PersLay: A Neural Network Layer for Persistence Diagrams and New Graph Topological Signatures

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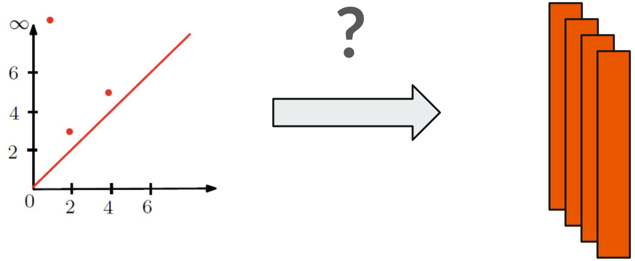
1. Introduction + Related Work
2. Paper Contributions
3. Network and Training
4. Results
5. Discussion

1. Introduction

Context: persistence diagrams are one of the main topological features, but they are difficult to use in machine learning pipeline due to the lack of structure of the space.



→ Solution: **vectorization** of the persistence diagrams

Related works:

- Real-valued functions on graphs
- Already existing vectorisation
- Deep Sets network [Zaheer, M., Kottur, S., Ravanbakhsh, S., Poczos, B., Salakhutdinov, R., & Smola, A.. *Deep sets.*]

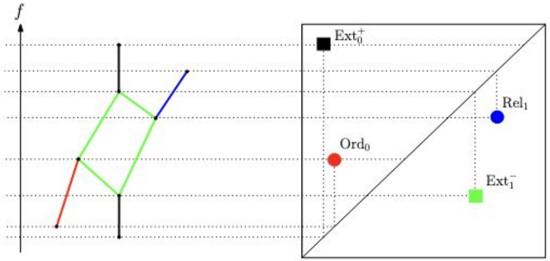
Current limitations:

- Few trainable parameters
- Hard to know choose vectorisation for a specific task
- Kernel methods are not optimized in terms of computation times

1. Introduction

Solution proposed by the paper:

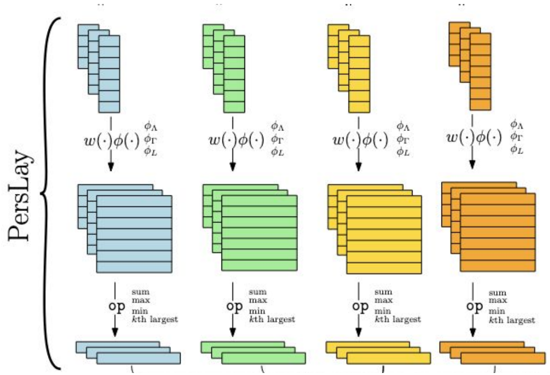
→ A framework to learn the vectorisation adapted to the task generalizing some of the vectorisation already existing.



Extended persistence diagrams

$$hks_{G,t} : \nu \mapsto \sum_{k=1}^{n} exp(-t\lambda_k)\psi_k(\nu)^2$$

Heat kernel signatures



PersLay: a new neural network layer

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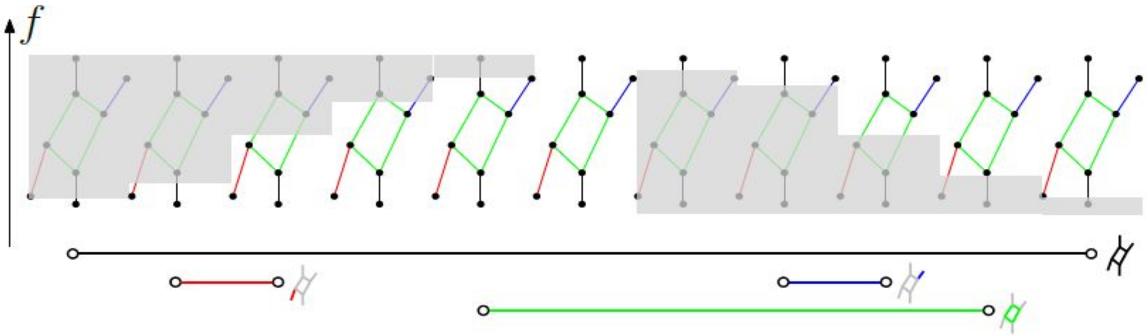
2. Extended persistence diagram



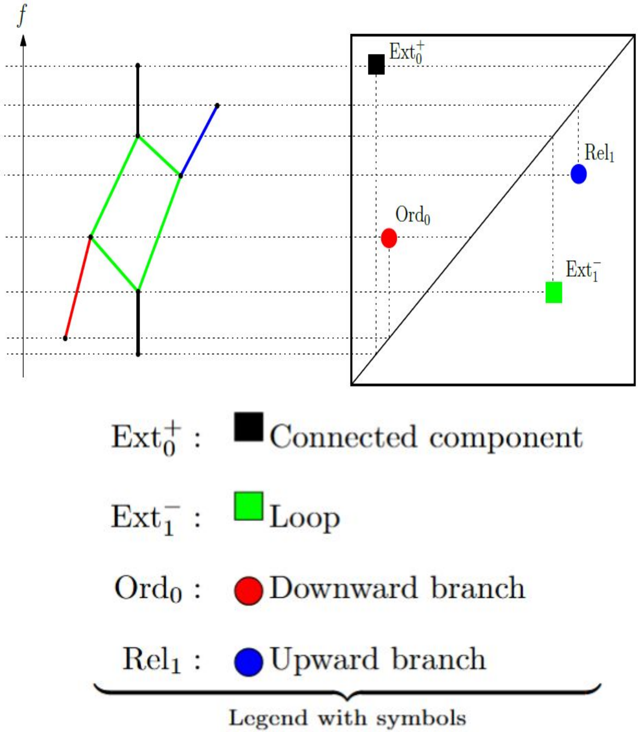
Filtration with up and sub levels

Up level :

$$[G=(V,E)][G_\alpha=(V_\alpha,E_\alpha)][V_\alpha=\{v\in V: f(v)\leq\alpha\}][E_\alpha=\{(v_1,v_2)\in E: v_1,v_2\in V_\alpha\}]$$

Sub level :

$$[X=(V,E)][X^\alpha=\{x\in X: f(x)\geq\alpha\}][E^\alpha=\{(x_1,x_2)\in E: x_1,x_2\in X^\alpha\}]$$



2. Heat Kernel Signatures on graphs

$$L_\omega = I - A^{-1/2} D A^{-1/2}$$

$$hks_{G,t} : \nu \mapsto \sum_{k=1}^{n} exp(-t\lambda_k)\psi_k(\nu)^2$$

λ_k Eigenvalues of the graph Laplacian

ψ_k Eigenfunctions of the graph Laplacian

t Diffusion parameter

Property :

- Stability w.r.t **graph perturbation** $d_B(Dg(G,t), Dg(G',t)) \leq C(G,t)||W||_F$
- Stability w.r.t **parameter t** $d_B(Dg(G,t), Dg(G,t')) \leq 2|t - t'|$

[Sun, J., Ovsjanikov, M., and Guibas, L. A concise and provably informative multi-scale signature based on heat diffusion.]

2. PersLay

$$\textsc{PersLay}(\mathrm{Dg}) := \mathsf{op}\left(\{w(p)\cdot\phi(p)\}_{p\in\mathrm{Dg}}\right)$$

any permutation invariant operation (sum, min...)

weight function (learnable)

point transformation function

Point transformation function:
Pour p un point du diagramme:

- Triangle point transformation: $\Lambda_p : t \to \max\{0,\, y - |t - x|\}$
- Gaussian point transformation: $\Gamma_p : t \to exp\left(-\, \|p - t\|_2^2 / \left(2\sigma^2\right)\right)$
- Line point transformation : $\mathbf{L}_\Delta : p \to \langle p, e_\Delta\rangle + b_\Delta$

Example with a triangle point transformation:

$$\phi : \mathbb{R}^2 \to \mathbb{R}^q$$

$$p \longrightarrow \begin{array}{c}\Lambda_p(t_1)\\ \Lambda_p(t_2)\\ \cdots\\ \Lambda_p(t_q)\end{array}$$

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3. Network

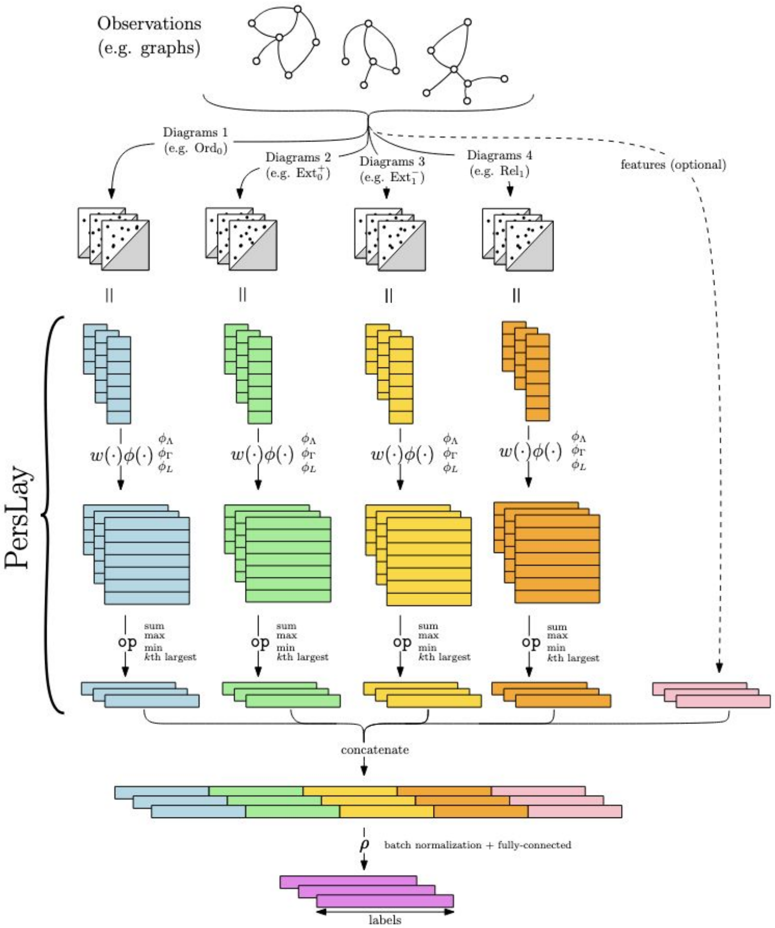
Network:

- 2 layers (PersLay + Fully connected layer)

Hyperparameters set-up:

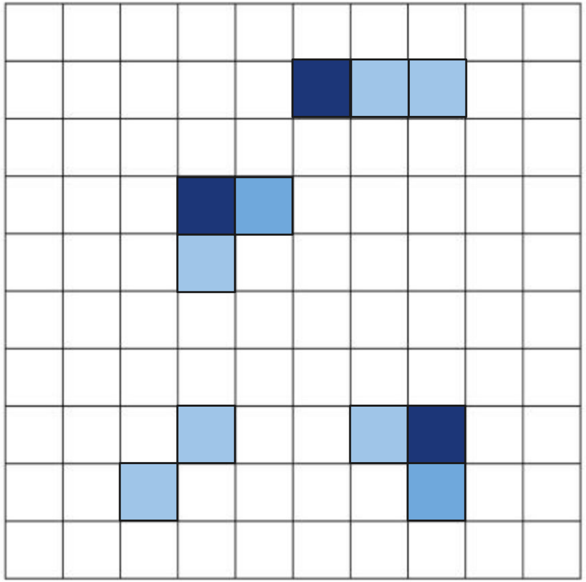
PersLay layer:

- op is the sum
- phi is the sum of the point transformation function



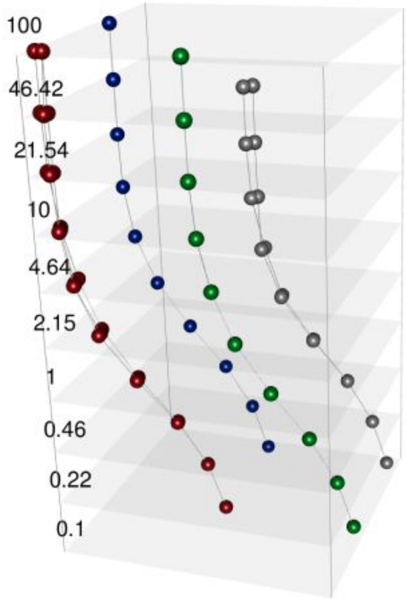
3. Choice of hyperparameters

How to set ω ?



Can we optimize t ?

The choice of t does not affect classification performance



Evolution of $t \mapsto Dg(G,t)$ for one graph from the MUTAD dataset

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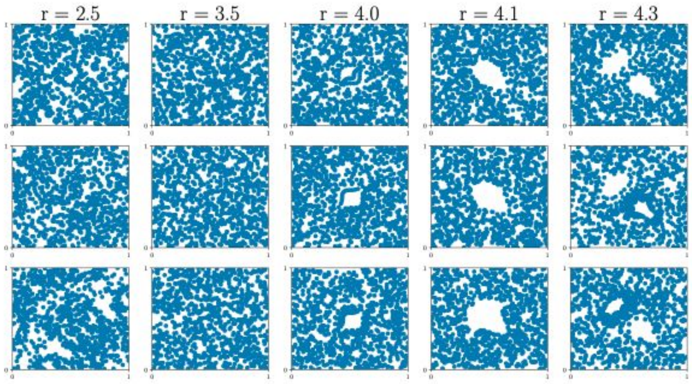
4. A proof of concept: Perslay results with AlphaComplex filtration

- **ORBIT5K : Improve results** compared to state-of-the-art method
- **ORBIT100K :** Capable of handling large-scale datasets where kernel method fail

Orbits generated by differents choice of r :



Dataset	PSS-K	PWG-K	SW-K	PF-K	PersLay
ORBIT5K	72.38(±2.4)	76.63(±0.7)	83.6(±0.9)	85.9(±0.8)	**87.7(±1.0)**
ORBIT100K	—	—	—	—	**89.2(±0.3)**

4. Results

Ablation studies :

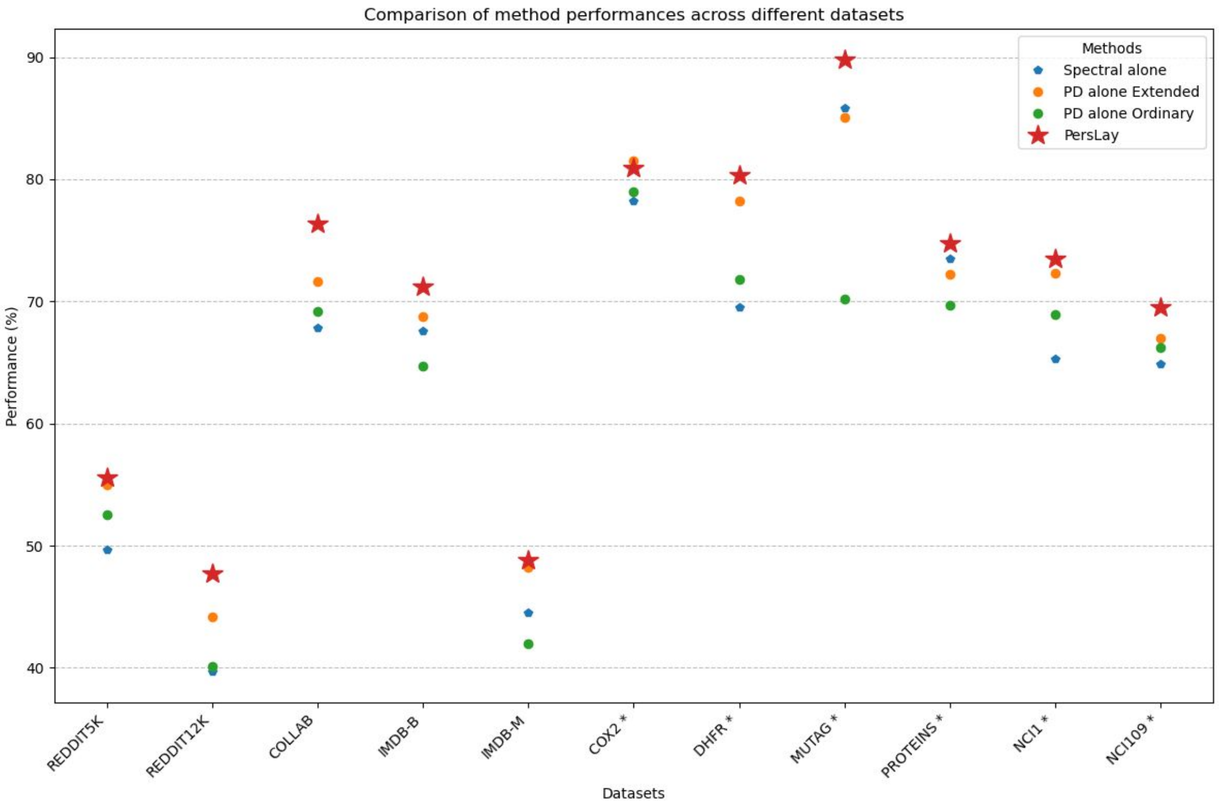
- Choice of the grid size is not a key parameter however too large grid size lead to overfitting
- The best choice of point transformation differs from one dataset to another.
- The sum permutation operator give better results

		Grid size for trainable weights w(p)					
		None	2×2	5×5	10×10	20×20	50×50
MUTAG	Train/Test acc (%)	92.3/88.9	91.1/88.8	91.7/89.6	92.3/**89.9**	93.7/88.3	94.1/87.7
COLLAB	Train/Test acc (%)	76.5/75.3	78.6/75.8	79.0/76.2	80.0/**76.5**	83.5/73.9	94.0/71.3

		Point transformation ϕ			Perm op	
		Gaussian	line	triangle	Sum	Max
MUTAG	Train/Test acc (%)	92.5/**89.7**	89.2/84.2	91.5/85.0	92.3/**89.5**	91.9/87.4
COLLAB	Train/Test acc (%)	79.7/75.3	79.9/**76.1**	79.4/74.7	80.0/**76.4**	78.8/75.0

4. Results

Ablation studies :



5. Discussion

Conclusion :

- Great improvement to add the graph topology for classification
- Important value added with the extended diagram to capture loops geometry
- Vectorization with reduction of the computational cost

To go further:

- The paper focuses on graph only, an extension can be the utilisation of PersLay to other applications.

MERCI

6. Our implementation

Appendice :

The adjacency matrix A of a graph G with vertex set : $V = \{v_1, v_2, ..., v_n\}$

$$A := \left(\mathbf{1}_{(v_i, v_j) \in E}\right)_{i,j}$$

Degree matrix : $D_{i,j} = \sum_j A_{i,j}$

Results - comparing to top five graphs

Dataset	SV[1]	RetGK* [2]	FGSD [3]	GCNN [4]	GIN [5]	PersLay	
						Mean	Max
REDDIT5K	—	56.1	47.8	52.9	57.0	55.6	56.5
REDDIT12K	—	48.7	—	46.6	—	47.7	49.1
COLLAB	—	81.0	80.0	79.6	80.1	76.4	78.0
IMDB-B	72.9	71.9	73.6	73.1	74.3	71.2	72.6
IMDB-M	50.3	47.7	52.4	50.3	52.1	48.8	52.2
COX2*	78.4	80.1	—	—	—	80.9	81.6
DHFR*	78.4	81.5	—	—	—	80.3	80.9
MUTAG*	88.3	90.3	92.1	86.7	89.0	89.8	91.5
PROTEINS*	72.6	75.8	73.4	76.3	75.9	74.8	75.9
NCI1*	71.6	84.5	79.8	78.4	82.7	73.5	74.0
NCI109*	70.5	—	78.8	—	—	69.5	70.1

Learning the weights