Apparent pairs and optimal cycles

Ulrich Bauer

Technical University of Munich (TUM)

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The geometric realization of AATRN

IMSI Institute, Chicago

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DFG Deutsche Forschungsgemeinschaft
German Research Foundation

SFB TRR 109 Discretization in Geometry and Dynamics

MDSI

mcml Munich Center for Machine Learning

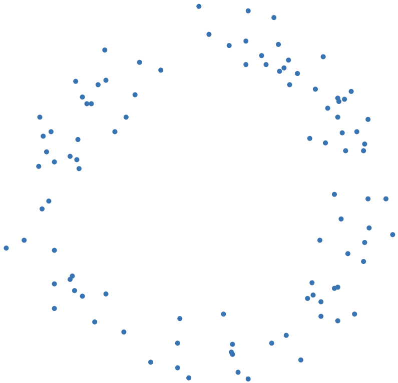
Technical University of Munich TUM

Ripser shortcuts

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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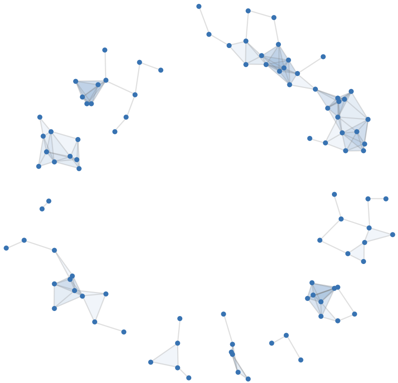

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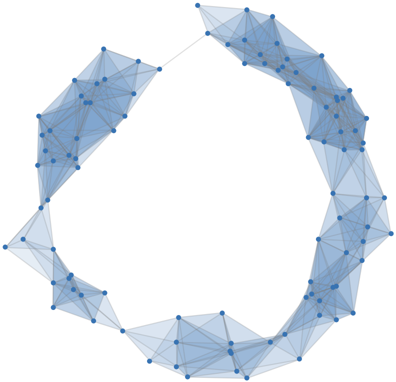

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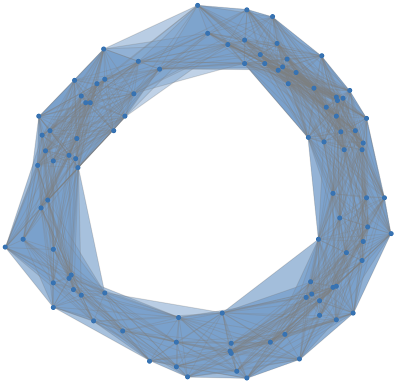

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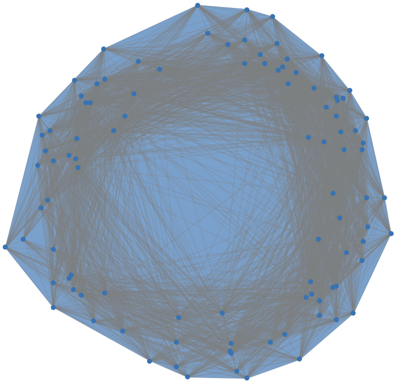
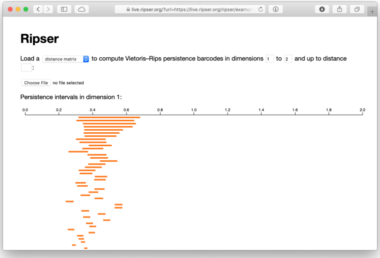
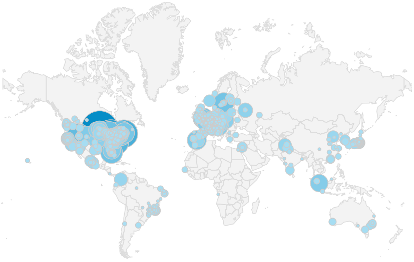


Ripser: software for computing Vietoris–Rips persistence barcodes

Open source software (`ripser.org`)





Ripser users worldwide

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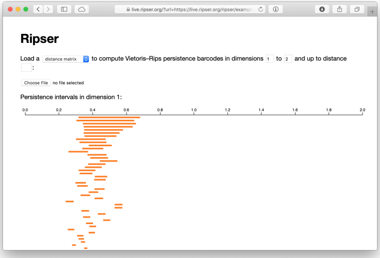

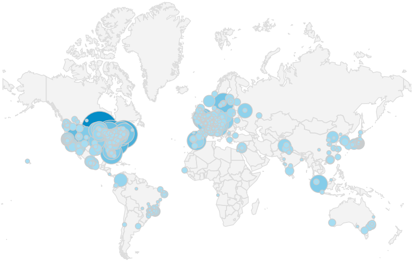

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Efficient matrix algorithm based on

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

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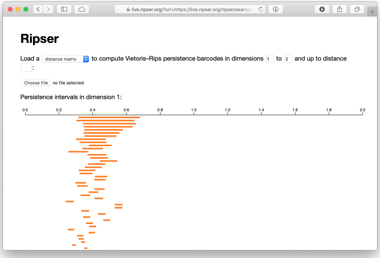

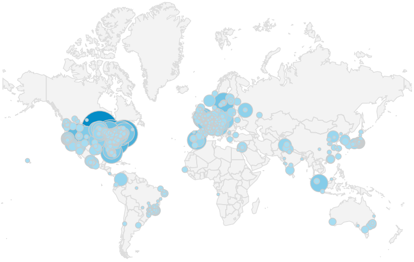

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Efficient matrix algorithm based on

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Computational improvements based on

- *implicit matrix representations*, avoiding storage of boundary matrix
- *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 many times

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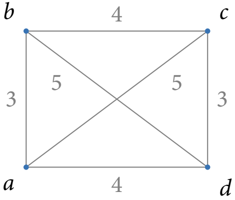
Proposition (B 2021)

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



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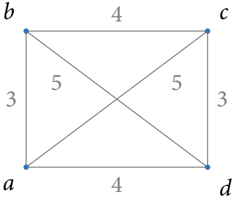

$$
\partial_1 = \begin{array}{cccccccc}
 & (a,b){:}3 & (c,d){:}3 & (a,d){:}4 & (b,c){:}4 & (a,c){:}5 & (b,d){:}5 & \\
\left(\begin{array}{c} \\ \\ \\ \\ \end{array}\right. & 1 & & 1 & & 1 & & \left.\begin{array}{c} \\ \\ \\ \\ \end{array}\right) \; (a) \\
 & \mathbf{1} & & & 1 & & 1 & (b) \\
 & & 1 & & 1 & 1 & & (c) \\
 & & \mathbf{1} & 1 & & & 1 & (d)
\end{array}
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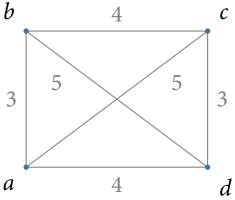

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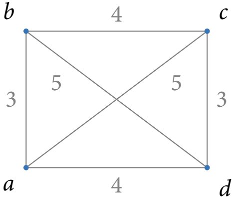
$$\partial_2 = \begin{array}{c} \begin{array}{cccc} (a,b,c){:}5 & (a,b,d){:}5 & (a,c,d){:}5 & (b,c,d){:}5 \end{array} \\ \begin{pmatrix} 1 & 1 & & \\ & & 1 & 1 \\ & 1 & 1 & \\ 1 & & & 1 \\ \mathbf{1} & & 1 & \\ & \mathbf{1} & & 1 \end{pmatrix} \end{array} \begin{array}{c} \\ (a,b){:}3 \\ (c,d){:}3 \\ (a,d){:}4 \\ (b,c){:}4 \\ (a,c){:}5 \\ (b,d){:}5 \end{array}$$

Apparent pairs of the diameter-lexicographic filtration



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$$\partial_3 = \begin{array}{c} (a,b,c,d) \\ \left(\begin{array}{c} 1 \\ 1 \\ 1 \\ \mathbf{1} \end{array}\right) \end{array} \begin{array}{c} \\ (a,b,c) \\ (a,b,d) \\ (a,c,d) \\ (b,c,d) \end{array}$$

A shortcut for finding pivots

$$
\begin{array}{cc}
(a,b,c) & \\
\begin{pmatrix} 1 \\ 1 \\ \\ 1 \\ \\ \end{pmatrix} &
\begin{matrix} (a,b) \\ (a,c) \\ (a,d) \\ (b,c) \\ (b,d) \\ (c,d) \end{matrix}
\end{array}
\qquad\qquad
\begin{array}{cc}
(a,b,c){:}5 & \\
\begin{pmatrix} \\ \\ \\ \\ \\ \end{pmatrix} &
\begin{matrix} (a,b){:}3 \\ (c,d){:}3 \\ (a,d){:}4 \\ (b,c){:}4 \\ (a,c){:}5 \\ (b,d){:}5 \end{matrix}
\end{array}
$$

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

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$$
\begin{array}{cl}
(a,b,c) & \\
\begin{pmatrix} 1 \\ 1 \\ \\ 1 \\ \\ \end{pmatrix} &
\begin{array}{l} (a,b) \\ (a,c) \\ (a,d) \\ (b,c) \\ (b,d) \\ (c,d) \end{array}
\end{array}
\longrightarrow
\begin{array}{cl}
(a,b,c){:}5 & \\
\begin{pmatrix} \\ \\ \\ 1 \\ \\ \end{pmatrix} &
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\end{array}
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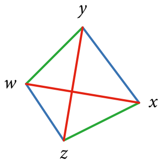
Hyperbolic collapses

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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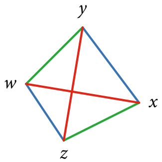

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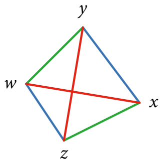

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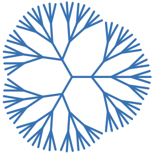
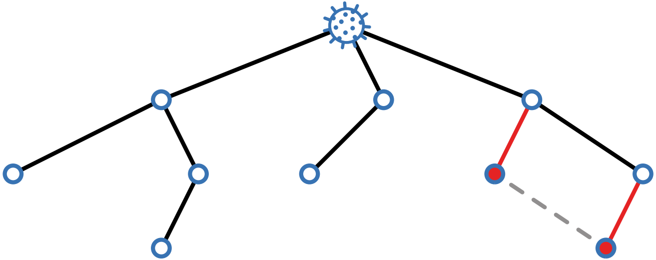
- Metric trees and their subspaces are precisely the 0-hyperbolic spaces.



Topology of viral evolution



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

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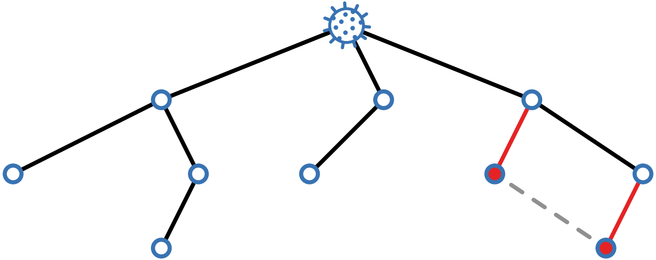

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Observation: Ripser runs unusually fast on genetic distance data

- 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)

Rips complexes of hyperbolic spaces

Theorem (Rips; Gromov 1988)

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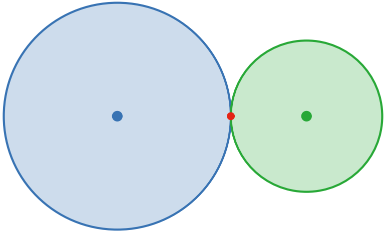
Theorem (B, Roll 2022)

Let X be a δ-hyperbolic ν-almost geodesic space. Then there is a discrete gradient encoding the collapses

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

for all $u > t \geq 4\delta + 2\nu$.

Geodesic defect



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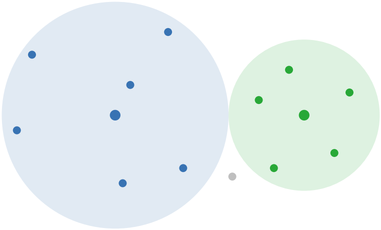

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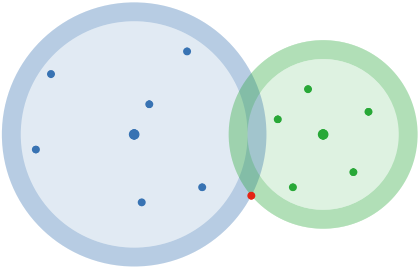

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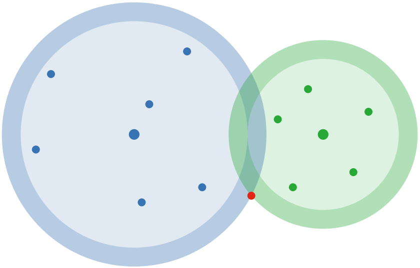
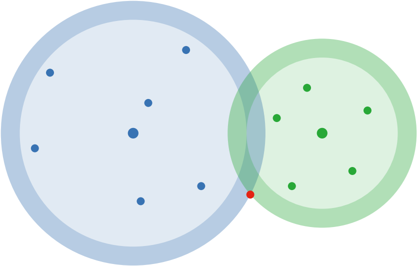


Definition (Bonk, Schramm 2000)

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

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

Geodesic defect



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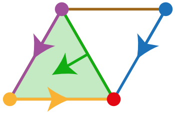
We call the infimum of all such ν the *geodesic defect* of X.

Discrete Morse theory

Definition (Forman 1998)

A *discrete vector field* on a cell complex is a partition of the set of simplices into



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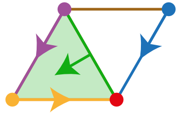

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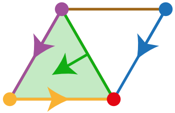

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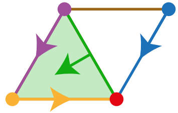

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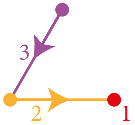

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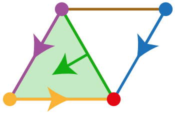

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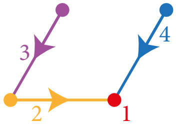

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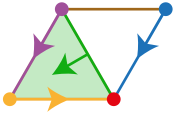

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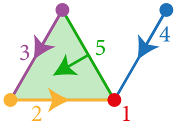

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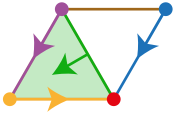

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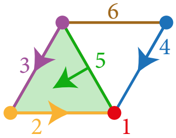

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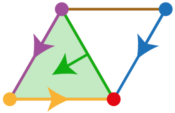

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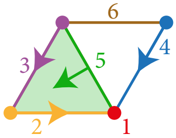

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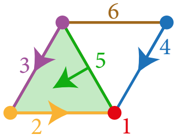

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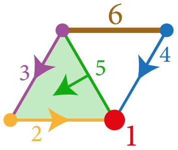

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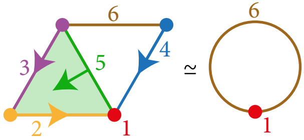

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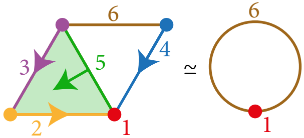

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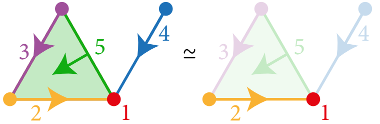

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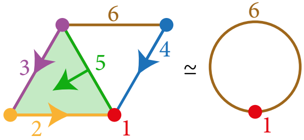

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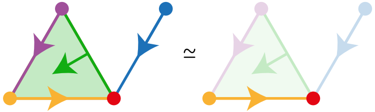

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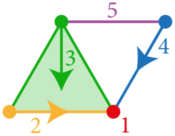

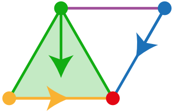

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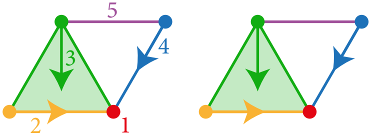

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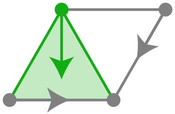

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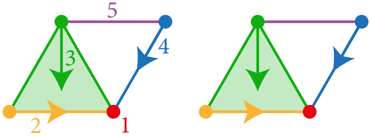

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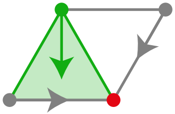

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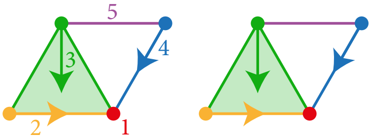

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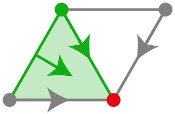

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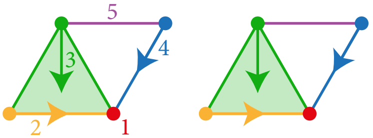

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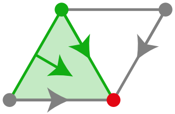

Proposition (B, Roll 2022)

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 $\operatorname{diam}\colon \Delta(V) \to \mathbb{R}$ *is a generalized discrete Morse function.*

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

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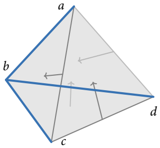

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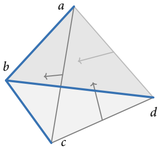

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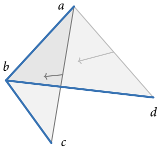

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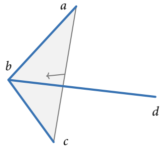

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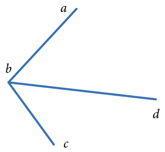

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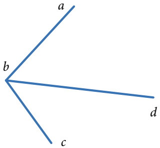

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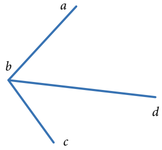

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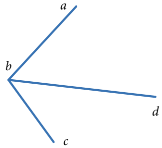

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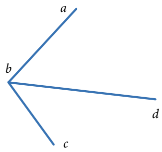

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- *apparent pairs* (based on a tree vertex ordering; refines the perturbed gradient)

Wrapping cycles

Morse theory for Čech and Delaunay complexes

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The Čech complexes and the Delaunay complexes (alpha shapes) are sublevel sets of (generalized) discrete Morse functions. Both functions have the same critical simplices/values.

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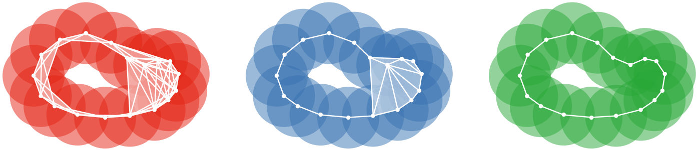
Theorem (B, Edelsbrunner 2017)

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:

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



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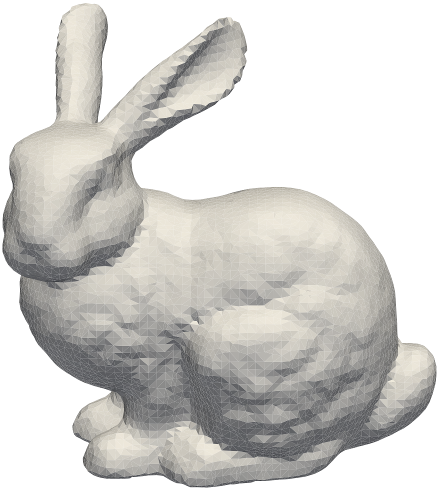
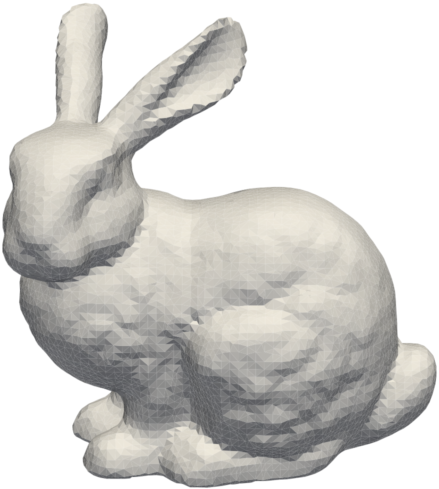


From Delaunay to Wrap complexes



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

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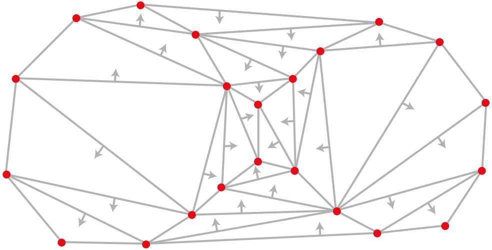

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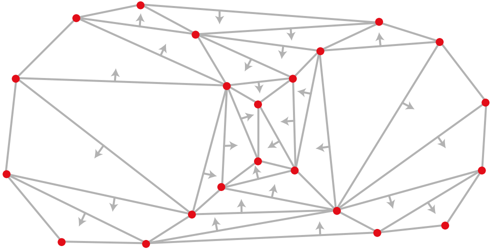

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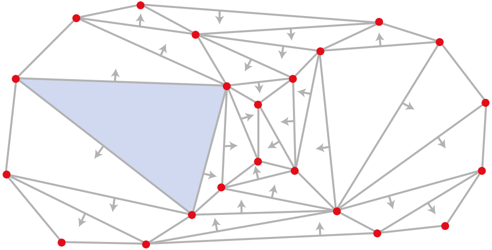

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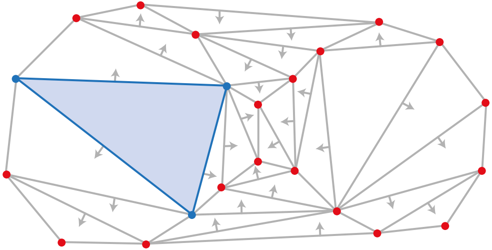

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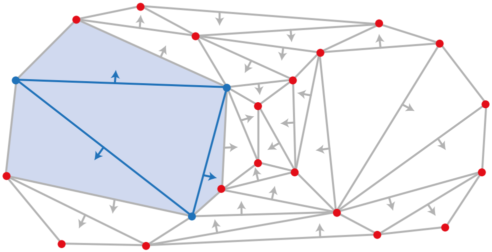

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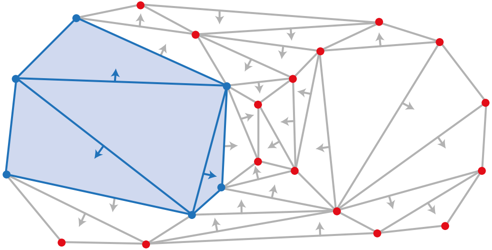

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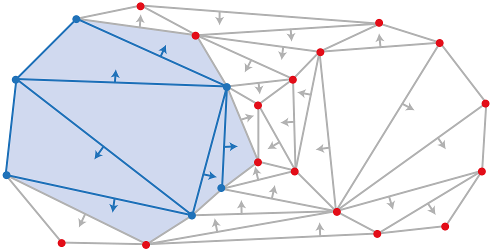

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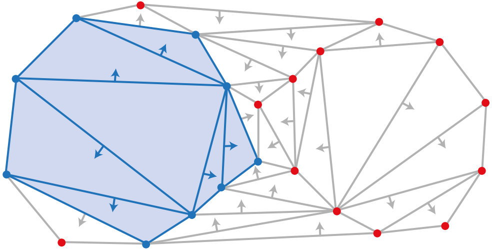

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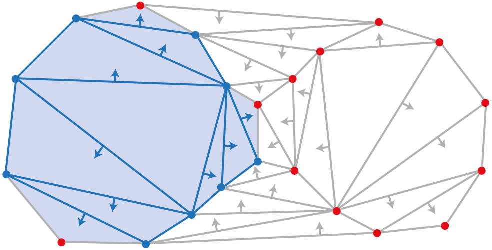

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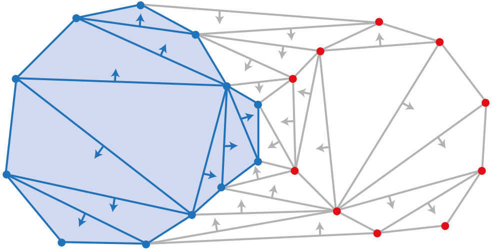

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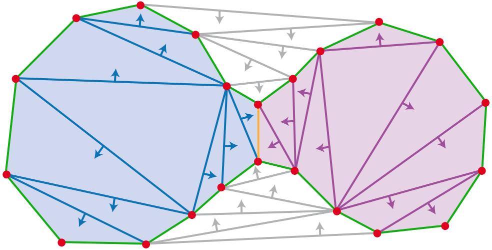

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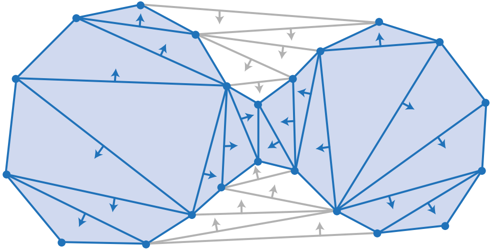

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Computing persistent homology via matrix reduction

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 $\mathrm{pivot}\, R_i = \mathrm{pivot}\, R_j$ **do**
      add column R_i to column R_j $\quad\triangleright$ eliminate the nonzero entry in row $\mathrm{pivot}\, R_i$
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Proposition

The resulting columns R_j are lexicographically minimal cycles within their homology class $[R_j] \in K_{j-1}$.

Standard reduction and exhaustive reduction

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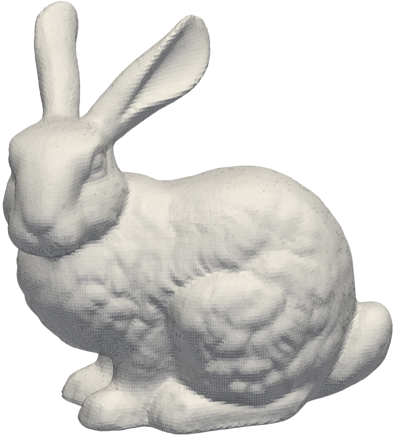

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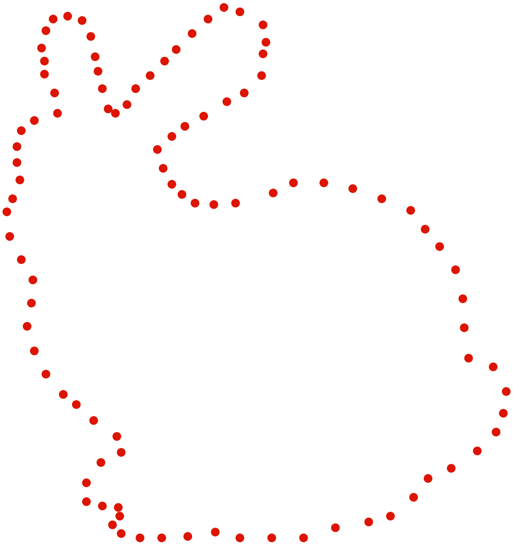

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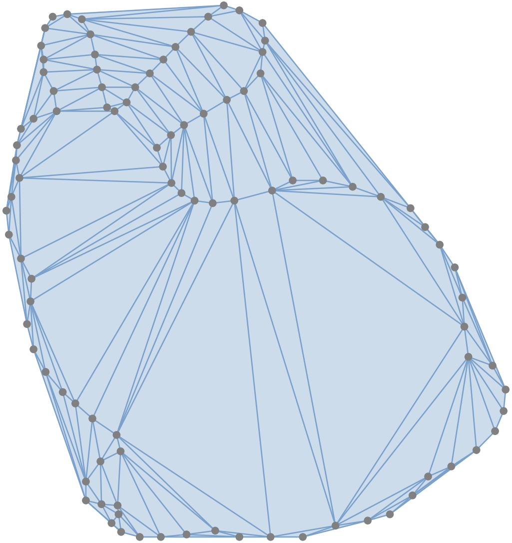

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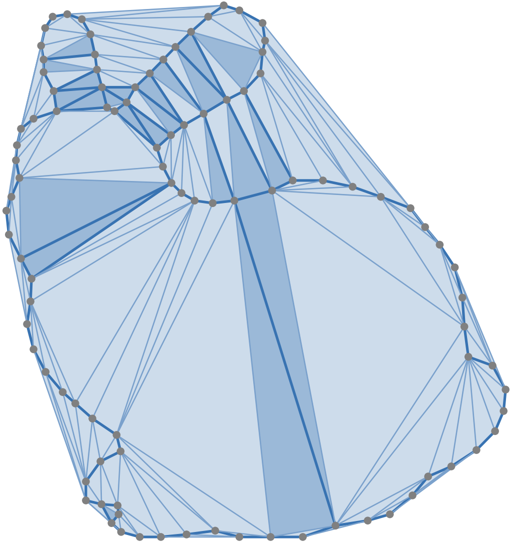

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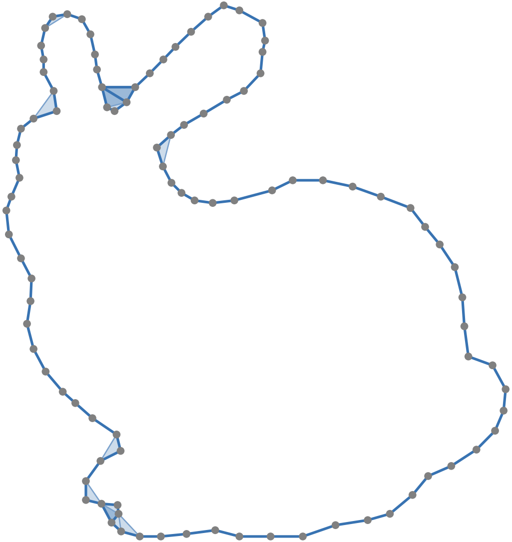

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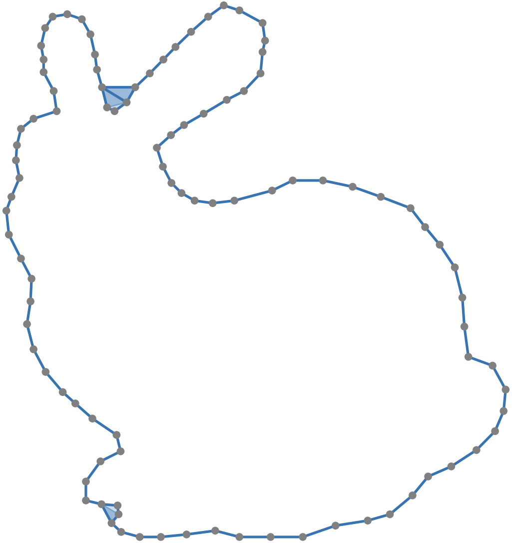

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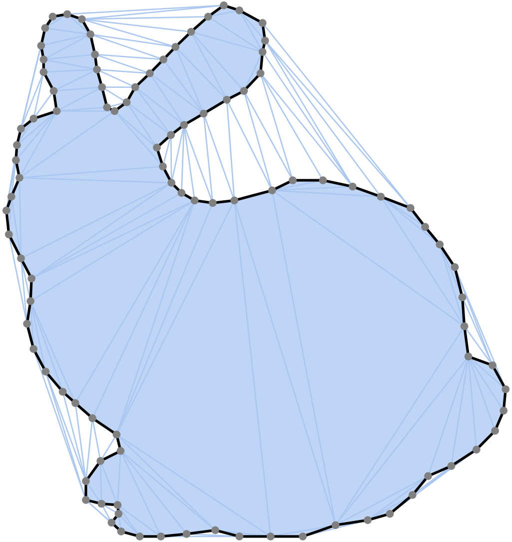

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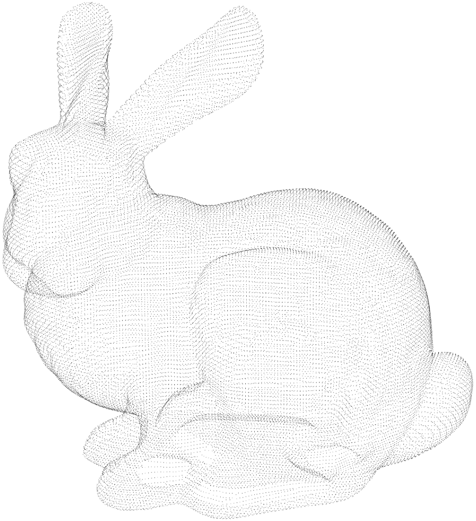

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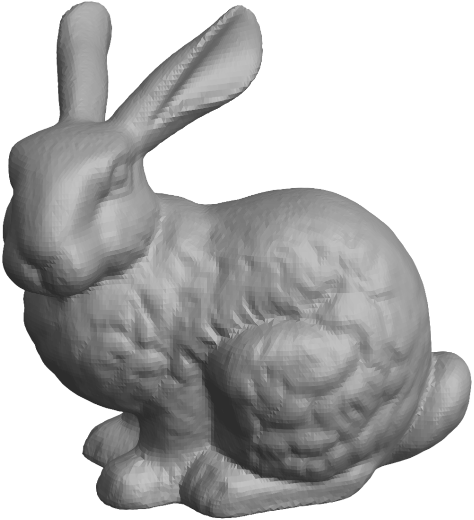
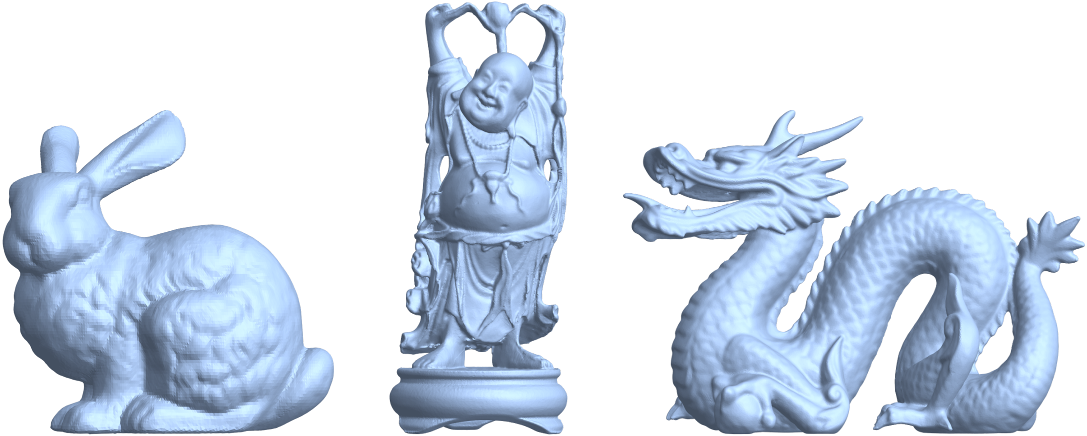


Surface reconstruction with minimal cycles

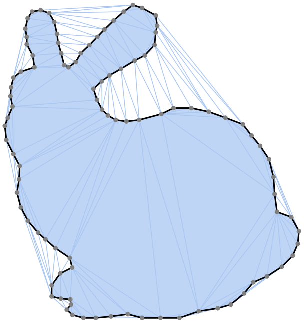


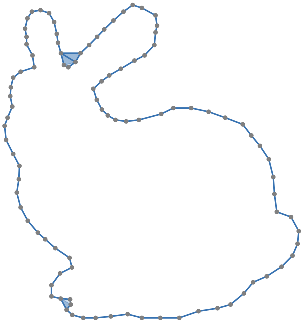
Wrap complexes support minimal cycles

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





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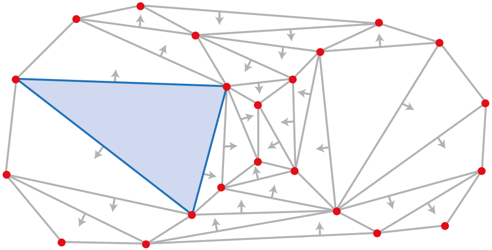

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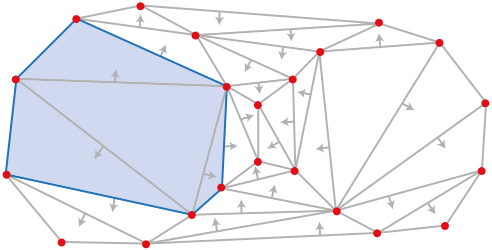

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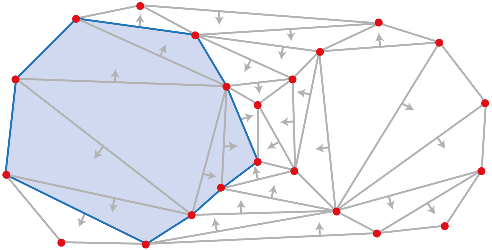

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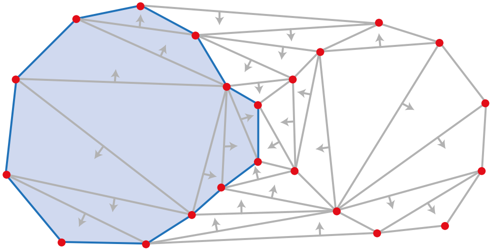

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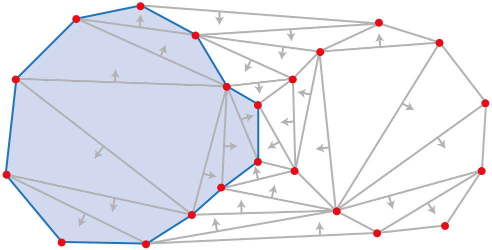

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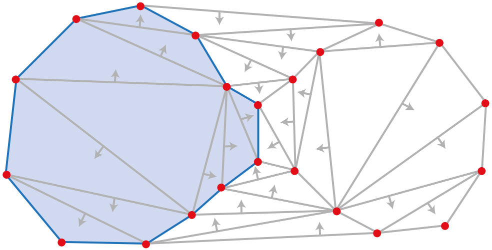

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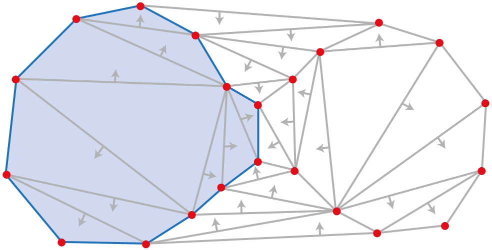

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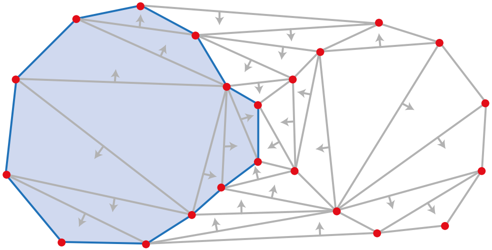

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This generalized Forman's theory for cell complexes:

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- All further definitions of discrete Morse theory apply verbatim.

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

Different angles on wrapping cycles

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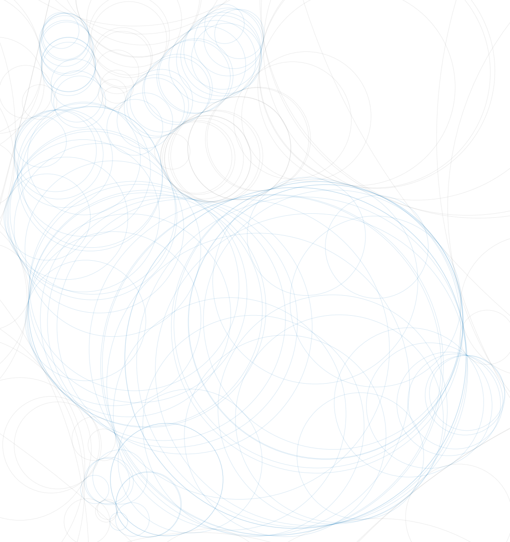
Thanks for your attention!



http://ulrich-bauer.org/apparent-pairs-talk-imsi.pdf

Thanks for your attention!

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