Topological data analysis and persistent homology

Developing an outlier detector based on persistent homology

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Outline

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- Look for correlations between radiomic features and treatment response

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UAB

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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).

Prior work

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This is persistence

Outline

The elevator pitch

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

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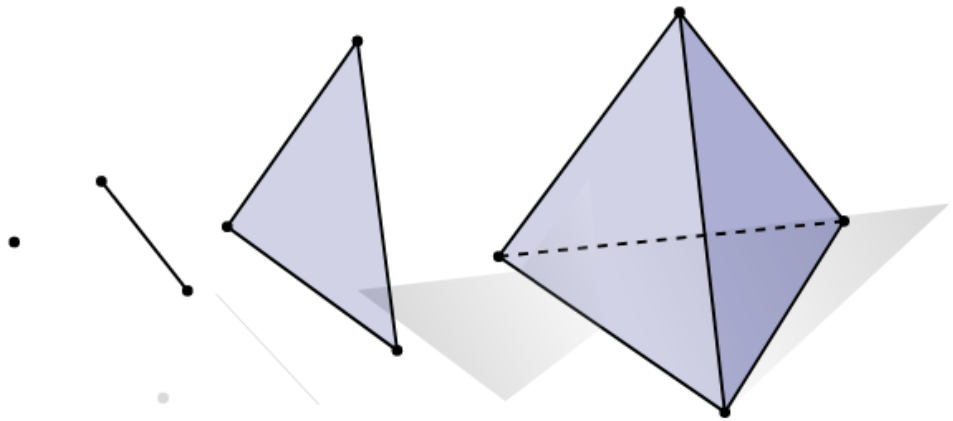
They come in many flavours, the simplest one is *simplicial homology*, which works for *simplicial complexes*.

The ingredients of homology

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



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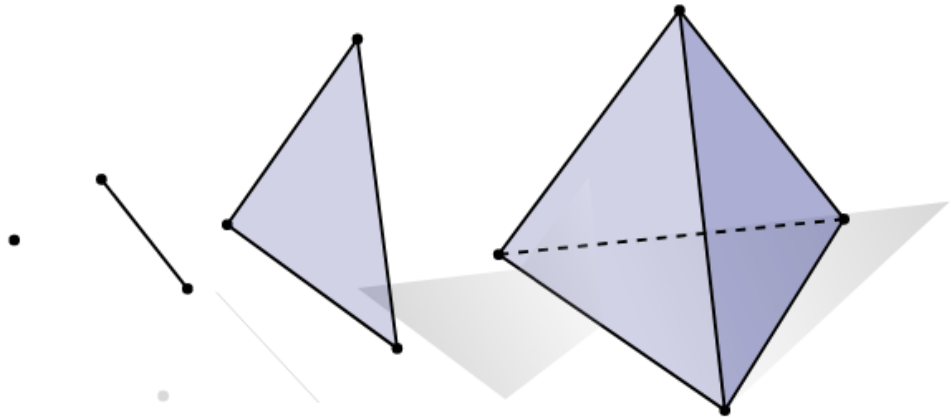

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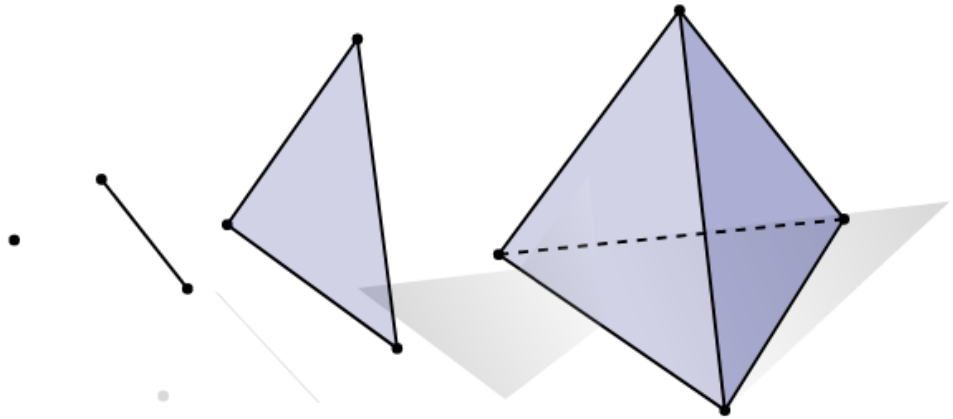

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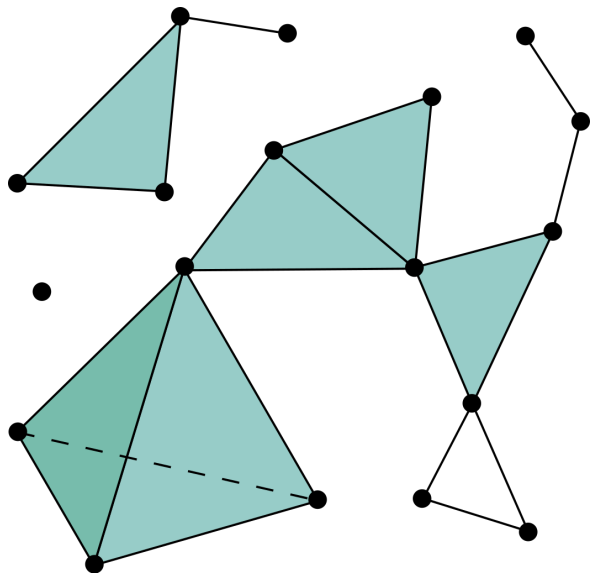

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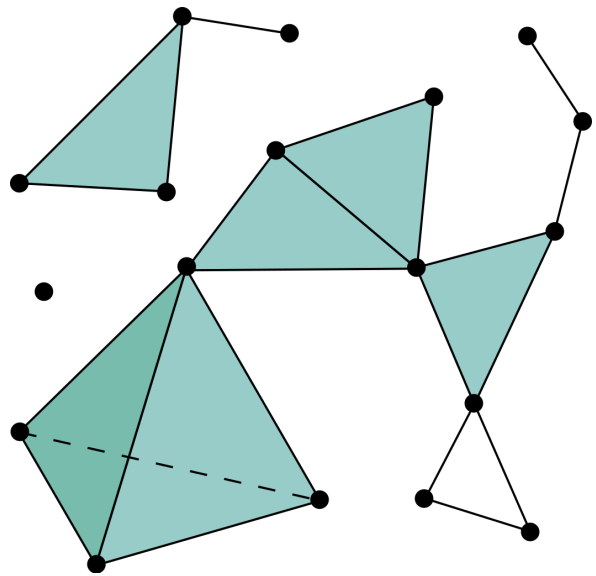

Remark

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

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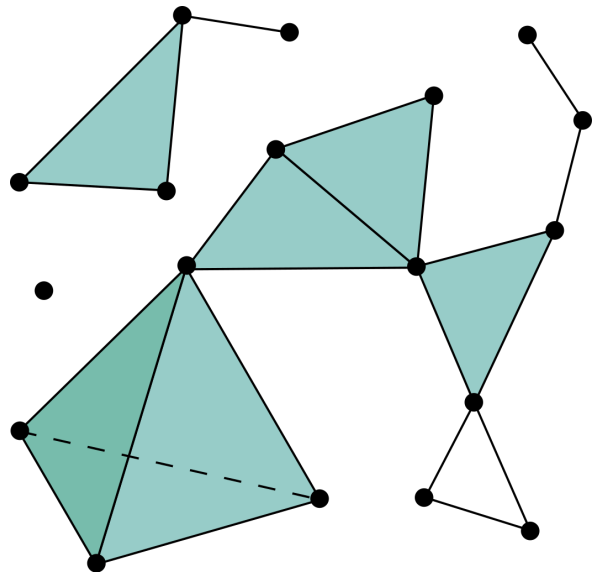

Remark

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 $p_0, \ldots, p_n$ is written $[p_0, \ldots, p_n]$. 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!

The boundary morphisms

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

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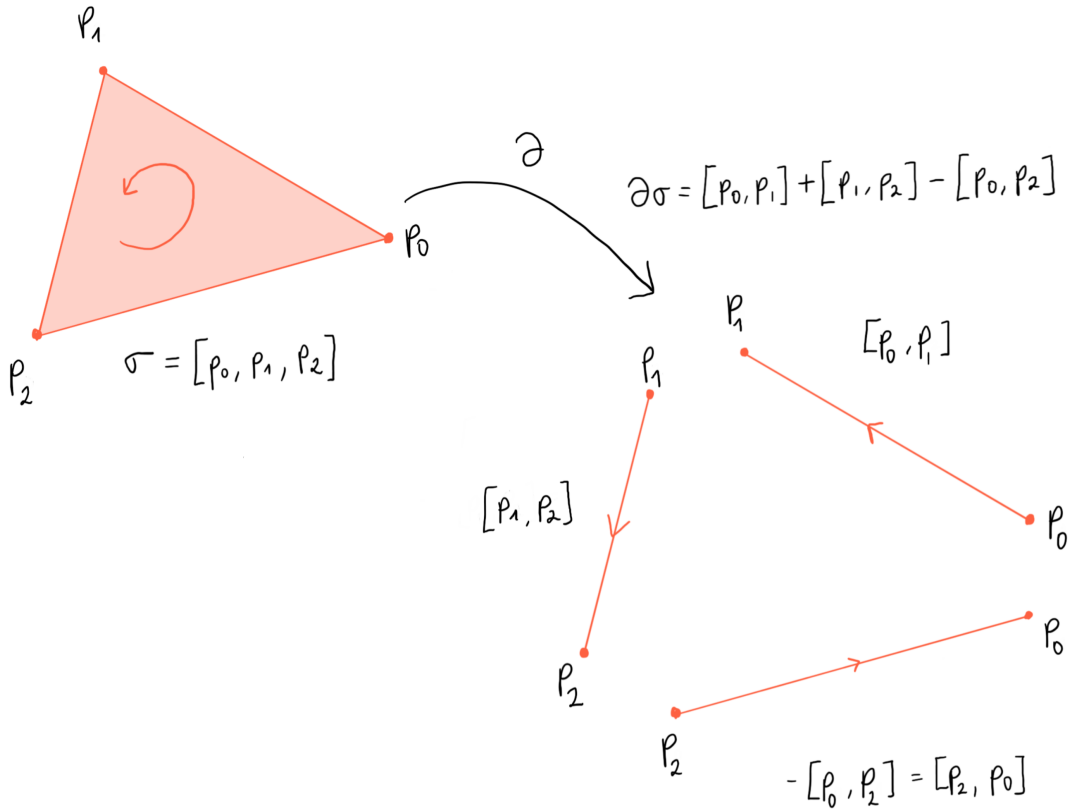

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Fact

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

so boundaries are always cycles.

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

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The steps of the filtration can be thought of as time

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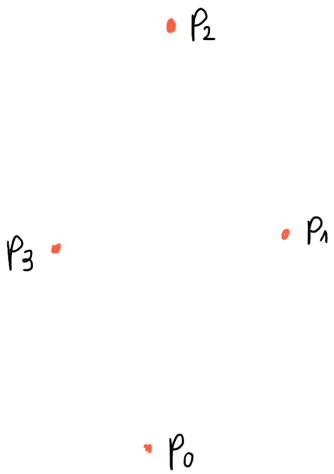
At each step, classes can be born (not in the image of f_i^{i+1}), die (in the kernel of f_i^{i+1}) or merge (have the same image through f_i^{i+1}).

An example



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

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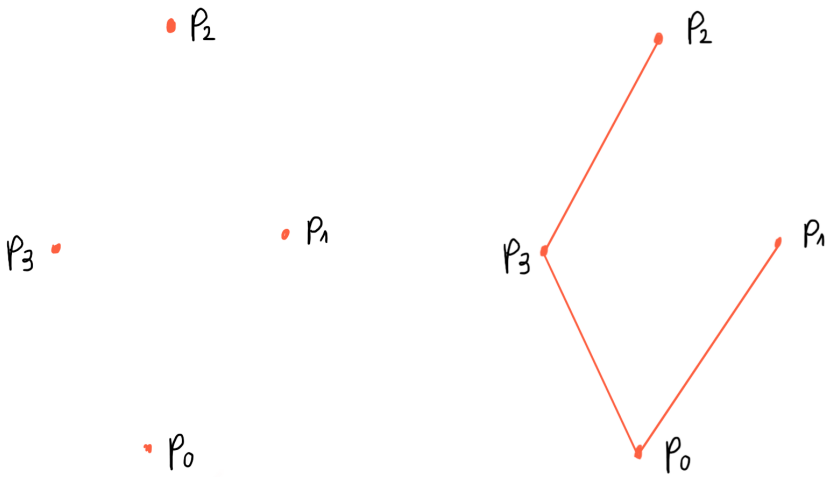

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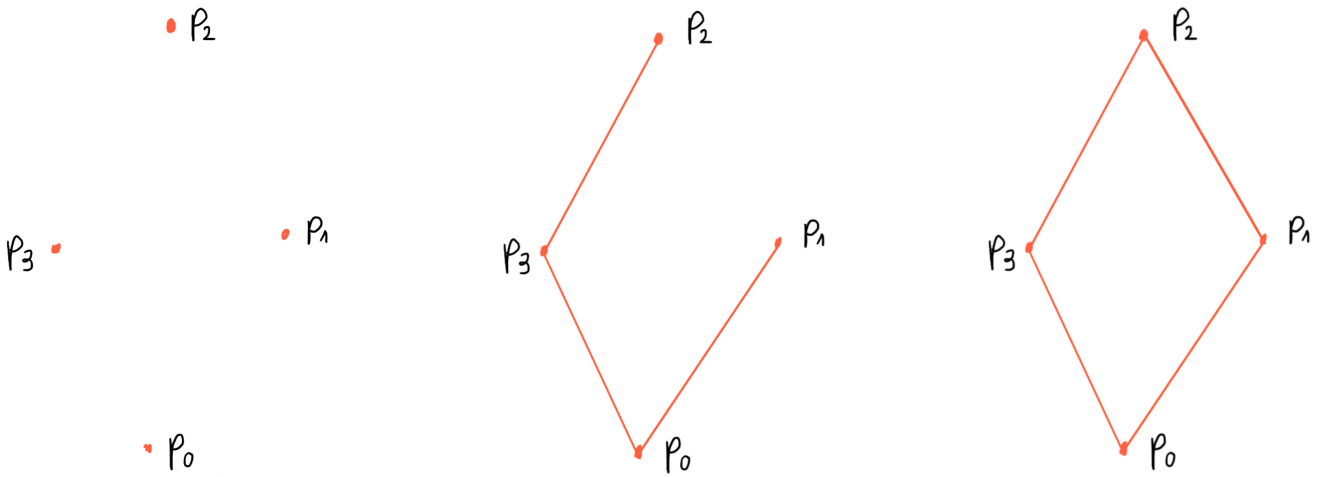

The cycle $[p_0, p_1] + [p_1, p_2] + [p_2, p_3] + [p_3, p_4]$ is born.

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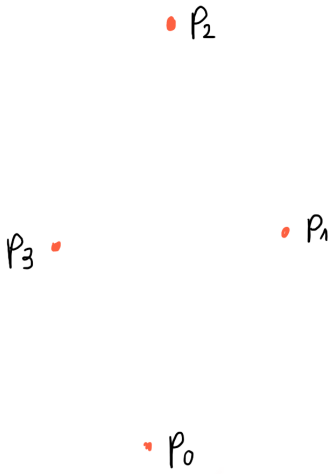
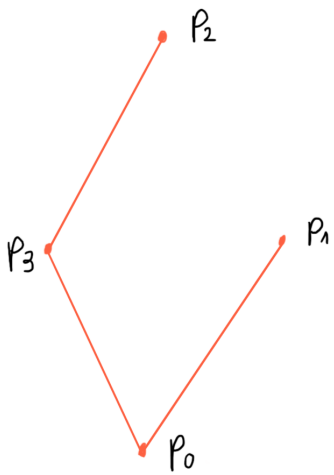
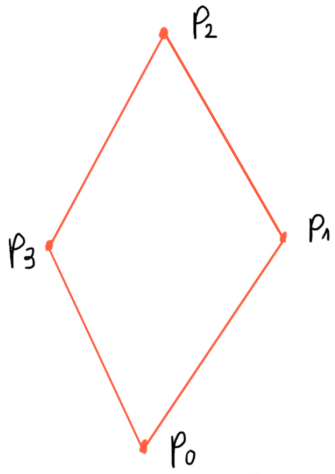
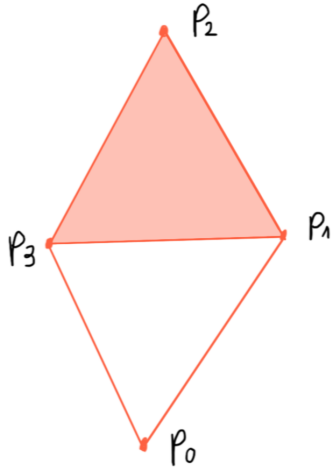






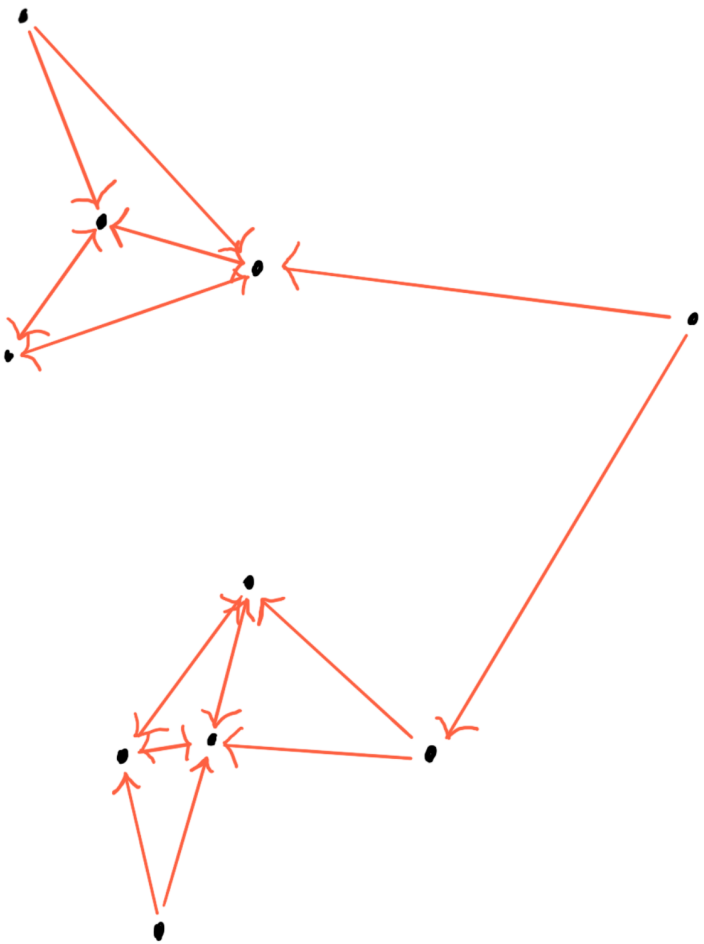


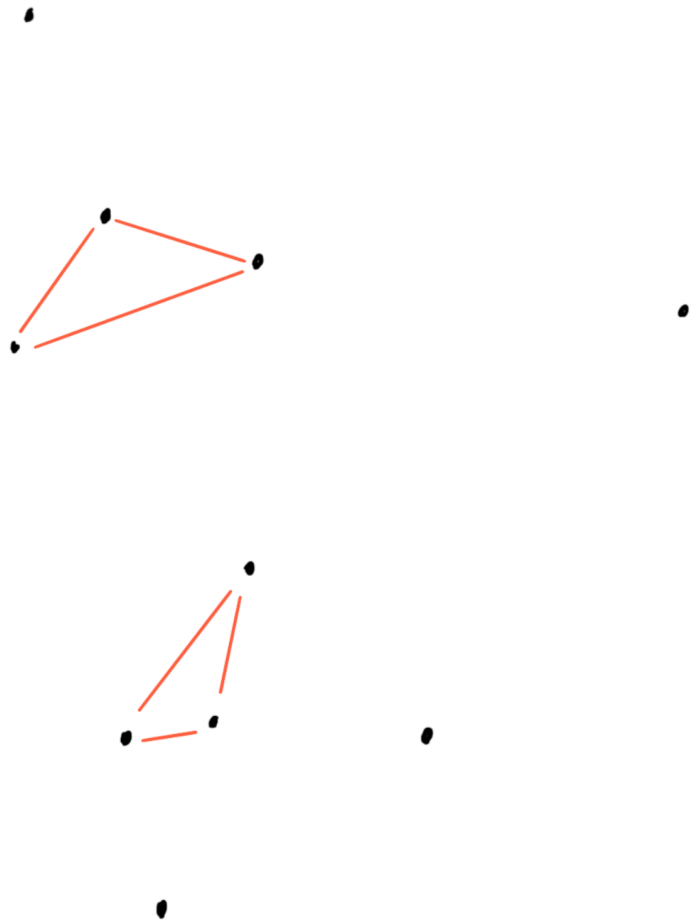
The cycle does not die.

Outline

Why the MkNN graph?

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`.

The class `Cloud`

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- The adjacency matrix of the the MkNN graph is

$$M = A \odot A^\top$$

where $\odot$ is the entrywise product.

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Once σ 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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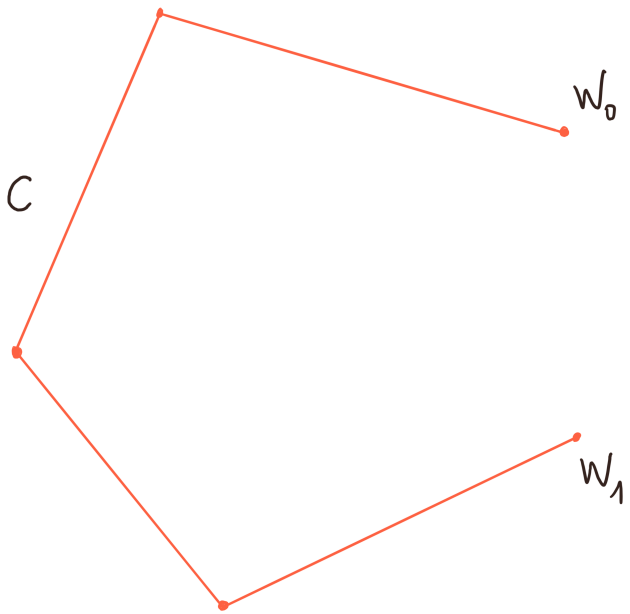

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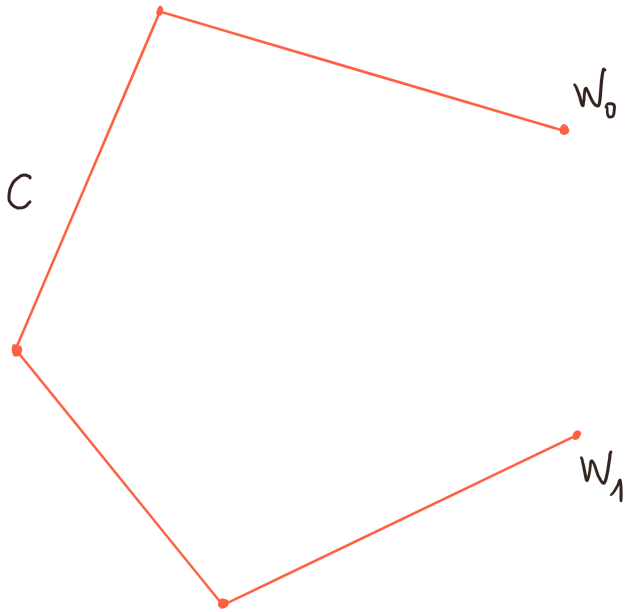

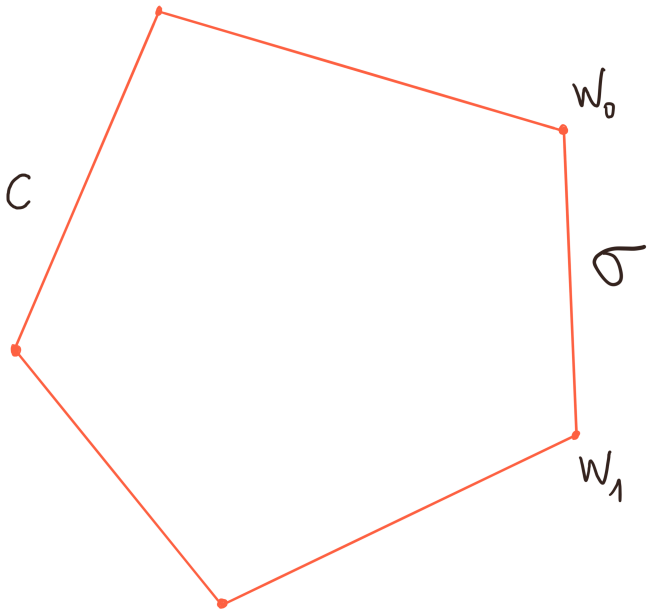

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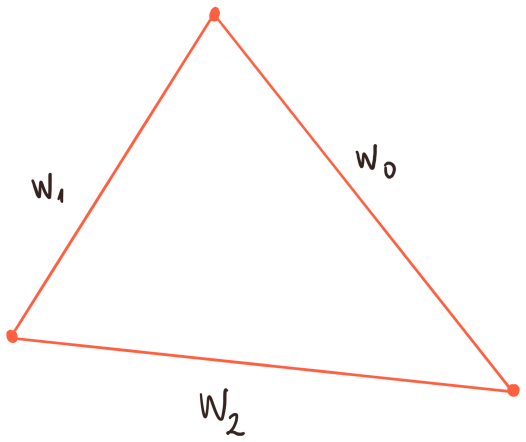

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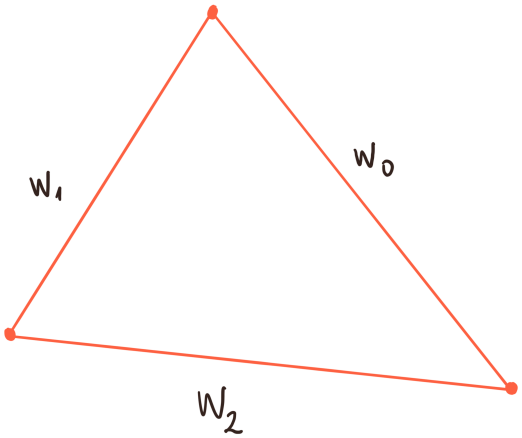

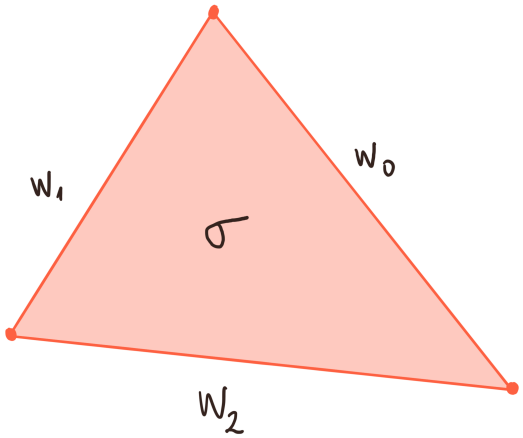

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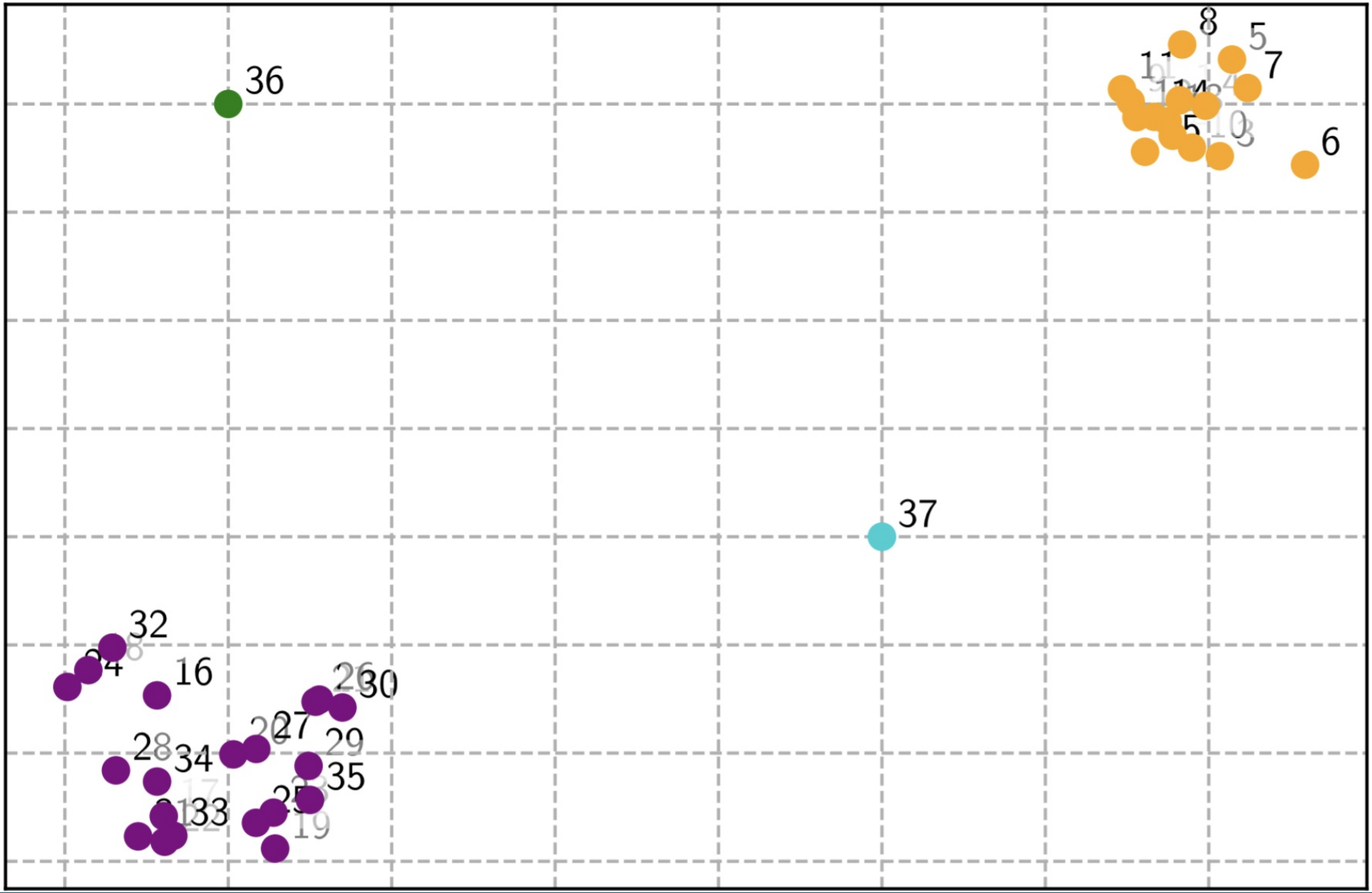
Outline

A run with toy data



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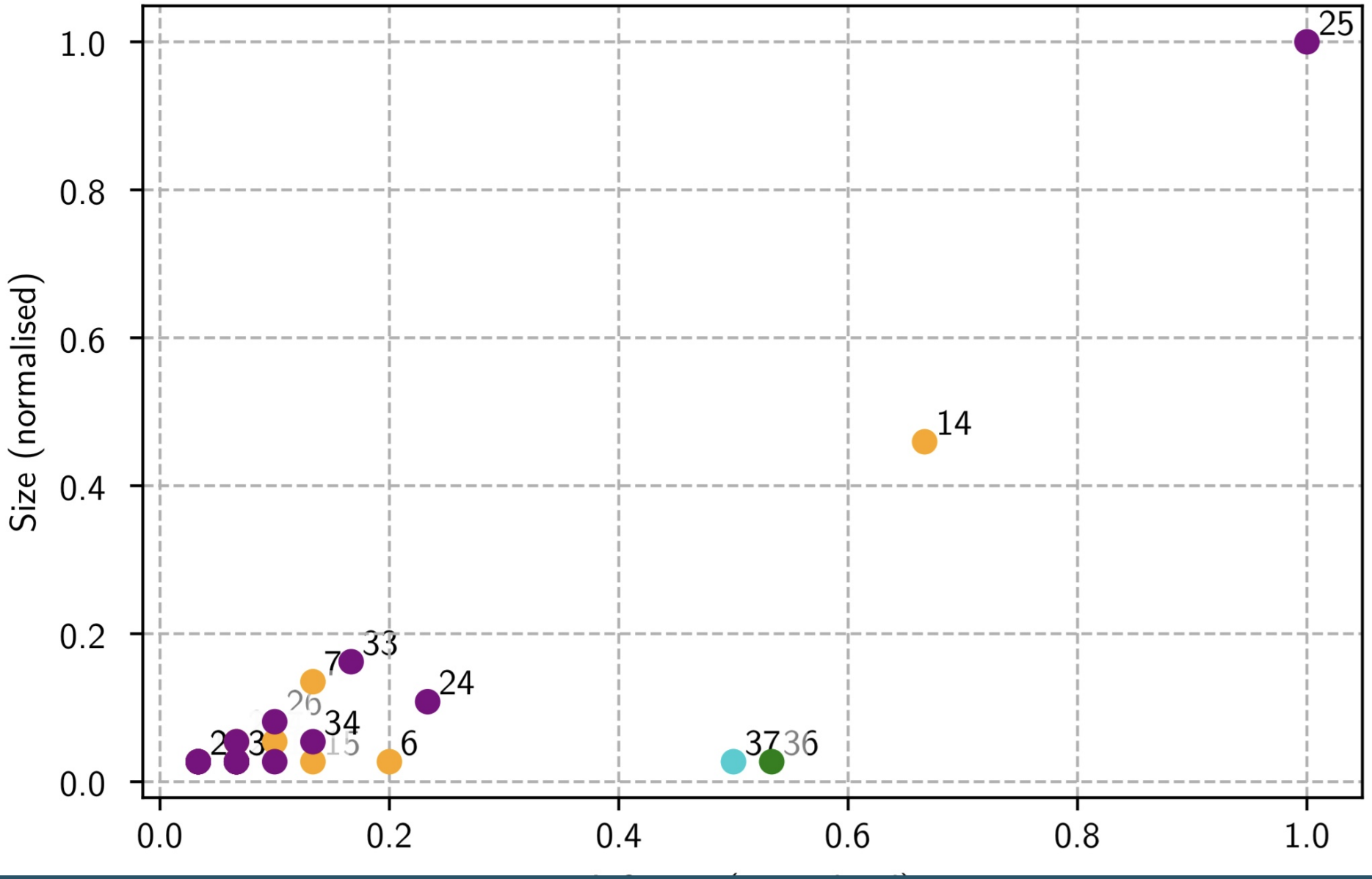

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- There are also genomic features corresponding to the same 20 patients.
- The detector was run on both sets to compare the clustering structure.

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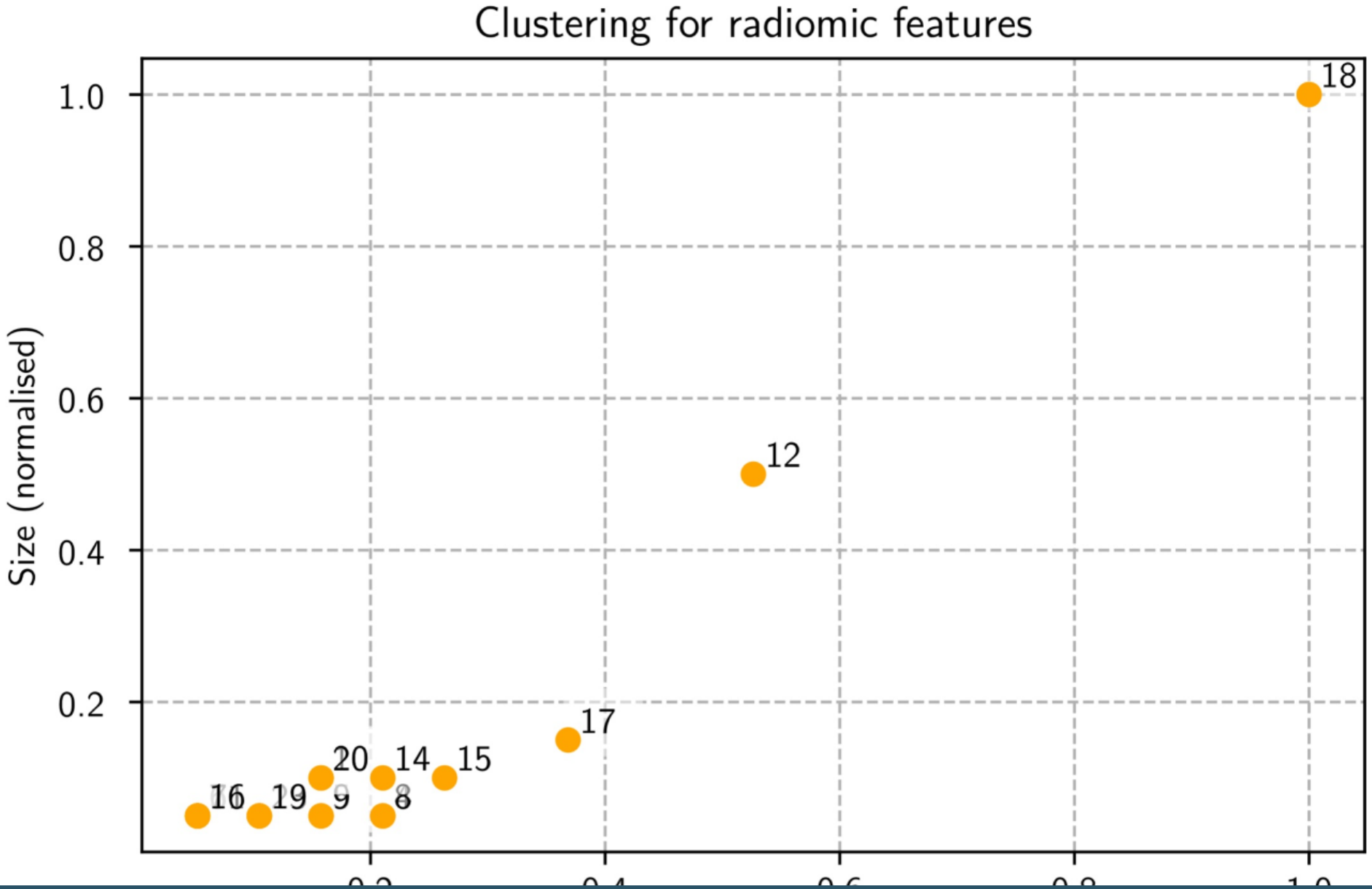
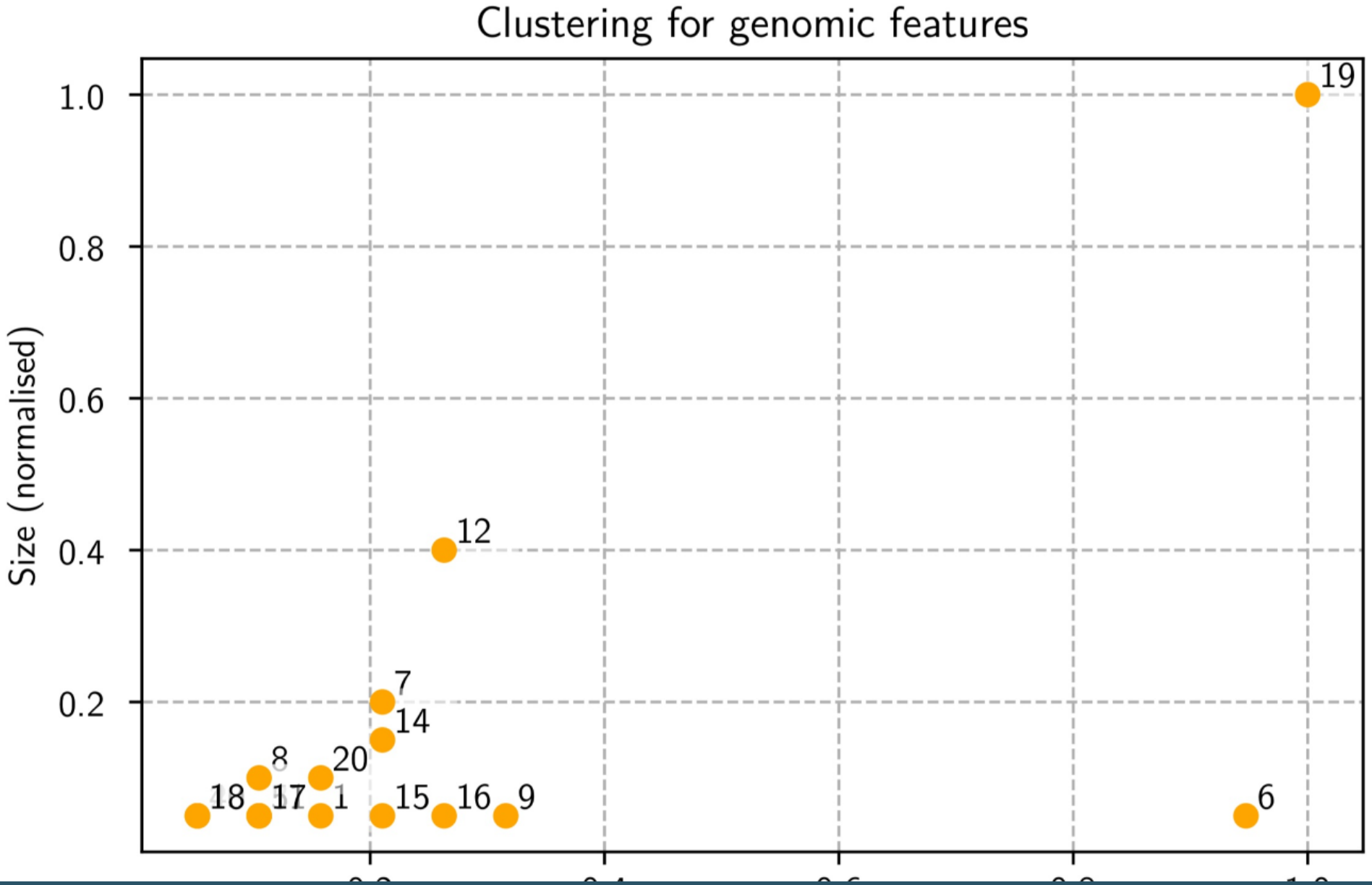


A run with real data



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

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
September 3rd 2020

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