

# Topological data analysis and persistent homology

Developing an outlier detector based on persistent homology

Arnau Mas

*Supervised by*  
Dr Albert Ruiz

Universitat Autònoma de Barcelona  
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Universitat Autònoma  
de Barcelona

- ① The problem
- ② An overview of homology
- ③ The detector
- ④ The results

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- Look for correlations between radiomic features and treatment response

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- Quantitative

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## Drawbacks

- May be hard to reproduce
- High dimensional feature spaces
- Limited number of cases





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- Main aim: early detection of patients with strange radiomic signatures, *outliers*, for whom standard treatments could fail.
- Use *topological data analysis*, hence TOPiomics (topological radiomics).

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This is persistence

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Algebraic topology studies topological spaces by computing algebraic invariants, namely with functors

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$$\text{Top} \rightarrow \text{Ab}$$

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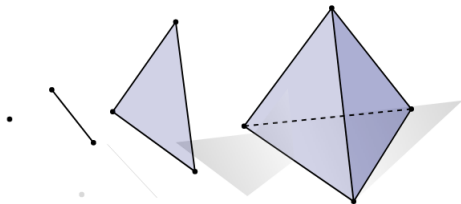
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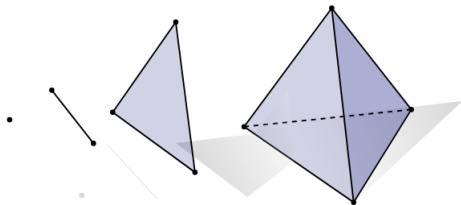
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They come in many flavours, the simplest one is *simplicial homology*, which works for *simplicial complexes*.

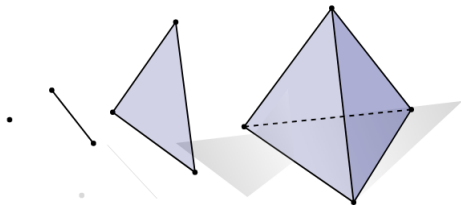
- *Simplex*. The convex hull of a set of points.



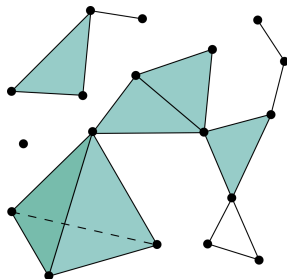
- *Simplex*. The convex hull of a set of (geometrically independent) points.



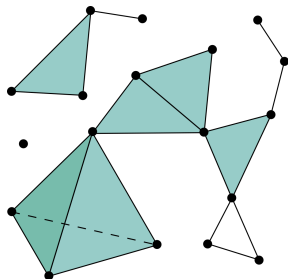
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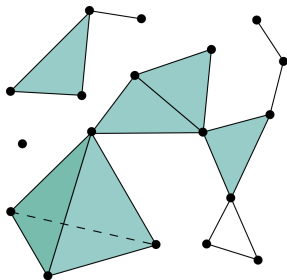


## Remark

In the combinatorial picture, the geometrical requirements are dropped and one speaks of *abstract* simplices, *abstract* simplicial complexes, etc.



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## Remark

Free abelian groups are equivalent to  $\mathbb{Z}$ -modules. Alternatively, one can also consider the vector spaces generated by the chains, for instance over  $\mathbb{F}_2$ .

## Orientation

The simplex generated by  $p_0, \dots, p_n$  is written  $[p_0, \dots, p_n]$ . The ordering determines an orientation, and we require that flipping orientation implies a change of sign in  $C_n(K)$ , e.g.

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The chain groups are not really free!

Define the boundary morphism  $\partial_n: C_n(K) \rightarrow C_{n-1}(K)$  by

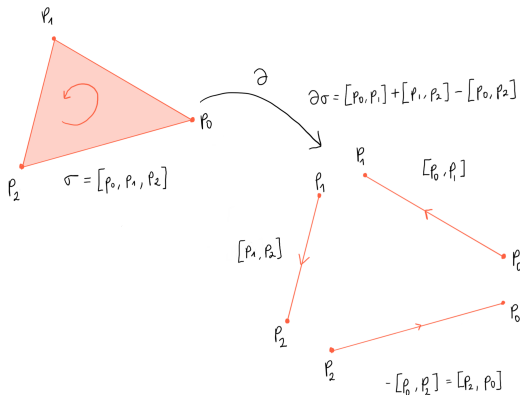
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## Fact

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

so boundaries are always cycles.



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Homology is invariant under homotopy, weaker than invariance under homeomorphism.

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The steps of the filtration can be thought of as time

Because of functoriality, there are maps between the different steps of homology,

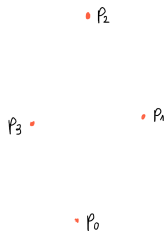
$$f_i^j: H_d^i(K) \rightarrow H_d^j(K).$$



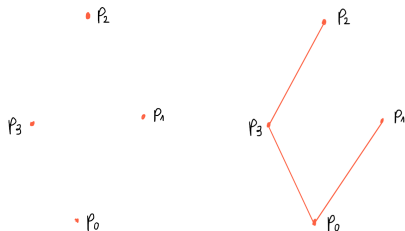
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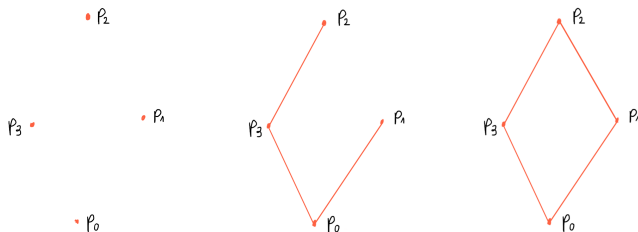
At each step, classes can be born (not in the image of  $f_i^{i+1}$ ), die (in the kernel of  $f_i^{i+1}$ ) or merge (have the same image through  $f_i^{i+1}$ ).



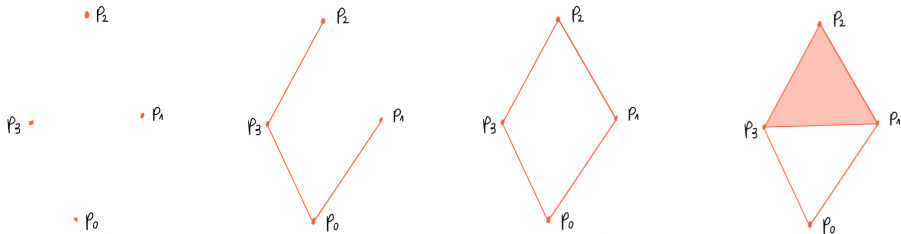
$[p_0], [p_1], [p_2], [p_3]$  are born.



$[p_0], [p_1], [p_2], [p_3]$  merge.



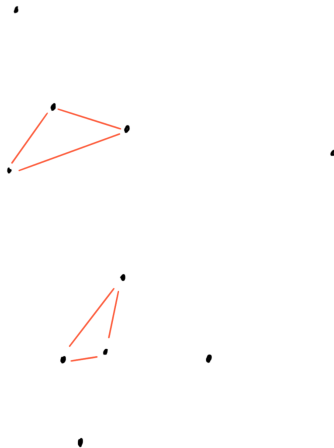
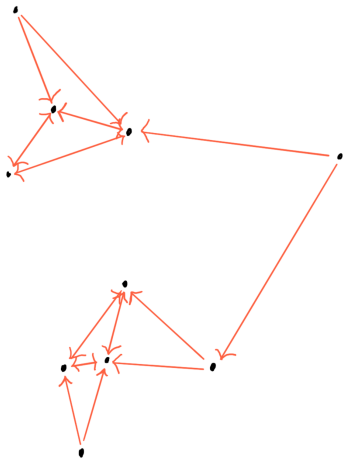
The cycle  $[p_0, p_1] + [p_1, p_2] + [p_2, p_3] + [p_3, p_4]$  is born.



The cycle does not die.

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It is good for detecting clusters in a data set.



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All of the Python code is available at  
[github.com/arnaumas/mknn-homology](https://github.com/arnaumas/mknn-homology).

- Store the cloud of  $N$  points in  $\mathbb{R}^d$  as a NumPy array of shape  $(N, d)$ .

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- The adjacency matrix of the the M $k$ NN graph is

$$M = A \odot A^T$$

where  $\odot$  is the entrywise product.



- The package NetworkX can compute the cliques of a graph. These correspond to the simplices of the *graph complex* associated to the  $MkNN$  graph of the cloud.

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- The simplices are ordered by order of appearance and dimension, which ensures any simplex is always preceded by its faces.

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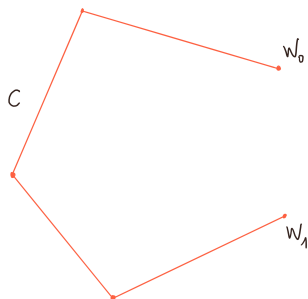
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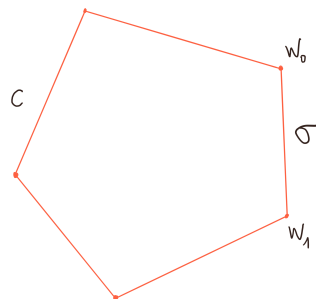
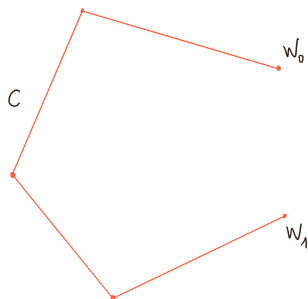
$$w_0 + \cdots + w_n = \partial c.$$

Once  $\sigma$  is added,

$$w_0 + \cdots + w_n = \partial c = \partial \sigma$$

so  $\partial(\sigma + c) = 0$ , which means  $\sigma + c$  is a new cycle.

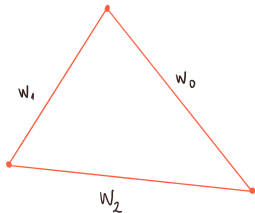




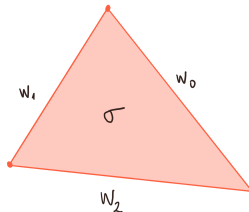
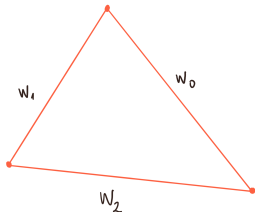
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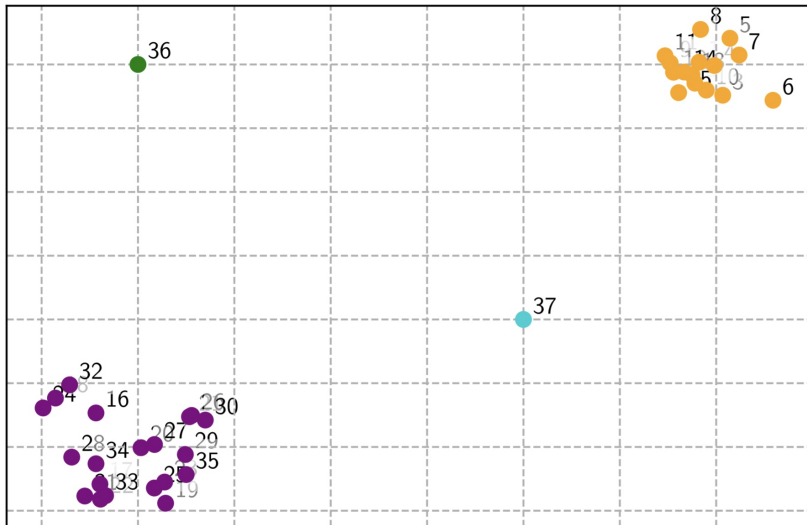


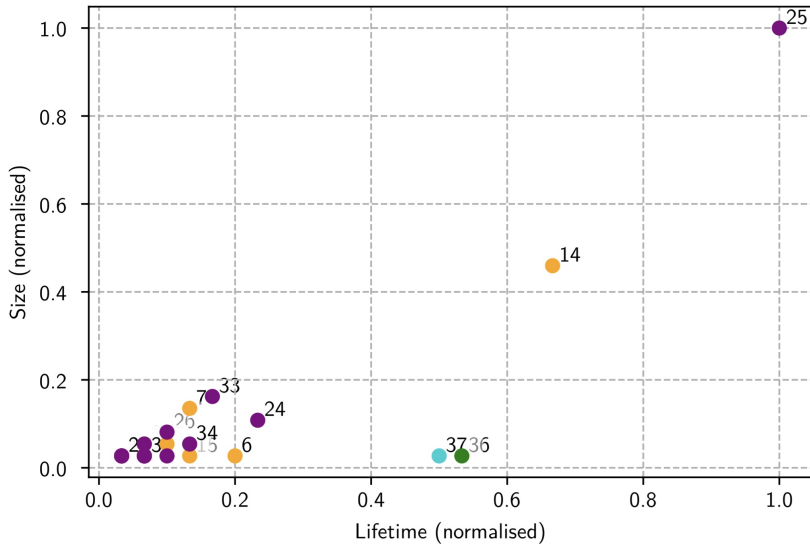
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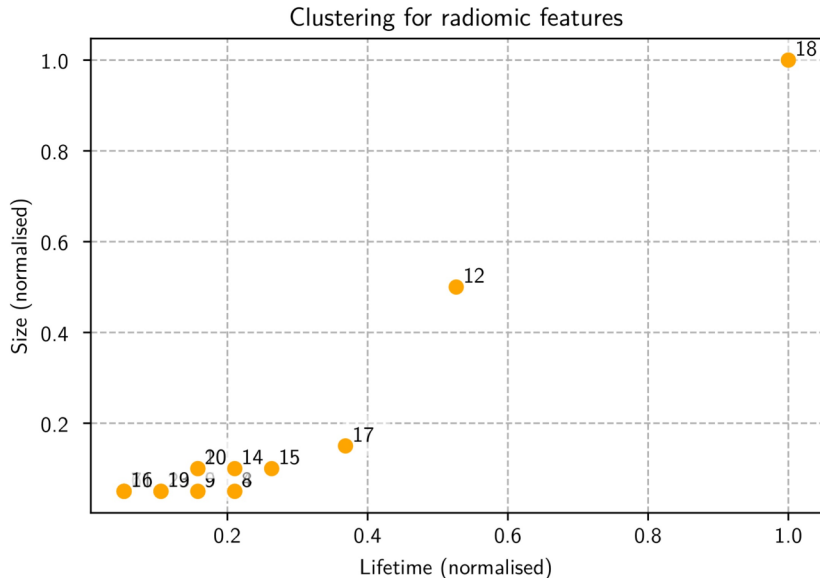




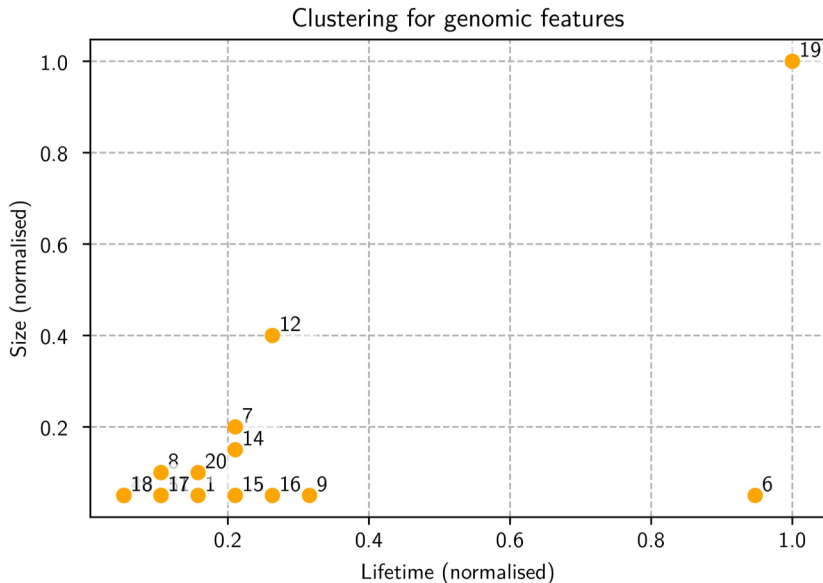
- The detector was run with a data set consisting of 26 radiomic features measured from 20 different patients. These are the result of a previous study carried out at VHIO.

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- There are also genomic features corresponding to the same 20 patients.
- The detector was run on both sets to compare the clustering structure.







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- Further considerations: efficiency, edgecase testing, higher dimensional homology.

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