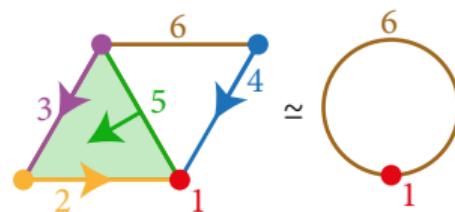
Discrete Morse functions – and their gradients – encode collapses of sublevel sets:



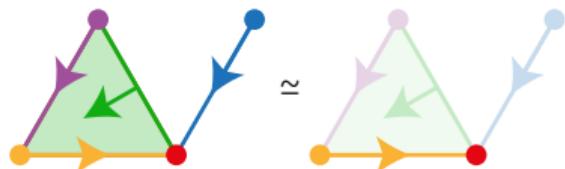
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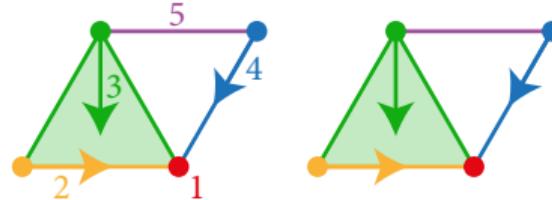


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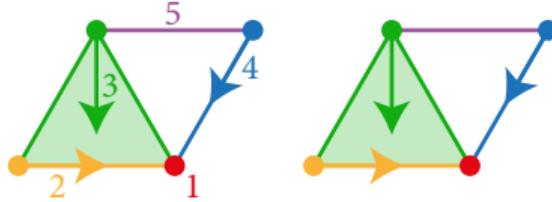
Generalizing discrete Morse theory

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

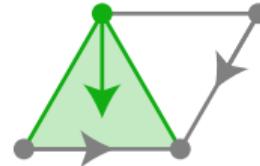


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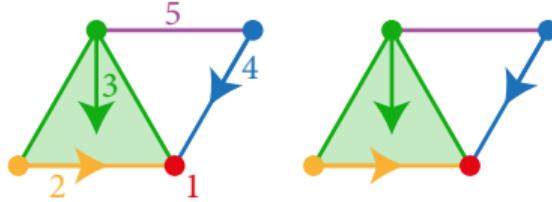


- A generalized vector field V can always be refined to a vector field.

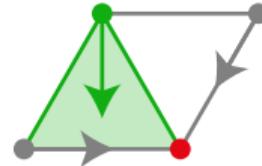


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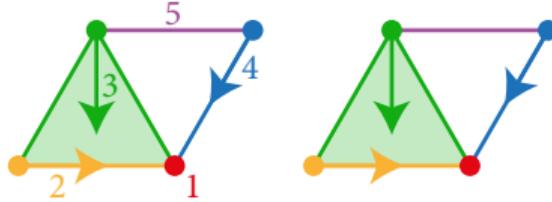


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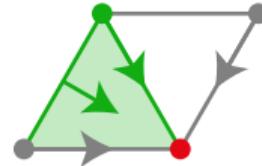


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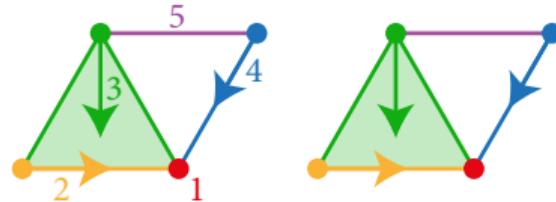


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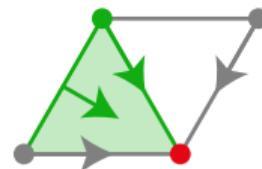


Generalizing discrete Morse theory

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- A generalized vector field V can always be refined to a vector field.



Proposition (B, Roll 2022)

Let f be a generalized discrete Morse function, breaking ties lexicographically.

Then the apparent pairs of zero persistence form a gradient that

- refines the gradient of f and
- has the same critical simplices.

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 $\text{diam}: \Delta(V) \rightarrow \mathbb{R}$ is a generalized discrete Morse function.

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- The apparent pairs (lexicographic refinement, based on arbitrary vertex order) refine this gradient.

The diameter function of generic trees

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

- The critical simplices are the tree simplices, $V \cup E$.
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In particular, the persistent homology is trivial in degrees > 0 .

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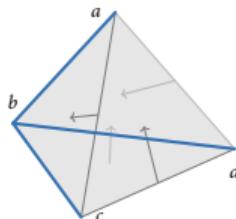
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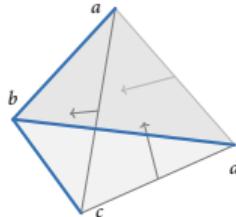
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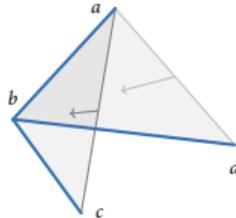
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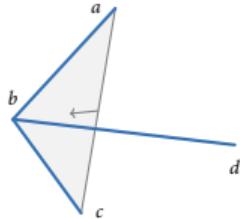
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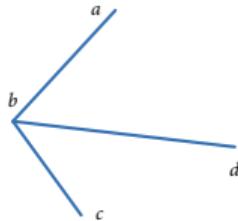
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Morse theory for Čech and Delaunay complexes

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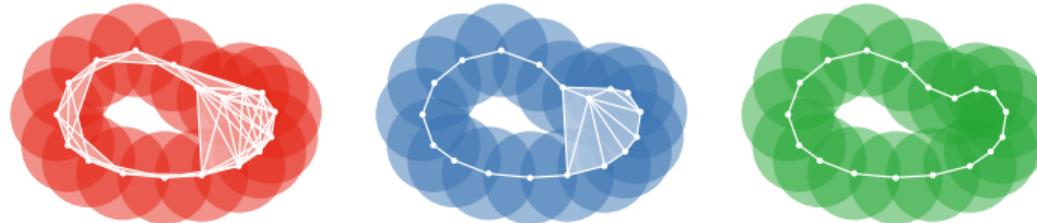
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Theorem (B, Edelsbrunner 2017)

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:

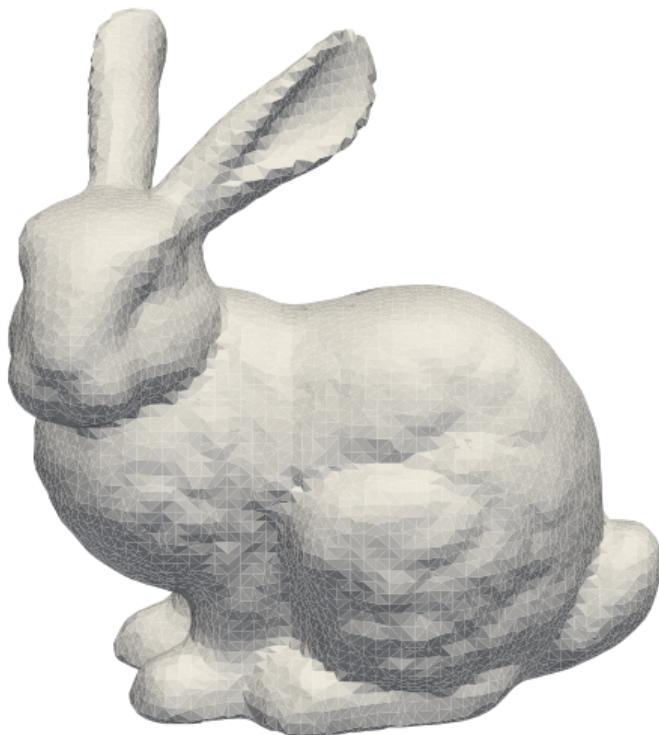
$$\text{Cech}_r X \searrow \text{Del}_r X \searrow \text{Wrap}_r X.$$



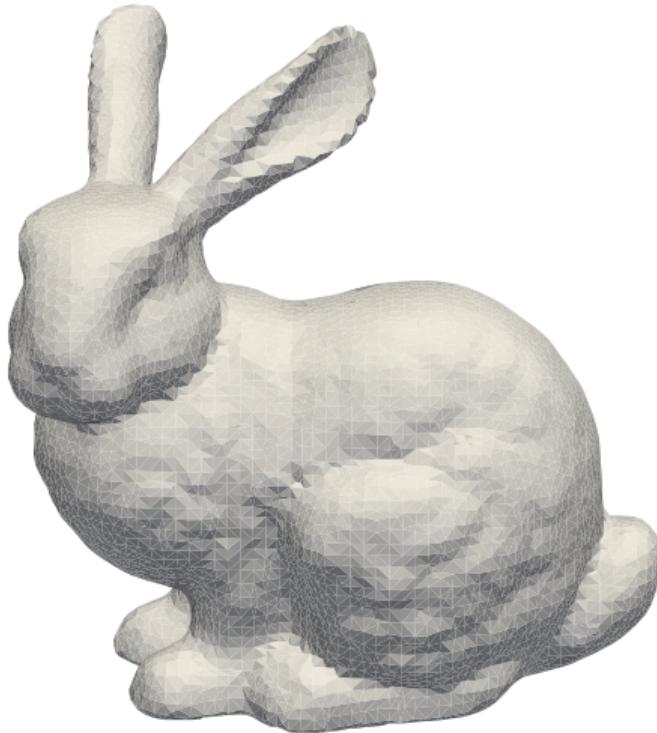
From Delaunay to Wrap complexes



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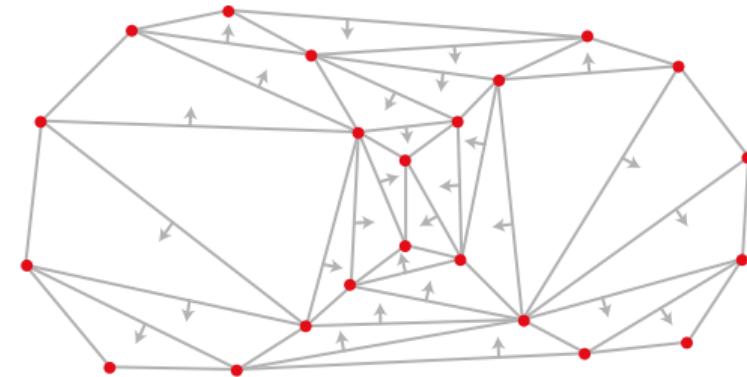
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Foundation of the surface reconstruction software *Wrap* (Edelsbrunner 1995, Geomagic)

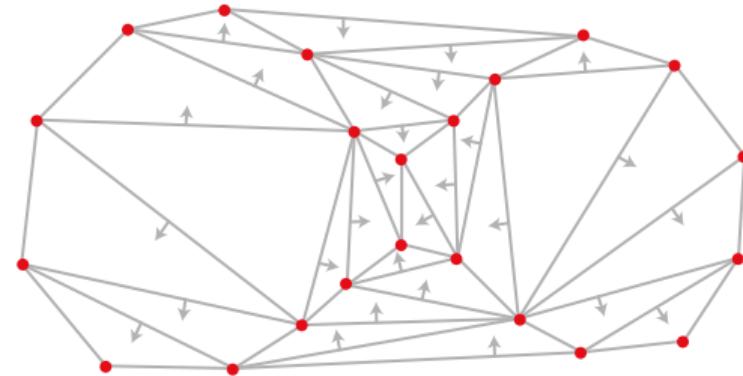
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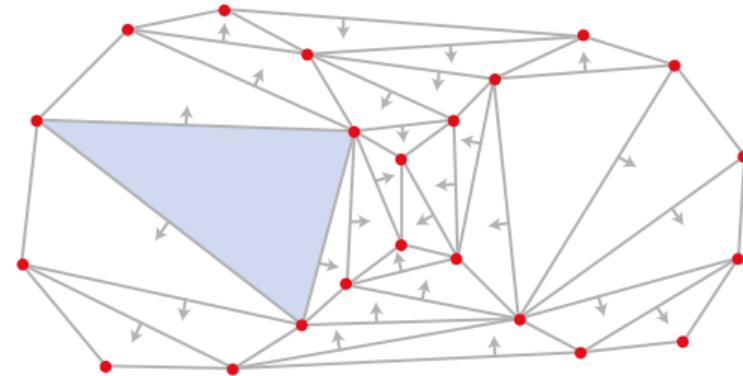
Definition (Edelsbrunner 1995; B, Edelsbrunner 2017)

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

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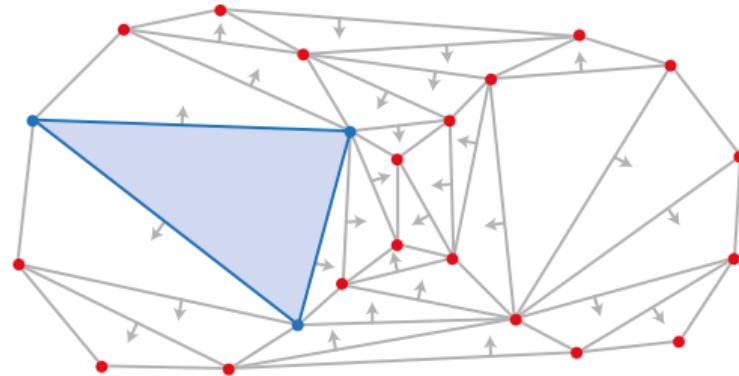
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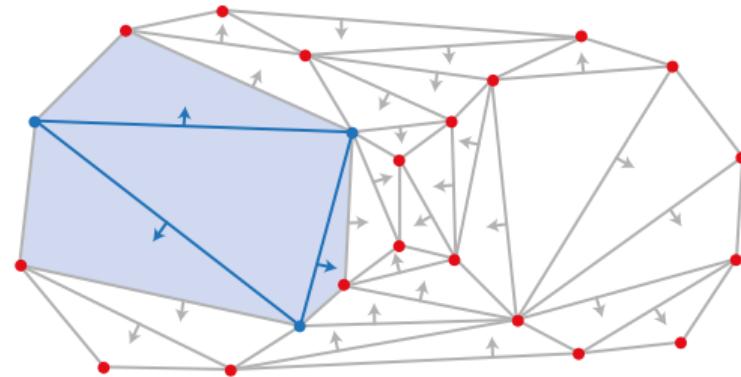
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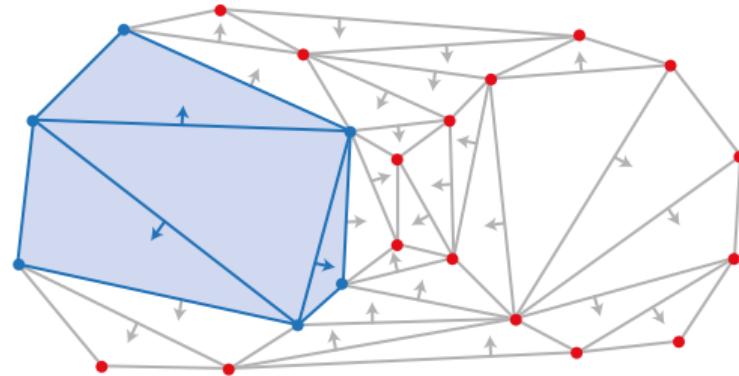
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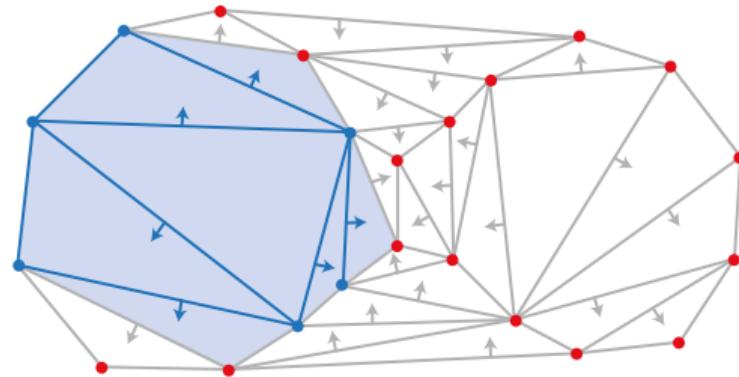
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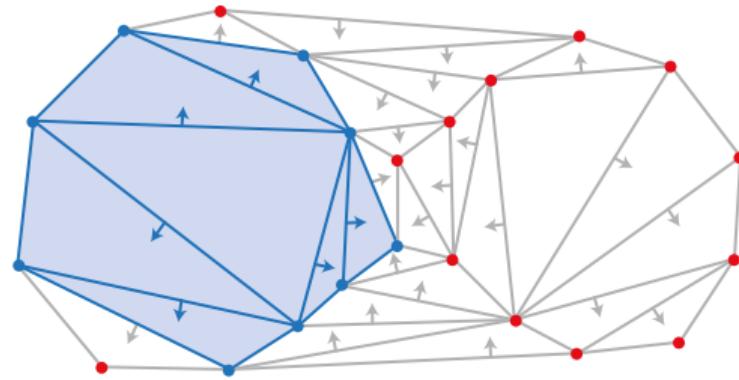
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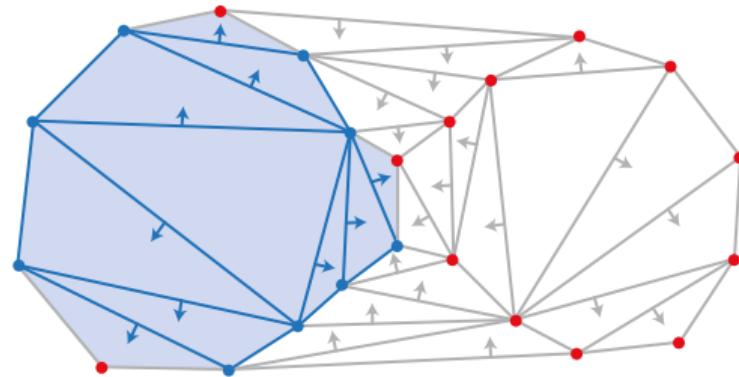
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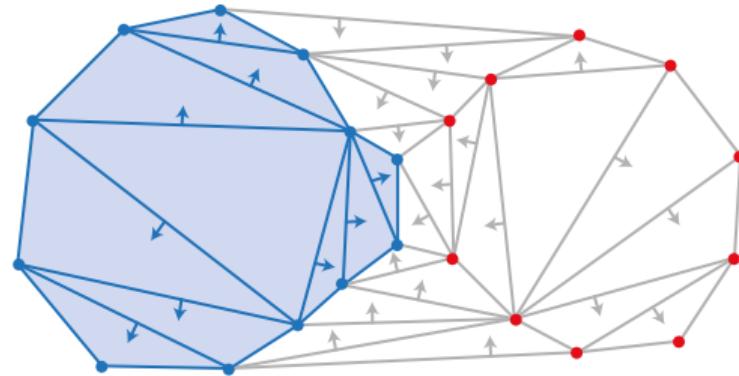
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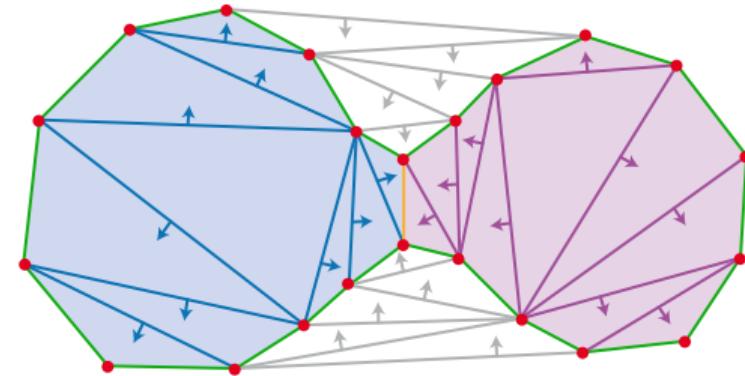
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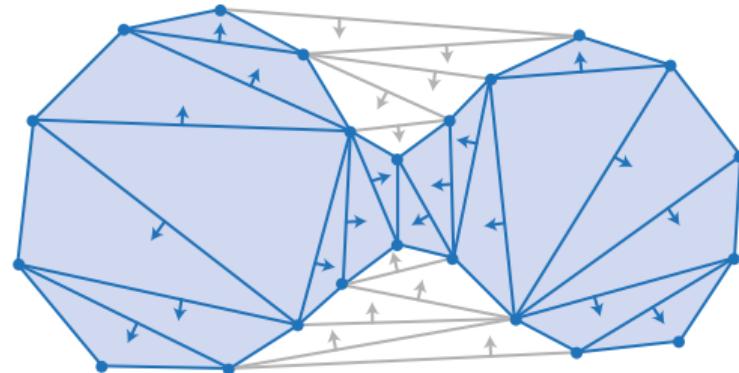
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Computing persistent homology via matrix reduction

Algorithm (matrix reduction; a variant of Gauss elimination)

Require: D : $m \times n$ matrix

Ensure: V is full rank upper triangular, $R = D \cdot V$ has unique column pivots

function Reduce(D)

$$R = D$$

$$V = I(n)$$

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

add column R_i to column R_j

▷ eliminate the nonzero entry in row pivot R_i

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return R, V

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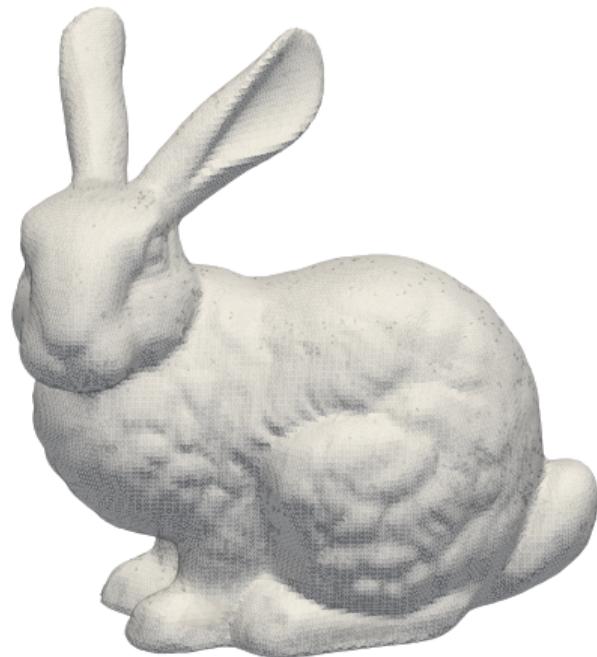
Proposition

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

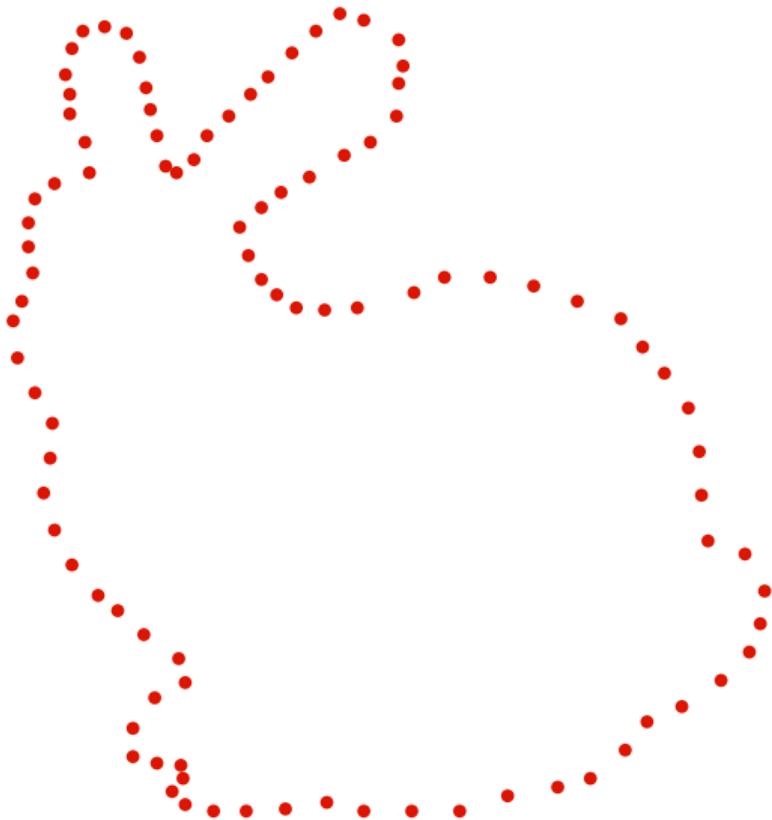
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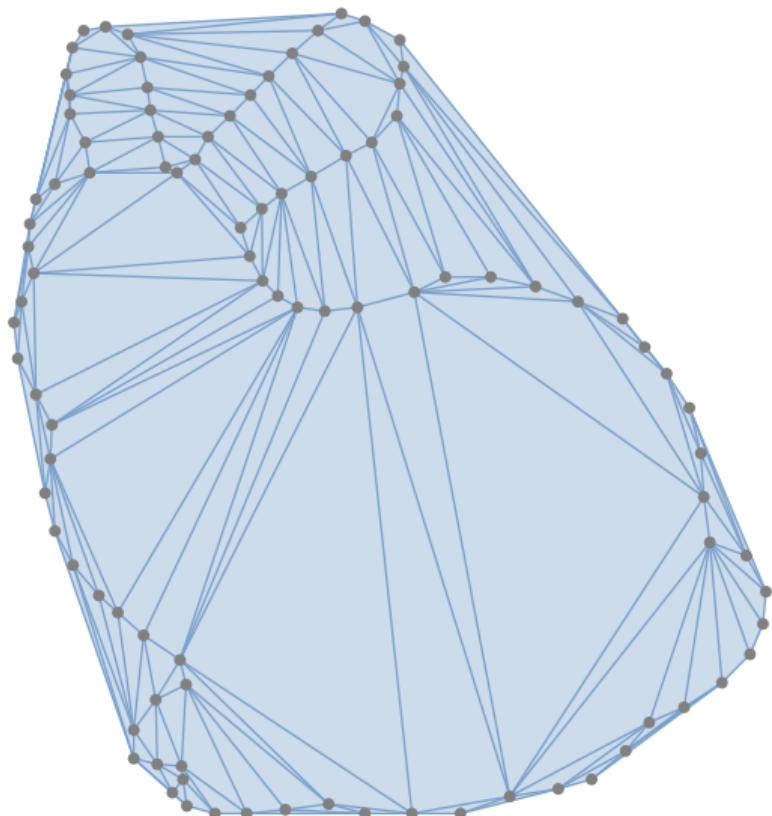
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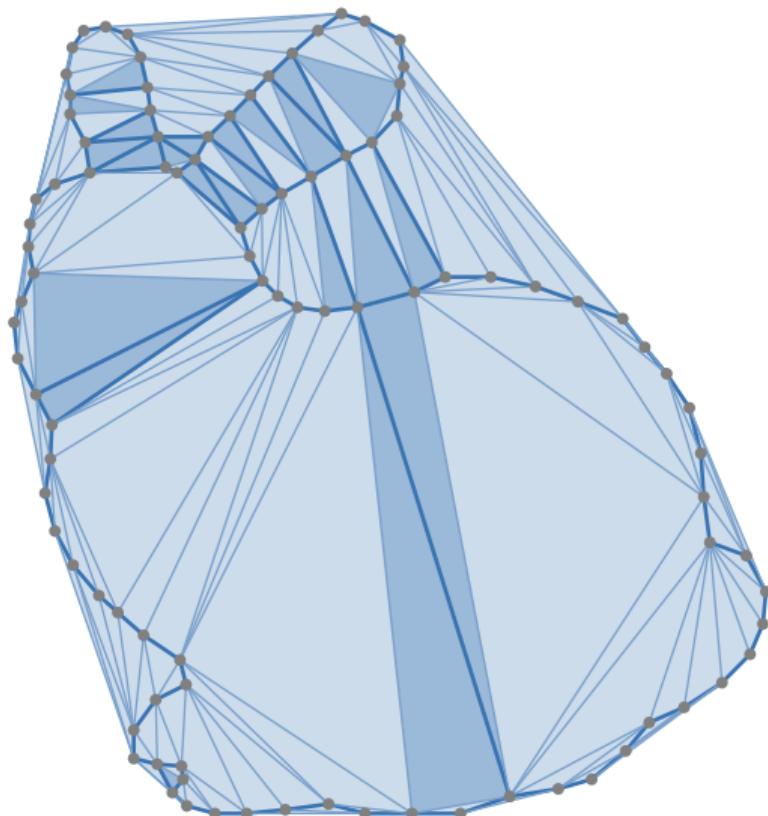
Wrap complexes and lexicographically minimal cycles



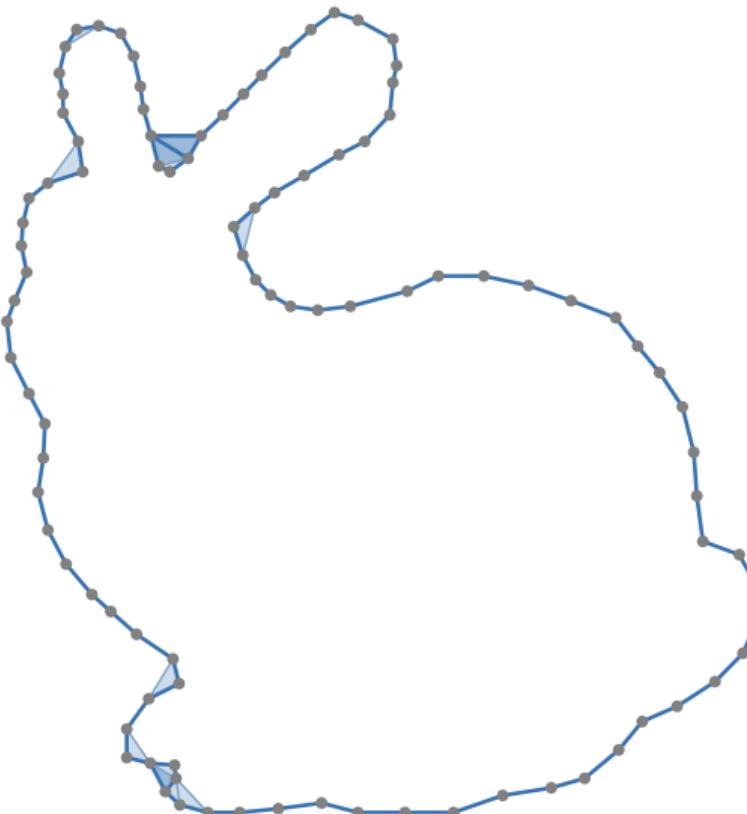
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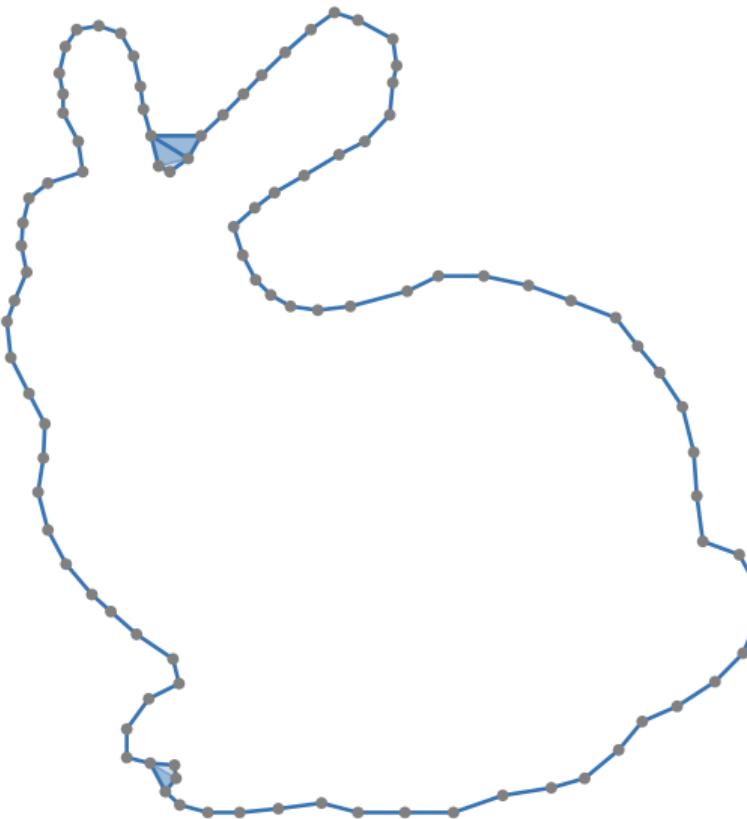
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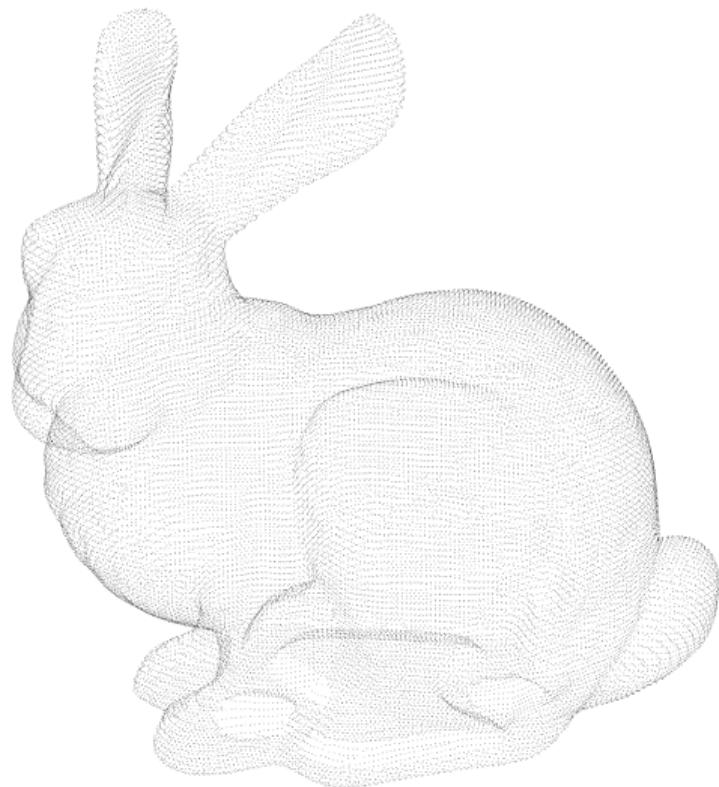
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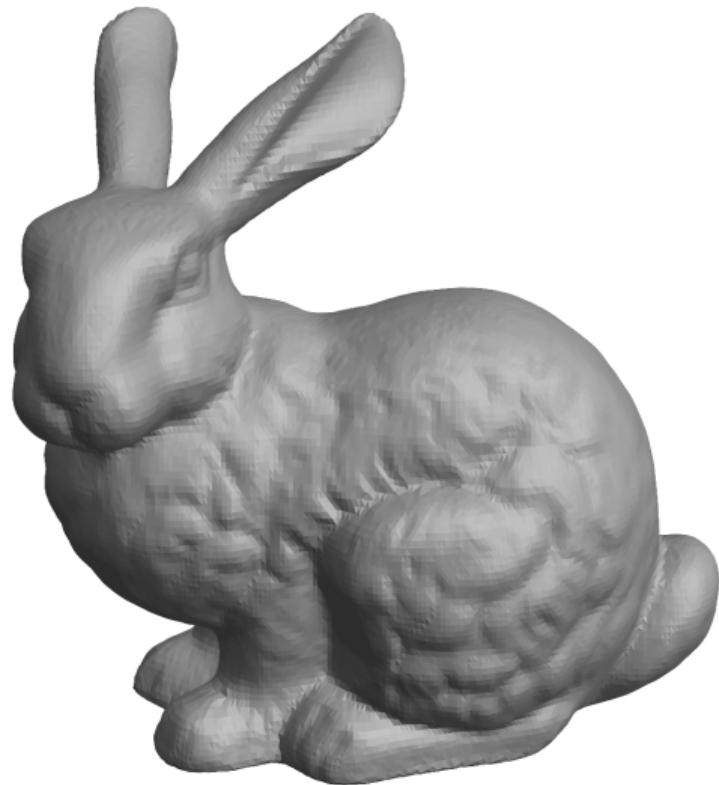
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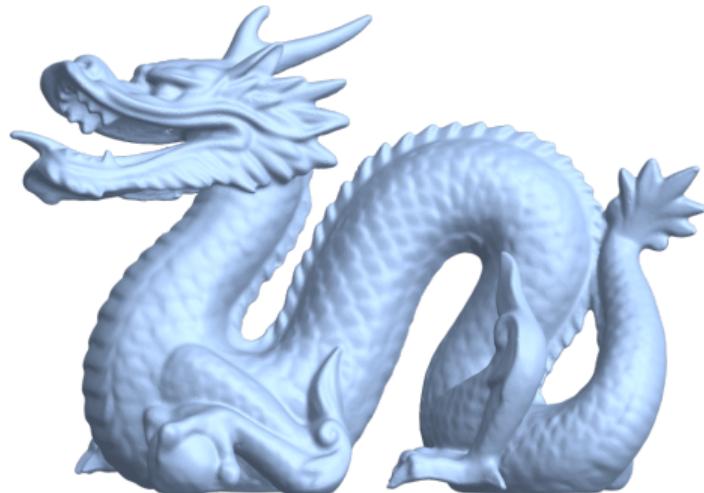
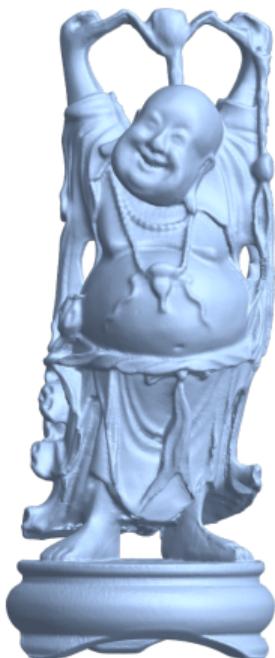
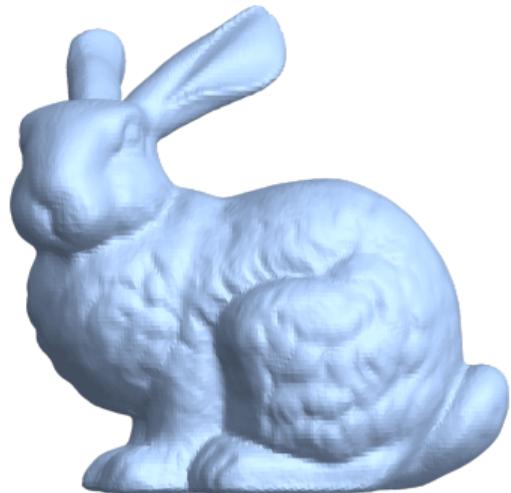
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Point cloud reconstruction with minimal cycles

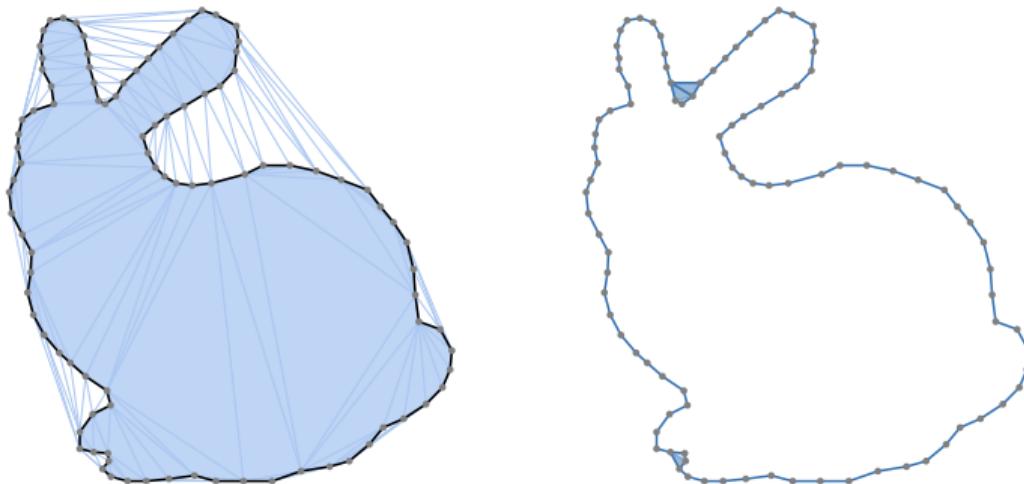


Wrap complexes support minimal cycles

Theorem (B, Roll 2024)

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 $\text{Del}_r(X)$ is supported on $\text{Wrap}_r(X)$.



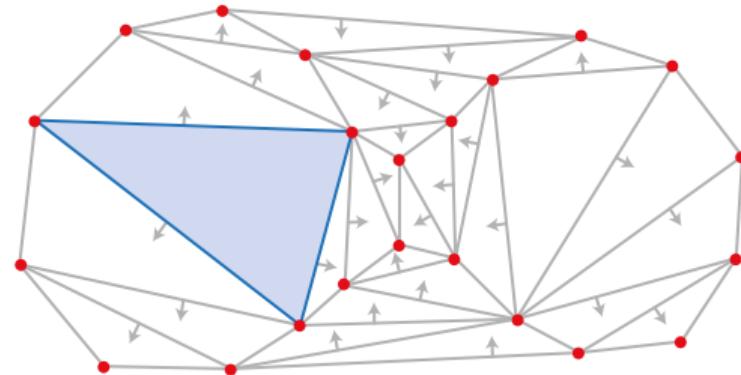
Algebraic gradient flows and persistent homology

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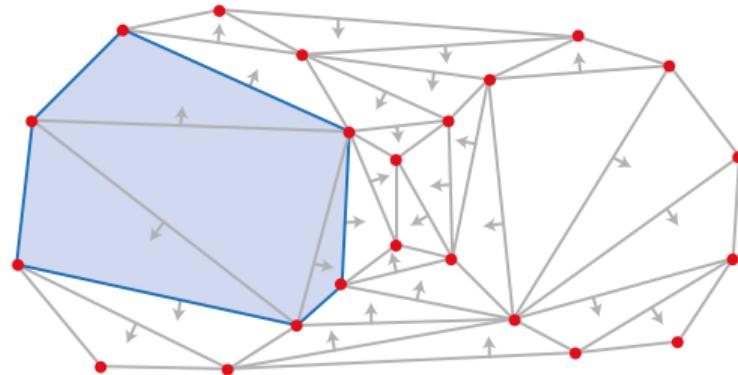
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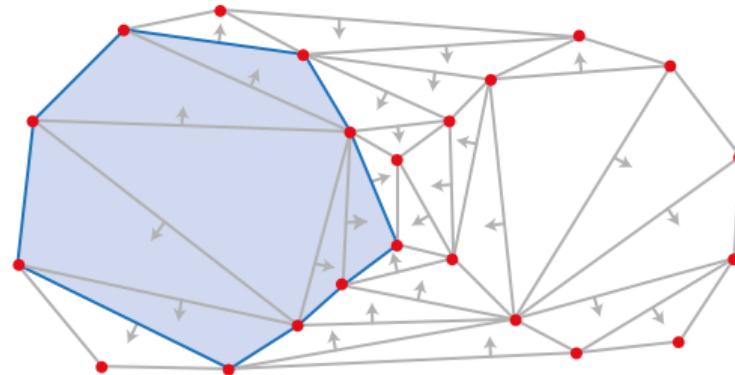
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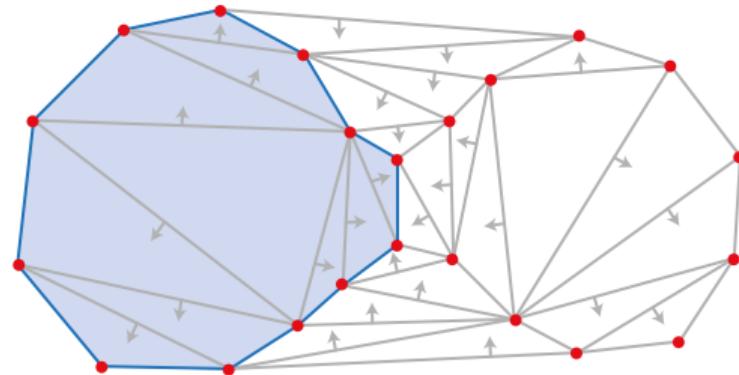
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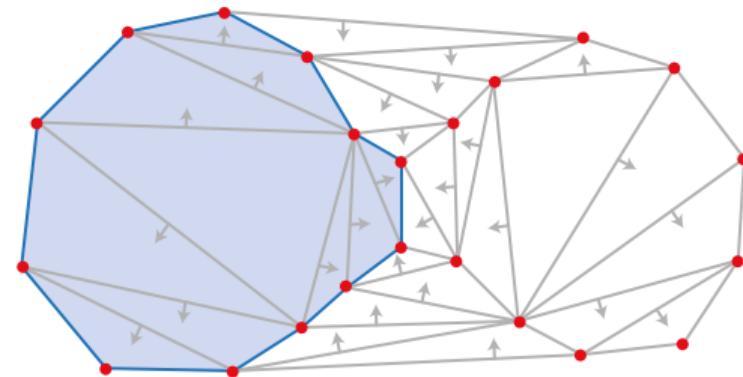
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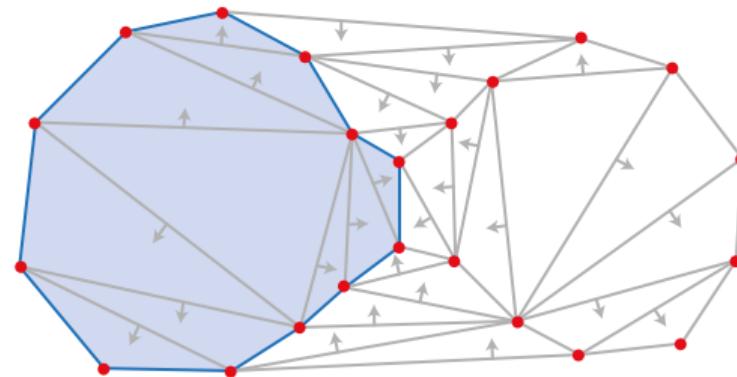


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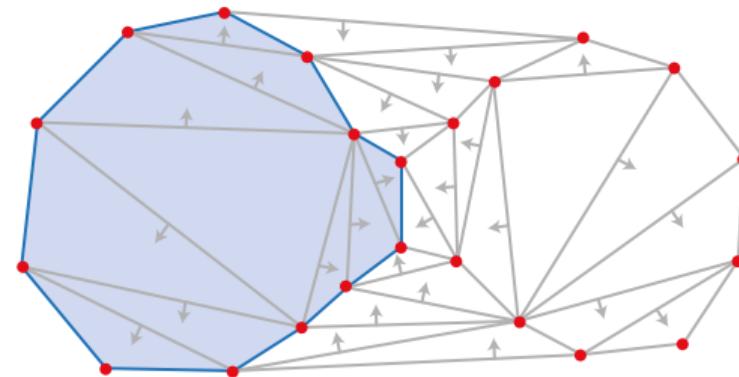
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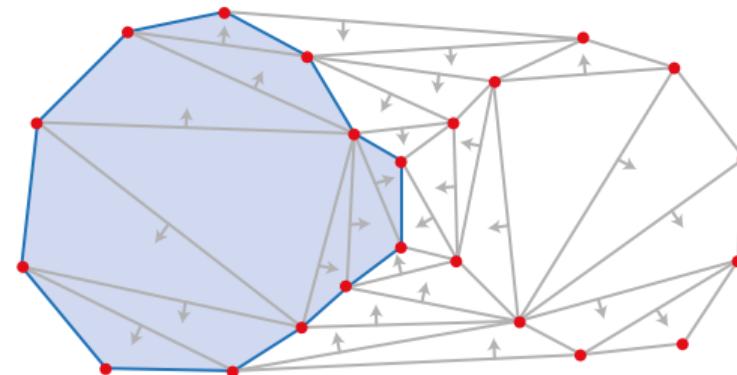
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- Matrix reduction (exhaustive) corresponds to gradient flow

Making discrete Morse theory algebraic

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This generalized Forman's theory for cell complexes:

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- All further definitions of discrete Morse theory apply verbatim

Algebraic gradients from persistent homology

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- Thus the apparent pairs gradient is a subset of the reduction gradient.

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For a cycle $z \in Z_*(K_i)$ in a simplexwise filtration $(K_i = \{\sigma_1, \dots, \sigma_i\})_i$, the following are equivalent:

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- z is invariant under the flow induced by the reduction gradient.

Key insights leading to the theorem

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 - Thus, a flow invariant cycle is also supported on the Wrap complex.

Thanks for your attention!

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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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Transactions of the AMS, 2017. doi:10.1090/tran/6991



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Ripser: efficient computation of Vietoris–Rips persistence barcodes

Journal of Applied and Computational Topology, 2021. doi:10.1007/s41468-021-00071-5