Topological Techniques for Working With Data

Michelle H. Feng, mhfeng@caltech.edu

Outline

Algebraic Topology

Applied Topology

Persistent Homology

- Simplicial Complexes (and other complexes)
- Persistent Homology

Algebraic Topology

A Brief History

- How do you reduce a topological space down into invariants?
- Used to be called combinatorial topology (Betti numbers, Euler characteristics)
- Emmy Noether: we can work with algebraic objects like groups instead
- These days, much of the field have gone down the categorical rabbit hole

What is it good for?

Key insight: sometimes, we care less about the precise shape of an object than the way it's put together. Using this, we can:

- classify topological spaces (up to homeomorphism)
- understand what types of vector fields can exist on a manifold
- understand fixed points and their existence

Why should we care? It's useful to think about how data is put together!

Applied Topology

Some applications

- Impossibility theorems
- Data structure
- Knot theory
- Circuit topology

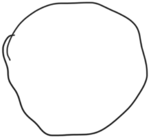
Data

- Connectedness
- “Shape”
- Patterns and cycles

Persistent Homology

Persistent Homology (PH)

- One of the most popular tools in TDA
- Applies homology theory to point clouds (usually)
- Loosely, characterizes the shape of a data set at a variety of different scales



S_1

What is the shape of a point cloud?

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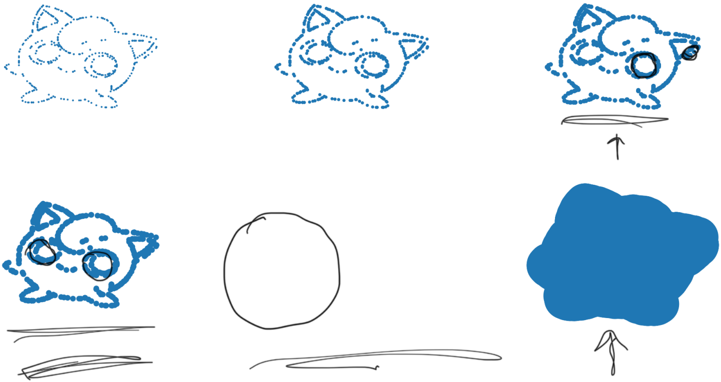


Why do we care about persistence?

Features that exist across a variety of scales are the "truest"

Basic workflow

Data set $\longrightarrow$ Topological object $\xrightarrow{\text{Homology computation}}$ Homology groups

Data set
- point cloud
- Graph/network
- Images

Topological object
- Simplicial complexes

Simplicial complexes

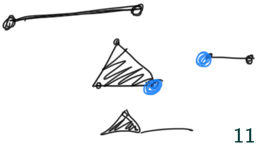
Definition

A *k-simplex* is a k-dimensional polytope which is the convex hull of its $k+1$ vertices.

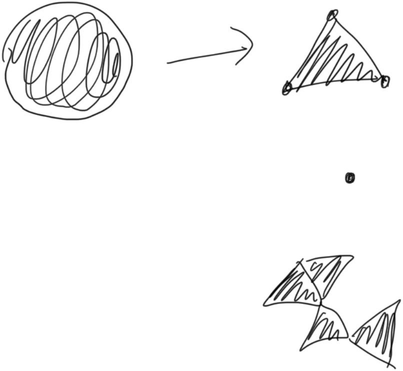
An *m-face* of a k-simplex is a subset of size $m+1$, and is an m-simplex itself.

A simplicial complex S is a set of simplices that satisfies the following conditions:

1. Every face of a simplex from S is also in S
2. The non-empty intersection of any two simplices $\sigma_1, \sigma_2 \in S$ is a face of both σ_1 and σ_2.



What do simplicial complexes look like?

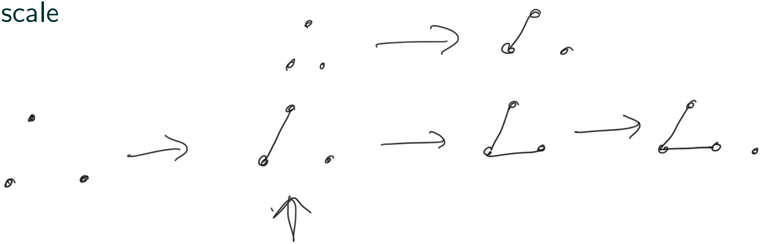


Filtered simplicial complexes

A filtered simplicial complex is a series

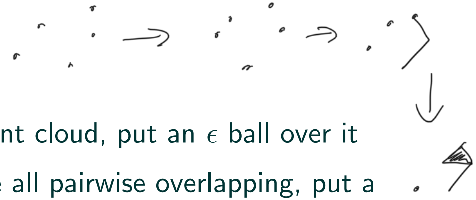
$$S_0 \subseteq S_1 \subseteq S_2 \subseteq \ldots \subseteq S_n$$

Intuitively, think of each S_i as being a glimpse of your object at a different scale

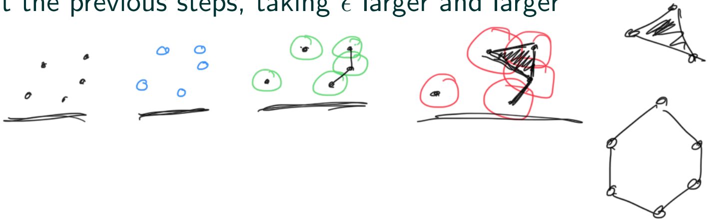


Vietoris–Rips

Constructed as follows:

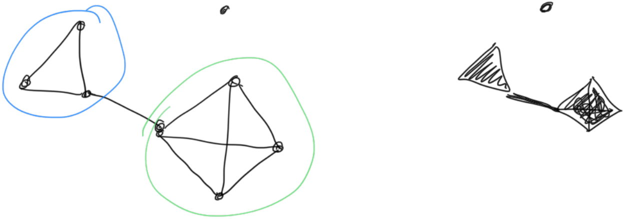


1. Fix ϵ
2. For every point in your point cloud, put an ϵ ball over it
3. Whenever $k+1$ ϵ balls are all pairwise overlapping, put a create a k-simplex
4. The resulting collection of simplices is a simplicial complex (call it S_ϵ)
5. Repeat the previous steps, taking ϵ larger and larger



Clique complex

Let G be a graph. The clique complex $X(G)$ of G is a simplicial complex formed by the sets of vertices in the cliques of G. Alternatively, $X(G)$ is a topological space in which each clique of k vertices is represented by a $(k-1)$-simplex.



Gotta go fast

- Alpha complexes: Delaunay triangulations for fun and profit
- Witness complexes: Sampling is your friend
- Flag complexes

Get creative!

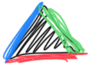
Homology theories

- Associate a sequence of algebraic objects to topological spaces
- Give us a way to rigorously define and categorize holes in a manifold
- Can compute homology on a variety of different topological objects
  - Simplicial
  - Cubical
  - Others

Homology

Let X be a simplicial complex. We construct a chain complex on X, which is a sequence of abelian groups $C_0, C_1, \ldots$ connected by homomorphisms $\partial_n : C_n \to C_{n-1}$, which are called boundary operators. We do this in such a way that

$$\partial_n \circ \partial_{n+1} = 0$$



Then the n-th homology group of X is

$$H_n(X) := \ker(\partial_n)/\mathrm{im}(\partial_{n+1})$$

$$C_2 \xrightarrow{\partial_2} C_1 \xrightarrow{\partial_1} C_0$$

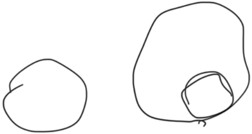
Key takeaway: **The n-th homology group of X is entirely determined by what n-simplices and $n+1$-simplices in X look like**

$$
\begin{tikzcd}
S_0 \arrow[r, "i"] \arrow[d] & S_1 \arrow[r] \arrow[d] & \cdots \arrow[r] & S_n \arrow[d] \\
H_i(S_0) \arrow[r] & H_i(S_1) \arrow[r] & \cdots \arrow[r] & H_i(S_n)
\end{tikzcd}
$$

What comes out of a PH computation?

Usually, a list of features, which correspond to elements of the homology groups, with some additional information:

For $x \in H_m(S_i)$, we get:



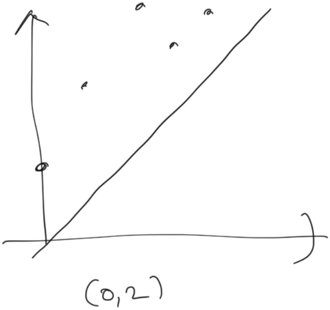
- Dimension m of the feature
- Non-unique generators of x
- A time b_x, called the "birth" of x, which is the lowest value such that $x \in H_m(S_{b_x})$
- A time d_x, called the "death" of x, which is the lowest value greater than b_x such that $x \notin H_m(S_{d_x})$ $\quad x \to x \to x \to x \to 0$
- Note that a feature can theoretically live forever, in which case we sometimes say it dies at ∞

Barcodes

- Represents each feature x with a bar stretching across $[b_x, d_x)$
- Usually use arrows or something similar to represent infinite persistence
- Handle different dimensions in a variety of ways (separate barcodes, colors, etc)

Persistence Diagrams (PDs)

- Plot each feature x at the point (b_x, d_x)
- Can compute distances between PDs (bottleneck, Wasserstein)



Persistence Images (PIs)

- Turns a PD into a vector
- Very roughly, perform a transformation which maps each feature to $(b_x, d_x - b_x)$, replace the point with a probability distribution, and discretize into an image
- The PI for each dimension is a vector
- PIs for all dimensions can be concatenated, resulting in a vector format for persistence

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