#### Complexes from point clouds Geometry, topology, algebra, and combinatorics

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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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- 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

















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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:

$$[L, U] = \{Q \mid L \subseteq Q \subseteq U\}$$

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• indicated by an arrow from L to U

A generalized discrete Morse function  $f : K \to \mathbb{R}$  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*)





A generalized vector field V can be refined to a vector field. For each non-critical face interval  $[L, U] \in V$ :



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- choose an arbitrary vertex  $x \in U \setminus L$
- partition [L, U] into pairs  $(Q \setminus \{x\}, Q \cup \{x\})$  for all  $Q \in [L, U]$ .



# Morse theory for Čech and Delaunay complexes

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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

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Problem (Homology inference) Determine the homology  $H_*(X)$ .

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This can work, but requires strong assumptions:

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

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## Homology inference using persistence

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- Apply homology  $H_* : \mathbf{Top} \to \mathbf{Vect}$
- Persistent homology is a diagram M = H<sub>\*</sub> ∘ K : R → Vect (persistence module):

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### Barcodes: the structure of persistence modules

#### Theorem (Crawley-Boevey 2015)

Any persistence module  $M : \mathbf{R} \to \mathbf{vect}$  (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<sub>i</sub>*: *i*th column of matrix *R*
- pivot R<sub>i</sub>: maximal row index with nonzero entry in column R<sub>i</sub>

Matrix reduction algorithm (variant of Gaussian elimination):

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$$R = D, V = I$$

- while  $\exists i < j$  with pivot  $R_i = \text{pivot } R_j$ 
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Result:

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



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Stability

# Stability of persistence barcodes for functions

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

- Consider the sublevel set filtrations  $f^{-1}(\infty, t]$  and  $g^{-1}(\infty, t]$ , and
- take the resulting persistence barcodes.

Then there exists a  $\delta$ -matching between the barcodes, meaning that:



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



Data

point cloud

 $P \subset \mathbb{R}^d$ 













# Interleavings

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



 $\forall t \in \mathbb{R}.$ 

# 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  $B(N) \rightarrow B(M)$  such that if J is mapped to I, then

- I and J are aligned below, and
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Dually, there is an injection  $B(M) \hookrightarrow B(N)$  for monomorphisms  $M \hookrightarrow N$ .

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<u> </u>		

### Induced matchings

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

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gives an induced matching between their barcodes:

• compose the injections  $B(M) \leftrightarrow B(\operatorname{im} f) \hookrightarrow B(N)$  from before to a matching  $B(M) \not\Rightarrow B(N)$ 



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  $\delta \ge 0$ , find a function  $f_{\delta}$  with the minimal number of critical points subject to  $||f_{\delta} - f||_{\infty} \le \delta$ .











### 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)

## Persistence and Morse theory

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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*

For a Morse function:

• critical points correspond to endpoints of barcode intervals

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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  $||g - f||_{\infty} \le \delta$ .

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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  $||f_{\delta} f||_{\infty} \leq \delta$  and
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Does not generalize to higher-dimensional manifolds!

**Functional topology** 

# When was persistent homology discovered?

- H. Edelsbrunner, D. Letscher, and A. Zomorodian Topological persistence and simplification Foundations of Computer Science, 2000
  - V. Robbins

Computational Topology at Multiple Resolutions. PhD thesis, University of Colorado Boulder, 2000

P. Frosini

A distance for similarity classes of submanifolds of a Euclidean space

Bulletin of the Australian Mathematical Society, 1990.

### 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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Annals of Mathematics Vol. 41, No. 2, April, 1940

#### 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 satisfied. The critical limits cluster at most at  $\pm \infty$ : the critical points are<sup>33/58</sup>

#### When was persistent homology discovered first?

Web Images	More	Sign in
Google		Q
Scholar	9 results (0.02 sec)	Ny Citations
All citations	Rank and span in functional topology	
Articles	Search within citing articles	
Case law My library	Exact homomorphism sequences in homology theory JL Kelley, E Pitcher - Annals of Mathematics, 1947 - JSTOR	ed.ac.uk [PDF]
Any time	The developments of this paper stem from the attempts of one of the authors to deduce relations between homology groups of a complex and homology groups of a complex which is its image under a simplicial map. Certain relations were deduced (see [EP 1] and [EP 2]	
Since 2016	Cited by 46 Related articles All 3 versions Cite Save More	
Since 2015		
Since 2012	Marston Morse and his mathematical works	ams.org [PDF]
Custom range	R Bott - Bulletin of the American Mathematical Society, 1980 - ams.org American Mathematical Society. Trus Morse grew to maturity just at the time when the subject of Analysis Situs was being shaped by such masters2 as Poincaré, Vebien, LEJ Broyuer, CR Ditkhoff, Jefschetz and Alexanderr and it was Morse's nenits and dhetinu to	
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	Unstable minimal surfaces of higher topological structure	
include citations	M Morse, CB Tompkins - Duke Math. J, 1941 - projecteuclid.org	
Create alert	<ol> <li>Introduction. We are concerned with extending the calculus of variations in the large to multiple integrals. Therproblem of the existence of minimal surfaces of unstable type contains many of the typical difficulties, especially those of a topological nature. Having studied this</li> </ol>	
	Cited by 19 Related articles All 2 versions Cite Save	
	por Persistence in discrete Morse theory U Bauer - 2011 - Citeseer	psu.edu [PDF]
	The goal of this thesis is to bring together two different theories about critical points of a scalar function and their relation to topology: Discrete Morse theory and Persistent homology While the goals and fundamental techniques are different there are certain	

# 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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Solution by Douglas (1930):

- identifies minimal surfaces with critical points of the Douglas
  - *.* . .

Existence of unstable minimal surfaces

#### Theorem (Morse, Tompkins 1939; Shiffman 1939)

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



# Existence of unstable minimal surfaces

#### Theorem (Morse, Tompkins 1939; Shiffman 1939)

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  $M : \mathbf{R} \to \mathbf{vect}$  is *q*-tame if for every s < t the structure map  $M_s \to M_t$  has finite rank.

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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  $f: X \to \mathbb{R}$  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  $f: X \to \mathbb{R}$  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  $f: X \to \mathbb{R}$  are compact and HLC, then their persistent homology is q-tame.

• f is not required to be continuous

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- *f* is not required to be continuous
- Conditions are satisfied by the Douglas functional
- Fixes the gap in Morse/Tompkins' proof

Persistence of Vietoris–Rips complexes



















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

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

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 <u>live.ripser.org</u>



### **Apparent pairs:**

Ripser uses the following construction for a computational shortcut:

#### Definition

In a simplexwise filtration  $(K_i = {\sigma_1, ..., \sigma_i})_i$ , a pair of simplices  $(\sigma, \tau)$  is an *apparent pair* if

- $\sigma$  is the latest proper face of  $\tau$ , and
- *τ* is the earliest proper coface of *σ*.

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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



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

(Columbia), M. Carrière (INRIA)



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Observation: Ripser runs unusually fast on genetic distance data

• SARS-CoV2 spike protein: 25556 data points (2.8  $\times$  10<sup>12</sup> 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  $t \ge 4\delta$ .

- 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

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



• 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  $u > t \ge 4\delta + 2v$ , 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  $r, s \ge 0$ with r + s = d(x, y) we have

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

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:

$$v \ge \frac{1}{2} \min_{x \neq y \in X} d(x, y)$$

• upper bound:

 $v \leq d_H(X, Z)$ 

for  $X \subseteq Z$  an ambient geodesic space

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for  $X \subseteq Z$  an ambient geodesic space

Possible ambient spaces for X:

•  $\ell^{\infty}(X)$  (functions  $X \to \mathbb{R}$ )

• Kuratowski embedding  $e: X \to \ell^{\infty}(X), x \mapsto (d_x = d(x, -): X \to \mathbb{R}$ 

• 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) = \{f: X \to \mathbb{R} \mid f(x) + f(y) \ge d(x, y), f(x) = \sup_{y \in X} (d(x, y) - f(y))\},\$$

equipped with the metric induced by the sup-norm.

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**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  $t > 4\delta + 2\nu$ .

#### Proof outline.

- Rips<sub>t</sub>(X) = Cech<sub>r</sub>(e(X), E(X)) (hyperconvexity)
- For  $r > 2\delta + v$ :  $(B_r(x))_{x \in e(X)}$  is a good cover of E(X) (density)
- $\operatorname{Cech}_r(e(X), E(X)) \simeq E(X)$  (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  $[e, \Delta_e]$ , where
  - $e \in \binom{V}{2} \setminus E$  is any non-tree edge
  - $\Delta_e$  is the unique maximal cofaces with diam  $\Delta_e = l(e)$
- Only vertices V and edges E are critical

#### Corollary (B, Roll 2021)

The discrete gradient induces collapses

Rips\_t(X)  $\searrow T_t$ for all  $t \in \mathbb{R}$ , withRips\_t(X)  $\searrow T \searrow \{*\}$ for all  $t \ge \max l(E)$ , andRips\_u(X)  $\searrow$  Rips\_t(X)for all  $(t, u] \cap l(E) = \emptyset$ .

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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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

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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- 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

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

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



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

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