

Topological data analysis

Lecture 4

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A principal incompatibility between “topology” and “applied”.

- Data analysis and machine learning deal with real numbers and real optimization.
- Topological invariants are discrete. There is no space with 2.3457 many connected components or $\frac{5}{6}$ many holes.
- How can one make Topology “applied”?

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- Data analysis and machine learning deal with real numbers and real optimization.
- Topological invariants are discrete. There is no space with 2.3457 many connected components or $\frac{5}{6}$ many holes.
- How can one make Topology “applied”?

Introduce “topological processes”!

Let X_t be a space depending on time $t \in \mathbb{R}$. If $t_1 \leq t_2$, we assume there is a map

$$f_{t_1 \leq t_2}: X_{t_1} \rightarrow X_{t_2},$$

such that $f_{t \leq t} = \text{id}_{X_t}$ and $f_{t_2 \leq t_3} \circ f_{t_1 \leq t_2} = f_{t_1 \leq t_3}$.

Compare this with stochastic processes...

Idea of applied topology

Topological process

Let X_t be a space depending on time $t \in \mathbb{R}$ and there are maps $f_{t_1 \leq t_2} : X_{t_1} \rightarrow X_{t_2}$.

Usually, all connecting maps $f_{t_1 \leq t_2}$ are inclusions. In this case the process is called a **filtration**.

Idea

- We may average topological invariants along all values of time t .
- This gives real-valued invariants which can be optimized using methods of machine learning.

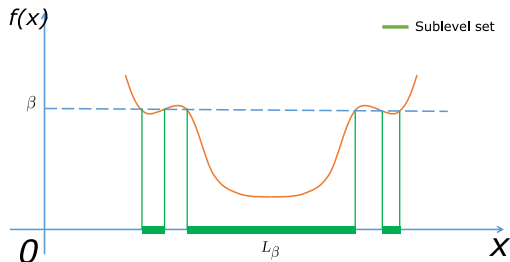
Important construction

Sublevel set filtration

Let $f: \mathbb{R}^d \rightarrow \mathbb{R}$ be a function. Consider sublevel sets of f

$$X_t^f = \{x \in \mathbb{R}^d \mid f(x) \leq t\}$$

This is a filtration.



Another important construction

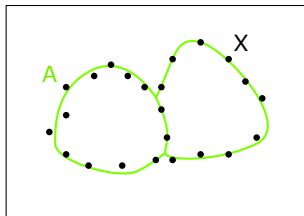
Čech filtration

Let $X = \{x_1, \dots, x_m\} \subset \mathbb{R}^d$ be a finite set (point cloud). Itself, the space X is not interesting topologically. But we may surround each point with a ball of variable radius $t/2$, and see how topology evolve:

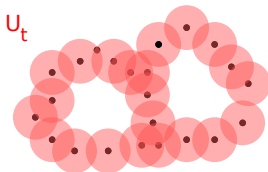
$$X_t = \bigcup_{i=1}^m B_{t/2}(x_i)$$

This is a filtration defined for $t \geq 0$.

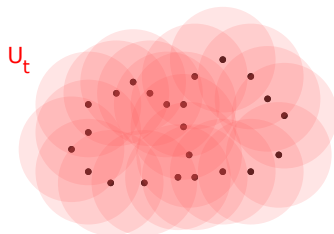
Čech filtration



$t \approx 0$



t is nice



$t \gg 0$

Toy example: average number of components

Let $X = \{x_1, \dots, x_m\} \subset \mathbb{R}^d$ be a point cloud and X_t its Čech filtration. Let $\text{nc}(X_t)$ be the number of connected components of X_t .

A new invariant

Define the number

$$\overline{\text{nc}}(X) = \int_0^{+\infty} (\text{nc}(X_t) - 1) dt.$$

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$$\overline{\text{nc}}(X) = \int_0^{+\infty} (\text{nc}(X_t) - 1) dt.$$

Question: any guess what $\overline{\text{nc}}(X)$ is?

Demonstration: press to play in browser

Toy example: evolution of components

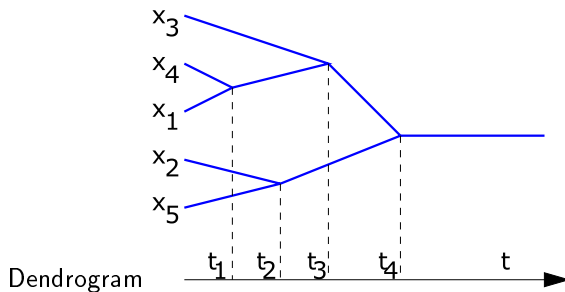
Answer:

$\overline{\text{nc}}(X)$ equals the length of the minimal spanning tree of X . Guess why.

Toy example: evolution of components

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Open question: how can we encode such dendrograms?

Persistent homology

Homology

Homology = higher dimensional analogue of counting connected components.

$\beta_i(X)$ = number of i -dimensional holes in X .

Persistent homology

How the number of holes in a filtration changes in time.

Filtration

A chain of simplicial complexes

$$K_0 \subset K_1 \subset K_2 \subset \cdots \subset K_m = K$$

is called a **filtration**.

For each j , it induces the chain of linear maps

$$H_j(K_0) \rightarrow H_j(K_1) \rightarrow H_j(K_2) \rightarrow \cdots \rightarrow H_j(K_m)$$

of \mathbb{k} -vector spaces.

Definition

A **persistence module** is a chain of finite dimensional \mathbb{k} -vector spaces and linear maps

$$V_0 \rightarrow V_1 \rightarrow V_2 \rightarrow \cdots \rightarrow V_m \rightarrow \cdots$$

If, for some m , $V_m = V_{m+1} = \cdots$, we say that persistence module **stabilizes**.

Main example: j -th homology of a filtration is a stabilizing persistence module. It is called **the persistence homology module** of a filtration:

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Exercise: prove that persistence module is the synonym for “graded module over the polynomial ring $\mathbb{k}[x]$ ” if you understand this phrase.

Interval modules and the structure theorem

Example: An interval module $I_{[b;d)}$ is the following module

$$0 \rightarrow \cdots \rightarrow 0 \rightarrow \underset{b}{\mathbb{k}} \xrightarrow{=} \cdots \xrightarrow{=} \mathbb{k} \rightarrow \underset{d}{0} \rightarrow 0 \rightarrow \cdots$$

where $b \in \mathbb{Z}_+$ is called **the birth-time** of a module and $d \in \mathbb{Z}_+ \sqcup \{+\infty\}$ is **the death-time**.

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Main Structural Theorem (about persistence modules)

Every stabilizing persistence module is isomorphic to a direct sum of interval modules. The summands are determined uniquely up to permutation.

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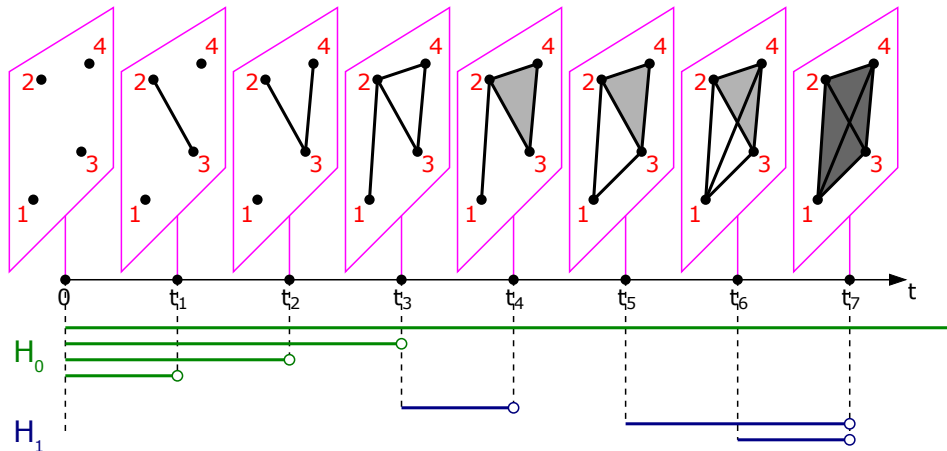
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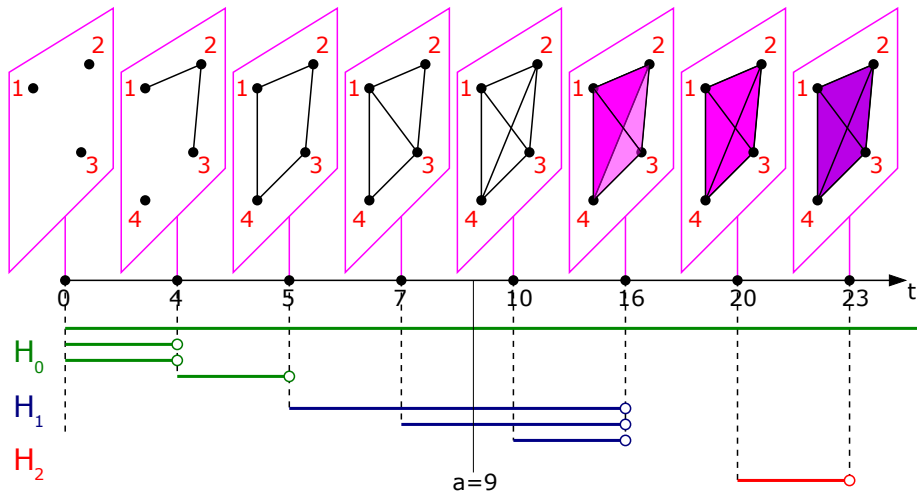
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Remark: This is actually an instance of **the classification theorem for finitely generated modules over PID** (the ring $\mathbb{k}[x]$ is a principal ideal domain).

Persistence homology decomposed into interval summands



Persistence homology decomposed into interval summands



Persistent homology of a filtration

Filtration:

$$K_0 \subset K_1 \subset K_2 \subset \cdots \subset K_m = K$$

j -th persistent homology module:

$$H_j(K_0) \rightarrow H_j(K_1) \rightarrow H_j(K_2) \rightarrow \cdots \rightarrow H_j(K_m).$$

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Should we compute all homology $H_j(K_i)$ separately, and then merge them to get interval decomposition?

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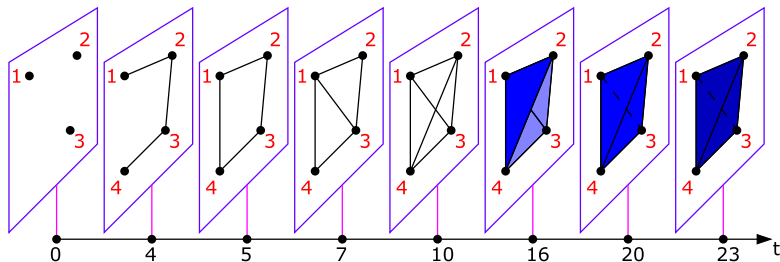
Main question

Should we compute all homology $H_j(K_i)$ separately, and then merge them to get interval decomposition?

Luckily, no! We need to store our filtration in an optimal form.

How to treat filtrations

Instead of $K_0 \subset K_1 \subset K_2 \subset \dots \subset K_m = K$ let us store the list of all simplices of K together with their birth times.



$\{1\}:0, \{2\}:0, \{3\}:0, \{4\}:4$

$\{1,2\}:4, \{1,3\}:7, \{1,4\}:5, \{2,3\}:4, \{2,4\}:10, \{3,4\}:4$

$\{1,2,3\}:16, \{1,2,4\}:16, \{1,3,4\}:16, \{2,3,4\}:20$

$\{1,2,3,4\}:23$

How to treat filtrations

We have two lists: **BirthTimes** and **Simplices**. We assume they satisfy the following:

- Their indices agree: $\text{BirthTimes}[i]$ is the time of appearance of $\text{Simplices}[i]$ in the filtration.

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Last condition assures that $K^i = \{\text{Simplices}[j] \mid j \leq i\}$ is always a **simplicial complex**.

How to treat filtrations

Last condition assures that $K^i = \{\text{Simplices}[j] \mid j \leq i\}$ is always a simplicial complex. We get new filtration

$$K^0 \subset K^1 \subset K^2 \subset \dots \subset K^N$$

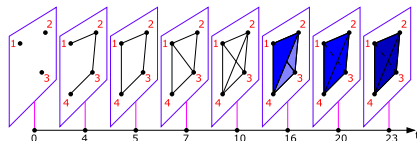
where N is the total number of simplices.

What is good

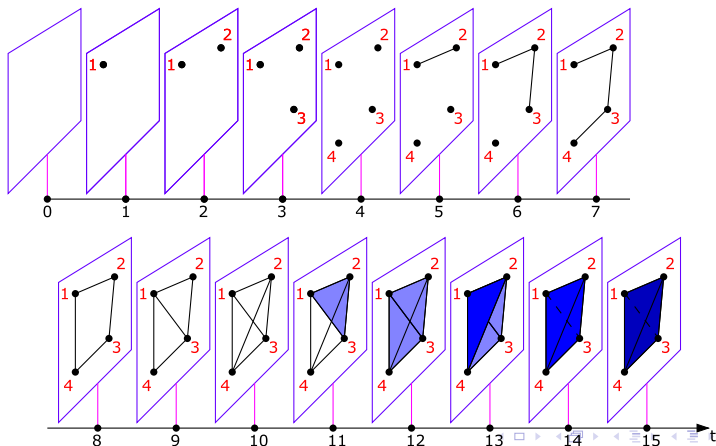
At each step of this new filtration, exactly one simplex is added. Namely $\text{Simplices}[i]$ is added at i -th step.

How to treat filtrations

Old filtration



New filtration



What happens with homology at each step

Proposition

Assume that $L \subset K$ and $K \setminus L$ is a single j -dim simplex. Then we have an alternative:

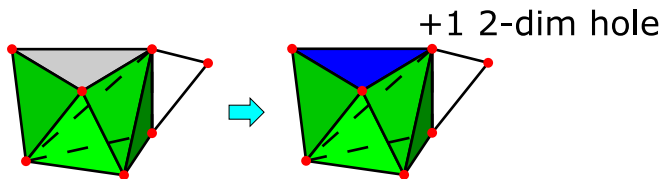
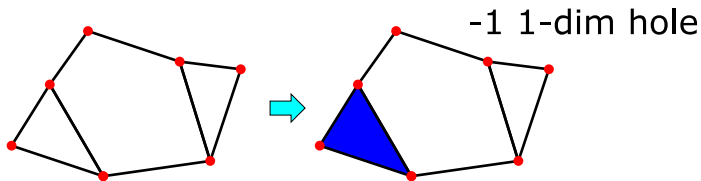
- $(j - 1)$ -th Betti number reduces by 1.
- j -th Betti number increases by 1.

Other Betti numbers do not change.

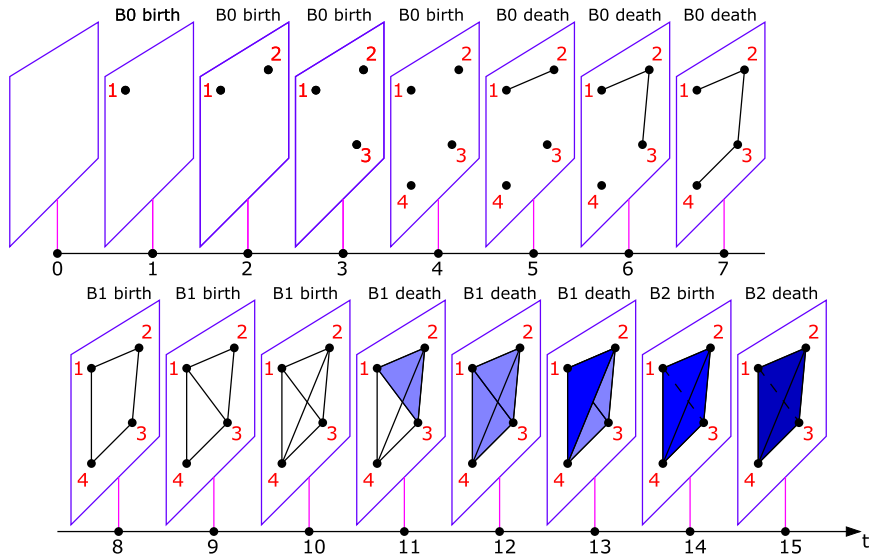
Adding a j -simplex, we either **seal up a $(j - 1)$ -hole**, or **create a j -hole**.

Exercise: prove it.

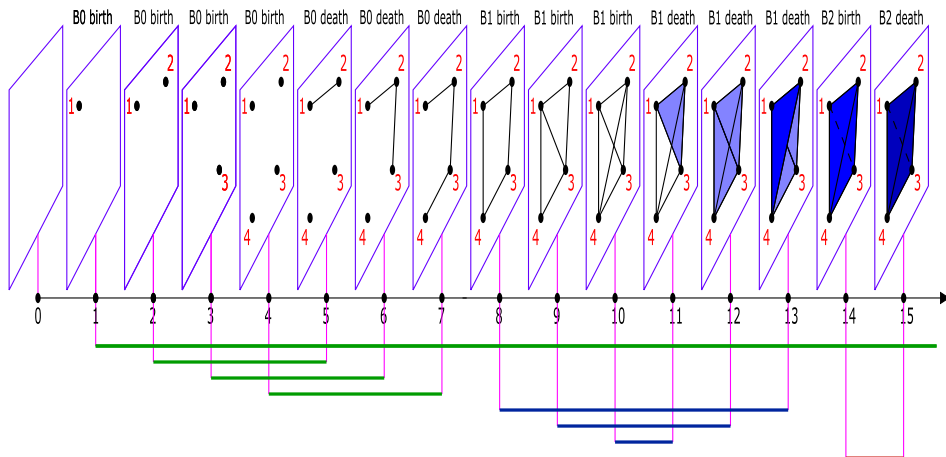
Adding a 2-simplex








Our detailed filtration



Our detailed filtration



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