Topological Graph Neural Networks

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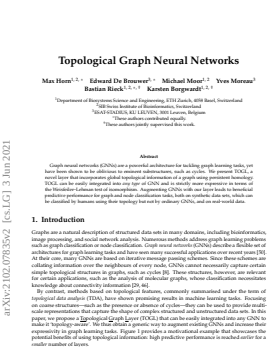
Topological layers for graph classification

TOGL



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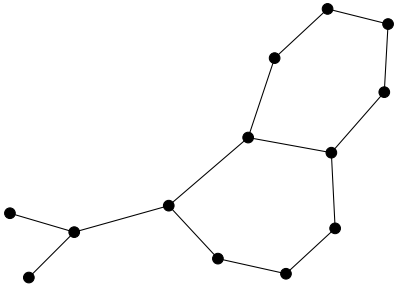
M. Horn†, E. De Brouwer†, M. Moor, Y. Moreau, B. Rieck†‡ and K. Borgwardt‡, 'Topological Graph Neural Networks', *ICLR*, 2022, arXiv: `2102.07835 [cs.LG]`

How to represent graphs?



- Graph $\mathrm{G} = \{V, E\}$
- Two graphs G and G' can have a *different* number of vertices.
- Hence, we require a *vectorised representation* $f : \mathcal{G} \to \mathbb{R}^d$ of graphs.
- Such a representation f needs to be *permutation-invariant*.

Graph neural networks in a nutshell

- Learn node representations h_v based on aggregated attributes a_v.
- Aggregate them over neighbourhoods.
- Iteration k contains information up to k hops away.
- Repeat procedure K times.

$$a_v^{(k)} := \texttt{aggregate}^{(k)}\left(\left\{h_u^{(k-1)} \mid u \in \mathcal{N}_{\mathrm{G}}(v)\right\}\right)$$

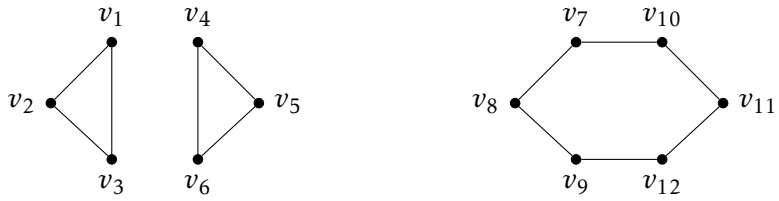
$$h_v^{(k)} := \texttt{combine}^{(k)}\left(h_v^{(k-1)}, a_v^{(k)}\right)$$

$$h_{\mathrm{G}} := \texttt{readout}\left(\left\{h_v^{(K)} \mid v \in \mathcal{V}_{\mathrm{G}}\right\}\right)$$

This terminology follows K. Xu, W. Hu, J. Leskovec and S. Jegelka, 'How Powerful are Graph Neural Networks?', *ICLR*, 2019.

Status quo

- GNNs are *at most* as expressive as the Weisfeiler–Lehman test for graph isomorphism, commonly abbreviated as WL[1][1].
- Graphs are topological objects.
- But GNNs are *incapable* of recognising certain topological structures!



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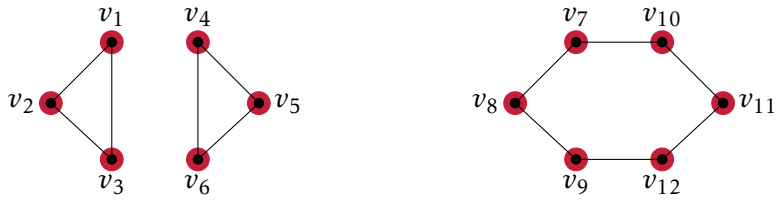

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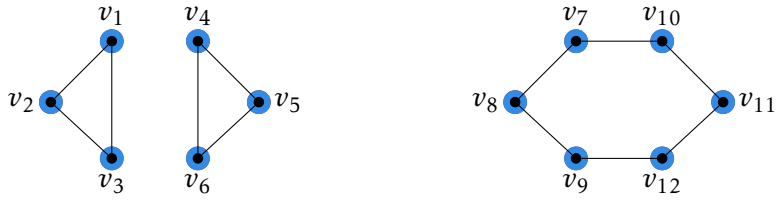
- Graphs are topological objects.
- But GNNs are *incapable* of recognising certain topological structures!
- **What can we gain when imbuing them with knowledge about the topology?**



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Graphs as simplicial complexes

$G = \{V, E\}$ as a simplicial complex K

- Let $K_k = \{\sigma \in K : dim(\sigma) = k\}$, and $\partial_k : K_k \rightarrow C_{k-1}(K) \quad \sigma \rightarrow \sum_{\substack{\tau:\tau\subset\sigma \\ dim(\tau)=k-1}} \tau$
- Topological features as the rank of the homolgy groups $H_k = \ker\partial_k / \text{im}\partial_{k+1}$

$K_0 = V, \quad K_1 = E$

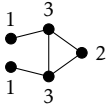
$\rightarrow \text{rank}(H_0) = \beta_0$: number of connected components and $\text{rank}(H_1) = \beta_1$: number of edges.

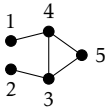
The expressivity of a filtration

Let $f : \mathbb{R}^d \to \mathbb{R}$ with $f^{(1)} < \cdots < f^{(n)}$.

Filtration $\emptyset = G^{(0)} \subseteq G^{(1)} \subseteq \cdots \subseteq G^{(n)} = G = (V, E)$

$V^{(i)} := \left\{ v \in V \mid f\left(x^{(v)}\right) \leq f^{(i)} \right\}$, $E^{(i)} := \left\{ v, w \in E \mid \max\left\{ f\left(x^{(v)}\right), f\left(x^{(w)}\right) \right\} \leq f^{(i)} \right\}$.





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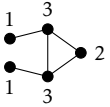
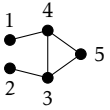


$G^{(1)}$



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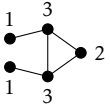
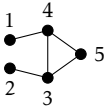


$G^{(2)}$



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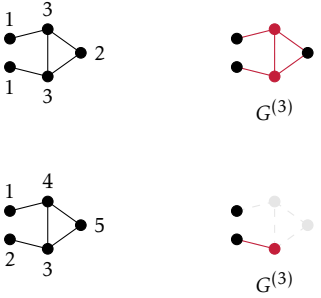

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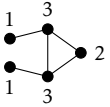
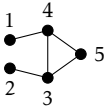


$G^{(3)}$



$G^{(4)}$

The expressivity of a filtration

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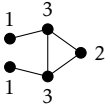

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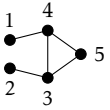


$G^{(5)}$

Persistence Diagrams

$$\emptyset \subset G^{(0)} \subset G^{(1)} \subset ... \subset G^{(N)} \subset G$$

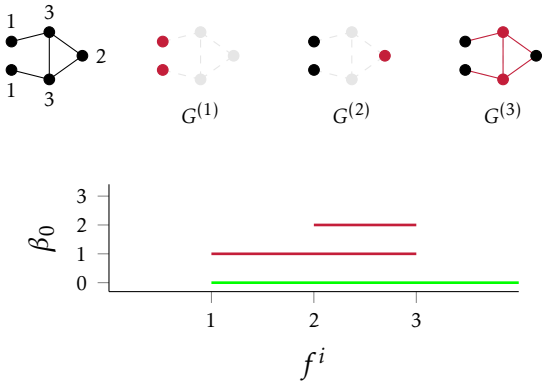
Let $\beta_k^{i,j}$ the *k-th persistent* Betti number, that is the number of topological features of dimension k that *persist* from $G^{(i)}$ to $G^{(j)}$.

- $k = 0$: number of connected components
- $k = 1$: number of cycles

We can build a *persistence diagram* by storing each point (f_i, f_j) with multiplicity

$$\mu_k^{i,j} = (\beta_k^{i,j-1} - \beta_k^{i,j}) - (\beta_k^{i-1,j-1} - \beta_k^{i-1,j}) \quad (1)$$

Persistence Diagrams

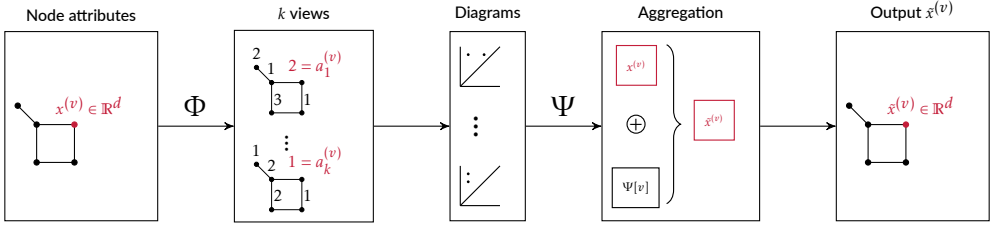


We know how to *learn* a filtration[2], can we create a **layer** that neatly integrates with arbitrary GNNs?

[2] C. D. Hofer, F. Graf, B. Rieck, M. Niethammer and R. Kwitt, 'Graph Filtration Learning', *ICML*, 2020, pp. 4314–4323.

Topological graph neural networks

Overview



- Use a node map $\Phi\colon \mathbb{R}^d \to \mathbb{R}^k$ to create k different filtrations of the graph.
- Use a coordinatisation function Ψ to create *compatible* representations of the node attributes.

Expressivity of a GNN

Typical GNN architectures are *no more expressive* than the Weisfeiler–Lehman test.

Theorem

Persistent homology is *at least* as expressive as WL[1], i.e. if the WL[1] label sequences for two graphs G and G' diverge, there exists an injective filtration f such that the corresponding persistence diagrams $\mathcal{D}_0$ and $\mathcal{D}'_0$ are not equal.

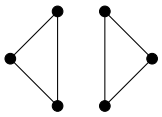
Proof sketch.

We first show how to construct an appropriate filtration function f from a WL[1] label sequence. Since f is not necessarily injective, we show that there is an injective function $\tilde{f}$ that is arbitrarily close to f and whose corresponding persistence diagrams $\widetilde{\mathcal{D}_0}$, $\widetilde{\mathcal{D}'_0}$ do *not* coincide. ■

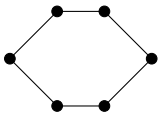
Expressivity of a GNN

There's more!

There are non-isomorphic graphs that WL[1] cannot distinguish, but persistent homology can:



G



G′

We have $\beta_0(\mathrm{G}) = \beta_1(\mathrm{G}) = 2$, because G consists of two connected components and two cycles, whereas $\beta_0(\mathrm{G}') = \beta_1(\mathrm{G}') = 1$ as G' only consists of one connected component and one cycle.

Experiments

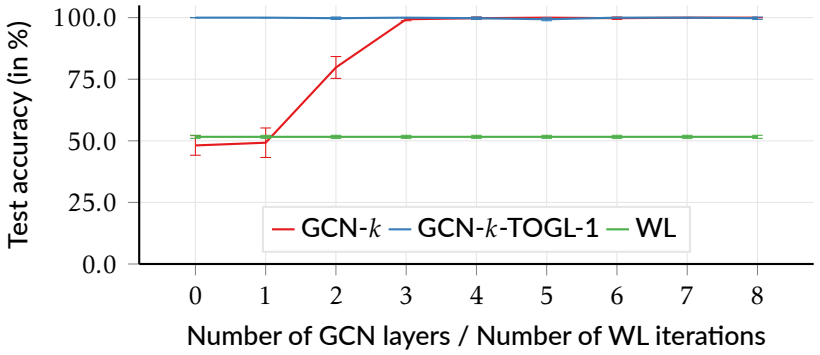
- ☆ Take GCN architecture with 4 convolutional layers (GCN-4).
- ☆ Replace second layer by TOGL.

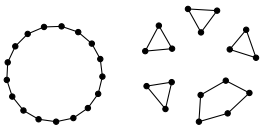
Plan

1. Assess expressivity on synthetic data sets.
2. Assess predictive performance on data sets without node features.
3. Assess predictive performance on benchmark data sets.

Expressivity

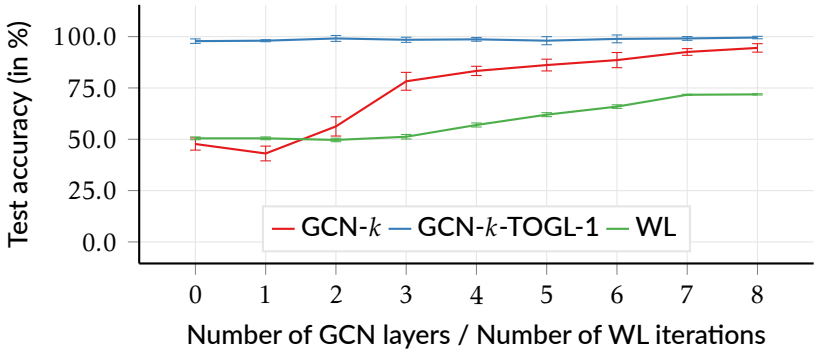
`Cycles` data set





Expressivity

Necklaces data set



Classifying graphs/nodes based on structural features alone

Existing data sets tend to 'leak' information into node attributes, thus decreasing the utility of topological features. Hence, we replaced all node features by random ones.

	Graph classification				*Node classification*
Method	DD	ENZYMES	MNIST	PROTEINS	Pattern
GCN-4	68.0±3.6	22.0±3.3	76.2± 0.5	68.8± 2.8	85.5 ± 0.4
GCN-3-TOGL-1	**75.1±2.1**	**30.3±6.5**	**84.8± 0.4**	**73.8± 4.3**	**86.6 ± 0.1**
GIN-4	75.6±2.8	21.3±6.5	83.4± 0.9	**74.6± 3.1**	84.8 ± 0.0
GIN-3-TOGL-1	**76.2±2.4**	**23.7±6.9**	**84.4± 1.1**	73.9± 4.9	**86.7 ± 0.1**
GAT-4	63.3±3.7	21.7±2.9	63.2±10.4	67.5± 2.6	**73.1 ± 1.9**
GAT-3-TOGL-1	**75.7±2.1**	**23.5±6.1**	**77.2±10.5**	**72.4± 4.6**	59.6 ± 3.3

Classifying benchmark data sets

While we improve baseline classification performance, the best performance is *not* driven by the availability of topological structures!

	Graph classification							*Node classification*
Method	CIFAR-10	DD	ENZYMES	MNIST	PROTEINS-full	IMDB-B	REDDIT-B	CLUSTER
GATED-GCN-4	**67.3 ± 0.3**	72.9 ± 2.1	65.7 ± 4.9	**97.3 ± 0.1**	**76.4 ± 2.9**	—	—	60.4 ± 0.4
WL	—	77.7 ± 2.0	54.3 ± 0.9	—	73.1 ± 0.5	71.2 ± 0.5	78.0 ± 0.6	—
WL-OA	—	**77.8 ± 1.2**	58.9 ± 0.9	—	73.5 ± 0.9	74.0 ± 0.7	87.6 ± 0.3	—
GCN-4	54.2 ± 1.5	72.8 ± 4.1	**65.8 ± 4.6**	90.0 ± 0.3	*76.1 ± 2.4*	68.6 ± 4.9	**92.8 ± 1.7**	57.0 ± 0.9
GCN-3-TOGL-1	*61.7 ± 1.0*	*73.2 ± 4.7*	53.0 ± 9.2	95.5 ± 0.2	76.0 ± 3.9	*72.0 ± 2.3*	89.4 ± 2.2	*60.4 ± 0.2*
GIN-4	54.8 ± 1.4	70.8 ± 3.8	*50.0 ± 12.3*	*96.1 ± 0.3*	72.3 ± 3.3	72.8 ± 2.5	81.7 ± 6.9	58.5 ± 0.1
GIN-3-TOGL-1	*61.3 ± 0.4*	*75.2 ± 4.2*	43.8 ± 7.9	96.1 ± 0.1	*73.6 ± 4.8*	**74.2 ± 4.2**	89.7 ± 2.5	*60.4 ± 0.2*
GAT-4	57.4 ± 0.6	71.1 ± 3.1	26.8 ± 4.1	94.1 ± 0.3	71.3 ± 5.4	*73.2 ± 4.1*	44.2 ± 6.6	56.6 ± 0.4
GAT-3-TOGL-1	*63.9 ± 1.2*	*73.7 ± 2.9*	*51.5 ± 7.3*	*95.9 ± 0.3*	*75.2 ± 3.9*	70.8 ± 8.0	*89.5 ± 8.7*	*58.4 ± 3.7*

What did we learn ?

- When topological structure is important, the addition of a topology-aware layer boosts performance.
- The position of the topology layer is an hyper-parameter and does impact performance.
- Should we incorporate higher-order structures (such as cliques) ?
- What do we gain from learning a filtration function (compared to fixed filtration) ?

Thank you !

arxiv/2102.07835

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