HELMHOLTZ MUNICH

AIH Institute of AI for Health

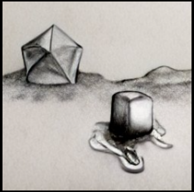
The Memory of Persistence

Bastian Rieck   Pseudomanifold

Induction

AI imitating art




Algebraic Topology: Counts & Calculations

What is algebraic topology?

Develop invariants that classify topological spaces up to homeomorphism.

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Use tools from algebra to study topological spaces.

What is algebraic topology?

Develop invariants that classify topological spaces up to homeomorphism.

Use tools from algebra to study topological spaces.

Understand shapes through calculations.

A first taste

Seven Bridges of Königsberg

Is there a walk through the city that crosses every bridge *exactly* once?

A first taste

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Seven Bridges of Königsberg

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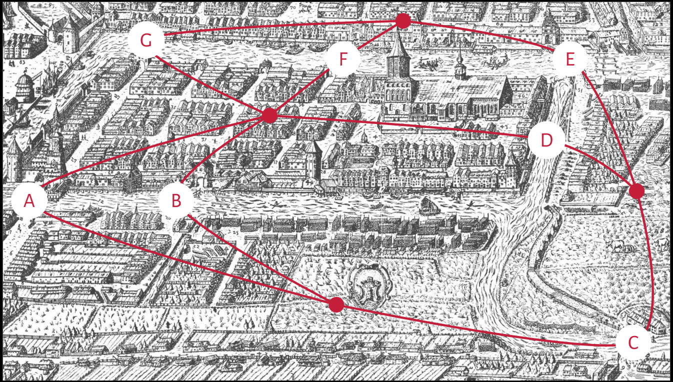

A first taste

Seven Bridges of Königsberg

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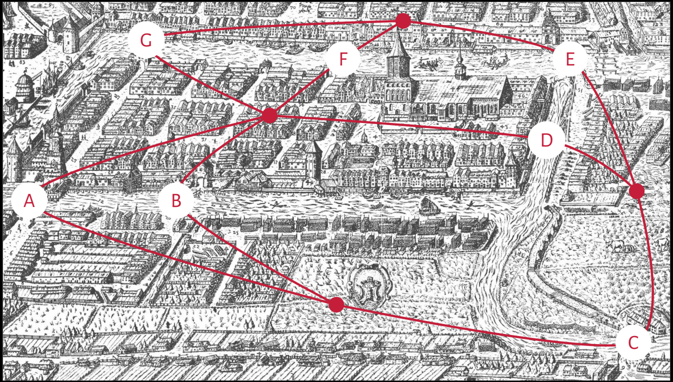


No such walk can exist because there are more than two vertices with *odd* degree!

Simple invariants

Euler characteristic

The *Euler characteristic* of a polyhedron is defined as $\chi := V - E + F$, where V is the number of vertices, E is the number of edges, and F is the number of faces, respectively.

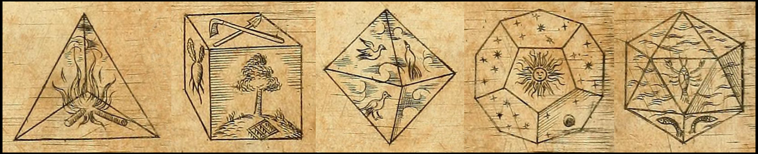
Simple invariants

Euler characteristic

The *Euler characteristic* of a polyhedron is defined as $\chi := V - E + F$, where V is the number of vertices, E is the number of edges, and F is the number of faces, respectively.

Theorem

The Euler characteristic of every Platonic solid is $\chi = 2$.



Simple invariants

Euler characteristic, continued

Space	V	E	F	χ

Simple invariants

Euler characteristic, continued

Space	V	E	F	χ
Tetrahedron	4	6	4	2

Simple invariants

Euler characteristic, continued

Space	V	E	F	χ
Tetrahedron	4	6	4	2
Hexahedron	8	12	6	2

Simple invariants

Euler characteristic, continued

Space	V	E	F	χ
Tetrahedron	4	6	4	2
Hexahedron	8	12	6	2
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Simple invariants

Euler characteristic, continued

Space	V	E	F	χ
Tetrahedron	4	6	4	2
Hexahedron	8	12	6	2
Octahedron	6	12	8	2
Dodecahedron	20	30	12	2

Simple invariants

Euler characteristic, continued

Space	V	E	F	χ
Tetrahedron	4	6	4	2
Hexahedron	8	12	6	2
Octahedron	6	12	8	2
Dodecahedron	20	30	12	2
Icosahedron	12	30	20	2

Simple invariants

Betti numbers

The d^{th} Betti number counts the number of d-dimensional holes. It can be used to distinguish between spaces.

$d = 0$: connected components

$d = 1$: cycles

$d = 2$: voids

Space	β_0	β_1	β_2

Simple invariants

Betti numbers

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- $d = 0$: connected components
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Space		β_0	β_1	β_2
Point	●	1	0	0

Simple invariants

Betti numbers

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Space		β_0	β_1	β_2
Point		1	0	0
Cube		1	0	1

Simple invariants

Betti numbers

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Cube		1	0	1
Sphere		1	0	1

Simple invariants

Betti numbers

The d^{th} Betti number counts the number of d-dimensional holes. It can be used to distinguish between spaces.

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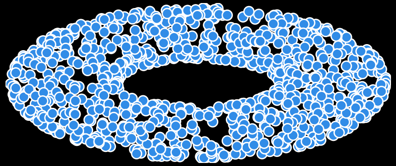
Space		β_0	β_1	β_2
Point		1	0	0
Cube		1	0	1
Sphere		1	0	1
Torus		1	2	1

Computational Topology: (Point) Cloud Atlas

Reality is often messy...



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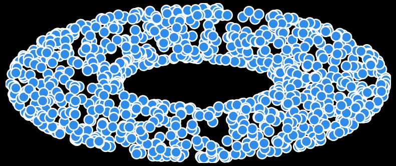


Representing spaces

Triangulations

Representing spaces

Triangulations

Representing spaces

Triangulations

Theorem

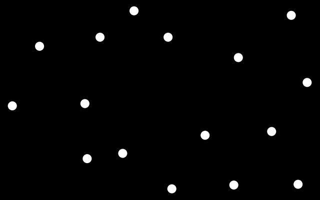
Every smooth manifold can be triangulated.

- S. S. Cairns, 'Triangulation of the Manifold of Class One', *Bulletin of the American Mathematical Society* 41.8, 1935, pp. 549–552
- J. H. C. Whitehead, 'On C^1-Complexes', *Annals of Mathematics* 41.4, 1940, pp. 809–824

Persistent homology

'Points cross scales like clouds cross the sky'

Approximate a point cloud at different scales and observe how topological features appear and disappear.



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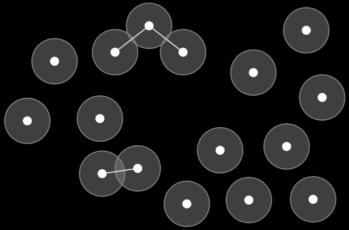

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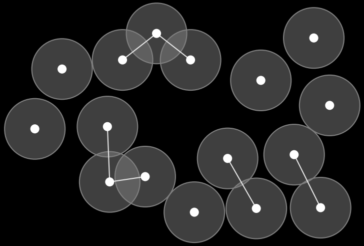

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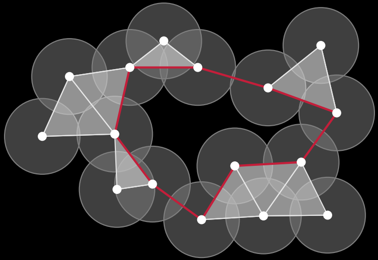

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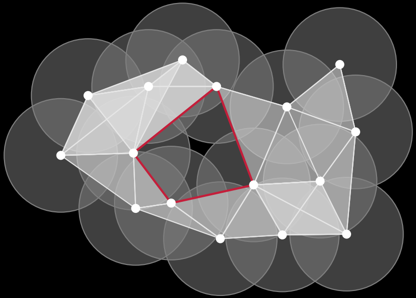

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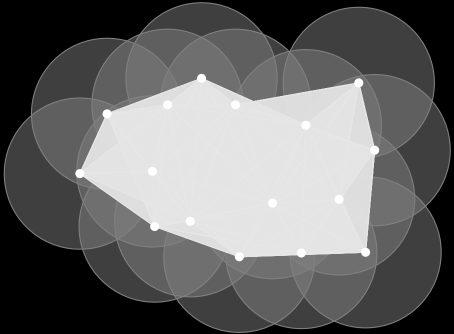
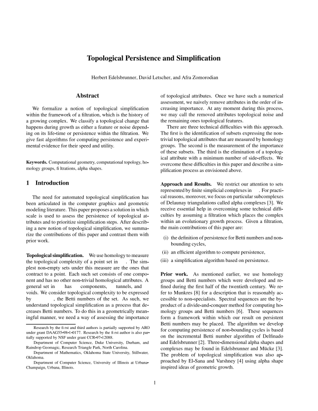


Persistent homology

Formalisation



Topological Persistence and Simplification

Herbert Edelsbrunner, David Letscher, and Afra Zomorodian

Abstract

We formalize a notion of topological simplification within the framework of a filtration, which is the history of a growing complex. We classify a topological change that happens during growth as either a feature or noise depending on its life-time or persistence within the filtration. We give fast algorithms for computing persistence and experimental evidence for their speed and utility.

Keywords. Computational geometry, computational topology, homology groups, filtrations, alpha shapes.

1 Introduction

The need for automated topological simplification has been articulated in the computer graphics and geometric modeling literature. This paper proposes a solution in which scale is used to assess the persistence of topological attributes and to prioritize simplification steps. After describing a new notion of topological simplification, we summarize the contributions of this paper and contrast them with prior work.

Topological simplification. We use homology to measure the topological complexity of a point set in . The simplest non-empty sets under this measure are the ones that contract to a point. Each such set consists of one component and has no other non-trivial homological attributes. A general set in has components, tunnels, and voids. We consider topological complexity to be expressed by , the Betti numbers of the set. As such, we understand topological simplification as a process that decreases Betti numbers. To do this in a geometrically meaningful manner, we need a way of assessing the importance of topological attributes. Once we have such a numerical assessment, we naively remove attributes in the order of increasing importance. At any moment during this process, we may call the removed attributes topological noise and the remaining ones topological features.

There are three technical difficulties with this approach. The first is the identification of subsets expressing the non-trivial topological attributes that are measured by homology groups. The second is the measurement of the importance of these subsets. The third is the elimination of a topological attribute with a minimum number of side-effects. We overcome these difficulties in this paper and describe a simplification process as envisioned above.

Approach and Results. We restrict our attention to sets represented by finite simplicial complexes in . For practical reasons, moreover, we focus on particular subcomplexes of Delaunay triangulations called alpha complexes [3]. We receive essential help in overcoming some technical difficulties by assuming a filtration which places the complex within an evolutionary growth process. Given a filtration, the main contributions of this paper are:

(i) the definition of persistence for Betti numbers and non-bounding cycles,

(ii) an efficient algorithm to compute persistence,

(iii) a simplification algorithm based on persistence.

Prior work. As mentioned earlier, we use homology groups and Betti numbers which were developed and refined during the first half of the twentieth century. We refer to Munkres [8] for a description that is reasonably accessible to non-specialists. Spectral sequences are the by-product of a divide-and-conquer method for computing homology groups and Betti numbers [6]. These sequences form a framework within which our result on persistent Betti numbers may be placed. The algorithm we develop for computing persistence of non-bounding cycles is based on the incremental Betti number algorithm of Delfinado and Edelsbrunner [2]. Three-dimensional alpha shapes and complexes may be found in Edelsbrunner and Mücke [3]. The problem of topological simplification was also approached by El-Sana and Varshney [4] using alpha shape inspired ideas of geometric growth.

Research by the fi rst and third authors is partially supported by ARO under grant DAAG55-98-1-0177. Research by the fi rst author is also partially supported by NSF under grant CCR-97-12088.

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Department of Mathematics, Oklahoma State University, Stillwater, Oklahoma.

Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, Illinois.

1

We formalize a notion of topological simplification within the framework of a filtration, which is the history of a growing complex. We classify a topological change that happens during growth as either a feature or noise depending on its life-time or persistence within the filtration. We give fast algorithms for computing persistence and experimental evidence for their speed and utility.

H. Edelsbrunner, D. Letscher and A. J. Zomorodian, 'Topological persistence and simplification', *Discrete & Computational Geometry* 28.4, 2002, pp. 511–533

Other formulations

On résiste à l'invasion des armées; on ne résiste pas à l'invasion des idées. (Victor Hugo)

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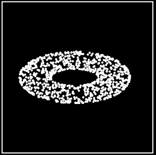
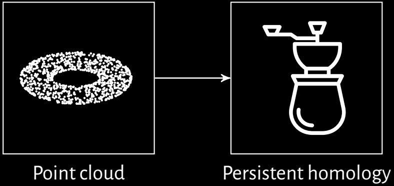
- P. Frosini, 'A Distance for Similarity Classes of Submanifolds of a Euclidean Space', *Bulletin of the Australian Mathematical Society* 42.3, 1990, pp. 407–415
- S. A. Barannikov, 'The Framed Morse Complex and its Invariants', *Advances in Soviet Mathematics* 21, 1994, pp. 93–115
- F. Cagliari, M. Ferri and P. Pozzi, 'Size Functions from a Categorical Viewpoint', *Acta Applicandae Mathematica* 67.3, 2001, pp. 225–235

One pipeline to rule them all?



Point cloud

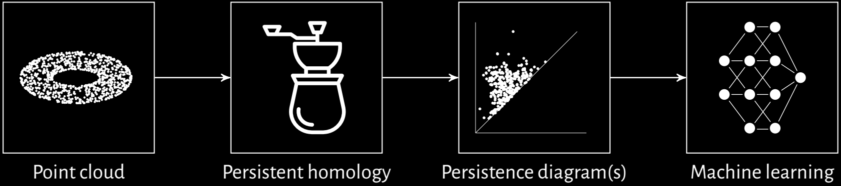
One pipeline to rule them all?



One pipeline to rule them all?

Point cloud　Persistent homology　Persistence diagram(s)

One pipeline to rule them all?



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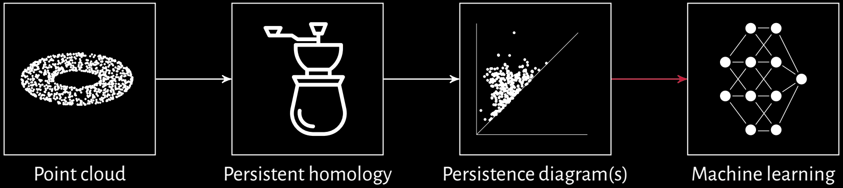

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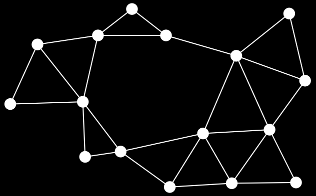
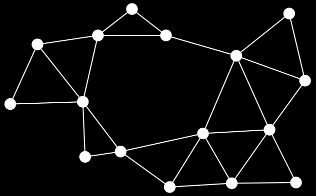
- M. Carrière, F. Chazal, M. Glisse, Y. Ike, H. Kannan and Y. Umeda, 'Optimizing persistent homology based functions', *Proceedings of the 38th International Conference on Machine Learning (ICML)*, 2021, pp. 1294–1303

But wait, there's more...



Graphs

But wait, there's more...



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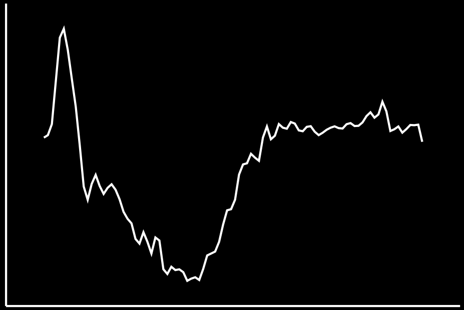

Time series

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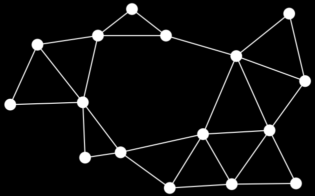
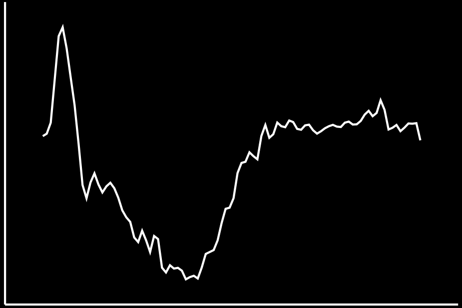


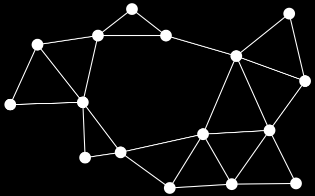
Graphs



Time series

Persistent homology provides us with a new paradigm for thinking about data.

But wait, there's more...



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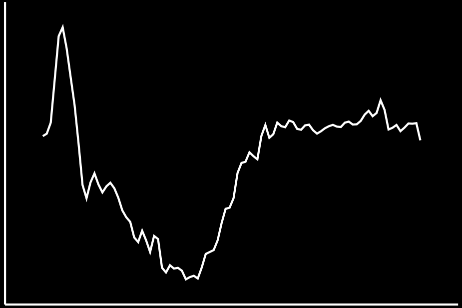


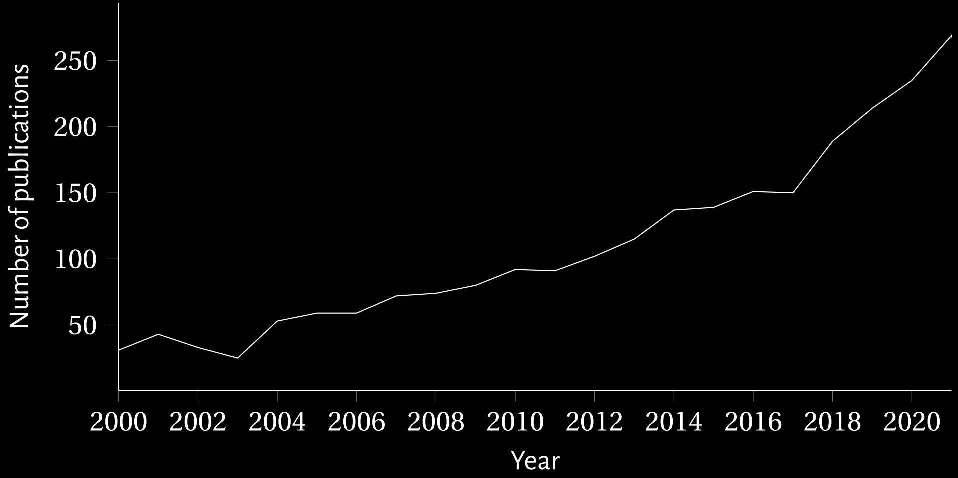
Time series

Persistent homology provides us with a new paradigm for thinking about data.

Data has shape, shape has meaning, and persistent homology helps us extract it.

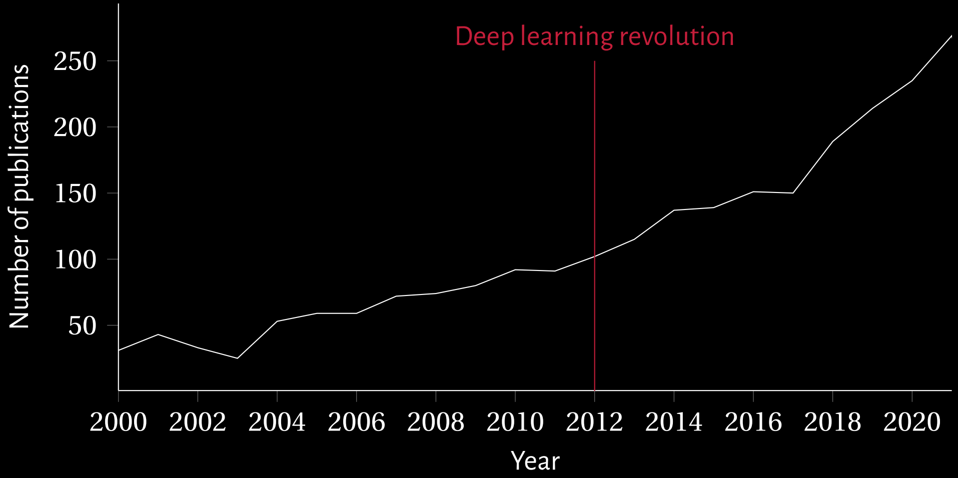
(paraphrasing Gunnar Carlsson)

Cambrian explosion?



Data taken from OpenAlex (`https://openalex.org`) for the concept of 'persistent homology.'

Cambrian explosion?



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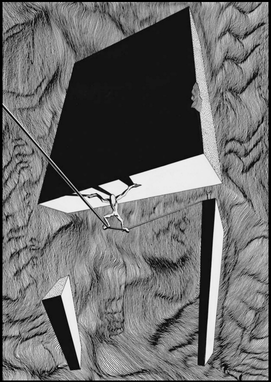
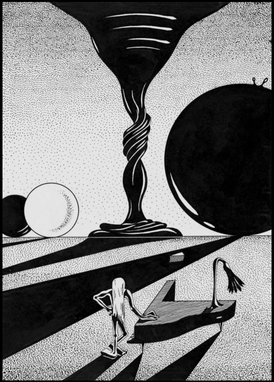
Challenges from a 2019 talk



Improving performance



Escaping flatland

First-class architectures

Images used with kind permission from Prof. A. T. Fomenko; these drawings are also found in the marvellous book *Homotopic Topology*.

Where are we now?

Performance

Persistent Homology Transform

Capturing shape without multifiltrations

Calculate filtration of a shape $M \subset \mathbb{R}^d$ for a 'height' $r \in \mathbb{R}$ as $M(v, r) := \{x \in M \mid \langle x, v \rangle \leq r\}$, where $v \in \mathbb{S}^{d-1}$ and $\langle \cdot, \cdot \rangle$ denotes an inner product.

Performance

Persistent Homology Transform

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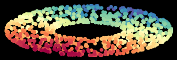

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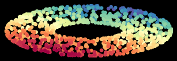

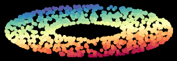

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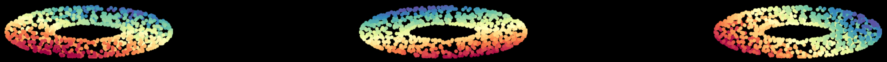
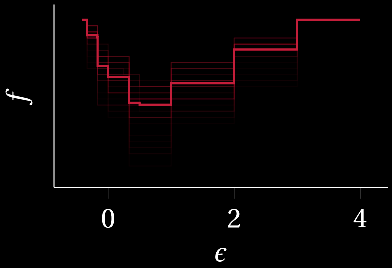


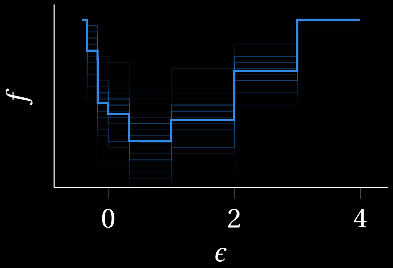
K. Turner, S. Mukherjee and D. M. Boyer, 'Persistent Homology Transform for Modeling Shapes and Surfaces', *Information and Inference* 3.4, 2014, pp. 310–344

Performance

Euler Characteristic Curves & Filtration Curves

We can evaluate a real-valued function f alongside a filtration, thus leading to a set of 'characteristic curves.'

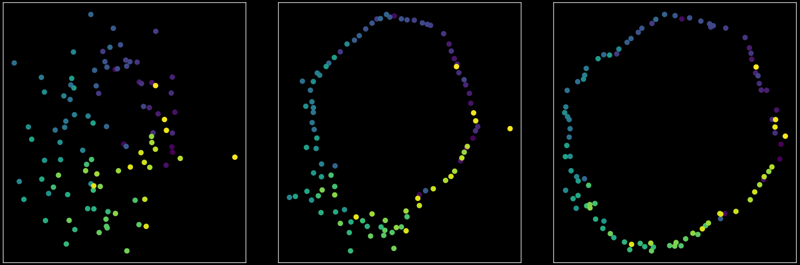




L. O'Bray*, **B. Rieck*** and K. Borgwardt, 'Filtration Curves for Graph Representation', *Proceedings of the 27th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining (KDD)*, New York, NY, USA: Association for Computing Machinery, 2021, pp. 1267–1275

Subsampling strategies

We can infer a lot of (topological) information from *random samples* of the data, and use this to perform topology-driven optimisation!



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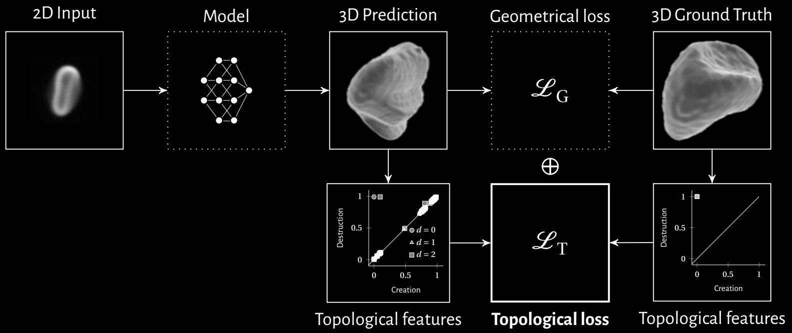
Escaping flatland (well, sort of...)

Using full 3D information to improve reconstruction tasks. Can we go higher?



D. J. E. Waibel, S. Atwell, M. Meier, C. Marr and **B. Rieck**, 'Capturing Shape Information with Multi-Scale Topological Loss Terms for 3D Reconstruction', *Medical Image Computing and Computer Assisted Intervention (MICCAI)*, 2022, arXiv: `2203.01703 [cs.CV]`, in press

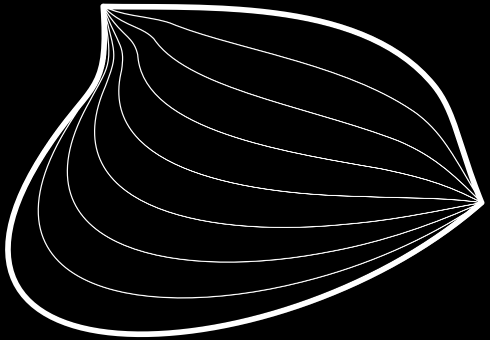
First-class architectures

- C. Hofer, R. Kwitt, M. Niethammer and A. Uhl, 'Deep learning with topological signatures', *Advances in Neural Information Processing Systems*, ed. by I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan and R. Garnett, vol. 30, Curran Associates, Inc., 2017, pp. 1633–1643
- M. Carrière, F. Chazal, Y. Ike, T. Lacombe, M. Royer and Y. Umeda, 'PersLay: A Neural Network Layer for Persistence Diagrams and New Graph Topological Signatures', *Proceedings of the 23rd International Conference on Artificial Intelligence and Statistics*, ed. by S. Chiappa and R. Calandra, vol. 108, Proceedings of Machine Learning Research, PMLR, 2020, pp. 2786–2796
- K. Kim, J. Kim, M. Zaheer, J. Kim, F. Chazal and L. Wasserman, 'PLLay: Efficient Topological Layer based on Persistent Landscapes', *Advances in Neural Information Processing Systems*, ed. by H. Larochelle, M. Ranzato, R. Hadsell, M. Balcan and H. Lin, vol. 33, Curran Associates, Inc., 2020, pp. 15965–15977

Lots of progress being made—can we now tackle *performance*?

The Beauty of Our Field

My personal journey into topology



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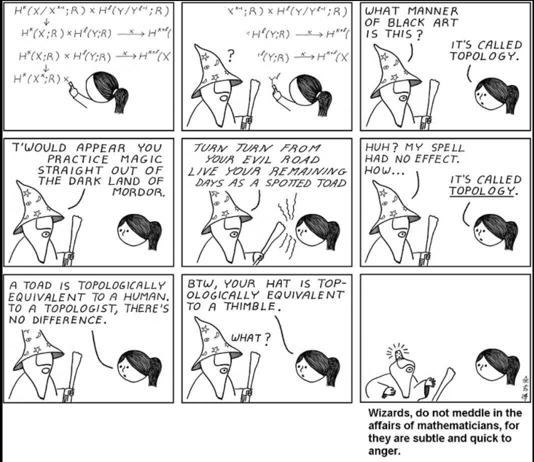

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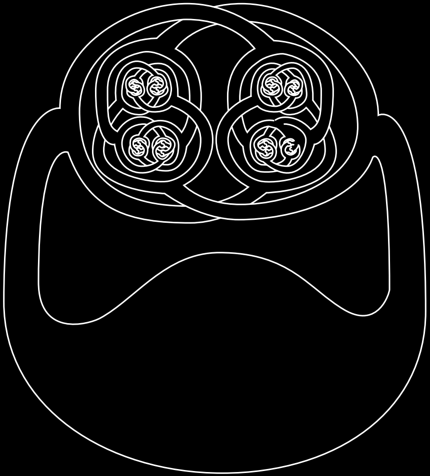
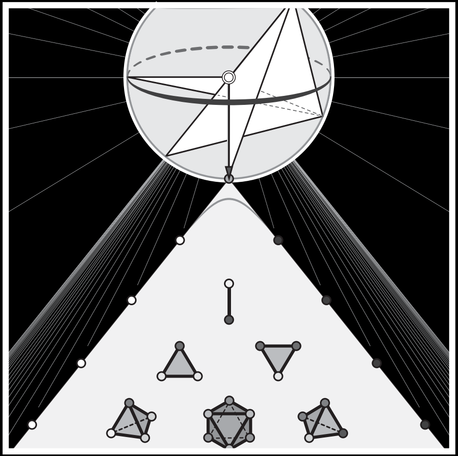
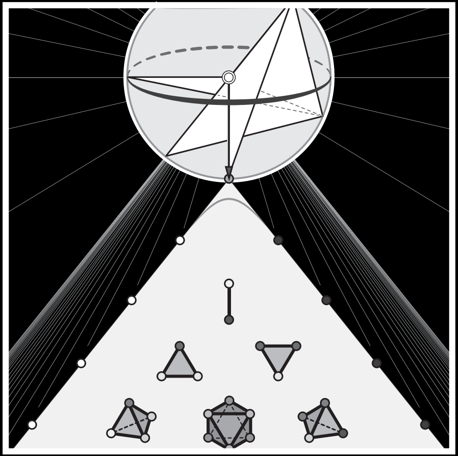


R. J. Daverman and G. A. Venema, *Embeddings in Manifolds*, vol. 106, Graduate Studies in Mathematics, Providence, RI, USA: American Mathematical Society, 2009



R. Ghrist, *Elementary Applied Topology*, 1.0, Createspace



R. Ghrist, *Elementary Applied Topology*, 1.0, Createspace

William Blake, 'The Ancient of Days'

The Next 20 Years

What we need

Our own data sets.

What we need

Our own data sets.

Harmonised frameworks and reporting.

What we need

Our own data sets.

Harmonised frameworks and reporting.

Users.

What to avoid

Round about the cauldron go;
In the persistent entrails throw.
Diagram that with many a pair
Makes the network look less bare.
Double, double toil and trouble;
GPU burn and cauldron bubble.

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The use of topological features should be *justified* and assessed carefully.

In M. Horn*, E. De Brouwer*, M. Moor, Y. Moreau, **B. Rieck**† and K. Borgwardt†, 'Topological Graph Neural Networks', *International Conference on Learning Representations (ICLR)*, 2022, arXiv: `2102.07835 [cs.LG]`, we showed that topological features are crucial for high predictive performance in graph learning problems.

Success stories

Michael Bronstein

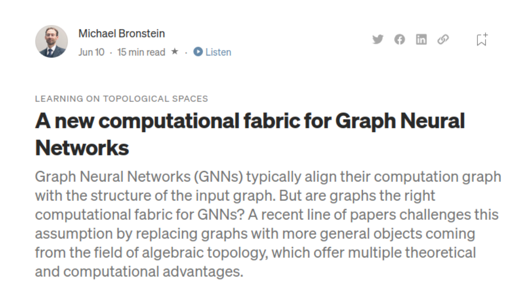
Jun 10 · 15 min read ★ · Listen

LEARNING ON TOPOLOGICAL SPACES

A new computational fabric for Graph Neural Networks

Graph Neural Networks (GNNs) typically align their computation graph with the structure of the input graph. But are graphs the right computational fabric for GNNs? A recent line of papers challenges this assumption by replacing graphs with more general objects coming from the field of algebraic topology, which offer multiple theoretical and computational advantages.

Success stories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Topological data analysis is starting to be picked up by other fields. **We need to highlight the value of a topological perspective.**

One way forward

Build bridges to ML topics (explainable ML, generative models, …).

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Dismantle obstacles to learning by investing in good explanations.

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Focus on intuition and good visualisations.

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Geometry and topology are not opposed to each other.

P. Bubenik, M. Hull, D. Patel and B. Whittle, 'Persistent homology detects curvature', *Inverse Problems* 36.2, 2020, p. 025008

Theory without practice is empty

Theory without practice is empty

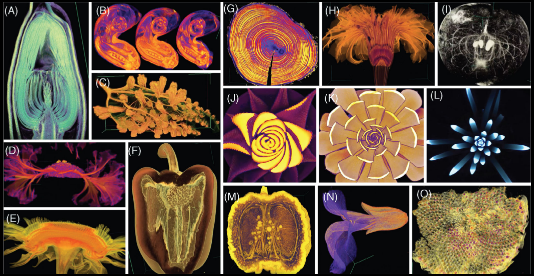
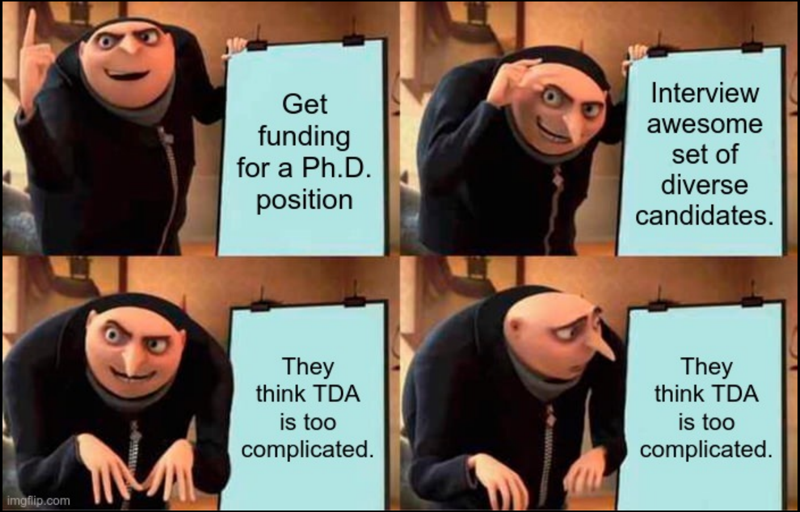


FIGURE 10 Endless forms most beautiful. X-ray Computed Tomography (CT) scans of biological specimens showing the diversity of morphology in the natural world. A, Magnolia bud, B, bean flowers, C, grapevine leaf with phylloxera galls, D, the fasciated meristem of a velvet flower, E, side view of a sunflower disc, F, bell pepper, G, tree rings, H, marigold flower, I, vasculature within an apple, J, Haworthia, K, Echeveria, L, Agave hybrid, M, citrus fruit, N, monkeyflower, O, archaeological sunflower disc specimen

E. J. Amézquita, M. Y. Quigley, T. Ophelders, E. Munch and D. H. Chitwood, 'The shape of things to come: Topological data analysis and biology, from molecules to organisms', *Developmental Dynamics* 249.7, 2020, pp. 816–833

Building a community



Building a community

Getting Started with Topological Data Analysis (TDA)

There are too many resources out there on TDA. And often people come to me and say "I'm overwhelmed and don't know how to get started." Well do I have a surprise for you. Here's the list of stuff I give to people who ask me. And before you send the hate mail… I have literally never taken algebra and I have literally never taken topology and I CERTAINLY have never taken algebraic topology. Other courses I have never taken include:

Source: Chad Topaz (`https://chadtopaz.com/getting-started-with-tda/`)

Building a community

Applied Algebraic Topology Research Network (AATRN)

‘Geometry & Topology in Machine Learning’ Slack

WinCompTop

Let’s build a diverse community! What can we do better? Let me know!

The end of the Möbius strip

Ten years ago, my first paper on TDA was published.

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Almost two years ago, I organised a TDA workshop at NeurIPS 2020.

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Thank you so much for having me!

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bastian.rieck.me
topology.rocks