Introduction to Topological Data Analysis
Part I: Topological Signatures from Point Clouds

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Overview of Topological Data Analysis (TDA)

Idea

Use ideas from the mathematical field of algebraic topology to describe structure of a dataset

- Connected components (a.k.a. clustering)
- "Holes" of various dimensions ("generalized clustering")

Benefits

Descriptions are

- Multiscale — get pictures of the data at multiple resolutions.
- Stable — topology is insensitive to noise.
- Flexible — topological methods apply to all types of data, can be used to get many types of insights.

Applications of TDA

Example application domains:

- Biomedicine
  - Discovered new subgroup of breast cancer [Nicolau et. al., 2013]
  - Predicts survival time for brain cancer patients [Crawford et. al., 2016]
- Shape Analysis
  - Used to classify 3D shapes for computer vision applications [Chazal et. al., 2009]
  - Applied to classify anatomical surfaces [Turner et. al., 2013]
- Machine Learning
  - Used to analyze structure of neural networks [Rieck et. al., 2018]
  - Topological features improve performance of neural networks [Carrière et. al., 2019]

Motivation: Hierarchical Clustering

Clustering data is a basic task in unsupervised learning.

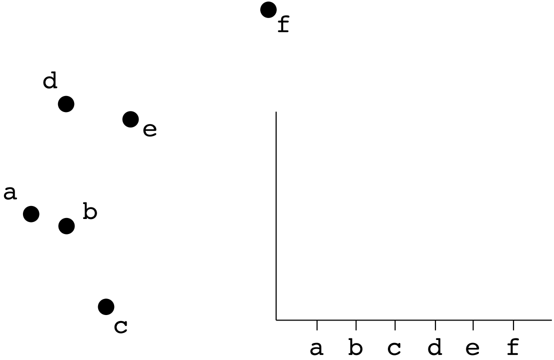
Methods like k-Means, DBSCAN, etc. partition data into clusters.

- Require parameter tuning.
- Produce one partition into clusters, potentially ignoring finer clustering structure.

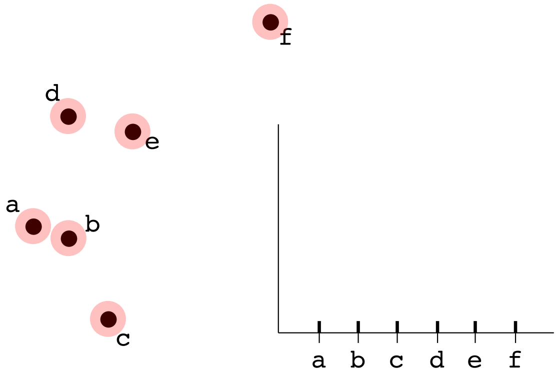
Hierarchical Clustering produces a multiscale summary of cluster structure, visualized as a dendrogram.

See Example 1 in accompanying Jupyter Notebook.

Example: Hierarchical Clustering



Example: Hierarchical Clustering



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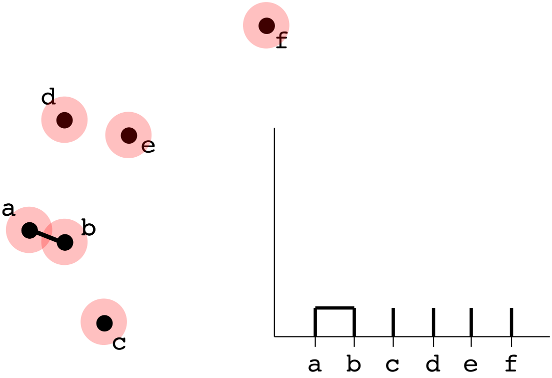
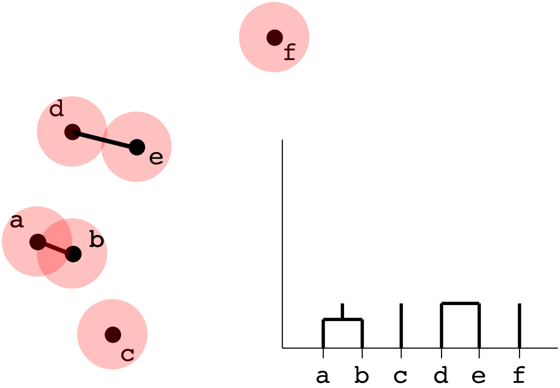
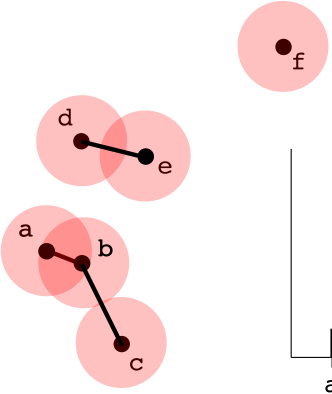
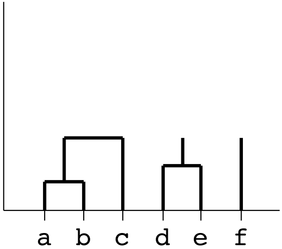


Example: Hierarchical Clustering

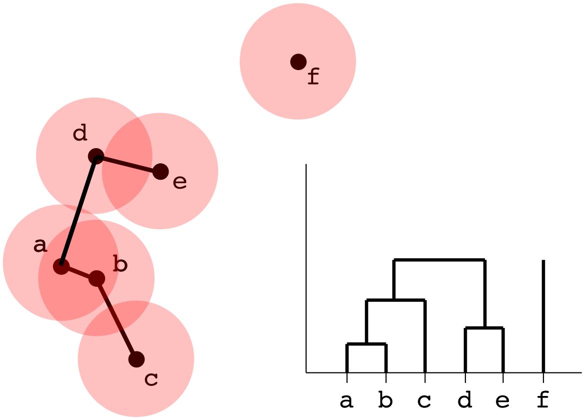


Example: Hierarchical Clustering

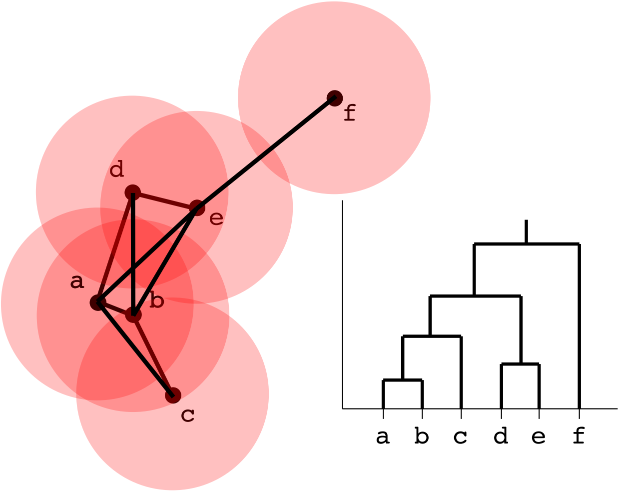




Example: Hierarchical Clustering



Example: Hierarchical Clustering



Concepts from Topology

Topology is a field of math which studies geometrical objects up to loose notions of "equivalence".

Each such object is called a (topological) space, denoted X.

Roughly, spaces are equivalent if one can be deformed into the other via stretching and bending, without creating or closing holes.

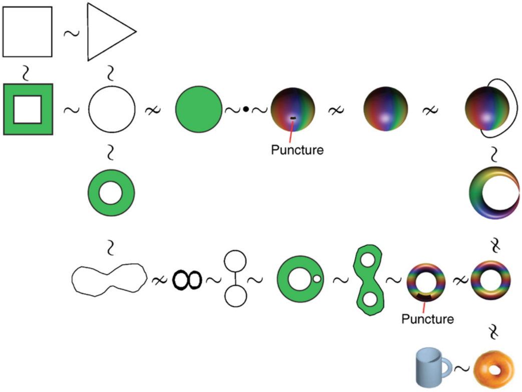


Figure: Homotopy equivalence, from Singh et. al. 2008.

Concepts from Topology

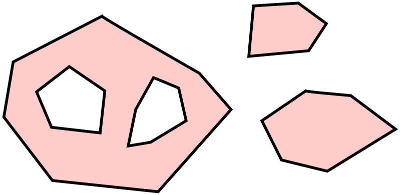
Algebraic topology is a subfield of topology where one computes invariants of a space which distinguish it from other spaces.

To each space X, we can associate a vector space $H_k(X)$ called the kth homology vector space of X.

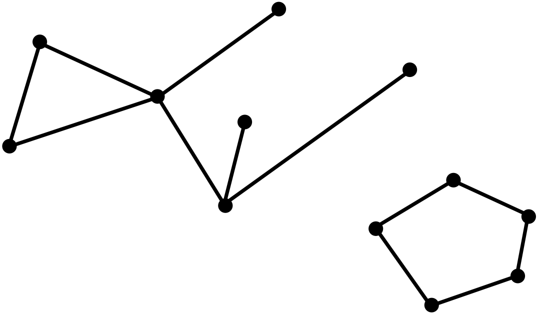
Its dimension $\beta_k(X)$ is called the kth Betti number of X.

The Betti number $\beta_k(X)$ counts "k-dimensional holes" in X:

- 0-dimensional — # of connected pieces
- 1-dimensional — # of unfilled loops
- 2-dimensional — # of unfilled "voids" (interior of a basketball)
- k-dimensional — well-defined concept we can't visualize



Examples of Betti Numbers



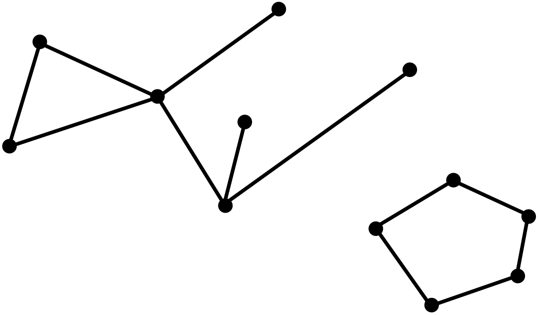
$\beta_0 =$

$\beta_1 =$

$\beta_2 =$

Figure: Disconnected graph.

Examples of Betti Numbers



$$\beta_0 = 2$$

$$\beta_1 = 1$$

$$\beta_2 = 0$$

Figure: Disconnected graph.

Examples of Betti Numbers

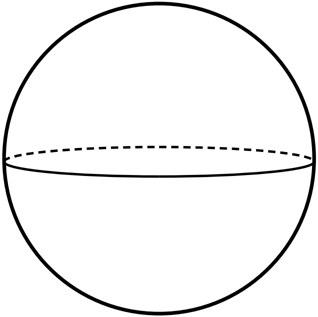


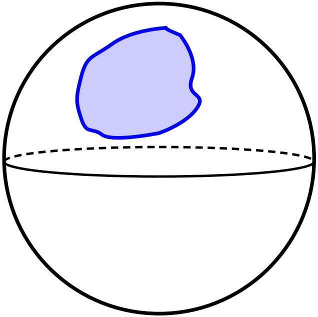
Figure: Surface of a sphere.

$\boldsymbol{\beta}_0 =$

$\boldsymbol{\beta}_1 =$

$\boldsymbol{\beta}_2 =$

Examples of Betti Numbers



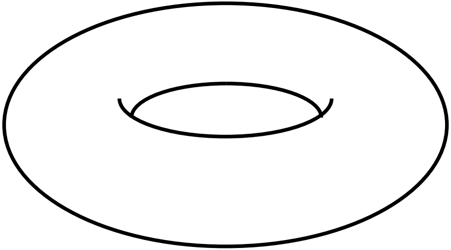
$\boldsymbol{\beta}_0 = 1$

$\boldsymbol{\beta}_1 = 0$

$\boldsymbol{\beta}_2 = 1$

Figure: Any loop on the sphere can be filled in with a disk.

Examples of Betti Numbers



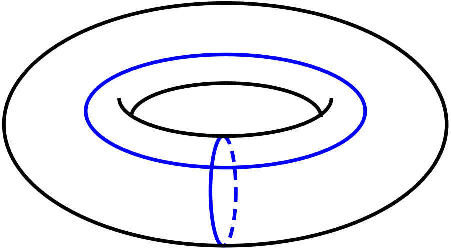
$\boldsymbol{\beta}_0 =$

$\boldsymbol{\beta}_1 =$

$\boldsymbol{\beta}_2 =$

Figure: Torus (surface of a donut).

Examples of Betti Numbers



$\beta_0 = 1$

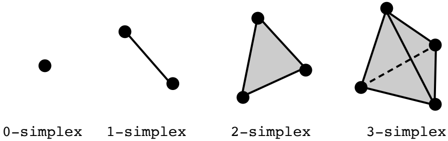
$\beta_1 = 2$

$\beta_2 = 1$

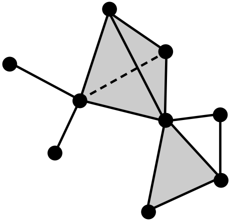
Figure: Blue loops can't be filled by disks that stay in the surface.

Simplicial Homology

A *k*-simplex is a *k*-dimensional generalization of a triangle.



A simplicial complex is a space obtained by gluing together simplices along lower-dimensional faces.

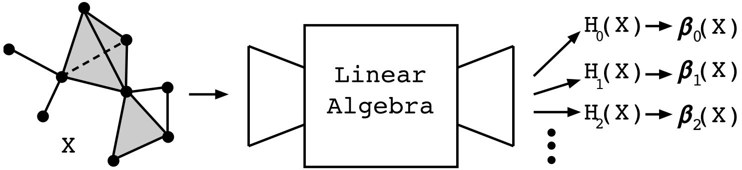


Simplicial Homology

Computing homology/Betti numbers of simplicial complexes is easy!

Boils down to linear algebra:

- Gluing process is described by linear maps.
- Homology is computed from kernels and images of these maps.



How Does This Apply to Data?

The most common type of data is a point cloud — a set of vectors $X = \{\vec{x}_1, \ldots, \vec{x}_N\}$, each $\vec{x}_j \in \mathbb{R}^d$.

This is a simplicial complex with only 0-dimensional simplices and no interesting topology; i.e.,

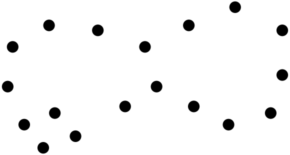
$$\beta_0 = N, \quad \beta_1, \beta_2, \ldots = 0.$$

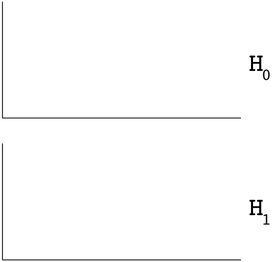
Idea

Construct a family of simplicial complexes following the example of hierarchical clustering.

This leads to the main tool in TDA: persistent homology.

Persistent Homology - An Example





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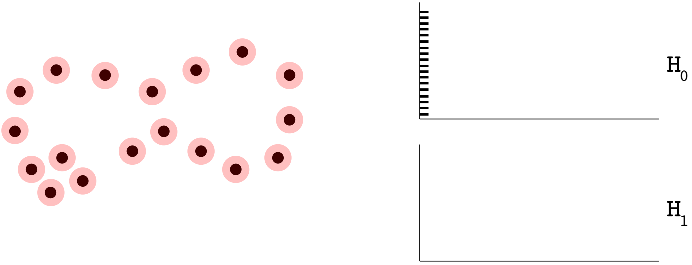

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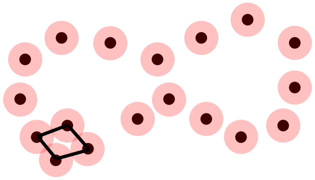

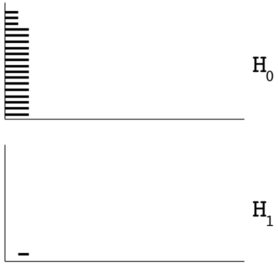

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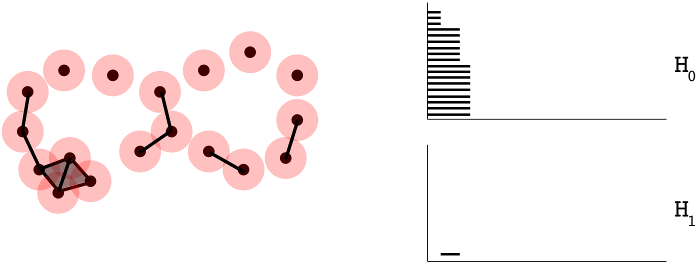

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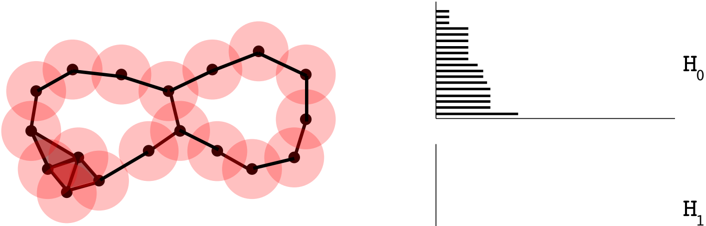

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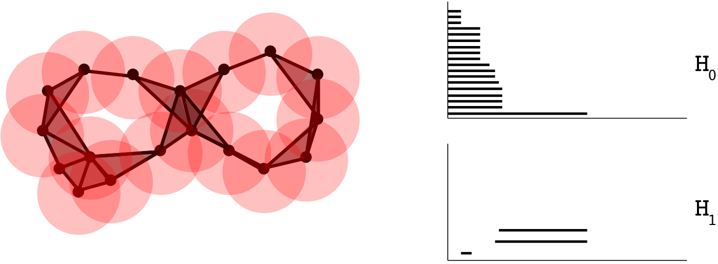

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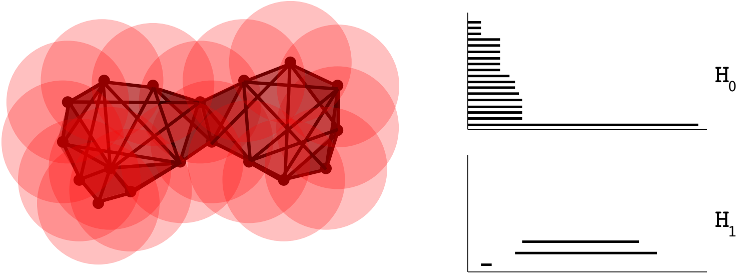
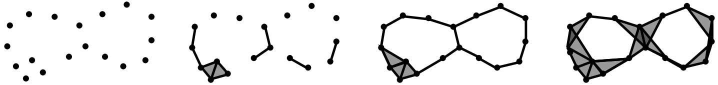


Terminology

Such a family is called a filtered simplicial complex.



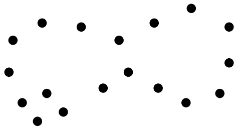
There are many techniques for creating them.

The previous example is called a Cech complex.

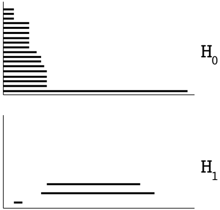
In computational examples, we'll use a related construction called a Vietoris-Rips complex.

Terminology

The topological signatures we get from persistent homology are called barcodes.



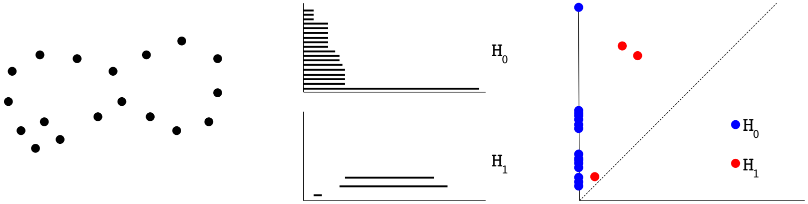
Dataset X



Barcodes for X

Terminology

We can record the "birth time" and "death time" of each topological feature to get a persistence diagram.

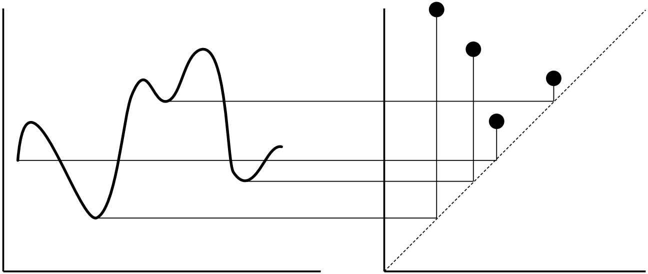


Dataset X   Barcodes for X   Persistence Diagram for X

See Example 2 in the accompanying Jupyter notebook.

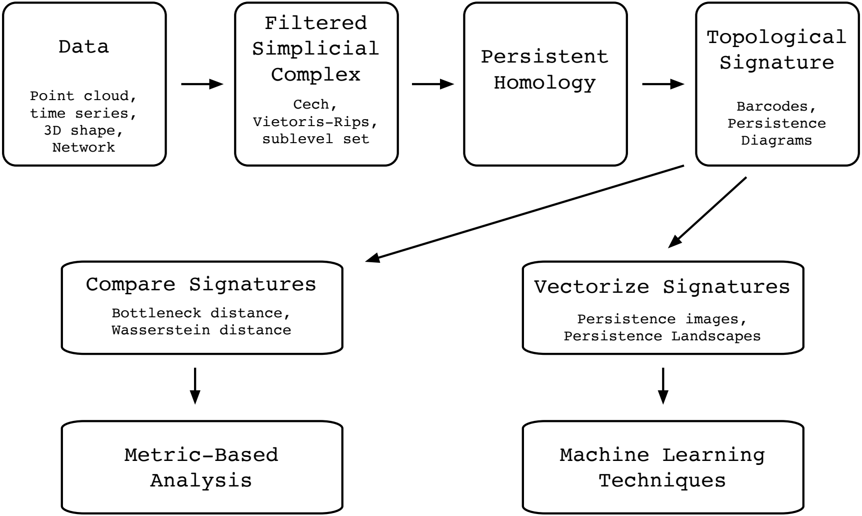
Terminology

Another common filtration is by sublevel sets of the graph of a function.



See Example 3 in the accompanying Jupyter notebook.

TDA Workflow



Next Time

- Comparing persistence diagrams via Bottleneck Distance
- Turning persistence diagrams into vectors for Machine Learning
- Applications:
  - Shape classification using persistence diagrams
  - Logistic regression on vectorized persistence diagrams