## Topology Tools for Explainable and Green Artificial Intelligence

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- 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

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

$$H_{1}(K_{1}) \longrightarrow H_{1}(K_{2}) \longrightarrow H_{1}(K_{3}) \longrightarrow H_{1}(K_{4}) \longrightarrow H_{1}(K_{5})$$

$$H_{1}(K) \longrightarrow V_{1} \xrightarrow{\rho_{1}^{2}} V_{2} \xrightarrow{\rho_{2}^{3}} V_{3} \xrightarrow{\rho_{4}^{4}} V_{4} \xrightarrow{\rho_{4}^{5}} V_{5} \longrightarrow 0$$
persistence module

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- Homology
- Vertex map, simplicial map
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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

 $(V_t, \rho_p^q)$ 

- $\rho_q^l \rho_p^q = \rho_p^l$  if  $0 \le p \le q \le l \le n+1$
- $\rho_p^p$  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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Example:  $B = \{([1,4], 1), ([2,3], 2), ([3,4], 1)\}$   $Rep B = \langle [1,4], [2,3], [2,3], [3,4] \rangle$  $SS = \{[1,4], [2,3], [3,4]\}$ 

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

- (abstract) Simplicial complexes
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- Persistence module
- Morphism between persistence modules



- 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  $VR(\mathbb{X}) \hookrightarrow VR(\mathbb{Y})$ .
- In turn, this induces a persistence morphism  $f: V \to U$ , where  $V = PH_n(VR(X))$  and  $U = PH_n(VR(Y))$

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- Partial matchings between barcodes
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#### Joint work with Manuel Soriano-Trigueros and Álvaro Torras-Casas



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#### A motivation

Stats is not enough:



Datasaurus dozen dataset

#### A motivation

A

0

2

Bottleneck distance is not enough:



#### <u>A motivation</u>

When can we say that a subset Y of a given a dataset X "samples" the same continuous space than X?



Why is it important?

- Data hungry
- Energy saving
- Storage saving
- Data is expensive



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Given  $B(V) = \{(I, m_I)\}$  and  $B(U) = \{(J, m_J)\}$ , we define a **partial matching** satisfying **block function** 

$$S_V = \{I\} \qquad S_U = \{J\}$$

$$\mathcal{M}: S_V \times S_U \longrightarrow \mathbb{Z}_{\geq 0}$$



The number of arrows leaving from an interval is smaller than its multiplicity

The number of arrows arriving to an interval is smaller than its multiplicity

Block function:

$$\mathcal{M} : S_V \times S_U \to \mathbb{Z}_{\geq 0} \qquad \sum_{J \in S_U} \mathcal{M} \ (I, J) \leq m_J$$

Example:

 $\mathsf{B}(\mathsf{V}) = \{([2,4],1), ([1,5],2)\} \text{ and } \mathsf{B}(\mathsf{U}) = \{([2,3],1), ([1,4],2)\}$ 

 ${\rm Consider}\ {\cal M} \quad \text{is zero except for} \quad$ 

$$\mathcal{M}([2,4],[1,4]) = 1 \text{ and } \mathcal{M}([1,5],[1,4]) = 2.$$

 $\ensuremath{\mathcal{M}}$  is a block function, since

$$\mathcal{M}([2,4],[1,4]) = 1 \le m_{[2,4]} \text{ and } \mathcal{M}([1,5],[1,4]) = 2 \le m_{[1,5]}$$

 $\mathcal{M}$  is not a partial matching

$$\mathcal{M}([2,4],[1,4]) + \mathcal{M}([1,5],[1,4]) = 3 \leq n_{[1,4]} = 2$$
.



The induced block function:  $\mathcal{M}_f: S_V \times S_U \to \mathbb{Z}_{\geq 0}$   $\sum_{J \in S_U} \mathcal{M}_f(I, J) \leq m_I$ 

$$V \xrightarrow{f} U$$

$$(I, m_I) \xrightarrow{} (J, m_J)$$

$$M_f(I; J)$$

The induced block function: 
$$\mathcal{M}_{f}: S_{V} \times S_{U} \to \mathbb{Z}_{\geq 0}$$
  $\sum_{J \in S_{U}} \mathcal{M}_{f}(I, J) \leq m_{I}$   
 $V \xrightarrow{f} U$   
 $\downarrow (I, m_{I}) \xrightarrow{f} (J, m_{J}) \downarrow$   
 $V \xrightarrow{f} (J, m_{J}) \downarrow$   
 $M_{f}(I, J) = \dim X_{IJt}$   
 $M_{f}(I, J) = \dim X_{IJt}$   
 $I \in I \cap J$   
 $X_{IJt} = \frac{fV_{It}^{+} \cap U_{Jt}^{+}}{fV_{It}^{-} \cap U_{Jt}^{+} + V_{It}^{+} \cap U_{Jt}^{-}}$ 

The induced block function: 
$$\mathcal{M}_f: S_V \times S_U \to \mathbb{Z}_{\geq 0}$$
  $\sum_{J \in S_U} \mathcal{M}_f(I, J) \leq m_I$   
Let  $I = [a, b]$  and  $J = [c, d]$ .  $\mathcal{M}_f(I, J) = \dim X_{IJd}$  if  $J \leq I$   
 $\mathcal{M}_f(I, J) = 0$  otherwise Otherwise determines of the set of

We say that  $J \leq I$  if  $c \leq a \leq d \leq b$ .

$$X_{IJt} = \frac{fV_{It}^{+} \cap U_{Jt}^{+}}{fV_{It}^{-} \cap U_{Jt}^{+} + V_{It}^{+} \cap U_{Jt}^{-}}$$

The induced block function: 
$$\mathcal{M}_f: S_V \times S_U \to \mathbb{Z}_{\geq 0}$$
  $\sum_{J \in S_U} \mathcal{M}_f(I, J) \leq m_I$   
 $\mathcal{M}_f(I, J) = \dim X_{IJd} \text{ if } J \leq I$   
 $\mathcal{M}_f(I, J) = 0$  otherwise Detween Persistence Modules. Computational Geometry, 112, 101985 (2023)  
• [a, b] and [c, d] are nested if  $a < c < d < b$ 

**Prop.:** If for any set of intervals  $S \subseteq S_V$  we have that

$$\sum_{I \in S} \mathcal{M}_f(I, J) > n_J,$$

then there exists a pair of nested intervals in  $S_V$ .

**Corollary:** If there are no two nested intervals in  $S_V$  then  $M_f$  is a partial matching.

Linearity of the induced block function:

Given a direct sum of morphisms of persistence modules

$$f^1 \oplus f^2 : V^1 \oplus V^2 \to U^1 \oplus U^2$$

we have that

$$\mathcal{M}_{f^{1} \oplus f^{2}}(I, J) = \mathcal{M}_{f^{1}}(I, J) + \mathcal{M}_{f^{2}}(I, J)$$
Example:  

$$U \qquad k \xrightarrow{\mathrm{Id}} k \longrightarrow 0$$

$$f \uparrow \simeq \uparrow ( \begin{pmatrix} 0 \\ 1 \end{pmatrix} \uparrow ) \uparrow \qquad \uparrow$$

$$V \qquad 0 \longrightarrow k^{2} \xrightarrow{\begin{pmatrix} 1 \\ 0 \end{pmatrix}} k$$

$$\mathcal{M}_{f} ?$$

Partial Matchings Induced by Morphisms between Persistence Modules. Computational Geometry, 112, 101985 (2023)

























Endpoint order:  $[a_1, b_1] \leq [a_2, b_2]$  iff  $b_1 < b_2$  or  $b_1 = b_2$  and  $a_1 \leq a_2$ 







Endpoint order:  $[a_1, b_1] \leq [a_2, b_2]$  iff  $b_1 < b_2$  or  $b_1 = b_2$  and  $a_1 \leq a_2$ 

#### Example:

- Sort both  $Rep B(S_1)$  and Rep B(T) by the endpoint order
- We have the matrix

$$F = \begin{bmatrix} 0.6, 1.3 & 0.5, 1.5 & 0.6, 1.5 \\ 0.4, 1.2 & 0 & 0 & 1 \\ 0.5, 1.2 & 1 & 1 & 0 \end{bmatrix}$$

• We obtain the matrices

$$F_{[0.6,1.3]} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \ F_{[0.5,1.5]} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \ F_{[0.6,1.5]} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix},$$

• Assignment:  $[0.6, 1.3] \mapsto [0.5, 1.2]$ ,  $[0.5, 1.5] \mapsto [0.5, 1.2]$  and  $[0.6, 1.5] \mapsto [0.4, 1.2]$ .

Endpoint order:  $[a_1, b_1] \leq [a_2, b_2]$  iff  $b_1 < b_2$  or  $b_1 = b_2$  and  $a_1 \leq a_2$ 

#### Example:

- Sort both  $Rep B(S_2)$  and Rep B(T) by the endpoint order
- We have the matrix

$$F = \begin{bmatrix} 0.6, 1.3 & 0.5, 1.5 & 0.6, 1.5 \\ 0.4, 1.2 & 0 & 1 & 1 \\ 0.5, 1.2 & 1 & 1 & 0 \end{bmatrix}$$

• We obtain the matrices

$$F_{[0.6,1.3]} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, F_{[0.5,1.5]} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, F_{[0.6,1.5]} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

• Assignment:  $[0.6, 1.3] \mapsto [0.5, 1.2]$  and  $[0.5, 1.5] \mapsto [0.5, 1.2]$ .

$$\begin{split} \mathcal{M}_{f}: S_{V} \times S_{U} \to \mathbb{Z}_{\geq 0} & \sum_{J \in S_{U}} \mathcal{M}_{f}(I, J) \leq m_{I} \\ \mathbb{M}_{f}(I, J) = \dim \lim_{t \in I \cap J} X_{IJt} \\ \end{split}$$
 Proof: Decorated points and persistence modules: 
$$\begin{split} & \sum_{J \in S_{U}} \mathcal{M}_{f}(I, J) \leq m_{I} \\ \mathbb{M}_{f}(I, J) = \dim \lim_{t \in I \cap J} X_{IJt} \\ & \underset{t \in (\cdot, 4]}{\overset{\bullet}{\longrightarrow}} & \underset{$$

$$\mathcal{M}_f: S_V \times S_U \to \mathbb{Z}_{\geq 0} \qquad \sum_{J \in S_U} \mathcal{M}_f(I, J) \leq m_I$$
$$\mathcal{M}_f(I, J) = \dim \lim_{t \in I \cap J} X_{IJt}$$

#### Proof:

A section of a vector space,  $\mathcal{V}$ , is a pair of vector spaces,  $(F^-, F^+)$ , such that

$$F^- \hookrightarrow F^+ \hookrightarrow \mathcal{V}$$

We say that a set of sections,  $\{(F_{\lambda}^{-}, F_{\lambda}^{+}) : \lambda \in \Lambda\}$ , of  $\mathcal{V}$  is **disjoint** if, for all  $\lambda \neq \mu$ ,  $F_{\mu}^{+} \hookrightarrow F_{\lambda}^{-}$  or  $F_{\lambda}^{+} \hookrightarrow F_{\mu}^{-}$ 

**Lemma.** If 
$$\{(F_\lambda^-,F_\lambda^+):\lambda\in\Lambda\}$$
 is a set of disjoint sections of  $\mathcal V$ , we have that

$$\bigoplus_{\lambda \in \Lambda} \left( F_{\lambda}^{+} / F_{\lambda}^{-} \right) \hookrightarrow \mathcal{V}$$

$$\mathcal{M}_f: S_V \times S_U \to \mathbb{Z}_{\geq 0}$$
$$\mathcal{M}_f(I, J) = \dim \lim_{t \in I \cap J} X_{IJt}$$

$$\sum_{J \in S_U} \mathcal{M}_f(I, J) \le m_I$$

Proof:

dim  $V^+_{(s,r) t}$ nº of intervals (a, b) such that  $t \in (a, b)$ ,<br/> $a \le s$  and  $b \le r$ dim  $V^-_{(s,r) t}$ nº of intervals (a, b) such that  $t \in (a, b)$ ,<br/>(a < s and  $b \le r)$  or  $(a \le s$  and b < r)

 $\begin{array}{l} V^-_{(s,r)\ t} \ \text{and} \ V^+_{(s,r)\ t} \ \text{are persistence submodules of } V \ \text{and} \ \text{, for each} \ t \ \text{,} \\ \left\{ \left( V^-_{(s,r)\ t}, V^+_{(s,r)\ t} \right) \right\}_{s < r} \ \text{are disjoint sections of} \ V_t \end{array}$ 

$$\bigoplus_{s < r} \left( V^+_{(s,r),t} / V^-_{(s,r),t} \right) \hookrightarrow V_t$$

Proof:  

$$\mathcal{M}_{f}: S_{V} \times S_{U} \to \mathbb{Z}_{\geq 0} \qquad \sum_{J \in S_{U}} \mathcal{M}_{f}(I, J) \leq m_{H}$$

$$\mathcal{M}_{f}(I, J) = \dim \lim_{t \in I \cap J} X_{IJt}$$

$$I = (a, b) \in S_{V} \qquad J = (c, d) \in S_{U}$$

$$A_{ct}^{d} := \frac{fV_{It}^{-} \cap U_{(c,d)t}^{+} + fV_{It}^{+} \cap U_{(c,d)t}^{-}}{fV_{It}^{-} \cap U_{(c,d)t}^{+}} \quad \text{and} \quad B_{ct}^{d} := \frac{fV_{It}^{+} \cap U_{(c,d)t}^{+}}{fV_{It}^{-} \cap U_{(c,d)t}^{+}}$$

$$\frac{B_{ct}^{d}}{A_{ct}^{d}} \simeq X_{IJt}$$

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$$\mathcal{M}_f: S_V \times S_U \to \mathbb{Z}_{\geq 0} \qquad \sum_{J \in S_U} \mathcal{M}_f(I, J) \leq m_I$$
$$\mathcal{M}_f(I, J) = \dim \lim_{t \in I \cap J} X_{IJt}$$

#### Proof:

$$\tilde{A}_{c}^{d} := \varinjlim_{t \in I \cap J} A_{ct}^{d} \qquad \qquad \tilde{B}_{c}^{d} := \varinjlim_{t \in I \cap J} B_{ct}^{d}$$

- For fixed d and variable c, they are persistence modules indexed by  ${f E}$
- They satisfies that

$$\frac{\tilde{B}_c^d}{\tilde{A}_c^d} \simeq \varinjlim_{t \in I \cap J} X_{IJt}$$

$$\mathcal{M}_f: S_V \times S_U \to \mathbb{Z}_{\geq 0} \qquad \sum_{J \in S_U} \mathcal{M}_f(I, J) \leq m_I$$
$$\mathcal{M}_f(I, J) = \dim \lim_{t \in I \cap J} X_{IJt}$$

Proof:

For each d,

 $\left\{ (\tilde{A}_{c}^{d}, \tilde{B}_{c}^{d}) : c \in \mathbf{E} \right\} \text{ is a disjoint set of sections of } \varinjlim_{c < d} \tilde{B}_{c}^{d}$   $\left( \bigoplus_{c < d} \varinjlim_{t \in I \cap J} X_{I(c,d)t} \right) \hookrightarrow \varinjlim_{c < d} \tilde{B}_{c}^{d} \hookrightarrow \varinjlim_{t \in (-\infty,d)} \left( fV_{It}^{+}/fV_{It}^{-} \right)$   $\underbrace{\tilde{B}_{c}^{d}}_{\tilde{A}_{c}^{d}}$ 



## Links

https://doi.org/10.1016/j.comgeo.2023.101985

https://arxiv.org/abs/2306.02411

Decomposition of pointwise finite-dimensional persistence modules. W. Crawley-Boevey.

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