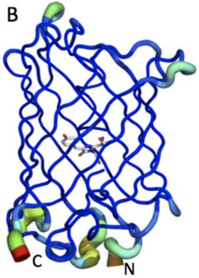
An Introduction to Topological Data Analysis

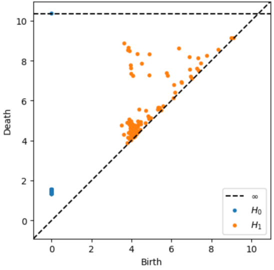
October 14, 2024

The Big Picture



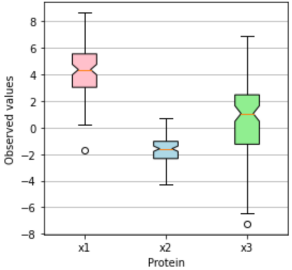
Raw Data

Point clouds
Networks
X-ray CT scans



Topological Summary

Mapper graphs
Persistence Diagrams
Euler Characteristic



Analysis

Statistics
Machine Learning
Prediction

Shape is Data, and Data has Shape

Main goal of TDA: Provide summaries of the shape of data that are

quantifiable

- Rigorously describe qualitative properties

comparable

- Establish a distance metric to compare any two summaries

robust

- A small change in the data set should result in a small change in the summary

concise

- Summaries should simplify the data

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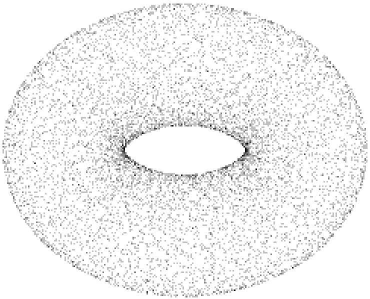
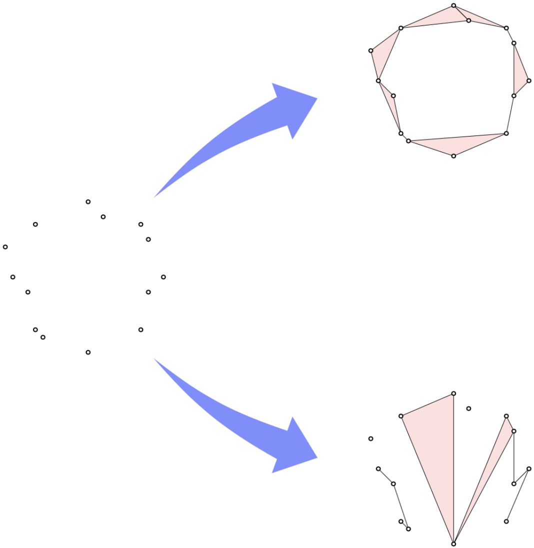
What is Topological Data Analysis?

Topological data analysis (TDA) uses techniques from topology to analyze the underlying structure of data.



Persistent Homology

Simplicial Complex



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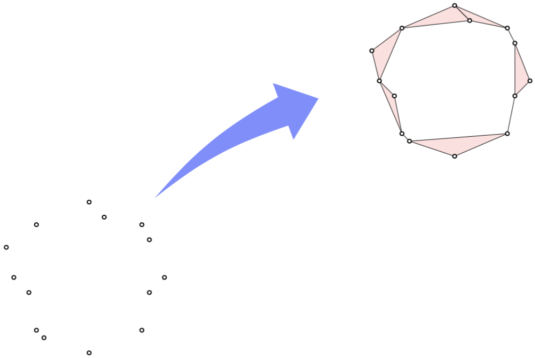
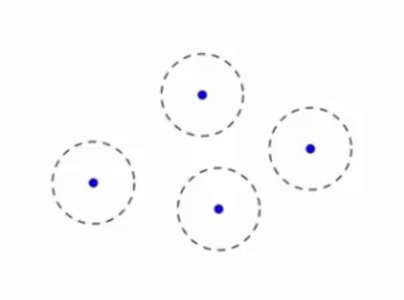


Čech Complex

We need a way to construct a simplicial complex from point cloud data.

- Draw a small ball around each point.
- Expand the balls according to time r.
- When n balls intersect, draw an $n-1$-simplex between their vertices.
- As r increases, the simplicial complex changes.
- The resulting complexes are called Čech complexes. At time r, the given Čech complex is denoted $C(r)$.



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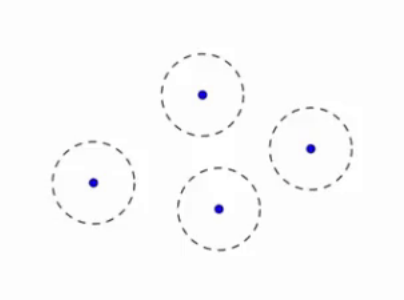

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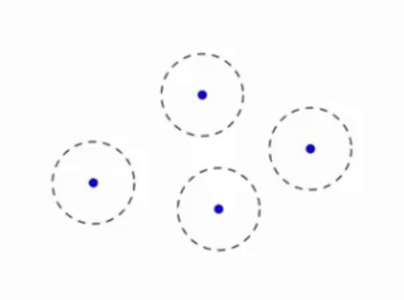

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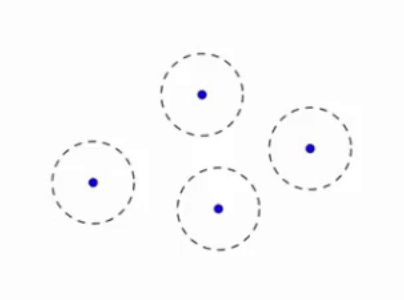

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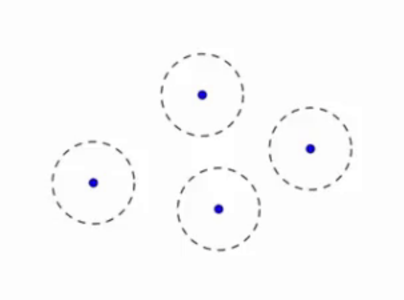

Vietoris-Rips Complex

There are many ways to create a simplicial complex from point cloud data

- Draw a small ball around each point.
- Expand the balls according to time r.
- When n balls pairwise intersect, draw an $n-1$-simplex between their vertices.
- As r increases, the simplicial complex changes.
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- Vietoris-Rips complexes can be computed more efficiently than Čech complexes
- At time r, the given Vietoris-Rips complex is denoted $VR(r)$.

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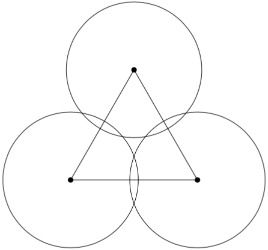
The Nerve Theorem

How do we know that the union of balls and the corresponding simplicial complex have the same topological structure?



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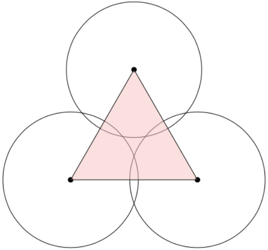


Vietoris-Rips complex

The Čech complex captures the hole but the Vietoris-Rips complex does not!

The Nerve Theorem

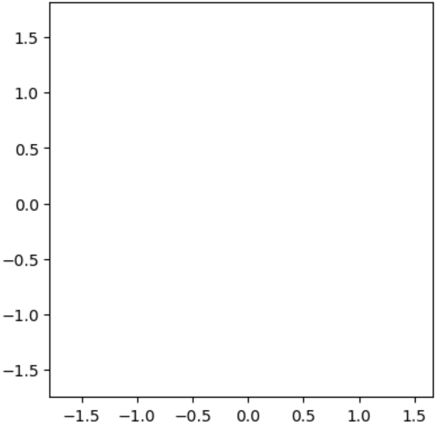
Let X be a set of point cloud data. Let $X(r)$ be the union of balls with radius r around the points of X, and let $C(r)$ be the corresponding Cech complex. Then $X(r)$ and $C(r)$ are homotopy equivalent.

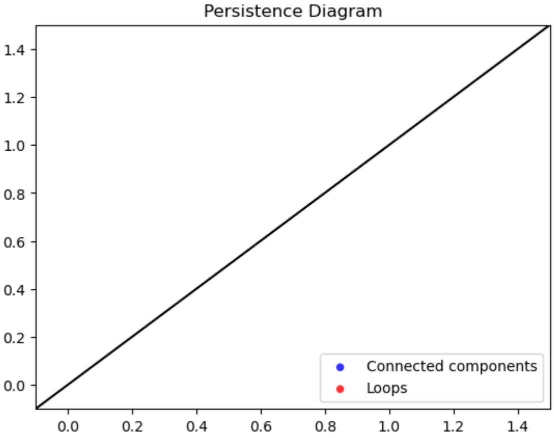
As we saw on the previous slide, the Nerve Theorem is not true for the Vietoris-Rips complex. However, we have the nice inclusion

$$C(r) \subset VR(r) \subset C(2r)$$

So if $C(r)$ and $C(2r)$ are good approximations of the structure of the point cloud data, then $VR(r)$ is as well.

Persistent Homology





Persistence Diagram

Persistent homology groups

Start with a filtration of simplicial complexes $\emptyset = K_0 \subseteq K_1 \subseteq \ldots \subseteq K_n = K$. Let $f_i \colon K_i \to K_{i+1}$ be the inclusion map. From this filtration, we obtain a sequence of homomorphisms $f_p^{i,j} \colon H_p(K_i) \to H_p(K_j)$.

Definition

The p-th persistent homology groups are the images of the homomorphisms induced by the inclusion $H_p^{i,j} = \operatorname{im} f_p^{i,j}$ for $0 \leq i \leq j \leq n$. The corresponding p-th persistent Betti numbers are $\beta_p^{i,j} = \operatorname{rank} H_p^{i,j}$.

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Birth and Death

Birth and Death

We say that a homology class $\gamma \in H_p(K_i)$ is born at K_i if

$$\gamma \notin H_p^{i-1,i} = \text{im}\, f_p^{i-1,i}$$

If γ is born at K_i, then it dies entering K_j if it merges with an older class as we go from K_{j-1} to K_j.

The Elder Rule

If γ is born at K_i and dies entering K_j, then the index persistence of γ is $j - i$. If γ is born at K_i and never dies, then the persistence index is infinity.

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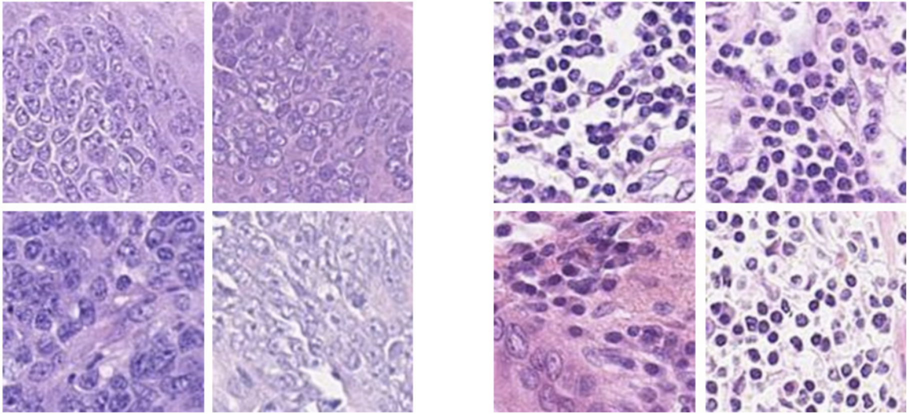
Application: Cancer



Tumor (left) and non-tumor (right) patches of colorectal tissue.

Application: Cancer

- Take images of tissue and divide them into patches.
- These images are processed into a greyscale image.
- Each pixel has a intensity value between 0 and 255. Let $B(n)$ be the union of all pixels with intensity $\leq n$. To form a filtration, let $K_i = B(i)$ for $0 \leq i \leq 255$.
- Nuclei in tumor regions lie much closer to each other than in non-tumor regions, so the homology of tumor regions does not change much compared to the homology of non-tumor regions.

This method was able to identify tumor tissue that expert analysis missed!

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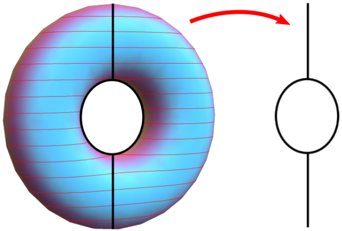
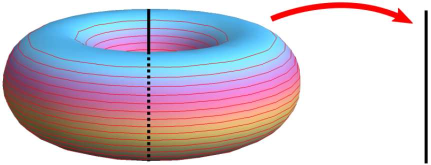
Reeb spaces

The Reeb Graph

Let S be a topological space, and let $f\colon S \to \mathbb{R}$ be a continuous function. The *Reeb graph* of f, denoted $\mathrm{Reeb}(f)$, is the space $S/\sim$, where $s_1 \sim s_2$ if and only if $f(s_1) = f(s_2)$ and s_1 and s_2 are in the same connected component of $f^{-1}(f(s_1)) = f^{-1}(f(s_2))$.

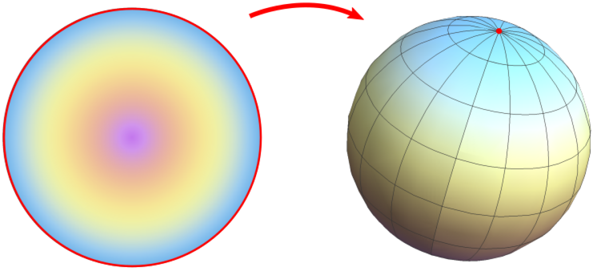




The Reeb graph depends both on the space X and the function f.

The Reeb space of a function

Let S and X be semi-algebraic sets, and let $f\colon S \to X$ be a semi-algebraic map continuous. The *Reeb space* of f, denoted $\mathrm{Reeb}(f)$, is the space $S/\sim$, where $s_1 \sim s_2$ if $f(s_1) = f(s_2)$ and s_1 and s_2 are in the same connected component of $f^{-1}(f(s_1)) = f^{-1}(f(s_2))$.



Letting $f\colon \mathbf{D}^2 \to \mathbf{S}^2$ be the map shown above, the resulting Reeb space is S^2.

Topological complexity

Dey et al. (2017)

If $f : X \to Y$ is a proper map and X is connected, then $\beta_1(\mathrm{Reeb}(f)) \leq \beta_1(X)$.

The previous example shows that this theorem does not generalize to $\beta(\mathrm{Reeb}(f))$. However, $\beta(\mathrm{Reeb}(f))$ can be bounded in terms of the complexity of the map f.

Theorem (Basu et al. (2018))

Let $S \subset \mathrm{R}^n$ be a bounded $\mathcal{P}$-closed semi-algebraic set, and $f = (f_1, \ldots, f_m) : S \to \mathrm{R}^m$ be a polynomial map. Suppose that $s = \mathrm{card}(\mathcal{P})$ and the maximum of the degrees of the polynomials in $\mathcal{P}$ and $f_1, \ldots, f_m$ is bounded by d. Then,

$$\beta(\mathrm{Reeb}(f)) \leq (sd)^{(n+m)^{O(1)}}.$$

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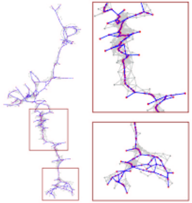
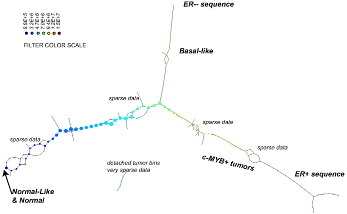
Applications of Reeb Graphs

- Ge et al. (2012) use the Reeb graph to obtain a skeleton graph of a metric graph.



- Nicolau et al. (2011) used Mapper, a discrete approximation of the Reeb graph, to analyze breast cancer tumor expression.



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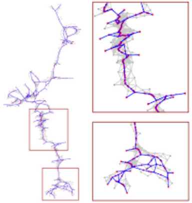

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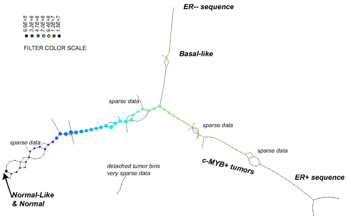

Mapper

The Mapper Algorithm Captures the Shape of Data

The Mapper algorithm produces a one-dimensional abstract graph that reflects the underlying structure of the input data.

Singh et al. (2007). Topological Methods for the Analysis of High Dimensional Data Sets and 3D Object Recognition. *PBG@Eurographics*.

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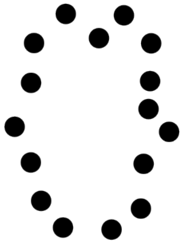

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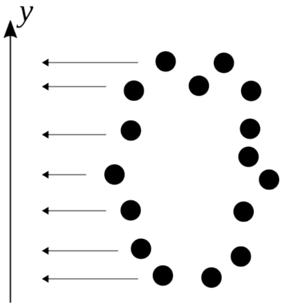

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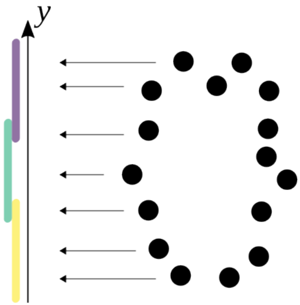

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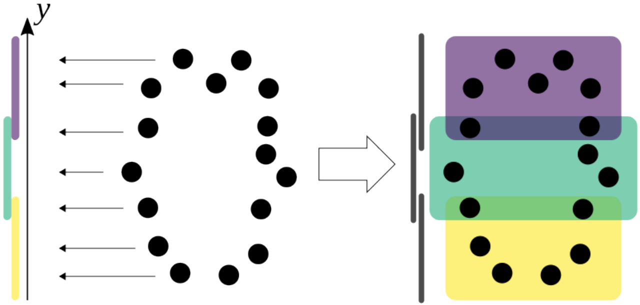

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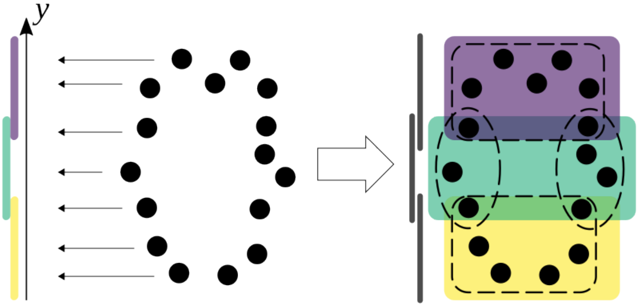

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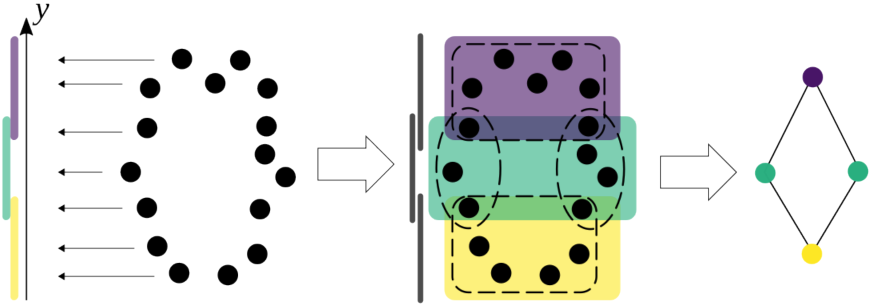

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