Topology Tools
for
Explainable and Green Artificial Intelligence

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Sixth EACA International School on Computer Algebra and its Applications

SANTIAGO DE COMPOSTELA, JULY 18-21, 2023

- Context: Green and Explainable artificial intelligence (REXASI-PRO)
- Computational topology tools: Persistent homology, barcodes, distance bottleneck, simplicial maps, Persistence modules, morphisms between persistence modules
- Partial matchings between barcodes
- Simplicial maps neural networks

Open position!!!

https://investigacion.us.es/investigacion/contratos-personal

Referencia: INV-IND-09-2023-I-015.

Relación de contratos convocados: 1.

Convocatoria: Convocatoria Indefinidos (IND) Septiembre 2023.

Dicho proyecto/ayuda/programa financiará el contrato por un período previsto desde **01/12/2023** hasta el **30/09/2025** (fecha fin del proyecto/ayuda/programa).

La actividad del presente contrato se desarrollará en el marco de una línea de investigación «*Computational Topology for Green Artificial Intelligence*», conforme a lo establecido en la convocatoria del proceso selectivo.

SOLICITUDES: del 08/09/2023 al 21/09/2023

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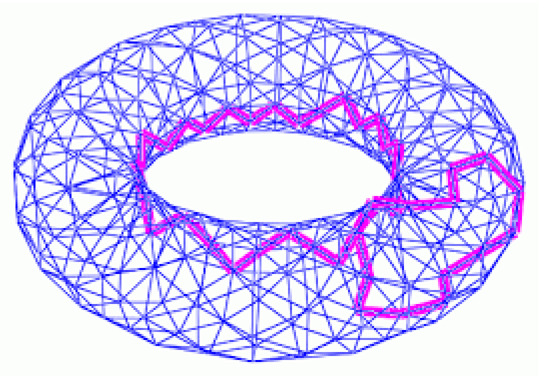

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Our goals within REXASI-PRO

Main goal

Use computational topology to design new methods to achieve **explainable and green artificial intelligence models.**

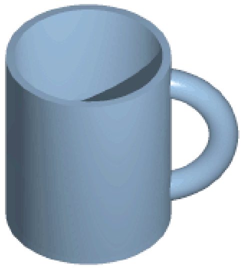
How to make greener the AI solution [WP6]

Specific Goals

1. Topology-aware reduce the input dataset.
2. Build explainable models based on topology.
3. Simplify the model preserving its learning capacity.
4. Create synthetic samples that can quickly train a model.

Why computational topology?

- Topology studies properties of spaces that are preserved against **continuous deformations.**
- Topological invariants can be used for deriving **equivalence classes**.
- **From local to global:** it allows to reveal hidden patterns that otherwise can not be pinpointed.

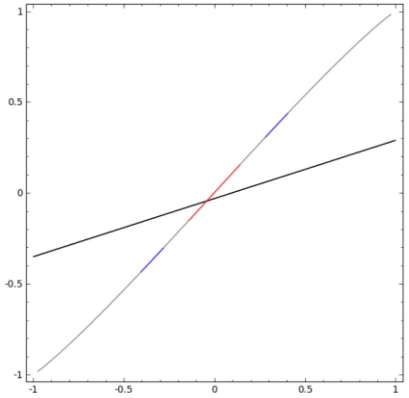


Why computational topology?

- Neural networks are compositions of **continuous functions**.

- The training process consists of **continuous deformations.**

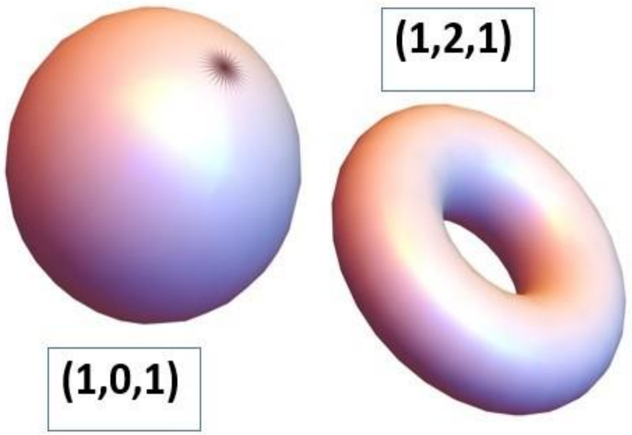
  The network *deforms* space so that, for example, data of different classes are separable by a hyperplane.



- Real-world high-dimensional data sets actually lie in low-dimensional **manifolds** (manifold hypothesis).

Why computational topology?

- **Topological space:** an object = a set endowed with a topology (a notion of nearness)
- **Algebraic topology:** the study of algebraic invariants that are preserved under homeomorphisms (bijective and bicontinuous functions between topological spaces)
- **Computational topology:** tools for computing algebraic invariants ***(over a field)***
- **Topological data analysis:** Analysis of the data using topology tools (mainly persistent homology)
- **Homology:** algebraic invariant that studies the number of *n*-holes in an object



0-hole: connected component

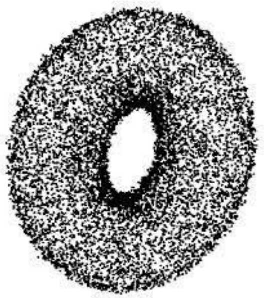
1-hole: tunnel

2-hole: cavity

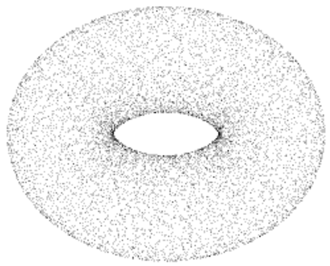
Conclusion: A torus and a sphere are not homeomorphic

Why computational topology?

- **From local to global**: it allows to *reveal hidden patterns* that otherwise can not be pinpointed (**topological data analysis**).



- **Stable invariants** can be used for *deriving classes of equivalence.*



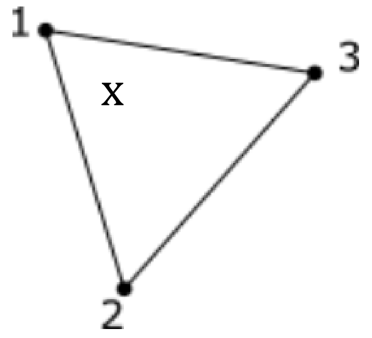
- **Detect changes** along the evolution of a system (without using any model)

Concepts from computational topology

- **(abstract) Simplicial complexes**

p-simplex $\sigma = \langle v_0, \dots, v_p \rangle$, v_i are the vertices of σ.

If $v_i \in R^n$ for $0 \le i \le n$ then $|\sigma|$ is the convex hull.



If $\mathrm{x} \in |\sigma|$ then there exists a unique vector

$$\left(\mathrm{b_o}(x), \dots, b_p(x)\right) \in R^{p+1}$$

such that $\sum_{i=0}^{p} b_i(x) = 1$, $b_j(x) \ge 0$ for all j, and $\mathrm{x} = \sum_{i=0}^{p} b_i(x) v_i$.

$$\partial_1 = \begin{array}{c} \\ \langle 1 \rangle \\ \langle 2 \rangle \\ \langle 3 \rangle \end{array} \begin{array}{c} \begin{array}{ccc} \langle 1,2 \rangle & \langle 1,3 \rangle & \langle 2,3 \rangle \end{array} \\ \begin{bmatrix} -1 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 1 \end{bmatrix} \end{array}$$

barycentric coordinates of x wrt σ

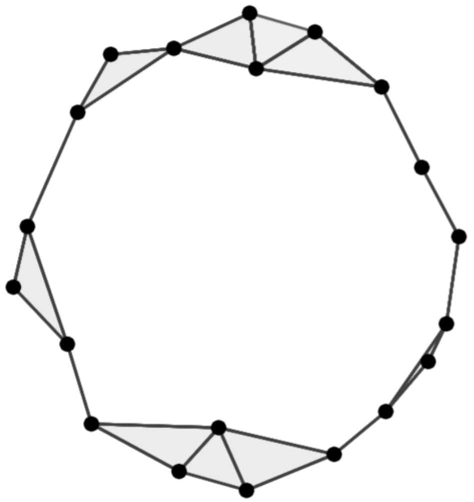
The boundary operator is defined as $\partial_p(\sigma) = \sum_{i=0}^{p} (-1)^i \langle v_0, \dots, \hat{v_i}, \dots, v_p \rangle$

Concepts from computational topology

- **(abstract) Simplicial complexes**

A simplicial complex K is a collection of simplices such that

1. Every face of a simplex of K is in K, and
2. The intersection of any two simplices of K is a face of each of them.



If all the vertices of K are in R^n, then $|K|$ is $\bigcup_{\sigma \in K} |\sigma|$.

A p-chain is a linear combination of simplices σ of dimension p, $c_p = \sum_{i=0}^{p} \alpha_i \sigma_i$, where coefficients lay on $\mathbb{Z}_2$ with the symmetric difference as addition operator.

Concepts from computational topology

- (abstract) Simplicial complexes
- **Homology** (over a field)

A p-cycle is a p-chain with an empty boundary $\partial_p c = 0$.

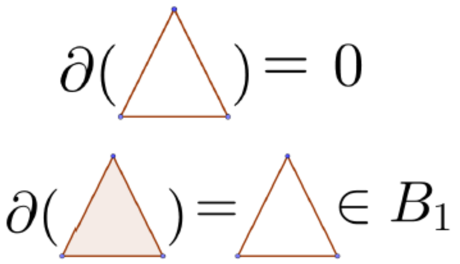
A p-boundary is a p-chain that is the boundary of a $(p + 1)$-chain.

Z_p group of p-cycles
B_p group of p-boundaries

$B_p \subset Z_p$

The p-homology group H_p is the quotient group Z_p / B_p

The p-th Betti number β_p is $rank(H_p)$



Computation of H_p : SNF
column operation (cycles),
row operations (boundaries)

$$\begin{bmatrix} \alpha_1 & 0 & 0 & & \dots & 0 \\ 0 & \alpha_2 & 0 & & & 0 \\ 0 & 0 & \ddots & & & \\ \vdots & & & \alpha_r & & \\ & & & & 0 & \\ 0 & & & & & \ddots \\ & & & & & & 0 \end{bmatrix}$$

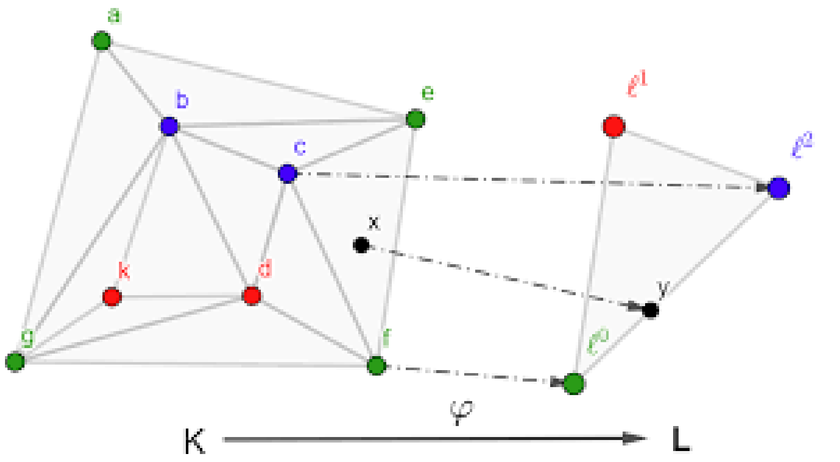
$\alpha_i \mid \alpha_{i+1}$ for all $1 \leq i < r$

$\alpha_i = 1$ **for all** $1 \leq i \leq r$
when working *over a field* .

Concepts from computational topology

- (abstract) Simplicial complexes
- Homology
- **Vertex map, simplicial map**

Given two simplicial complexes K and L, a vertex map $\varphi^{(0)} : K^{(0)} \to L^{(0)}$ is a function from the vertices of K to the vertices of L such that for any simplex $\sigma \in K$, the set $\varphi(\sigma) := \{v \in L^{(0)} \ : \ \exists u \in \sigma,\ \varphi^{(0)}(u) = v\}$ is a simplex of L.



The simplicial map $\varphi\colon |K| \to |L|$ induced by the vertex map $\varphi^{(0)}$ is a continuous function defined as

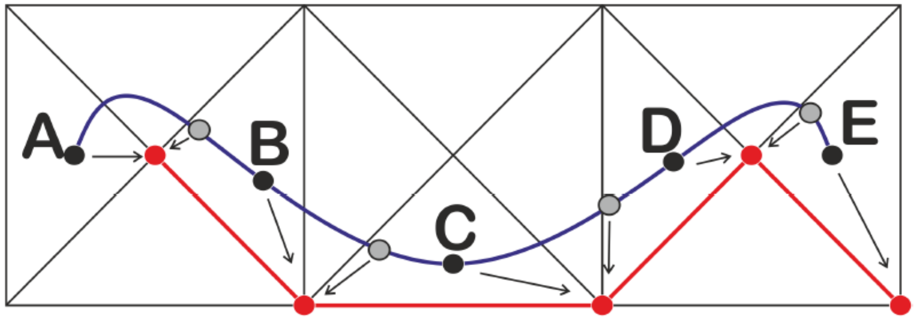
$$\varphi(x) = \sum_{i=0}^{n} b_i(x)\varphi^{(0)}(u_i)$$

where $(b_0(x), \dots, b_n(x))$ are the barycentric coordinates of x wrt $\sigma = \langle u_0, \dots, u_n\rangle \in K$ with $x \in \sigma$.

Concepts from computational topology

- (abstract) Simplicial complexes
- Homology
- Vertex map, simplicial map
- **Simplicial Approximation Theorem**

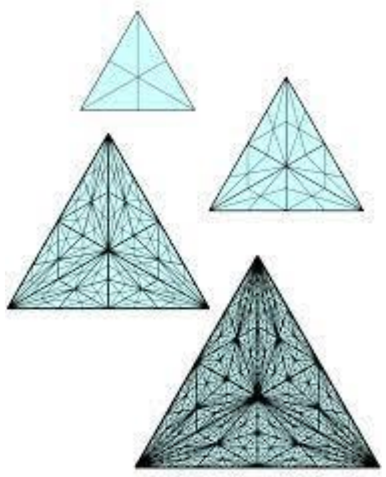
If $g : |K| \to |L|$ is a continuous function, then there exists a sufficiently large $t > 0$ such that $\varphi : |Sd^t K| \to |L|$ is a simplicial approximation of g.



$g(|\,\mathrm{st}\ v|) \subset |\,\mathrm{st}\ \varphi(v)|$ (star condition)

$Sd\ K$ = barycentric subdivision of K

$$Sd^t\ K = Sd^{t-1}\ Sd\ K$$

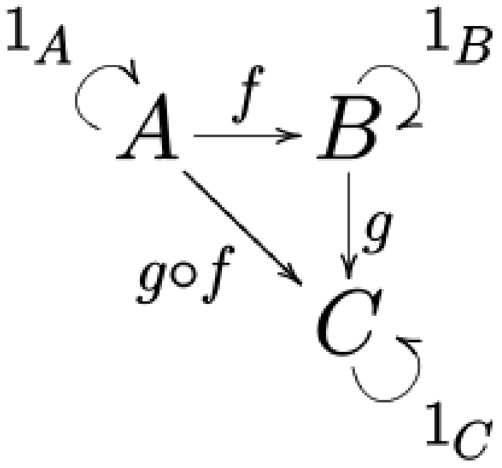


wikipedia

Concepts from computational topology

- (abstract) Simplicial complexes
- Homology
- Vertex map, simplicial map
- Simplicial Approximation Theorem
- **Category SpCpx : simplicial complexes, simplicial maps**

Category
Objects = $\{A, B, C\}$
Morphisms = $\{f, g\}$



Obs: Homology is functorial:

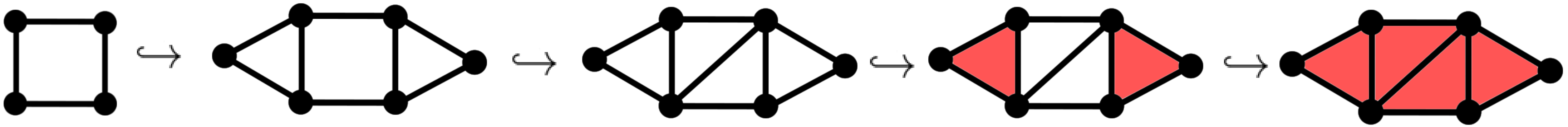
$$K_1 \xrightarrow{\alpha} K_2 \Longrightarrow H_n(K_1) \xrightarrow{H_n(\alpha)} H_n(K_2)$$

Simplicial map ⟹ linear map between vector spaces

Category SpCpx

Concepts from computational topology

- (abstract) Simplicial complexes
- Homology
- Vertex map, simplicial map
- Simplicial Approximation Theorem
- Category SpCpx : simplicial complexes, simplicial maps
- **Filtration**



Concepts from computational topology

- (abstract) Simplicial complexes
- Homology
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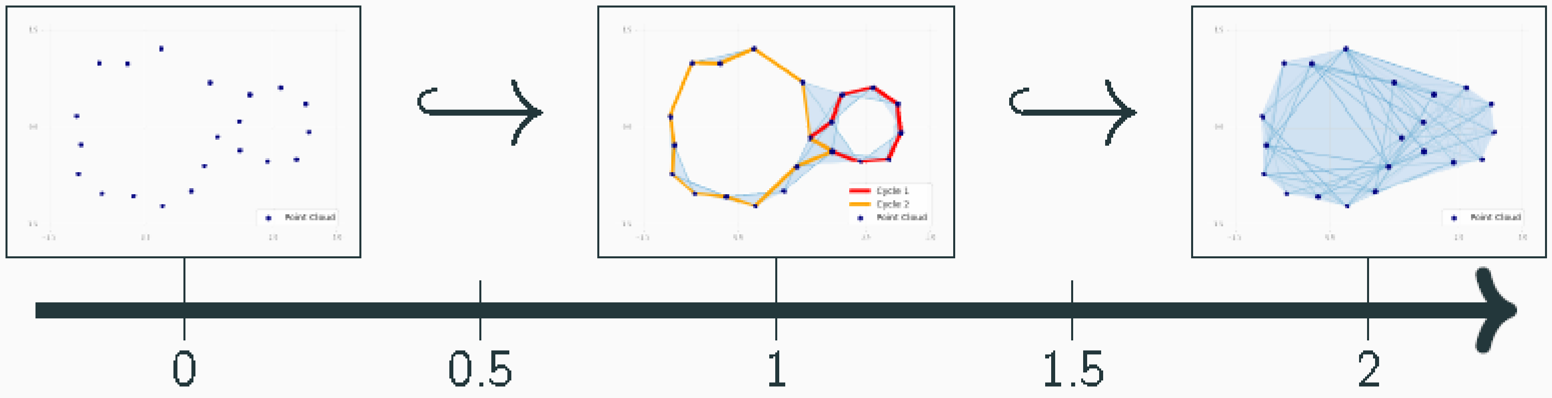
- Category SpCpx : simplicial complexes, simplicial maps
- **Filtration**

Example:
Filtration
Vietoris-Rips

- Consider a point sample $\mathbb{X} \subseteq \mathbb{R}^n$.
- Let $r \geq 0$, $\mathrm{VR}_r(\mathbb{X})$ is the **simplicial complex** with edges $[x, y] \in \mathrm{VR}_r(\mathbb{X}) \iff \|x - y\| \leq 2r$
- Given a sequence $a_0 < a_1 < \cdots < a_n$ from $\mathbb{R}$,

$$\mathrm{VR}_{a_0}(\mathbb{X}) \hookrightarrow \mathrm{VR}_{a_1}(\mathbb{X}) \hookrightarrow \cdots \hookrightarrow \mathrm{VR}_{a_n}(\mathbb{X})$$



- **Category R** : objects $a \in \mathbb{R}$, arrows $a \to b$ iff $a \leq b$
- **Filtered Complex** : $\mathrm{VR}(\mathbb{X}) : \mathbf{R} \to$ **SpCpx**

Concepts from computational topology

- (abstract) Simplicial complexes
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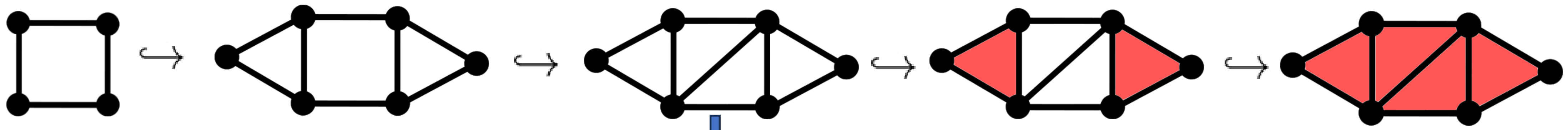
- Category SpCpx : simplicial complexes, simplicial maps
- Filtration
- **Persistent homology**



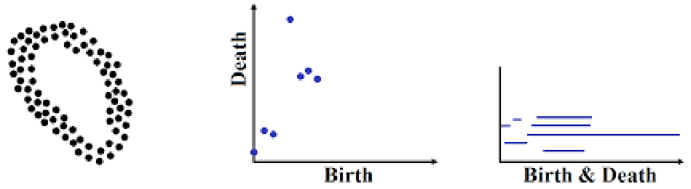
$\downarrow H_1$

$$H_1(K_1) \longrightarrow H_1(K_2) \longrightarrow H_1(K_3) \longrightarrow H_1(K_4) \longrightarrow H_1(K_5)$$

$$B = \{([1,4],1),([2,3],2),([3,4],1)\}$$

$$B = \{([1,4],1),([2,3],2),([3,4],1)\}$$

$$S = \{[1,4],[2,3],[3,4]\}$$



Barcode $\simeq$ persistence diagram

Concepts from computational topology

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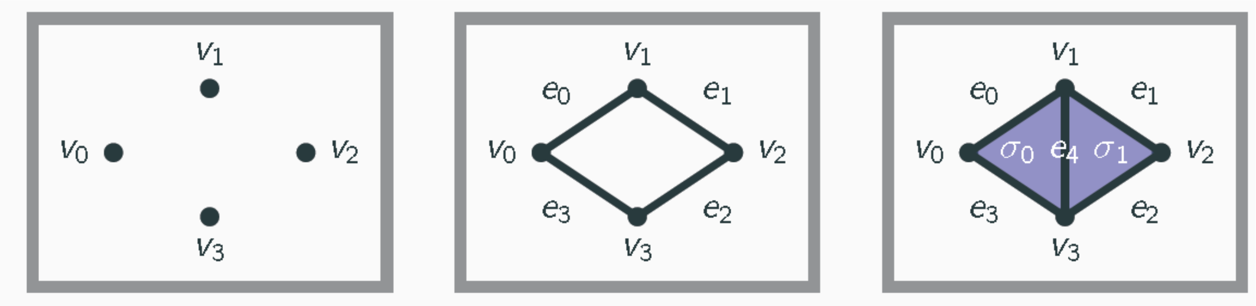
- **Persistent homology**



Boundary Matrix:

	e_0	e_1	e_2	e_3	e_4	σ_0	σ_1
v_0	-1	0	0	-1	0	0	0
v_1	1	-1	0	0	-1	0	0
v_2	0	1	-1	0	0	0	0
v_3	0	0	1	1	1	0	0
e_0	0	0	0	0	0	1	0
e_1	0	0	0	0	0	0	-1
e_2	0	0	0	0	0	0	-1
e_3	0	0	0	0	0	-1	0
e_4	0	0	0	0	0	1	1

Concepts from computational topology

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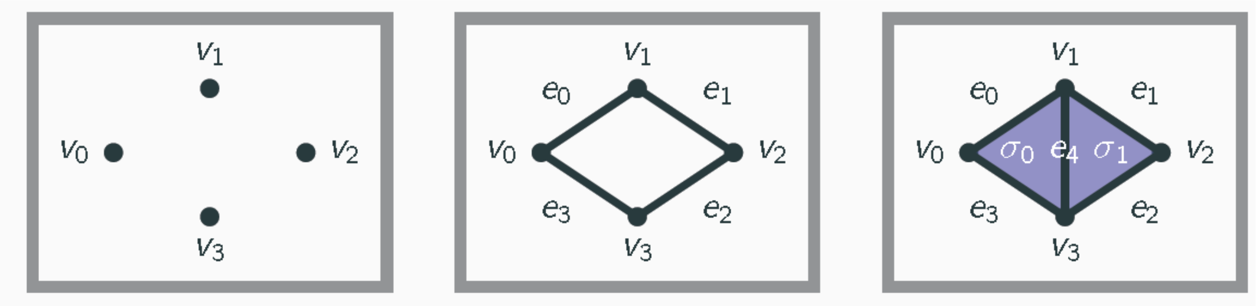
- **Persistent homology**



Reduced Boundary Matrix:

	e_0	e_1	e_2	e_3	e_4	σ_0	σ_1
v_0	-1	0	0	0	0	0	0
v_1	1	-1	0	0	0	0	0
v_2	0	1	-1	0	0	0	0
v_3	0	0	1	0	0	0	0
e_0	0	0	0	0	0	1	-1
e_1	0	0	0	0	0	0	-1
e_2	0	0	0	0	0	0	-1
e_3	0	0	0	0	0	-1	1
e_4	0	0	0	0	0	1	0

$\rightarrow$

Persistence Pairs

(v_1, e_0)
(v_2, e_1)
(v_3, e_2)
(e_4, σ_0)
(e_3, σ_1)

- For each pair (τ, σ), we obtain an interval $I = [\mathrm{filt}(\tau), \mathrm{filt}(\sigma)]$.
- I is nontrivial iff $\mathrm{filt}(\tau) < \mathrm{filt}(\sigma)$
- $\mathrm{filt}(\tau)$ is the **birth value** and $\mathrm{filt}(\sigma)$ is the **death value** of I.

Concepts from computational topology

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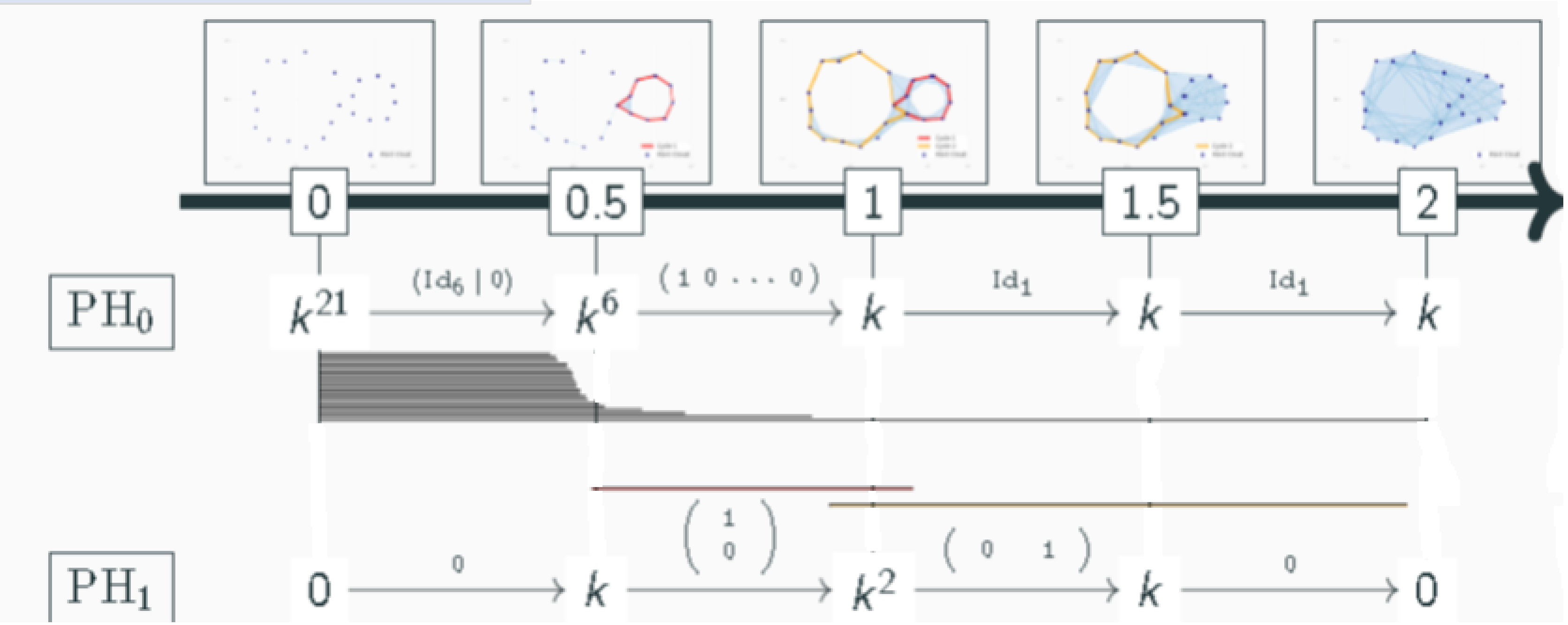
Example:
b a r c o d e

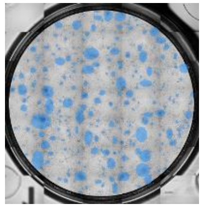


- **Homology:** H_0 “connected components”, H_1 “holes”, etc.
- **Persistent Homology** : $PH_n(X) := H_n(VR(X)) : \mathbf{R} \to \mathbf{Vect}_k$

Concepts from computational topology

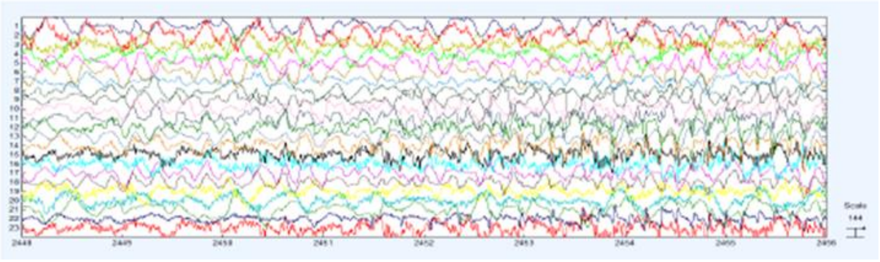
- **General pipeline:**

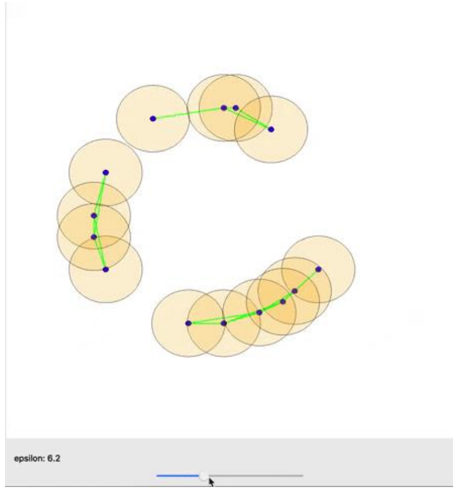
Data & aim → **Combinatorial structure & filtration** → **Topological features** → **Summarization**



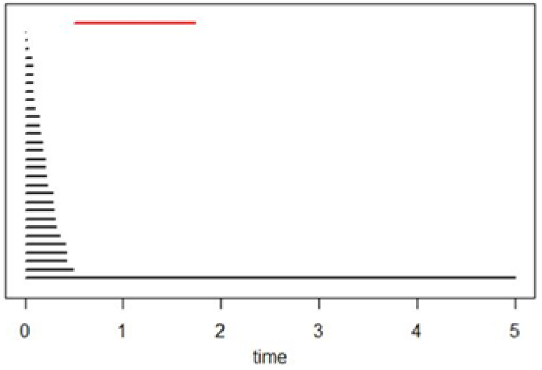
La más bella niña
De nuestro lugar,
Hoy viuda y sola
Y ayer por casar

	Sex	Race	Height	Income	Marital Status	Years of Educ.	Liberal-ness
R1001	M	1	70	50	1	12	1.73
R1002	M	2	72	100	2	20	4.53
R1003	F	1	55	250	1	16	2.99
R1004	M	2	65	20	2	16	1.13
R1005	F	1	60	10	3	12	3.81
R1006	M	1	68	30	1	9	4.76
R1007	F	5	66	25	2	21	2.01
R1008	F	4	61	43	1	18	1.27
R1009	M	1	69	67	1	12	3.25

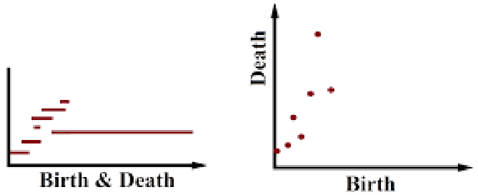




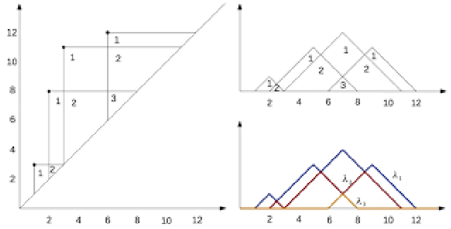
Vietoris-Rips filtration
Lower-star filtration
Clique complexes
…



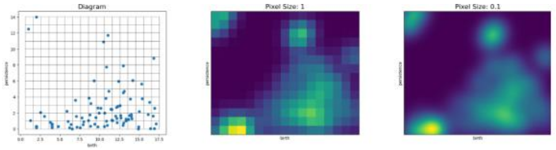
barcodes = persistence diagrams



$$E = -\sum_{i=1}^{n} \frac{\ell_i}{L} \log\left(\frac{\ell_i}{L}\right)$$



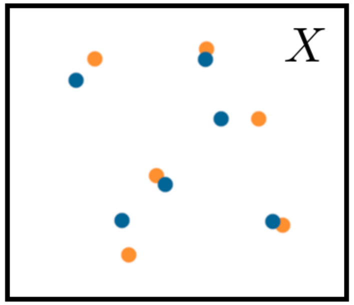
Persistent entropy
Persistence landscape
Persistence images



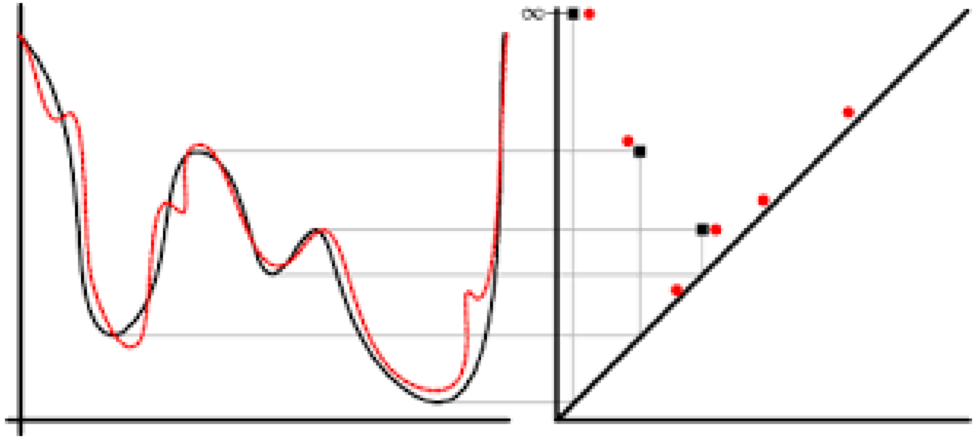
Concepts from computational topology

Stability of persistent homoloy

Stability: If P_1 and P_2 are "similar"



$$d\left(B\left(PH_n(VR(P_1))\right), B\left(PH_n(VR(P_2))\right)\right)$$ is ``small''



Stability: $f, g : X \to \mathbb{R}$

$$F_t = f^{-1}[0,t) \quad G_t = g^{-1}[0,t)$$

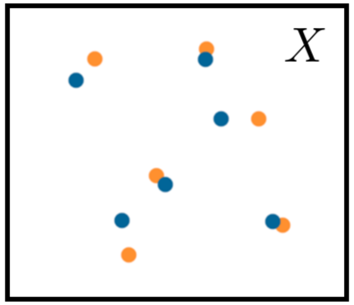
$$d_p(A,B) \leq c\left(\|f-g\|_\infty\right)^{1-\frac{k}{p}}$$

$$d_\infty(A,B) \leq \|f-g\|_\infty$$

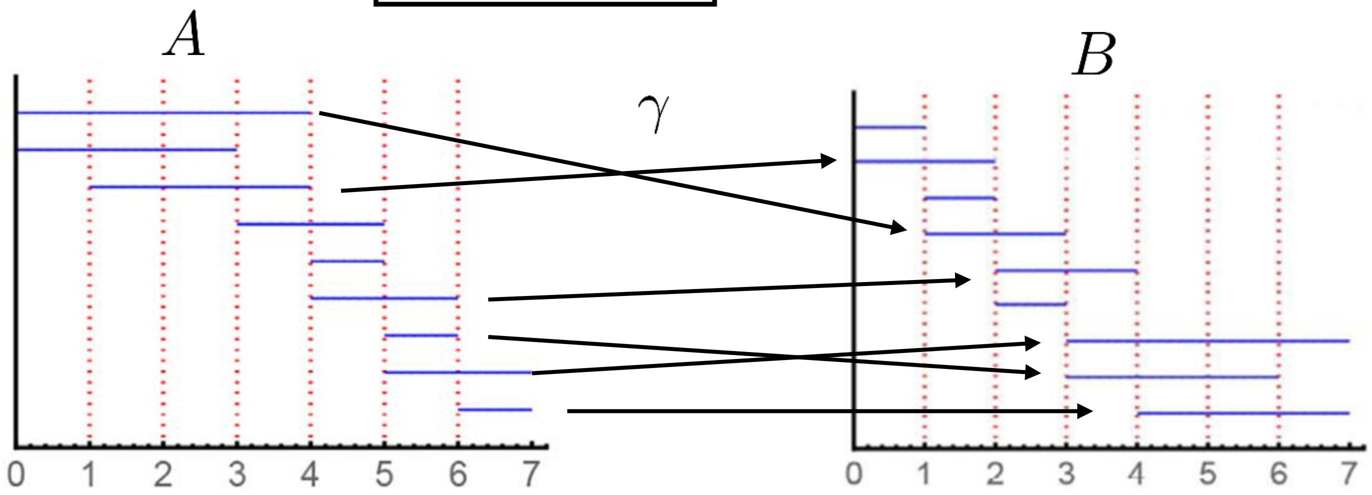
Concepts from computational topology

Stability of persistent homology

Stability: If P_1 and P_2 are "similar"



$d\left(B\left(PH_n(VR(P_1))\right), B\left(PH_n(VR(P_2))\right)\right)$ is ``small''



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$$d_\infty(A,B) \leq \|f-g\|_\infty$$

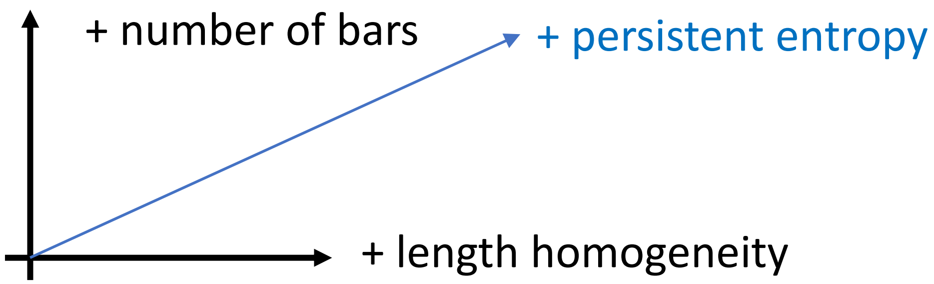
p-th Wasserstein distance: $d_p(A,B) = \min_\gamma \ d_{p\gamma}(A,B)$

Bottleneck distance: $d_\infty(A,B) = \min_\gamma \ d_{\infty\gamma}(A,B)$

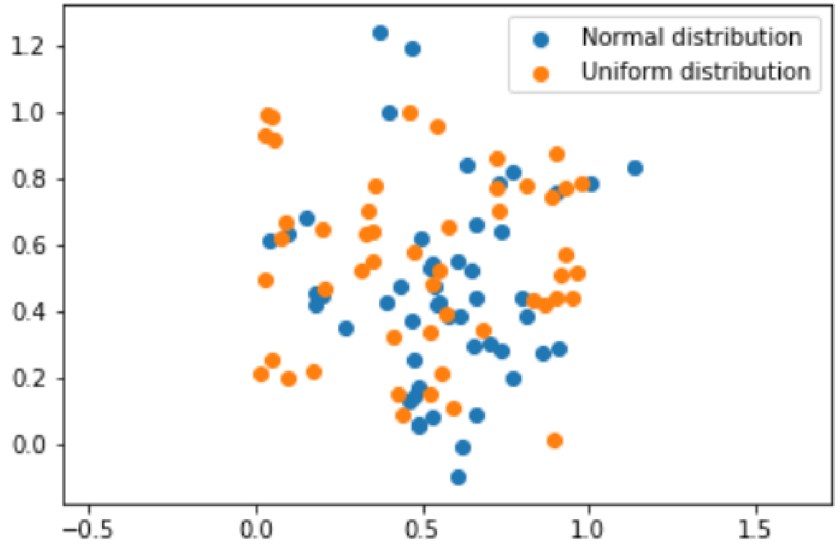
Concepts from computational topology

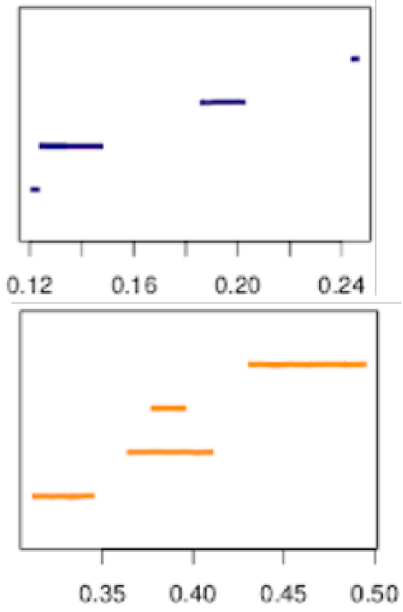
Stability of persistent entropy

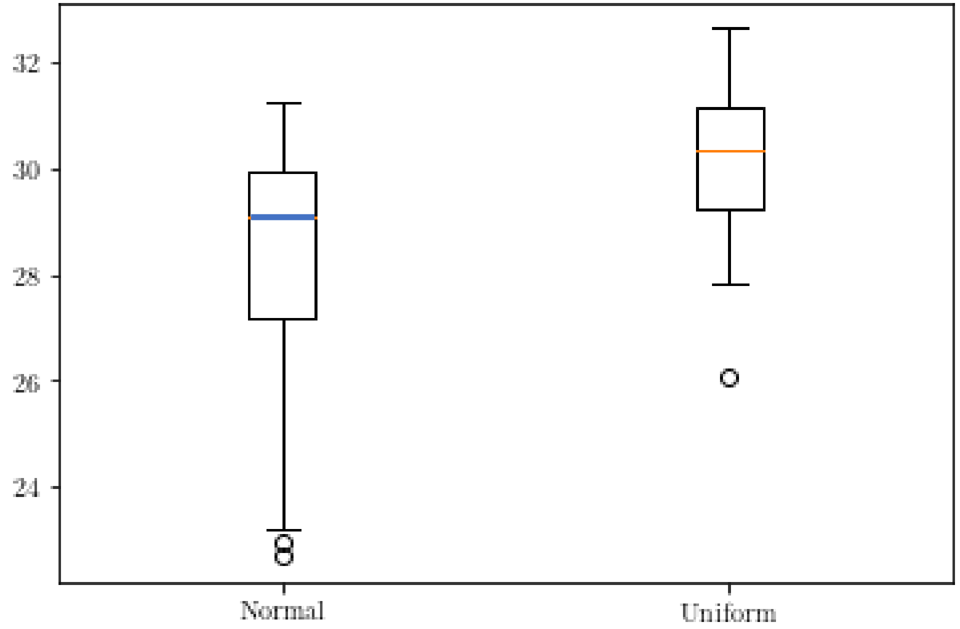
What is persistent entropy measuring?



On the stability of persistent entropy and new summary functions for topological data analysis. Pattern Recognition 107, 107509 (2020)

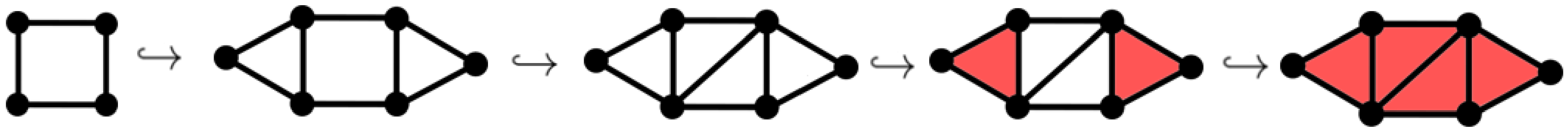






Concepts from computational topology

- (abstract) Simplicial complexes
- Homology
- Vertex map, simplicial map
- Simplicial Approximation Theorem
- Category SpCpx : simplicial complexes, simplicial maps
- Filtration
- Persistent homology
- **Persistence module**



$$H_1(K_1) \longrightarrow H_1(K_2) \longrightarrow H_1(K_3) \longrightarrow H_1(K_4) \longrightarrow H_1(K_5)$$

$V = PH_1(K)$

$$0 \longrightarrow V_1 \xrightarrow{\rho_1^2} V_2 \xrightarrow{\rho_2^3} V_3 \xrightarrow{\rho_3^4} V_4 \xrightarrow{\rho_4^5} V_5 \longrightarrow 0$$

persistence module

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- **Persistence module**

A persistence module can be seen as a functor from {1, … , n} to the category of vector spaces

This definition can be extended to any other totally ordered set

$$(V_t, \rho_p^q)$$

$$1 \leq 2 \leq \ldots \leq n$$

$$\Downarrow$$

$$0 \xrightarrow{\rho_0^1} V_1 \xrightarrow{\rho_1^2} V_2 \xrightarrow{\rho_2^3} \ldots \xrightarrow{\rho_{n-1}^n} V_n \xrightarrow{\rho_n^{n+1}} 0$$

- $\rho_q^l \rho_p^q = \rho_p^l$ if $0 \leq p \leq q \leq l \leq n+1$
- ρ_p^p is the identity map

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The category of persistence modules satisfies that

- The **direct sum** of persistence modules is a persistence module
- The **intersection** of persistence modules is a persistence module
- The **quotient** of persistence modules is a persistence module
- The notion of **submodule** is well defined

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$$V \simeq \bigoplus_{I \in S} \left(\oplus_{m_I} k_I \right)$$

Interval module $k_{I_t} = \begin{cases} 1 & \text{if } t \in I \\ 0 & \text{otherwise} \end{cases}$

$B = \{(I, m_I)\}$ $\quad$ $S = \{ \text{I} : \ldots \}$

Example: $B = \{([1,4], 1), ([2,3], 2), ([3,4], 1)\}$

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$$V \simeq \bigoplus_{I \in S} \left(\oplus_{m_I} k_I \right)$$

$I = [a, b]$ $\quad t \in I$

$$\mathrm{Im}^+_{at}(V) := \mathrm{im}\ \rho^t_a, \qquad \mathrm{Ker}^+_{bt}(V) := \ker\ \rho^{b+1}_t$$

$$\mathrm{Im}^-_{at}(V) := \mathrm{im}\ \rho^t_{a-1}, \qquad \mathrm{Ker}^-_{bt}(V) := \ker\ \rho^b_t$$

$$V^+_{It} := \mathrm{Im}^+_{at}(V) \cap \mathrm{Ker}^+_{bt}(V)$$

$$V^-_{It} := \mathrm{Im}^-_{at}(V) \cap \mathrm{Ker}^+_{bt}(V) + \mathrm{Im}^+_{at}(V) \cap \mathrm{Ker}^-_{bt}(V)$$

$$k_I \simeq \frac{V^+_{It}}{V^-_{It}} \qquad \mathrm{m_I} = \dim \frac{V^+_{It}}{V^-_{It}}$$

Example: $B = \{([1,4], 1), ([2,3], 2), ([3,4], 1)\}$

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- **Morphism between persistence modules**

$$\begin{array}{cccccccccccc} U & 0 & \longrightarrow & U_1 & \xrightarrow{\phi_1^2} & U_2 & \xrightarrow{\phi_2^3} & \cdots & \xrightarrow{\phi_{n-1}^n} & U_n & \longrightarrow & 0 \\ f\uparrow & & & f_1\uparrow & & f_2\uparrow & & & & f_n\uparrow & & \\ V & 0 & \longrightarrow & V_1 & \xrightarrow{\rho_1^2} & V_2 & \xrightarrow{\rho_2^3} & \cdots & \xrightarrow{\rho_{n-1}^n} & V_n & \longrightarrow & 0 \end{array}$$

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- **Morphism between persistence modules**

$$
\begin{array}{ccccccccc}
U & \quad & U_1 & \longrightarrow & U_2 & \longrightarrow & \dots & \longrightarrow & U_n \\
f \big\uparrow & & f_1 \big\uparrow & & f_2 \big\uparrow & & & & f_n \big\uparrow \\
V & & V_1 & \longrightarrow & V_2 & \longrightarrow & \dots & \longrightarrow & V_n
\end{array}
$$

Example:

- Let $\mathbb{X}$ and $\mathbb{Y}$ be two finite subsets from $\mathbb{R}^n$ such that $\mathbb{X} \subseteq \mathbb{Y}$.
- This induces an embedding $\mathrm{VR}(\mathbb{X}) \hookrightarrow \mathrm{VR}(\mathbb{Y})$.
- In turn, this induces a persistence morphism $f : V \to U$, where $V = \mathrm{PH}_n(\mathrm{VR}(\mathbb{X}))$ and $U = \mathrm{PH}_n(\mathrm{VR}(\mathbb{Y}))$

Links

- https://colah.github.io/posts/2014-03-NN-Manifolds-Topology/
- Elements of algebraic topology. Munkres
- Computational Topology: An Introduction. Edelsbrunner, Harer
- Topological Data Analysis with applications. Carlsson, Vejdemo-Johansson
- Decomposition of pointwise finite-dimensional persistence modules. W. Crawley-Boevey.

- https://lewtun.github.io/hepml/lesson06_persistent-homology/

- https://colab.research.google.com/github/lewtun/hepml/blob/master/notebooks/lesson06_persistent-homology.ipynb

- https://colab.research.google.com/github/shizuo-kaji/TutorialTopologicalDataAnalysis/blob/master/TopologicalDataAnalysisWithPython.ipynb

Our goals within REXASI-PRO

Main goal

Use computational topology to design new methods to achieve **explainable and green artificial intelligence models.**

UNIVERSIDAD DE SEVILLA

spinδox.LABS

How to make greener the AI solution [WP6]

Specific Goals

1. Topology-aware reduce the input dataset.
2. Build explainable models based on topology.
3. Simplify the model preserving its learning capacity.
4. Create synthetic samples that can quickly train a model.

Topology Tools
for
Explainable and Green Artificial Intelligence

Rocio Gonzalez-Diaz
rogodi@us.es

- Context: Green and Explainable artificial intelligence (REXASI-PRO)
- Computational topology tools: Persistent homology, barcodes, distance bottleneck, simplicial maps, Persistence modules, morphisms between persistence modules
- Partial matchings between barcodes
- Simplicial maps neural networks