# Complexes from point clouds 

# Geometry, topology, algebra, and combinatorics 

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TUM

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Combinatorial Coworkspace 2022


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## Geometry and topology of biomolecules



Gramicidin (an antibiotic functioning as an ion channel)

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## Čech complexes

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## Definition

Let $X$ be a topological space, and let $\mathcal{U}=\left(U_{i}\right)_{i \in I}$ be a cover of $X$. The nerve of $\mathcal{U}$ is the simplicial complex

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\operatorname{Nrv}(\mathcal{U})=\left\{J \subseteq I| | J \mid<\infty \text { and } \bigcap_{i \in J} U_{i} \neq \varnothing\right\}
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(R. U. Bauer, M. Kerber, F. Roll, and A. Rolle

A Unified View on the Functorial Nerve Theorem and its Variations
Preprint, arXiv:2203.03571, 2022

Delaunay complexes

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## Generalized discrete Morse theory

## Definition (Forman 1996, Chari 2000, Freij 2009)

A generalized discrete vector field on a simplicial complex $K$ is a partition of the simplices into intervals of the face poset:

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A generalized discrete Morse function $f: K \rightarrow \mathbb{R}$ satisfies:

- the sublevel sets $K_{t}=f^{-1}(-\infty, t]$ are subcomplexes (for all $t \in \mathbb{R}$ )
- the level sets $f^{-1}(t)$ form a generalized
 vector field (the discrete gradient of $f$ )


## Refining generalized vector fields

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For each non-critical face interval $[L, U] \in V$ :


- choose an arbitrary vertex $x \in U \backslash L$
- partition $[L, U]$ into pairs

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(Q \backslash\{x\}, Q \cup\{x\}) \text { for all } Q \in[L, U] .
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## Morse theory for Čech and Delaunay complexes

## Proposition (B, Edelsbrunner 2014)

The Čech complexes and the Delaunay complexes (alpha shapes) are sublevel sets of (generalized) discrete Morse functions.

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## Theorem (B., Edelsbrunner 2017)

Čech, Delaunay, and Wrap complexes are related by collapses

$$
\operatorname{Cech}_{r} X \searrow \operatorname{Del}_{r} X \searrow \operatorname{Wrap}_{r} X,
$$

encoded by a single discrete gradient field.


## Delaunay and Wrap complexes



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## Homology inference

## Inferring homology from samples

Given: finite sample $P \subset X$ of unknown shape $X \subset \mathbb{R}^{d}$
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- approximate $X$ by a thickening $P_{\delta}=\bigcup_{p \in P} B_{\delta}(p)$ that covers $X$

This can work, but requires strong assumptions:

## Homology reconstruction by thickening

Theorem (Niyogi, Smale, Weinberger 2006)
Let $X$ be a submanifold of $\mathbb{R}^{d}$. Let $P \subset X$ and $\delta>0$ be such that

- $P_{\delta}$ covers X, and
- $\delta<\sqrt{3 / 20} \operatorname{reach}(X)$.

Then $H_{*}(X) \cong H_{*}\left(P_{2 \delta}\right)$.

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Let $X \subset \mathbb{R}^{d}$. Let $P \subset X$ and $\delta>0$ be such that

- $P_{\delta}$ covers $X$,
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- A filtration is a certain diagram $K: \mathbf{R} \rightarrow$ Top of topological spaces, indexed over the poset of real numbers $\mathbf{R}:=(\mathbb{R}, \leq)$

- a topological space $K_{t}$ for each $t \in \mathbb{R}$
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- Apply homology $H_{*}$ : Top $\rightarrow$ Vect
- Persistent homology is a diagram $M=H_{\star} \circ K: \mathbf{R} \rightarrow$ Vect (persistence module):

$$
\cdots \cdots \cdots M_{s} \longrightarrow M_{t} \cdots \cdots \cdots \cdots
$$




## Barcodes: the structure of persistence modules

## Theorem (Crawley-Boevey 2015)

Any persistence module $M: \mathbf{R} \rightarrow$ vect (of finite dim. vector spaces over some field $\mathbb{F}$ ) decomposes as a direct sum of interval modules

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- The supporting intervals form the persistence barcode.



## Computation

## Homology by matrix reduction

Notation:

- $D$ : boundary matrix (with $\mathbb{Z}_{2}$ coefficients)
- $R_{i}$ : ith column of matrix $R$
- pivot $R_{i}$ : maximal row index with nonzero entry in column $R_{i}$

Matrix reduction algorithm (variant of Gaussian elimination):

- $R=D, V=I$
- while $\exists i<j$ with pivot $R_{i}=\operatorname{pivot} R_{j}$
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Result:

- $R=D \cdot V$ is reduced (each column has a unique pivot)
- $V$ is full rank upper triangular


## Persistent homology by matrix reduction




3

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5


|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 |  |  | 1 |  | 1 |  |  |
| 2 |  |  | 1 |  |  | 1 |  |
| 3 |  |  |  |  |  |  | 1 |
| 4 |  |  |  |  | 1 | 1 |  |
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| 3 |  |  |  |  |  |  | 1 |
| 4 |  |  |  |  | 1 | 0 |  |
| 5 |  |  |  |  |  |  | 1 |
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## Persistent homology by matrix reduction



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|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
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## Stability

## Stability of persistence barcodes for functions

Theorem (Cohen-Steiner, Edelsbrunner, Harer 2005)
Let $f, g: X \rightarrow \mathbb{R}$ with $\|f-g\|_{\infty}=\delta$ (and some regularity assumptions).

- Consider the sublevel set filtrations $f^{-1}(\infty, t]$ and $g^{-1}(\infty, t]$, and
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Then there exists a $\delta$-matching between the barcodes, meaning that:


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- unmatched intervals have length $\leq 2 \delta$.



## Persistence and stability: the big picture

Data
point cloud
$P \subset \mathbb{R}^{d}$

## Persistence and stability: the big picture



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| Data | point cloud | $P \subset \mathbb{R}^{d}$ |
| :---: | :---: | :---: |
|  | $\downarrow \text { distance }$ |  |
| Geometry | function | $f: \mathbb{R}^{d} \rightarrow \mathbb{R}$ |
| $\downarrow$ | $\downarrow$ sublevel sets |  |
| Topology | topological spaces (filtration) | $K: \mathbf{R} \rightarrow$ Top |
| $\downarrow$ | homology |  |
| Algebra | vector spaces (persistence module) | $M: \mathbf{R} \rightarrow \mathbf{V e c t}$ |

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| Algebra | vector spaces (persistence module) | $M: \mathbf{R} \rightarrow$ Vect |
| I | $\downarrow$ structure theorem |  |
| Combinatorics | intervals (persistence barcode) | $B: \mathbf{R} \rightarrow \mathbf{M c h}$ |

## Persistence and stability: the big picture



## Persistence and stability: the big picture



## Interleavings

Let $\delta=\|f-g\|_{\infty}$. Write $F_{t}=f^{-1}(-\infty, t]$ for the $t$-sublevel set of $f$.

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Applying homology, the persistence modules
$H_{*}(F), H_{*}(G): \mathbf{R} \rightarrow$ Vect are $\delta$-interleaved:


## Algebraic stability of persistence barcodes

Theorem (Chazal et al. 2009, 2012; B, Lesnick 2015)
If two persistence modules are $\delta$-interleaved, then there exists a $\delta$-matching of their barcodes.


## Structure of persistence sub-/quotient modules

## Proposition (B, Lesnick 2015)

Let $M \rightarrow N$ be an epimorphism of persistence modules.
Then there is an injection of barcodes $B(N) \hookrightarrow B(M)$ such that
if J is mapped to $I$, then

- I and are aligned below, and
- I bounds above.

This construction is functorial.

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This construction is functorial.
Dually, there is an injection $B(M) \hookrightarrow B(N)$ for monomorphisms $M \rightarrow N$.

## Induced matchings

For $f: M \rightarrow N$ a general morphism of pfd persistence modules, the epi-mono factorization

$$
M \rightarrow \operatorname{im} f \hookrightarrow N
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If $f$ is a $\delta$-interleaving morphism, then this is a $\delta$-matching.

## Simplification

## Topological simplification of functions

Consider the following problem:

## Problem (Topological simplification)

Given a function $f$ and a real number $\delta \geq 0$, find a function $f_{\delta}$ with the minimal number of critical points subject to $\left\|f_{\delta}-f\right\|_{\infty} \leq \delta$.






## Persistence and Morse theory

Morse theory (smooth or discrete):

- Relates critical points to homology of sublevel sets
- Provides a method for canceling pairs of critical points

(from Milnor: Lectures on the h-cobordism theorem, 1965)


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Persistent homology:
- Relates homology of different sublevel set
- Identifies pairs of critical points (birth and death of homology) and quantifies their persistence


## Combining persistence and Morse theory

For a Morse function:

- critical points correspond to endpoints of barcode intervals


## Combining persistence and Morse theory

For a Morse function:

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## Proposition

The critical points of $f$ with persistence $>2 \delta$ provide a lower bound on the number of critical points of any function $g$ with $\|g-f\|_{\infty} \leq \delta$.

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## Theorem (B, Lange, Wardetzky, 2011)

Let $f$ be a function on a surface and let $\delta>0$.
Canceling all pairs with persistence $\leq 2 \delta$ yields a function $f_{\delta}$

- satisfying $\left\|f_{\delta}-f\right\|_{\infty} \leq \delta$ and
- achieving the lower bound on the number of critical points.


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Does not generalize to higher-dimensional manifolds!

## Functional topology

## When was persistent homology discovered？

R H．Edelsbrunner，D．Letscher，and A．Zomorodian
Topological persistence and simplification
Foundations of Computer Science， 2000
國 V．Robbins
Computational Topology at Multiple Resolutions．
PhD thesis，University of Colorado Boulder， 2000
显
P．Frosini
A distance for similarity classes of submanifolds of a Euclidean space
Bulletin of the Australian Mathematical Society， 1990.
俥 S．A．Barannikov．
The framed Morse complex and its invariants．
In Singularities and bifurcations，Adv．Soviet Math．（vol．21）， 1994.

## When was persistent homology discovered first?

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## RANK AND SPAN IN FUNCTIONAL TOPOLOGY

By Marston Morse

(Received August 9, 1939)

## 1. Introduction.

The analysis of functions $F$ on metric spaces $M$ of the type which appear in variational theories is made difficult by the fact that the critical limits, such as absolute minima, relative minima, minimax values etc., are in general infinite in number. These limits are associated with relative $k$-cycles of various dimensions and are classified as 0 -limits, 1 -limits etc. The number of $k$-limits suitably counted is called the $k^{\text {th }}$ type number $m_{k}$ of $F$. The theory seeks to establish relations between the numbers $m_{k}$ and the connectivities $p_{k}$ of $M$. The numbers $p_{k}$ are finite in the most important applications. It is otherwise with the numbers $m_{k}$.

The theory has been able to proceed provided one of the following hypotheses is caticfiod The oritical limitc oluctor at most at $1 \infty$. the oritical ninte ar $3^{33 / 58}$

## When was persistent homology discovered first?

## Web Images

More.
Sign in


## Motivation and application: minimal surfaces

## Problem (Plateau's problem)

Find an immersed disk of least area spanned by a given closed Jordan curve.

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## Problem (Plateau's problem)

Find an immersed disk of least area spanned by a given closed Jordan curve.

(from Dierkes et al.: Minimal Surfaces, 2010)
Solution by Douglas (1930):

- identifies minimal surfaces with critical points of the Douglas


## Existence of unstable minimal surfaces

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Assume that a given curve bounds two separate stable minimal surfaces.


## Existence of unstable minimal surfaces

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Assume that a given curve bounds two separate stable minimal surfaces. Then there also exists an unstable minimal surface bounding that curve (a critical point that is not a local minimum).


## Q-tame persistence modules

## Definition (Chazal et al. 2009)

A persistence module $M: \mathbf{R} \rightarrow$ vect is $q$-tame if for every $s<t$ the structure $\operatorname{map} M_{s} \rightarrow M_{t}$ has finite rank.

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- A q-tame persistence module
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- A q-tame persistence module
- does not necessarily admit a barcode,
- but has a submodule at distance 0 that admits a barcode.
- Morse's goal, in modern language:
- Sufficient conditions for sublevel sets to have q-tame persistence,
- which are satisfied by the minimal surface functional


## Q-tameness from local connectivity

## Theorem (Morse, 1937)

If a function $f: X \rightarrow \mathbb{R}$ on a metric space $X$ is bounded below and the sublevel set filtration is compact and weakly locally connected, then it has $q$-tame persistent Vietoris homology.

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## Homologically locally small filtrations

## Definition

The sublevel set filtration of a function $f: X \rightarrow \mathbb{R}$ is homologically locally connected (HLC) if

- for any point $x \in X$, any values $f(x)<s<t$, and
- any neighborhood $V$ of $x$ in the sublevel set $f^{-1}(-\infty, t]$, there is
- a neighborhood $U \subseteq V$ of $x$ in the sublevel set $f^{-1}(-\infty, s]$
such that the inclusion $U \hookrightarrow V$ induces a zero map on homology.


## A sufficient condition for q-tame persistence

Theorem (B, Medina-Mardones, Schmahl 2021)
If the sublevel sets of a function $f: X \rightarrow \mathbb{R}$ are compact and $H L C$, then their persistent homology is $q$-tame.

- $f$ is not required to be continuous


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- Conditions are satisfied by the Douglas functional
- Fixes the gap in Morse/Tompkins' proof


# Persistence of Vietoris-Rips complexes 

## Vietoris-Rips complexes



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## Vietoris-Rips complexes

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

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

## An example computation

## Example data set:

- 192 points on $\mathbb{S}^{2}$
- homology up to dimension 2: over 56 mio. simplices in 3-skeleton


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Some previous software:

- javaplex (Stanford): 3200 seconds, 12 GB
- Dionysus (Duke): 615 seconds, 3.4 GB
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- try live.ripser.org



## Apparent pairs:

Ripser uses the following construction for a computational shortcut:
Definition
In a simplexwise filtration $\left(K_{i}=\left\{\sigma_{1}, \ldots, \sigma_{i}\right\}\right)_{i}$, a pair of simplices $(\sigma, \tau)$ is an apparent pair if

- $\sigma$ is the latest proper face of $\tau$, and
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## Proposition

The apparent pairs form a discrete gradient.

## Proposition

The apparent pairs form persistence pairs: the cycle $\partial \tau$ gives rise to an interval $[f(\sigma), f(\tau))$ in the persistence barcode.

## The diameter-lexicographic filtration

We use the lexicographic refinement of the Vietoris-Rips filtration:

- Choose a total order on the vertices
- Order simplices by diameter
- Order simplices with same diameter by lexicographic vertex order


## Topology of viral evolution



Joint work with: A. Ott, M. Bleher, L. Hahn (Heidelberg), R. Rabadan, J. Patiño-Galindo
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Observation: Ripser runs unusually fast on genetic distance data

- SARS-CoV2 spike protein: 25556 data points $\left(2.8 \times 10^{12}\right.$ simplices for $H_{1}$ )

Can we make it run even faster?

## The Rips Contractibility Lemma

Theorem (Rips; Gromov 1988)
Let $X$ be a $\delta$-hyperbolic geodesic metric space. Then $\operatorname{Rips}_{t}(X)$ is contractible for all $t \geq 4 \delta$.

- What about non-geodesic spaces?
- In particular, finite metric spaces?
- Connection to Ripser?


## Gromov-hyperbolicity

## Definition (Gromov 1988)

A metric space $X$ is $\delta$-hyperbolic if for all $w, x, y, z \in X$ we have

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



- The hyperbolic plane is $\ln$ 2-hyperbolic

- 0-hyperbolic spaces are subspaces of trees


## Rips contractibility for non-geodesic spaces

## Theorem (B, Roll 2021)

Let $X$ be a finite $\delta$-hyperbolic space. Then there is a discrete gradient encoding the collapses

$$
\operatorname{Rips}_{u}(X) \searrow \operatorname{Rips}_{t}(X) \searrow\{*\}
$$

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

## Geodesic defect



## Geodesic defect



## Geodesic defect



Definition (Bonk, Schramm 2000)
A metric space $X$ is $v$-geodesic if for all points $x, y \in X$ and all $r, s \geq 0$ with $r+s=d(x, y)$ we have

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

We call the infimum of all such $v$ the geodesic defect of $X$.

## Bounds on the geodesic defect

$v$ : geodesic defect of finite $(X, d)$

- lower bound:

$$
v \geq \frac{1}{2} \min _{x \neq y \in X} d(x, y)
$$

- upper bound:

$$
v \leq d_{H}(X, Z)
$$

for $X \subseteq Z$ an ambient geodesic space

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Possible ambient spaces for $X$ :

- $\ell^{\infty}(X)$ (functions $X \rightarrow \mathbb{R}$ )
- Kuratowski embedding $e: X \rightarrow \ell^{\infty}(X), x \mapsto\left(d_{x}=d(x,-): X \rightarrow \mathbb{R}\right.$
- injective hull (tight span): subspace of $\ell^{\infty}(X)$


## The tight span of a metric space

Given a metric space $(X, d)$, the injective hull is

$$
E(X)=\left\{f: X \rightarrow \mathbb{R} \mid f(x)+f(y) \geq d(x, y), f(x)=\sup _{y \in X}(d(x, y)-f(y))\right\},
$$

equipped with the metric induced by the sup-norm.

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equipped with the metric induced by the sup-norm.
Properties:

- geodesic
- hyperconvex (metric balls have the Helly property)
- injective (in the category of metric spaces)
[Aronszain-Panichpakdi 1956]
- contains the Kuratowski embedding $e(X): x \mapsto d_{x}$
- minimal space with above properties
- contractible [Isbell 1962]


## Density of Kuratowski embedding

## Theorem (Lang $2013+\epsilon$ )

Let $X$ be a $\delta$-hyperbolic $v$-geodesic metric space. Then the injective hull $E(X)$ is $\delta$-hyperbolic, and every point in $E(X)$ has distance at most $2 \delta+v$ to $e(X)$.

Corollary (Lim, Mémoli, Okutan $2020+\epsilon$ )
$\operatorname{Rips}_{t}(X)$ is contractible for all $t>4 \delta+2 v$.
Proof outline.

- $\operatorname{Rips}_{t}(X)=\operatorname{Cech}_{r}(e(X), E(X))$ (hyperconvexity)
- For $r>2 \delta+v:\left(B_{r}(x)\right)_{x \in e(X)}$ is a good cover of $E(X) \quad$ (density)
- $\operatorname{Cech}_{r}(e(X), E(X)) \simeq E(X) \quad$ (nerve theorem)
- $E(X) \simeq\{*\}$ (contractibility)


## Collapsing Vietoris-Rips complexes of generic trees

Consider a generic finite metric tree $T=(V, E)$ (distinct distances).

- diam: $2^{V} \rightarrow \mathbb{R}$ is a generalized discrete Morse function.
- The discrete gradient has the non-critical intervals $\left[e, \Delta_{e}\right]$, where
- $e \in\binom{V}{2} \backslash E$ is any non-tree edge
- $\Delta_{e}$ is the unique maximal cofaces with $\operatorname{diam} \Delta_{e}=l(e)$
- Only vertices $V$ and edges $E$ are critical


## Corollary (B, Roll 2021)

The discrete gradient induces collapses

$$
\begin{array}{lr}
\operatorname{Rips}_{t}(X) \searrow T_{t} & \text { for all } t \in \mathbb{R}, \text { with } \\
\operatorname{Rips}_{t}(X) \searrow T \searrow\{*\} & \text { for all } t \geq \max l(E), \text { and } \\
\operatorname{Rips}_{u}(X) \searrow \operatorname{Rips}_{t}(X) & \text { for all }(t, u] \cap l(E)=\varnothing .
\end{array}
$$

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

## Arbitrary tree metrics

Example: phylogenetic trees

- non-generic tree metric
- diam is not a generalized discrete Morse function


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Example: phylogenetic trees

- non-generic tree metric
- diam is not a generalized discrete Morse function

There is still a compatible gradient:

- independent of choices (canonical gradient)
- for generic trees: equals the diam gradient
- only $V, E$ critical
- induces the same collapses


## Symbolic perturbation

Tie breaking for non-distinct pairwise distances:

- Choose total order on vertices
- Order edges lexicographically
- Perturb metric symbolically w.r.t. edge order


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This results in a gradient structure like a generic tree metric


- The canonical gradient (from the previous slide) refines the perturbed gradient (for any choice of total order)
- Hence, the perturbed gradient induces the same collapses


## Collapsing Rips complexes of trees with apparent pairs

Let $X$ be the path length metric spaces for a weighted tree $T=(X, E)$.

- Choose a root and extend the tree order to a total order.


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## Theorem (B, Roll 2021)

The apparent pairs gradient has critical simplices only on the tree $T$. It induces the collapses

$$
\operatorname{Rips}_{u}(X) \searrow \operatorname{Rips}_{t}(X) \searrow T_{t}
$$

for all $u>t$ such that no tree edge $e \in E$ has length $l(e) \in(t, u]$.


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

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