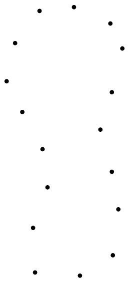
Geometric Complexes in Topological Data Analysis

Fabian Roll

Technical University of Munich

Persistent homology pipeline



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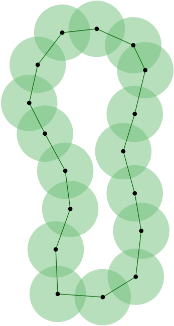

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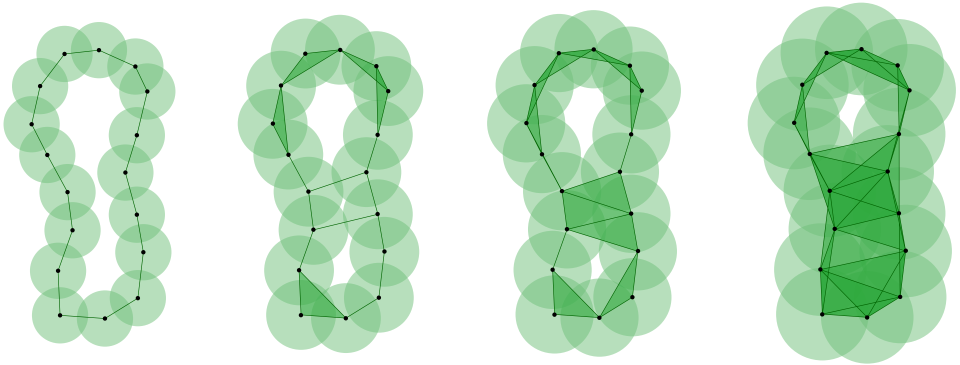

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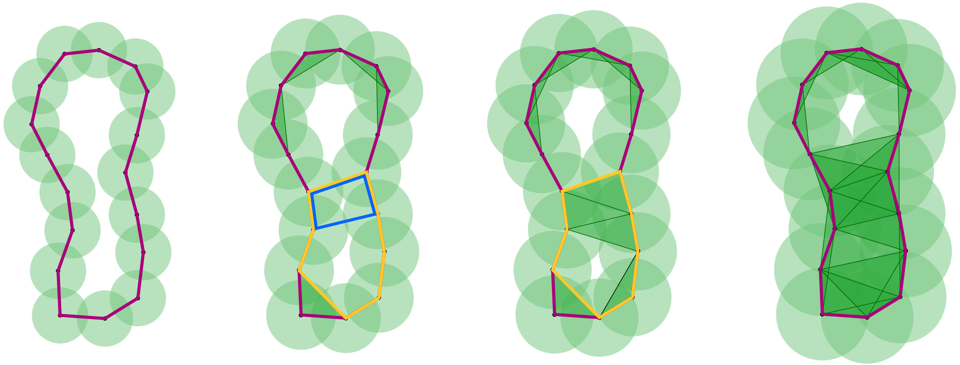

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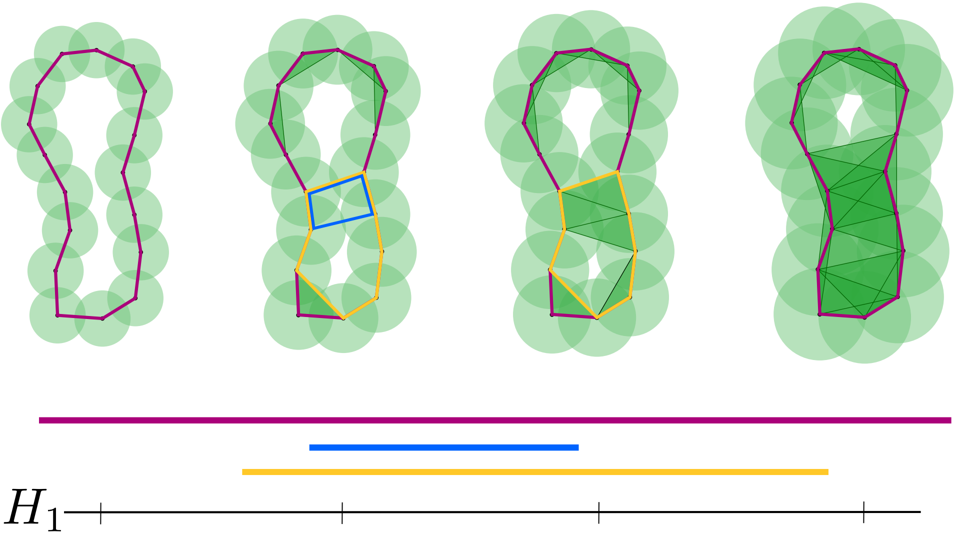
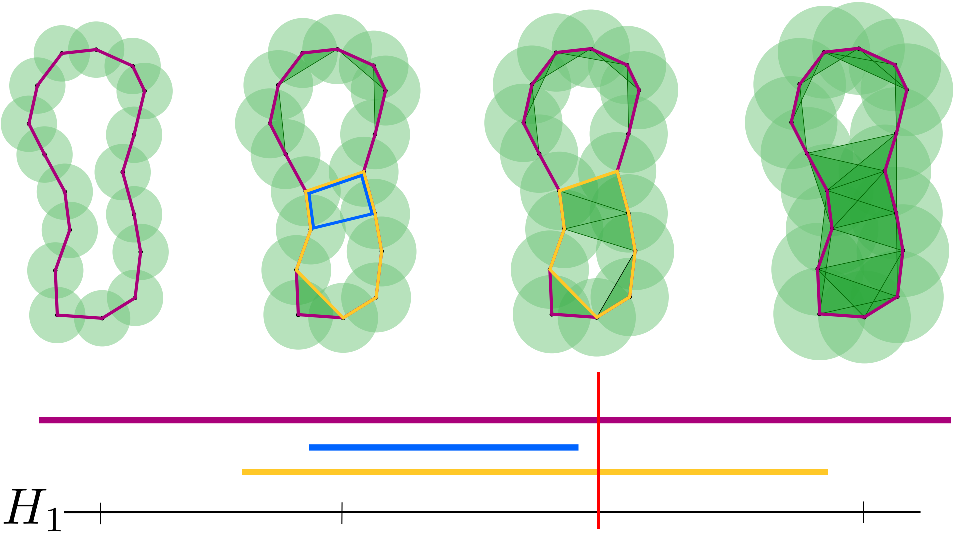


Research question about geometric complexes

What are interesting topological properties and how do they interact with the persistent homology pipeline?

Nerve theorems



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- no general-purpose and complete discussion of this topic in the literature that is tailored to the use cases in topological data analysis (e.g., functorial closed cover nerve theorems)

Nerve theorems - contributions

- provide a thorough overview to (functorial) nerve theorems for open/closed covers

$$\begin{tikzcd} {|\mathrm{Nrv}(\mathcal{U}_r)|} \arrow[r] \arrow[d, "\simeq"] \arrow[dr, phantom, "\circlearrowright ?"] & {|\mathrm{Nrv}(\mathcal{U}_l)|} \arrow[d, "\simeq"'] \\ X_r \arrow[r] & X_l \end{tikzcd}$$

U. Bauer, M. Kerber, F. Roll, and A. Rolle
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  - Quillen (1967): formalizes similarities between homotopy theory and homological algebra
- give various counterexamples that show the non-obvious subtleties of nerve theorems

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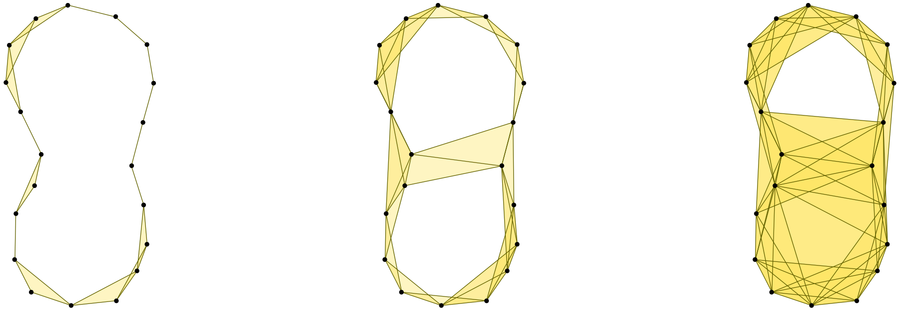
Vietoris–Rips complexes

Definition. Let X be a metric space. The Vietoris-Rips complex at scale r is the simplicial complex

$$\mathrm{Rips}_r(X) = \{S \subseteq X \text{ finite} \mid S \neq \emptyset,\ \operatorname{diam} S \leq r\}.$$



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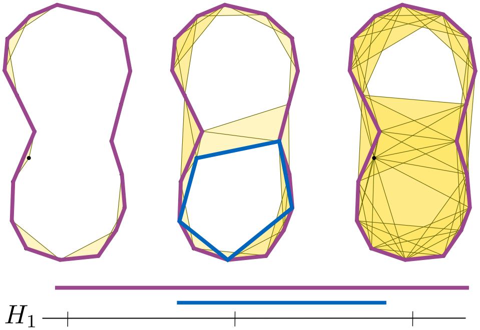
- For $r \to 0$: Used by Leopold Vietoris (1927) to extend homology theory to metric spaces.
- For $r \to \infty$: Used by Eliyahu Rips and Mikhael Gromov (1987) to study hyperbolic groups.
- For all $r > 0$: Used in topological data analysis (nowadays) in the context of persistent homology:



Application of Vietoris–Rips persistent homology

COVID-19 genetic evolution data

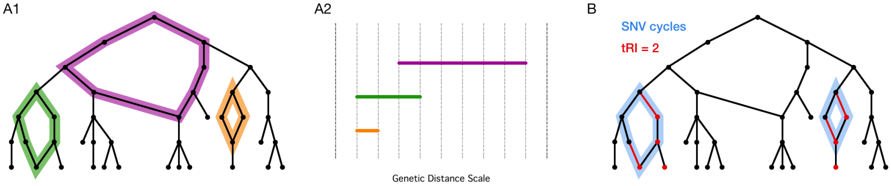


Figure 2. Topological data analysis quantifies convergent evolution. (A) Persistent homology detects reticulate events in viral evolution by means of a persistence barcode. Each bar in the barcode (A2) corresponds to a topological cycle in the reticulate phylogeny (A1). Bars at small genetic distance scales are expected to correspond mainly to homoplasies, while recombination events typically produce topological features at larger scales. (B) SNV cycles are topological cycles in the reticulate phylogeny for which adjacent sequences differ by single nucleotide variations (SNV) only. Under the assumption of single substitutions per site, any SNV in

M. Bleher, L. Hahn, M. Neumann, J. A. Patino-Galindo, M. Carriere, U. Bauer, R. Rabadan, and A. Ott
Topological data analysis identifies emerging adaptive mutations in SARS-CoV-2
Preprint, arXiv:2106.07292, 2023

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covid data (≈ 15000 points)	Ripser's runtime
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ordered reversed chronologically	2 min

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We address two questions:

1. What about non-geodesic spaces? Finite metric spaces?
2. Connections to Ripser?

Generalized contractibility lemma

Theorem (Bauer, R). Let X be a δ-hyperbolic metric space. Then there is a discrete gradient encoding the collapses

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

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

U. Bauer, F. Roll
Gromov Hyperbolicity, Geodesic Defect, and Apparent Pairs in Vietoris-Rips Filtrations
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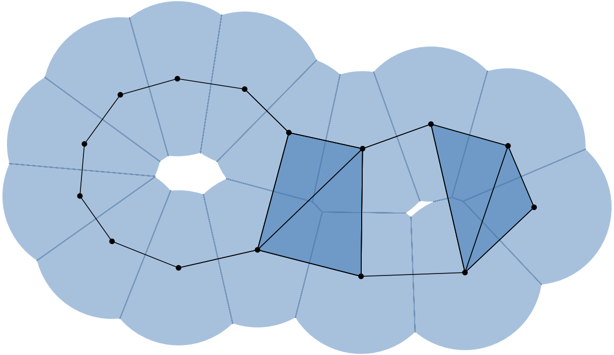
- In this case, Ripser computes the persistent homology without a single matrix operation.
  - Heuristically explains its outstanding performance on genetic distances (close to tree metrics).
- We use symbolic pertubation of edge lengths in the proof.
  - If X is generic, the diameter function is a generalized discrete Morse function.

Delaunay complexes

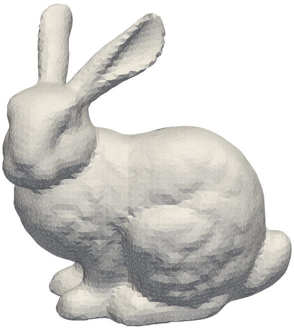
Definition. The *Delaunay complex* $\mathrm{Del}_r(X)$, or *alpha complex*, of $X \subseteq \mathbb{R}^d$ is the nerve of the cover by closed Voronoi balls of radius r centered at points in X.



Wrap

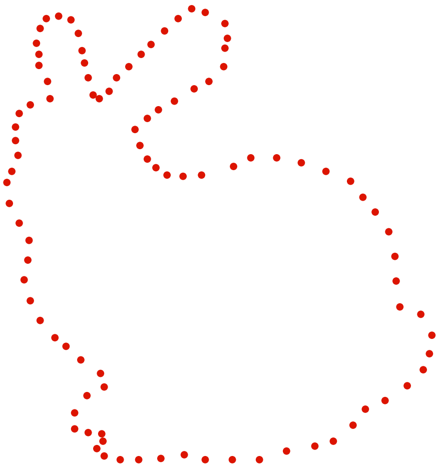
- Originally introduced by Edelsbrunner (1995) as a subcomplex of the Delaunay triangulation for surface reconstruction, using flow lines associated to Euclidean distance functions
- Redeveloped using discrete Morse theory (Forman 1998) by Bauer & Edelsbrunner (2014/17)

Delaunay complex



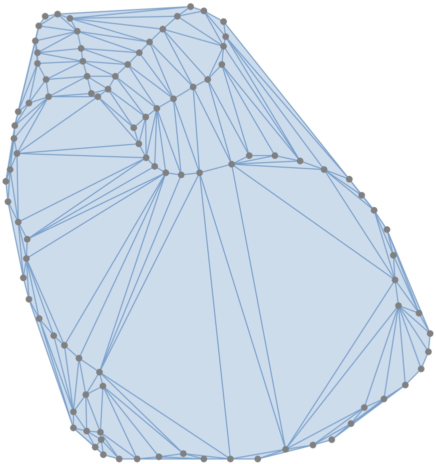
Wrap complex

Wrap complexes



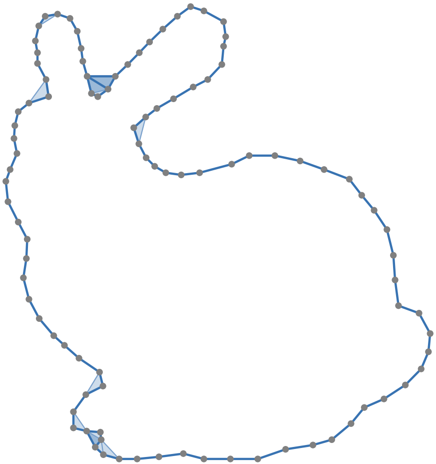
Point cloud

Wrap complexes



Delaunay triangulation

Wrap complexes



Delaunay complex

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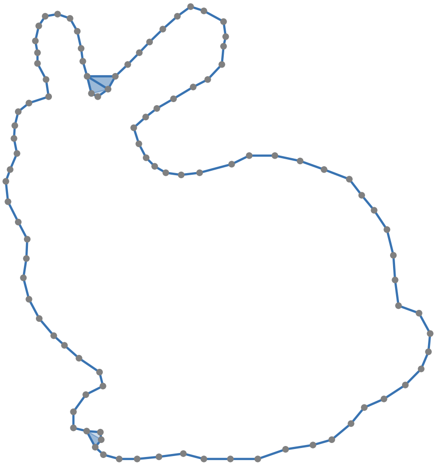
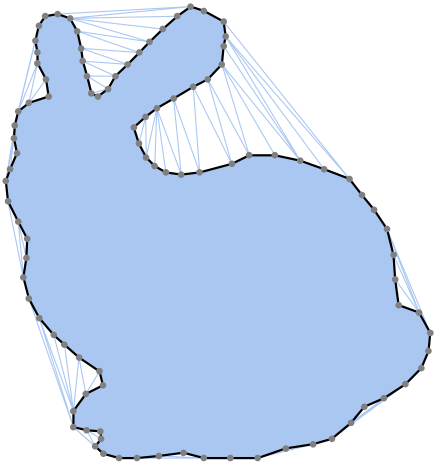


Wrap complex

Wrap complexes

Can we do better?

Exhaustively reduced cycles



Reduction process

Algebraic gradient flows and persistent homology

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  - using a slightly different total order on simplices refining the minimum enclosing radius function

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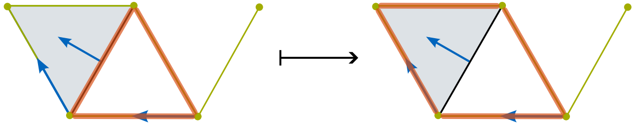
  - using a slightly different total order on simplices refining the minimum enclosing radius function
- Forman (1998) defines a *flow* $C_*(K) \to C_*(K)$ associated to a discrete gradient



Algebraic gradient flows and persistent homology

We interpret persistent homology in terms of algebraic Morse theory:

- persistence pairs form an algebraic gradient

U. Bauer, F. Roll,
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- exhaustive Matrix reduction corresponds to gradient flow
- the lexicographically minimal cycles are invariant under the algebraic gradient flow
- connects to generalized discrete Morse theory, and hence to the Wrap complex, through gradient refinements (by apparent pairs)

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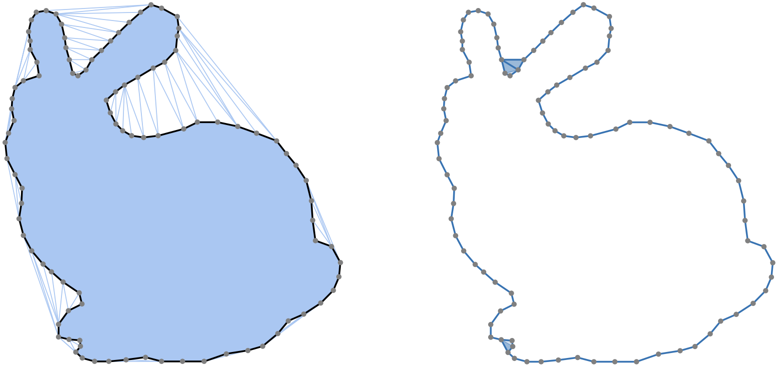
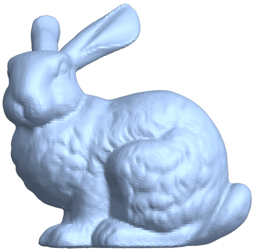
Minimal cycles and Wrap complexes

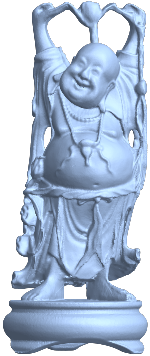
Theorem (Bauer, R). Let $X \subset \mathbb{R}^d$ be a finite subset in general position and let $r \in \mathbb{R}$. Then the lexicographically minimal cycles of $\mathrm{Del}_r(X)$, with respect to the Delaunay-lexicographic order on the simplices, are supported on $\mathrm{Wrap}_r(X)$.

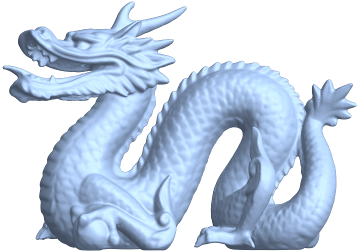


Point cloud reconstruction with most persistent features

The lexicographically minimal cycle, with respect to the Delaunay-lexicographic order on the simplices, corresponding to the interval in the persistence barcode of the Delaunay filtration with the largest death/birth ratio:







```
$ docker build -o output github.com/fabian-roll/wrappingcycles
```

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- Generalized Rips contractibility lemma and explained, in a special case, why the geometry and combinatorics of the input strongly influences the persistence computation time.
- Interpreted persistence in terms of algebraic Morse theory and established a strong connection between a Morse-theoretic and a homological approach to shape reconstruction.