

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., 2011]
- 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.

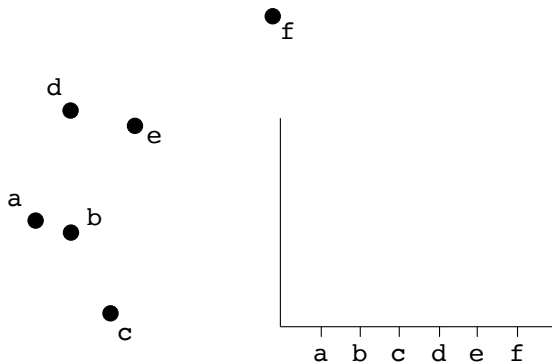
Methods like k -Means, DBSCAN, etc. partition data into clusters.

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

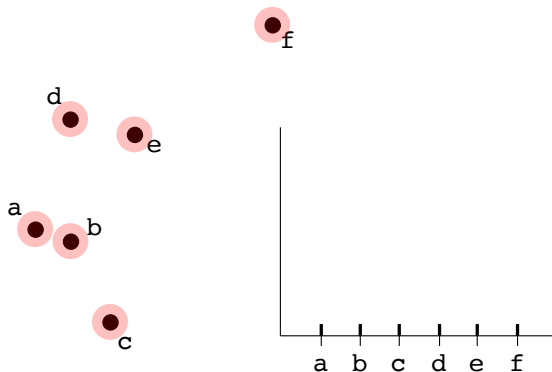
Hierarchical Clustering produces a multiscale summary of cluster structure, visualized as a **dendrogram**.

See Example 1 in accompanying Jupyter Notebook.

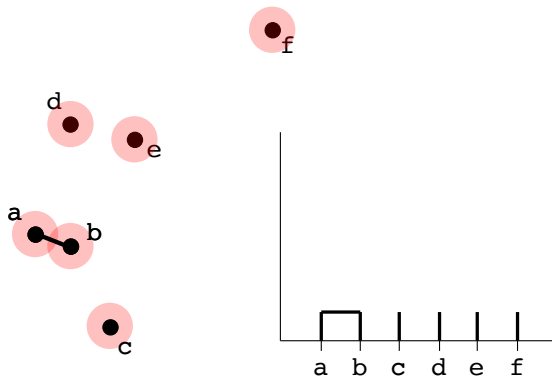
Example: Hierarchical Clustering



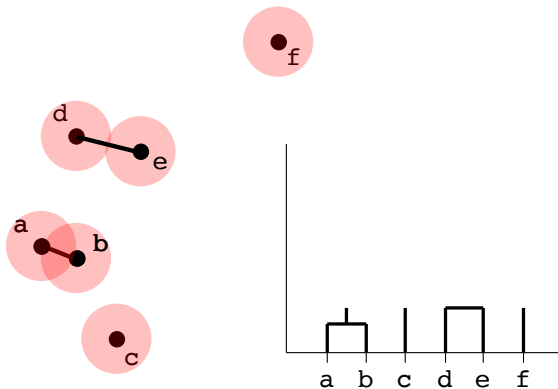
Example: Hierarchical Clustering



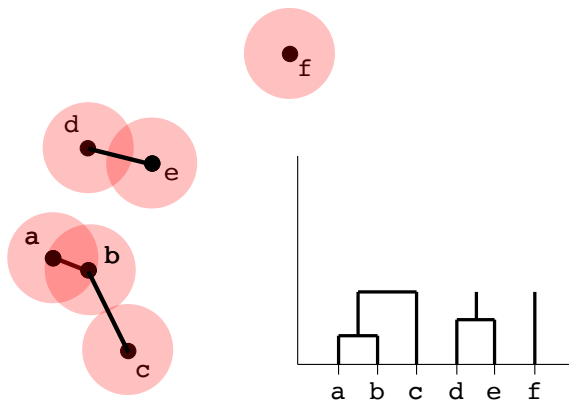
Example: Hierarchical Clustering



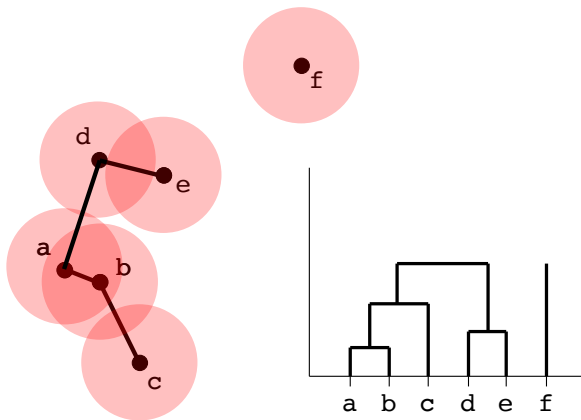
Example: Hierarchical Clustering



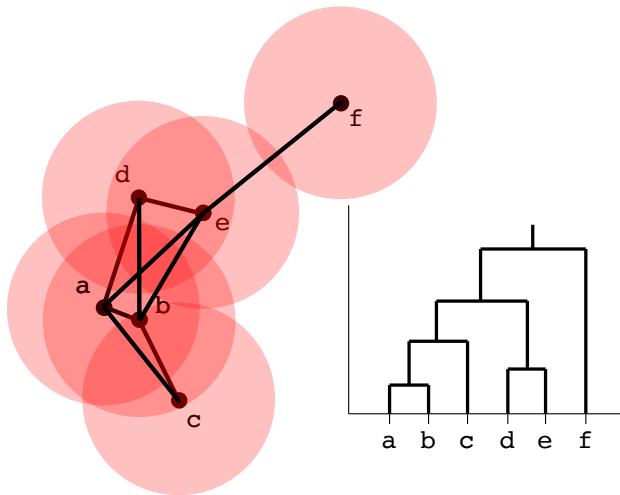
Example: Hierarchical Clustering



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.

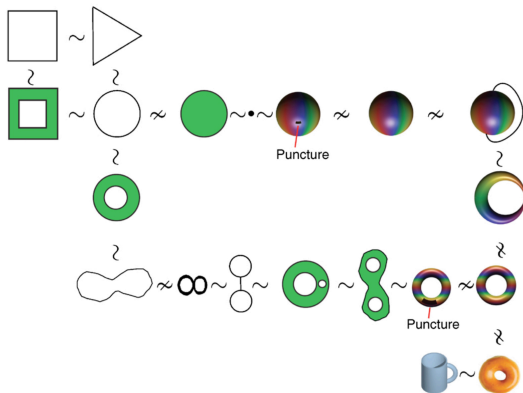


Figure: Homotopy equivalence, from Singh et. al. 2008.

Concepts from Topology

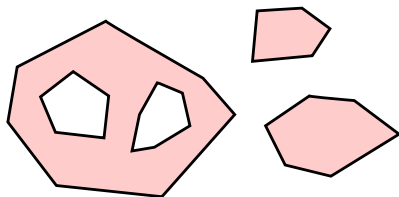
Algebraic topology is a subfield of topology where one computes invariants of a space which distinguish it from other spaces.

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

Its dimension $\beta_k(X)$ is called the **k th 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

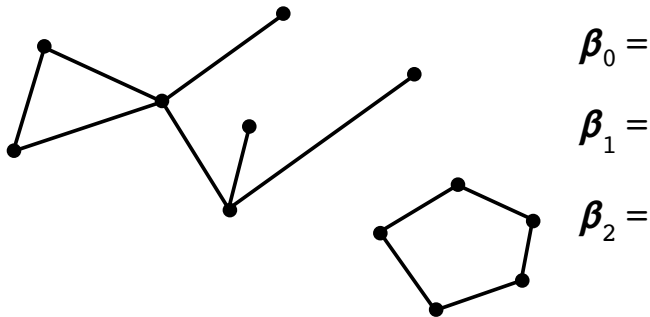
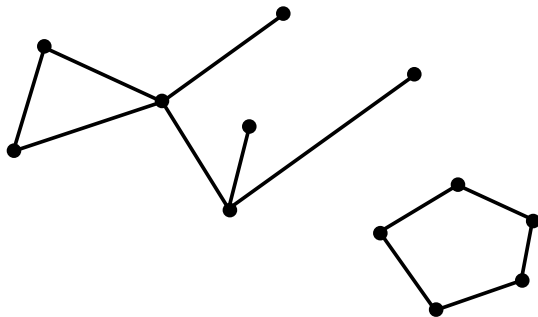


Figure: Disconnected graph.

Examples of Betti Numbers



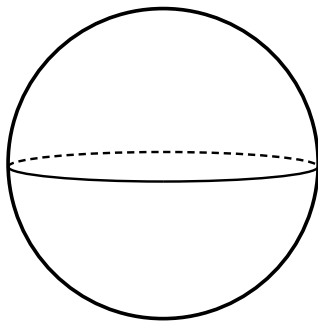
$$\beta_0 = 2$$

$$\beta_1 = 2$$

$$\beta_2 = 0$$

Figure: Disconnected graph.

Examples of Betti Numbers



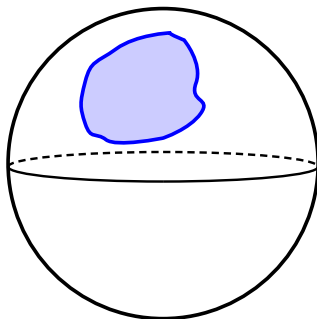
$$\beta_0 =$$

$$\beta_1 =$$

$$\beta_2 =$$

Figure: Surface of a sphere.

Examples of Betti Numbers



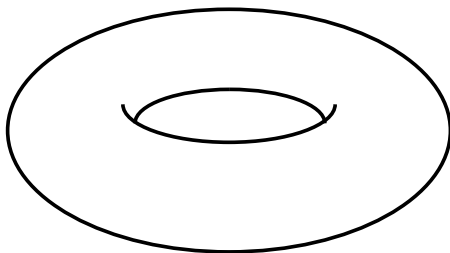
$$\beta_0 = 1$$

$$\beta_1 = 0$$

$$\beta_2 = 1$$

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

Examples of Betti Numbers



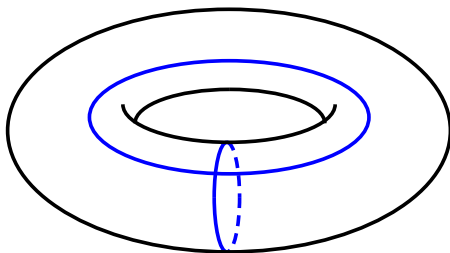
$$\beta_0 =$$

$$\beta_1 =$$

$$\beta_2 =$$

Figure: Torus (surface of a donut).

Examples of Betti Numbers



$$\beta_0 = 1$$

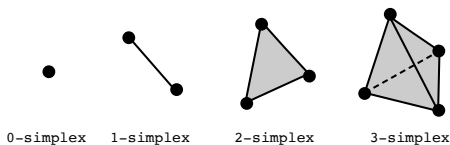
$$\beta_1 = 2$$

$$\beta_2 = 1$$

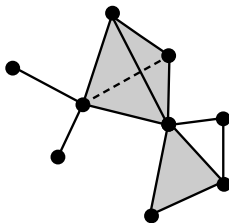
Figure: Blue loops can't be filled by disks that stay in the surface.

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.

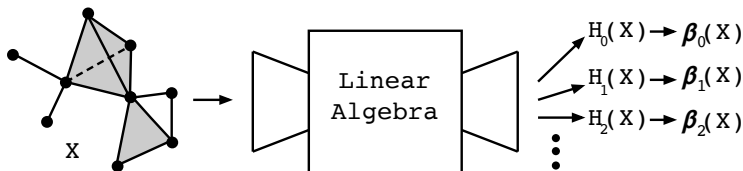


Simplicial Homology

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 $X = \{\vec{x}_1, \dots, \vec{x}_N\}$, each $\vec{x}_j \in \mathbb{R}^d$.

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

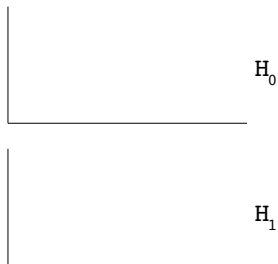
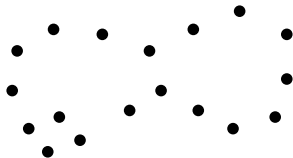
$$\beta_0 = N, \quad \beta_1, \beta_2, \dots = 0.$$

Idea

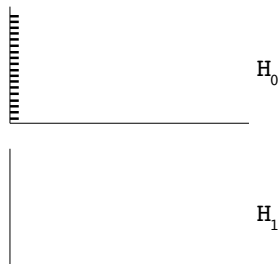
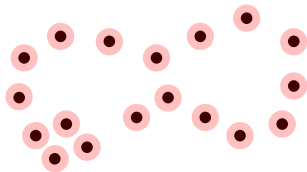
Construct a **family** of simplicial complexes following the example of hierarchical clustering.

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

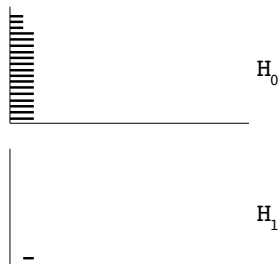
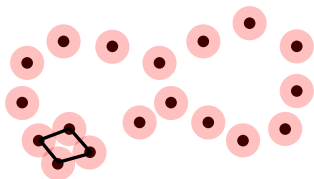
Persistent Homology - An Example



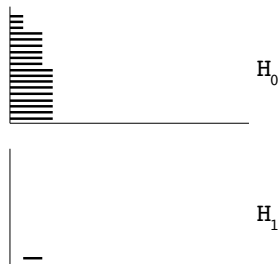
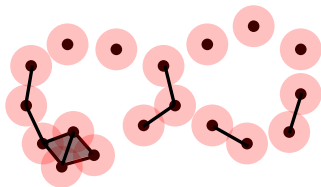
Persistent Homology - An Example



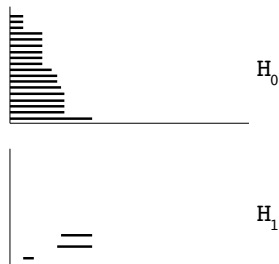
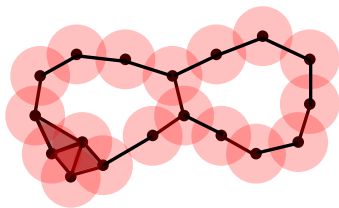
Persistent Homology - An Example



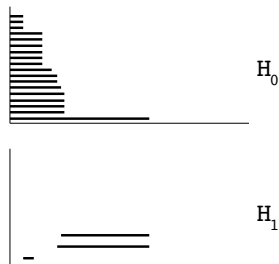
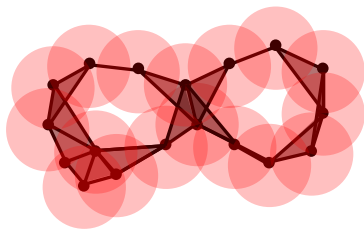
Persistent Homology - An Example



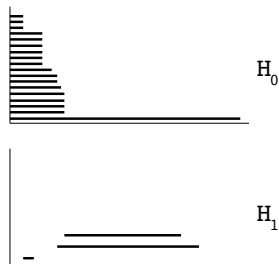
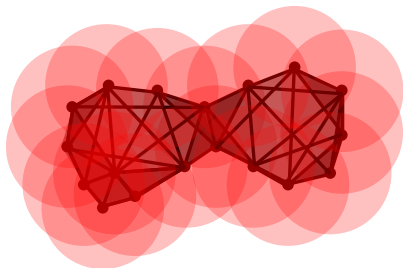
Persistent Homology - An Example



Persistent Homology - An Example

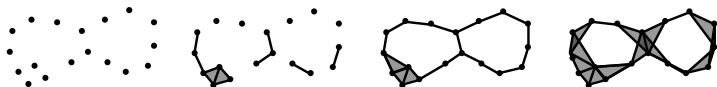


Persistent Homology - An Example



Terminology

Such a family is called a **filtered simplicial complex**.



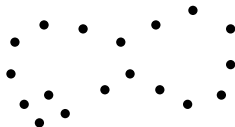
There are many techniques for creating them.

The previous example is called a **Cech complex**.

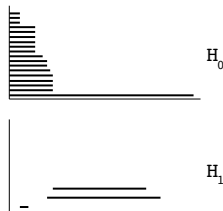
In computational examples, we'll use a related construction called a **Vietoris-Rips complex**.

Terminology

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



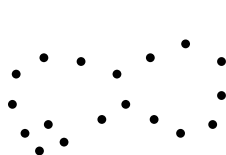
Dataset X



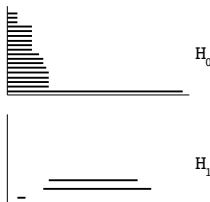
Barcodes for X

Terminology

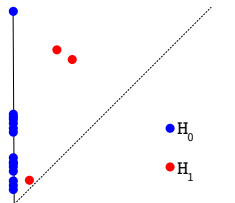
We can record the "birth time" and "death time" of each topological feature to get a **persistence diagram**.



Dataset X



Barcodes for X

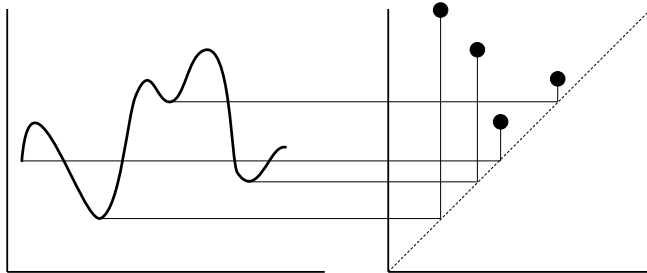


Persistence Diagram for X

See Example 2 in the accompanying Jupyter notebook.

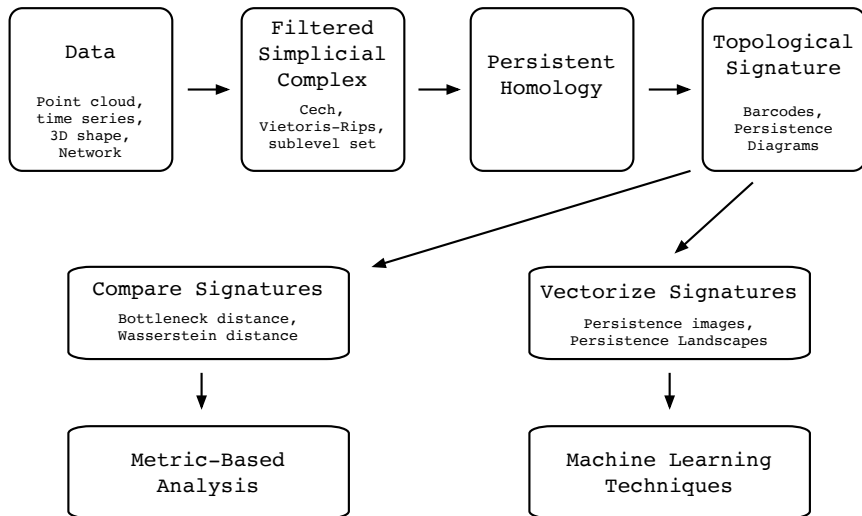
Terminology

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