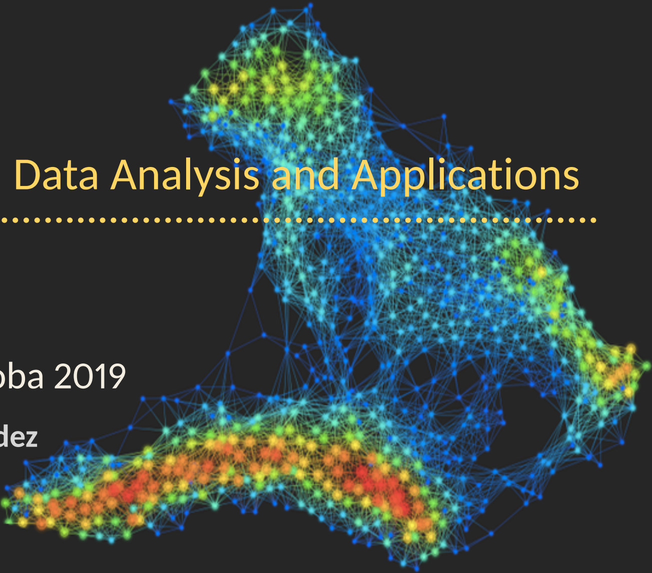
Topological Data Analysis and Applications



PyData Córdoba 2019

Ximena Fernández

Outline

Topological Data Analysis

Topo... what?

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Let $S = \{x_1, x_2, \cdots, x_n\}$ be a point cloud, that is, a sample of a space X (where X is a metric space, a manifold, a topological space). Our goal is to recover *(the topology of)* X.

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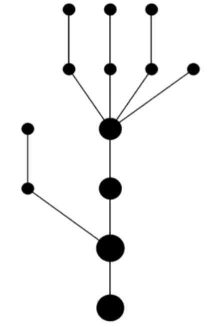

Reconstruction method

Simplicial complexes

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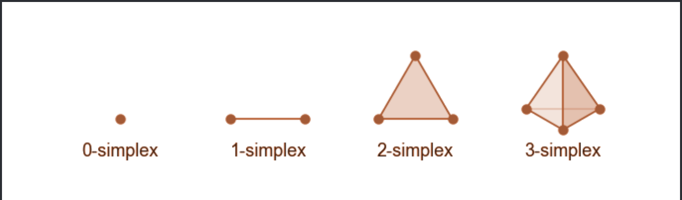

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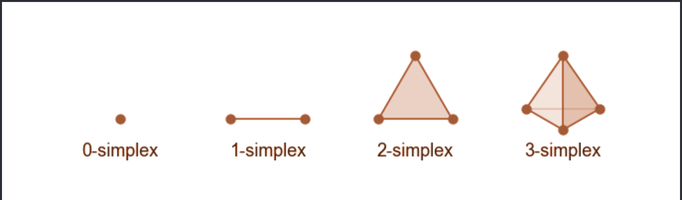

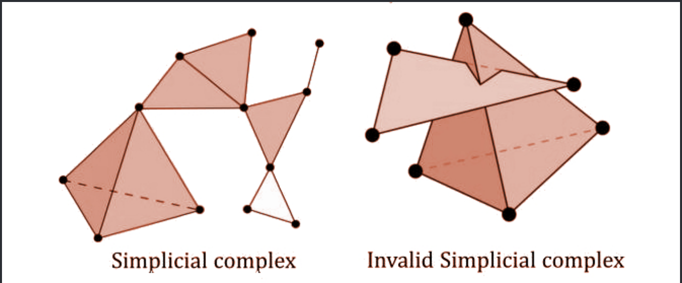

Reconstruction method

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Definition

Let X be a topological space, and let $\mathscr{U} = \{U_1, U_2, \cdots, U_m\}$ be a *cover* of X. The nerve of $\mathscr{U}$ is the simplicial complex $N(\mathscr{U})$ with:

- one **vertex** for each element in the cover
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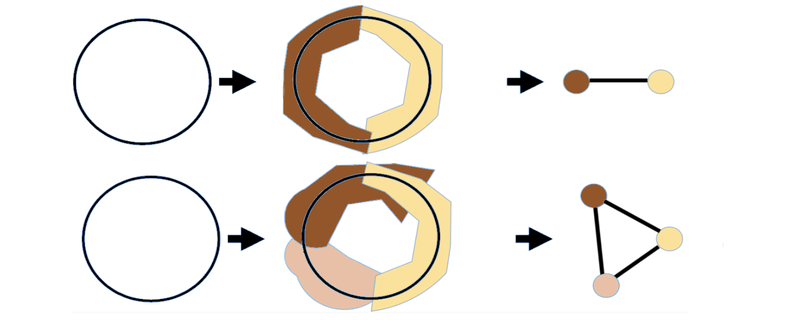


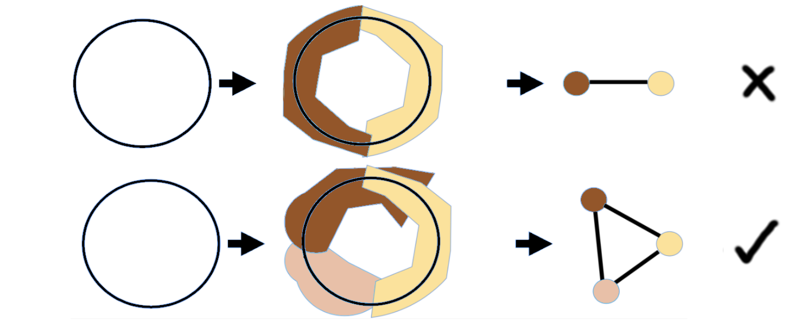
Reconstruction method

Nerve Theorem

Theorem

*Let X be a topological space, and let $\mathscr{U} = \{U_1, U_2, \cdots, U_m\}$ be a **good cover** of X by open sets.*

*Then X is **homotopically equivalent** to $N(\mathscr{U})$.*



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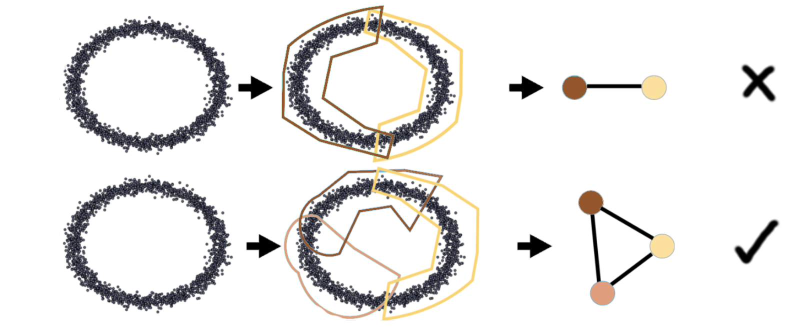


Reconstruction method

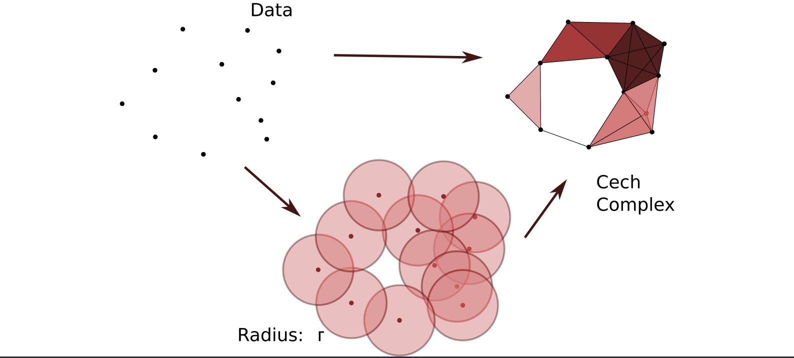
Reconstruction method

How can I select a (good) cover in a point cloud?

Reconstruction method

How can I select a (good) cover in a point cloud?

Let $S = \{x_1, x_2, \cdots, x_n\}$ a point cloud. Suppose you have a metric on S. Define the cover $\mathscr{U}$ as the collection of balls $B(x_1, r), B(x_2, r), \cdots, B(x_n, r)$ with center in the points $x_1, x_2, \cdots x_n$ of S and radius $r > 0$.



Reconstruction method

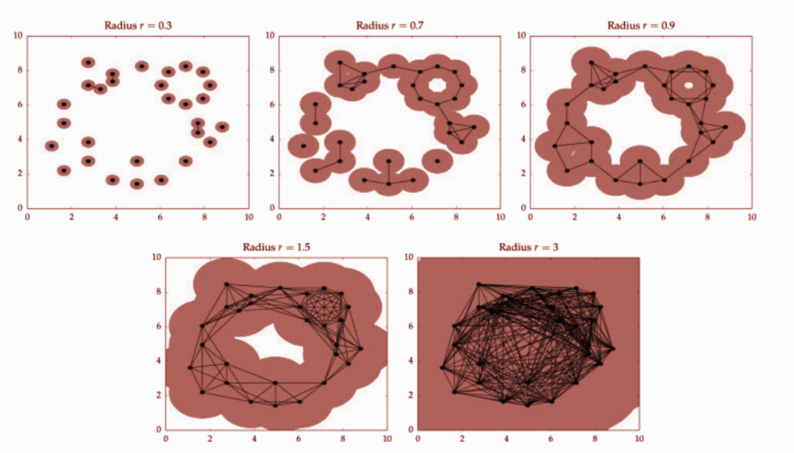
Which radius should I choose?

Reconstruction method

Which radius should I choose?

Problem

Different choices of r give rise to different topologies.



Persistent Homology

All radii

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Solution

Study the *geometry* of the data with a *multiscale resolution*.

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All radii

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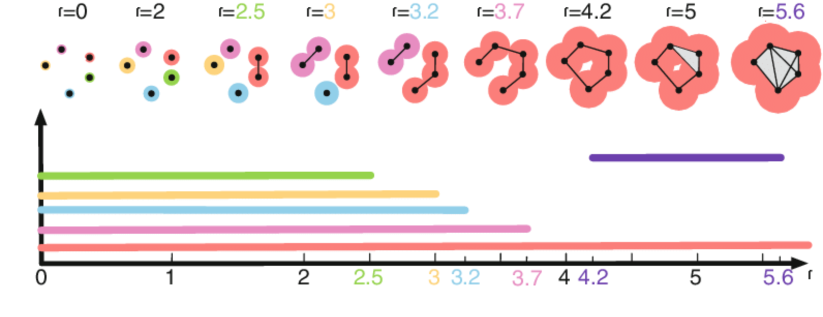
Study the *geometry* of the data with a *multiscale resolution*.
Specifically, compute the *evolution* of the homology of the nerve of a cover *with the radius* of the balls.



Dynamical systems

ft. Persistent Homology

- Maletic, S., Zhao, Y., Rajkovic, M. (2016). *Persistent topological features of dynamical systems*. Chaos, 26 5, 053105.

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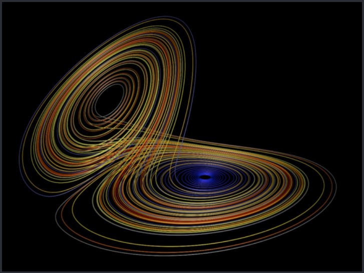


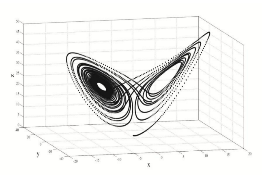
Classify the dynamical systems by identifying geometrical invariants of the *state space*. Concretely, perform a discrete simulation of the dynamical system and compute the persistent homology of this point cloud.

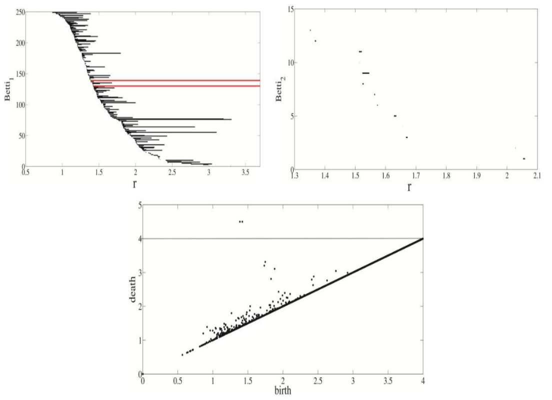
Dynamical systems

ft. Persistent Homology

Lorenz

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = rx - y - xz$$
$$\dot{z} = xy - bz$$





Dynamical systems

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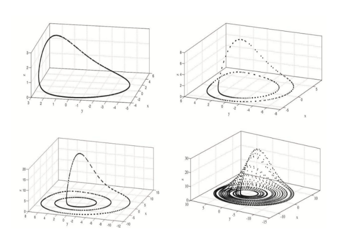
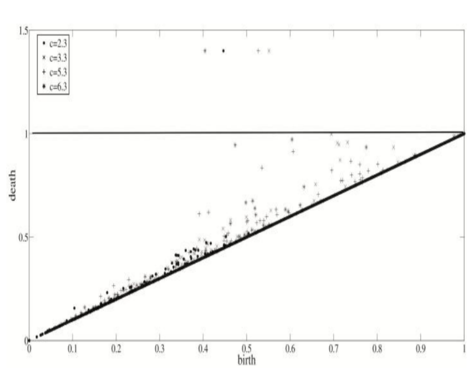
Rösler

$$\dot{x} = -\sigma(y+z)$$
$$\dot{y} = x + ay$$
$$\dot{z} = b + xz + cz$$





Uniform Manifold Approximation and Projection (UMAP)

Smart metric

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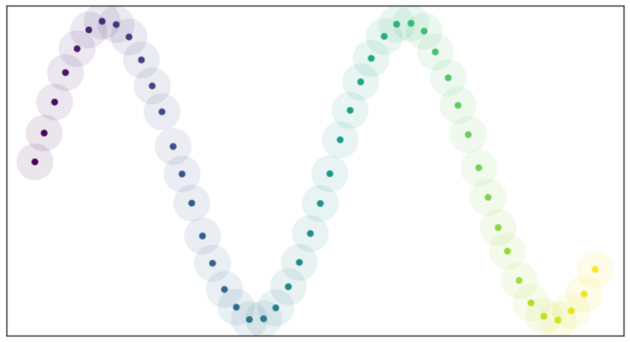
Expectation



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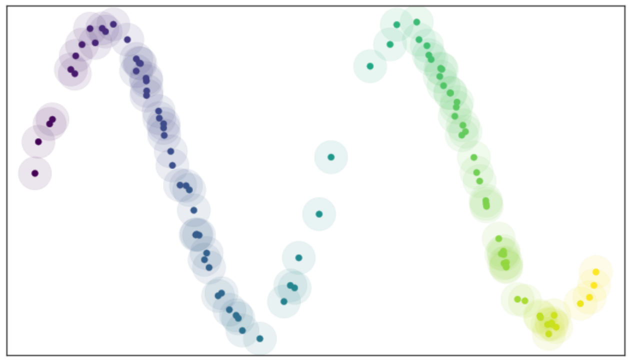
Reality



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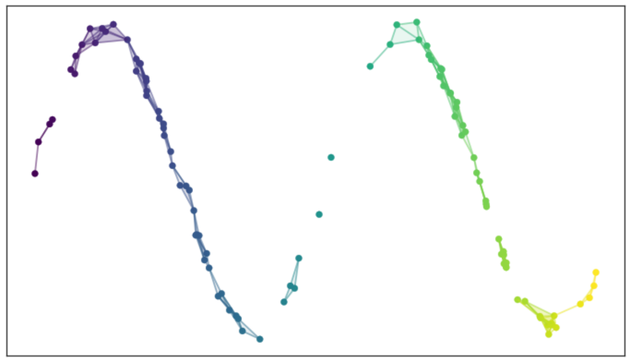

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We will **assume** that:

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- The Riemannian metric is locally constant (or can be approximated as such)
- The manifold is locally connected

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Let S be a point cloud in $\mathbb{R}^m$.

Define (an approximation of) a local notion of distance such that: a unit ball about each point in S stretches to the k-th nearest neighbor of the point (with k a parameter).

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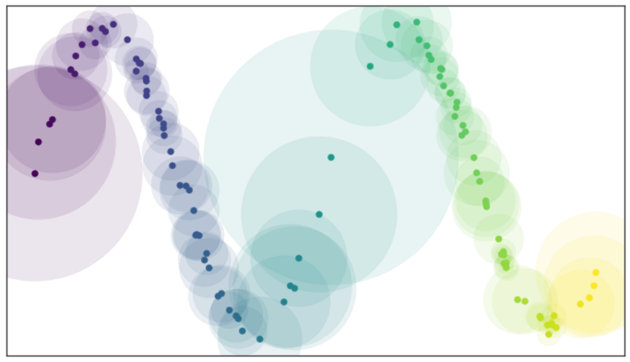

UMAP

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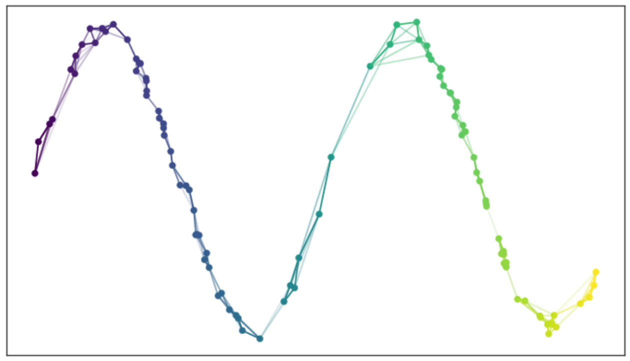
Make a compatibilization of this locally sense of distance.

Compute the nerve of that covering by unit balls.



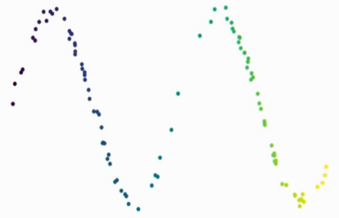
UMAP

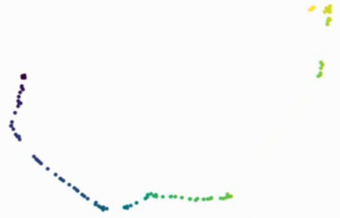
Projection

High dimensional representation ⟶ **Low dimensional representation**

Riemmanian manifold with varying metric

Low dimensional euclidean space with the euclidean metric





Single-cell RNA-sequences

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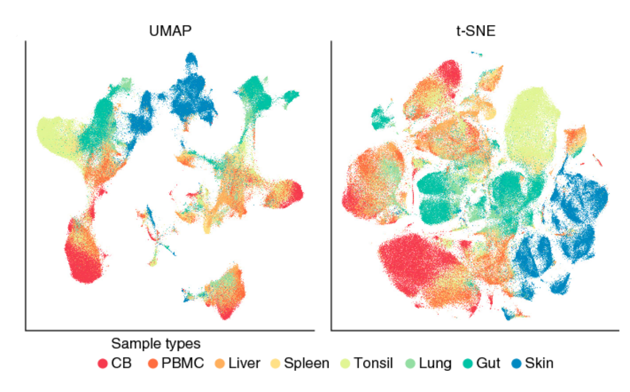
- Becht, E., McInnes, L., Healy, J., Dutertre, C., Kwok, I.W., Ng, L.G., Ginhoux, F., Newell, E.W. (2018). *Dimensionality reduction for visualizing single-cell data using UMAP*. Nature Biotechnology, 37, 38-44.



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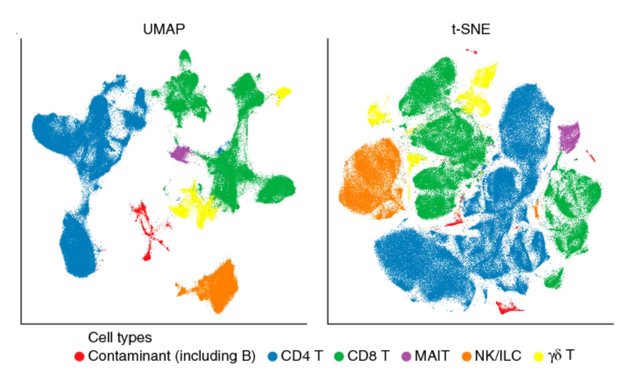

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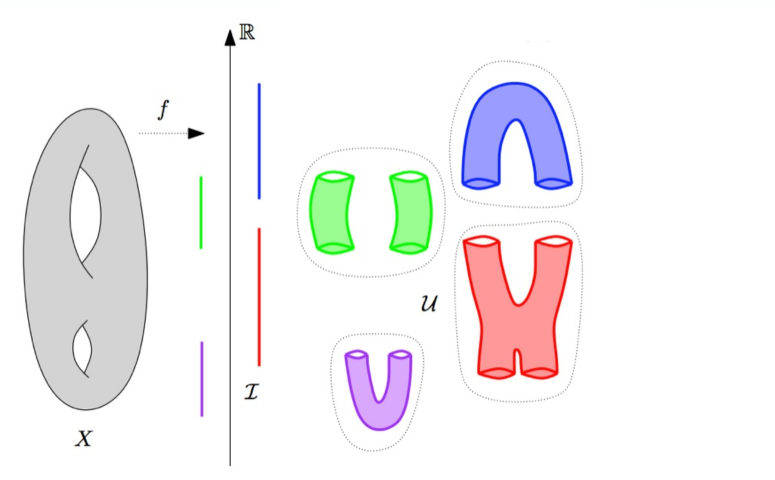
- Define $\mathscr{U}^{\pi_0}$ as the connected components of the preimage $f^{-1}(I_j)$ of each interval I_j of $\mathscr{I}$.
- $N(\mathscr{U}^{\pi_0})$ *recovers* the topology of X.

Mapper

Smart cover



Mapper

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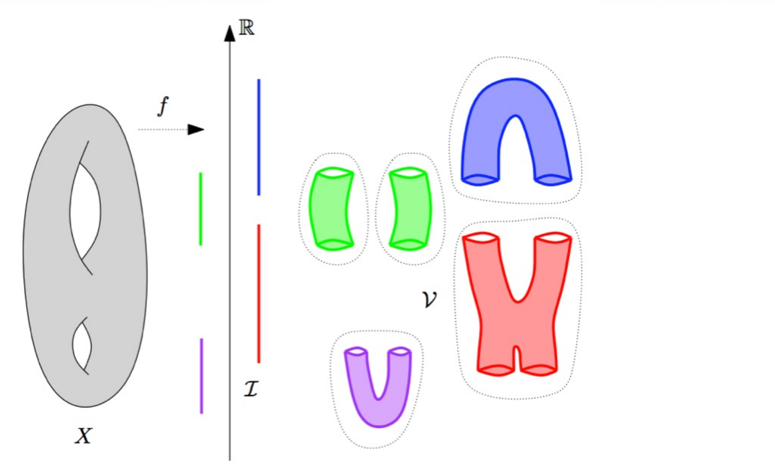

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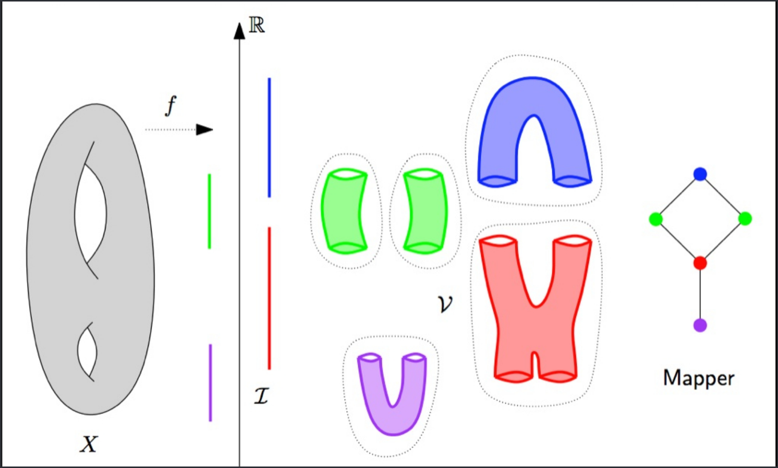

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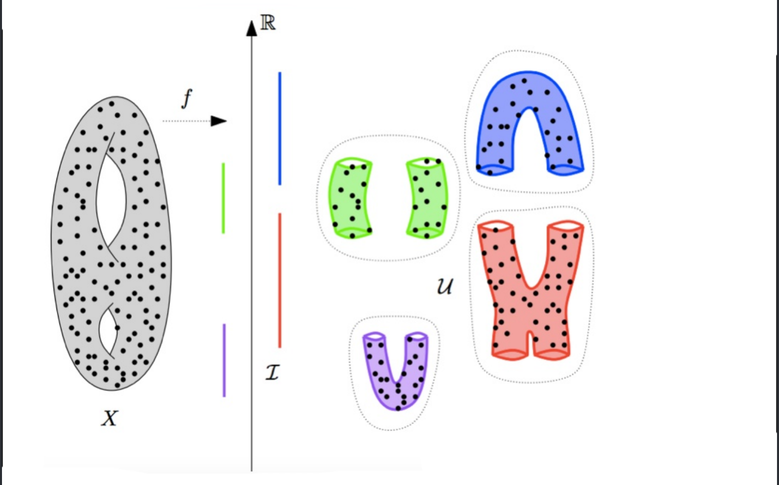

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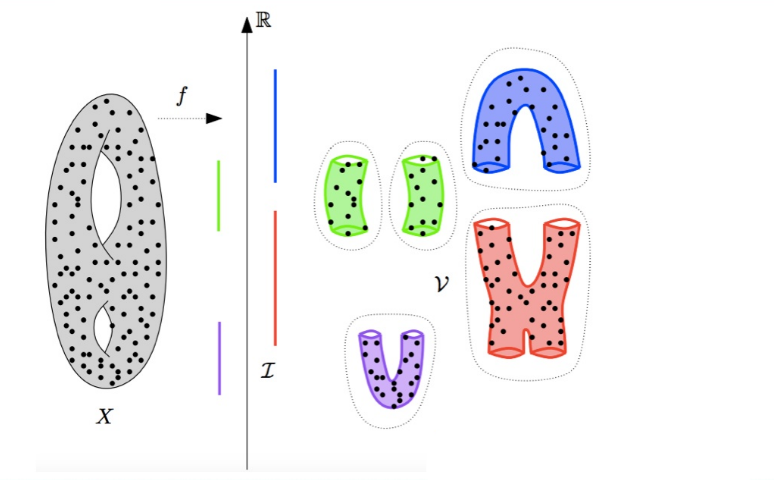

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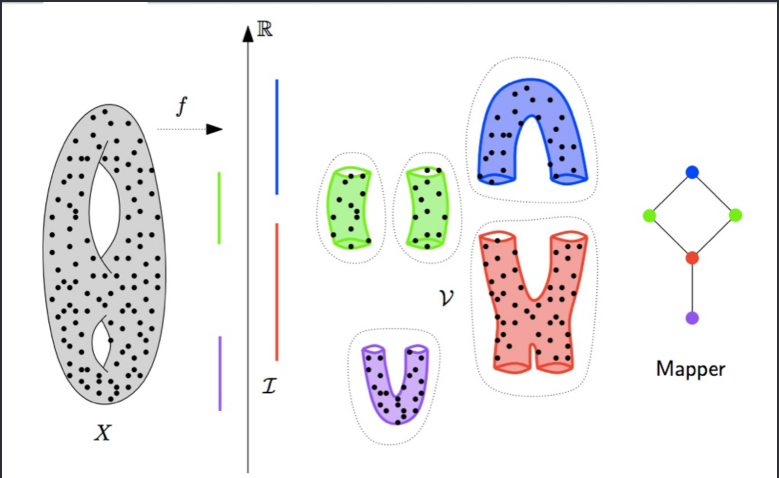
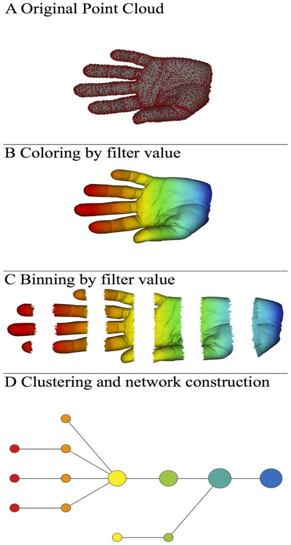


Mapper

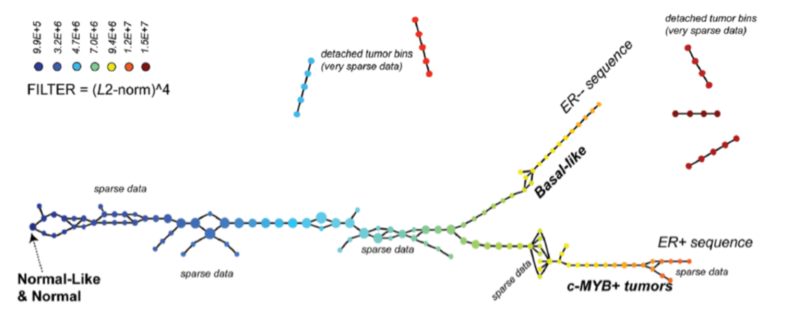
promise made is a debt unpaid



Cancer detection

ft. Mapper

- Nicolau, M., Levine, A.J., Carlsson, G. (2011). *Topology based data analysis identifies a subgroup of breast cancers with a unique mutational profile and excellent survival.* Proceedings of the National Academy of Sciences of the United States of America, 108 17, 7265-70.



Outline

Python Libraries

1. *Scikit-TDA*
   - *Installation:* `pip install sktda`
   - *Documentation: scikit-tda.org*
   - *Contribution: github.com/scikit-tda*

   1.1 *Persistent Homology*
      » *Installation:* `pip install ripser`
      » *Documentation: https://ripser.scikit-tda.org*

   1.2 *Kepler Mapper*
      » *Installation:* `pip install kmapper`
      » *Documentation: kepler-mapper.scikit-tda.org*

2. *UMAP*
   - *Installation:* `pip install umap-learn`
   - *Documentation: umap-learn.readthedocs.io*
   - *Contribution: github.com/lmcinnes/umap*

Code examples

Public repository:

`https://github.com/ximenafernandez/PyData2019_TDA`

Outline

Bibliography

Persistent Homology, *Mapper*, *UMAP* *and* *general theory*.

[1] Carlsson, G. (2009) *Topology and data.* Bulletin of the American Mathematical Society, 46(2):255–308.

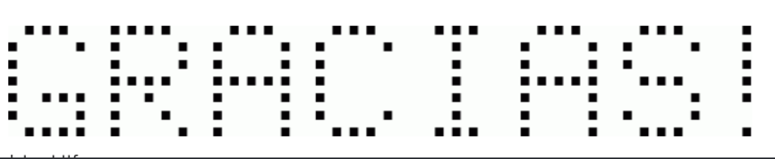
[2] Edelsbrunner, H., Letscher, D., Zomorodian, A. (2002) *Topological persistence and simplification.* Discrete Computational Geometry 28, pages 511–533.

[3] Fernandez, X. Minian, E. (2018). *The Cylinder of a Relation and Generalized Versions of the Nerve Theorem.* Discrete Computational Geometry.

[4] McInnes, L., Healy, J. (2018) *UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction*, ArXiv e-prints 1802.03426.

[5] Singh G., Mémoli F., Carlsson G. (2007) *Topological methods for the analysis of high dimensional data sets and 3d object recognition.* InSPBG, pages 91–100.

[6] Zomorodian, A. (2001) *Computing and Comprehending Topology: Persistence and Hierarchical Morse Complexes.* PhD thesis, University of Illinois at Urbana-Champaign.


GRACIAS!