Path-based GNNs* can count cycles and are incomparable to k-WL

***if nodes know their neighbors**

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The Expressive Power of Path-Based Graph Neural Networks

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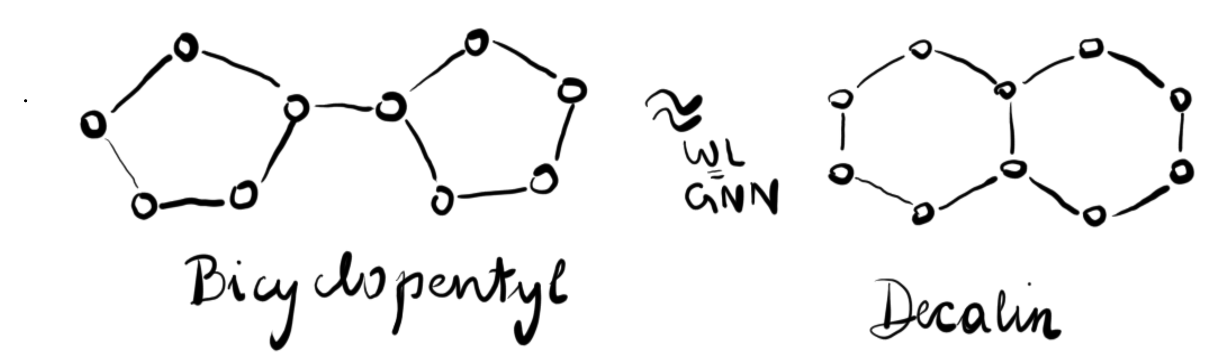
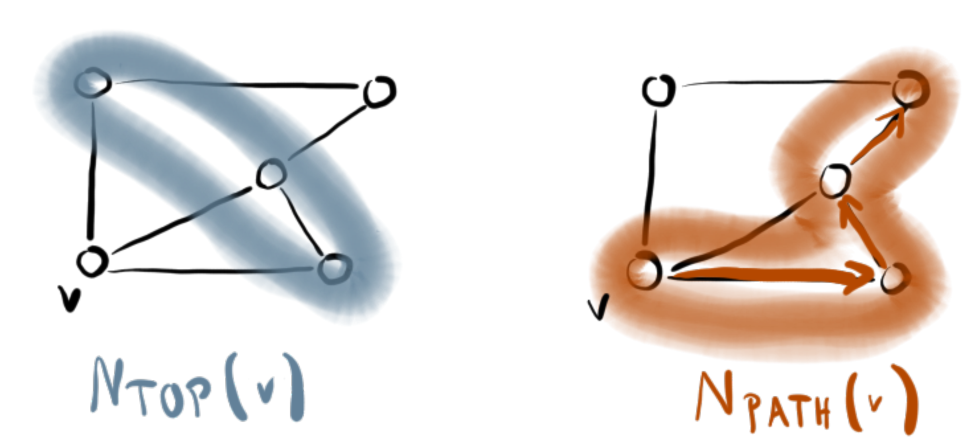
WHY SHOULD I CARE?

Standard message-passing graph neural networks (GNNs) are limited by the Weisfeiler-Leman (WL) graph isomorphism test.



We show that **path-based GNNs with distance encoding** form a **novel class of highly expressive GNNs.**



We introduce **d-PATH-WL,** where colors are refined as:

$$\mathbf{c}_v^{(i)} = \texttt{HASH}\left(d\text{-}\mathcal{P}_v^{\ell\,(i-1)}\right)$$

$\mathcal{P}_v^{\ell} = \{\{ p_v^k \mid k \leq \ell \}\}$

distance encoding

TIME COMPLEXITY. One iteration of **d-PATH-WL** takes $\mathcal{O}(nD^{\ell})$.

#of nodes ↗ ← maximum degree

MONOTONICITY OF EXPRESSIVE POWER. The expressive power of **d-PATH-WL** is non-decreasing with the distance encoding depth d and path length ℓ.

WHAT DID YOU SHOW?

We focused on two variants of **d-PATH-WL:**

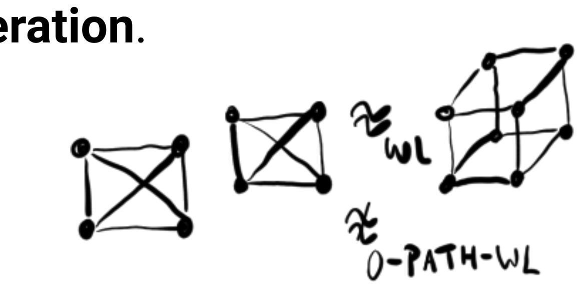
0-PATH-WL → no distance encoding

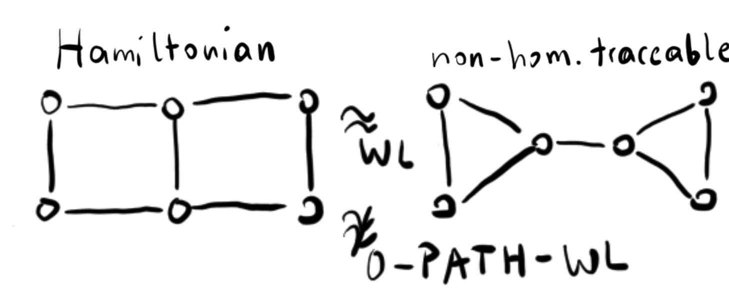
1-PATH-WL → nodes know their neighbors

THEOREM. 0-PATH-WL is **strictly more expressive** than 1-WL for $\ell \geq 2$.

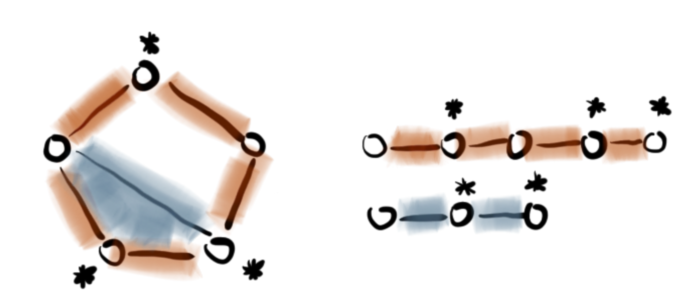
THEOREM. 0-PATH-WL can distinguish several graph families* with **only one iteration**.

*which 1-WL can't distinguish

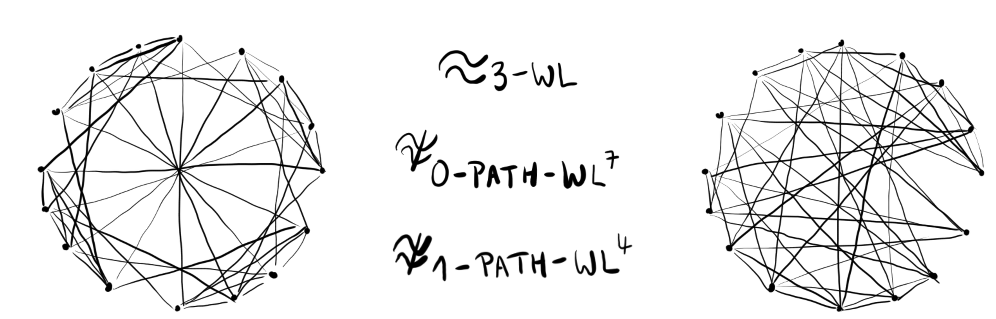




THEOREM. 1-PATH-WL can **count cycles.**



THEOREM. 1-PATH-WL is **incomparable** to k-WL for every k ≥ 3.



THEOREM. 1-PATH-WL is not less expressive than SubgraphGNN, Local 2-GNN, and Folklore k-GNN for every k ≥ 2.

(HOW) DOES IT WORK IN PRACTICE?

We propose **PAIN** (PAth Isomorphism Network), a GNN with expressive power equivalent to **d-PATH-WL**:

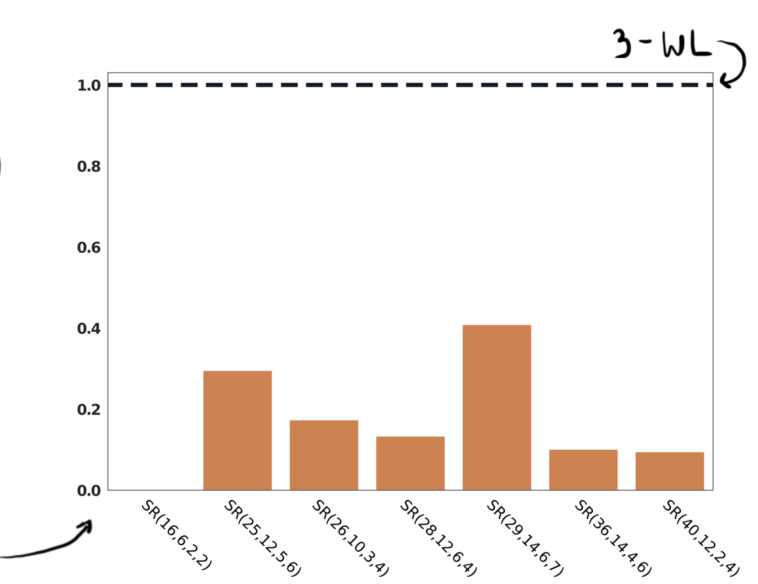
$$\mathbf{h}_v^{(i)} = \texttt{AGG}\left(\{\{\mathbf{z}_p^{(i-1)} \mid p \in d\text{-}\mathcal{P}_v^{\ell}\}\}\right)$$

$z_p^{(i-1)} = f((h_v^{(i-1)}, \ldots, h_{v_\ell}^{(i-1)}))$

We evaluate the expressive power of **PAIN** on the synthetic datasets **EXP**, **SR** and **CSL.**

0-PATH-WL with $\ell=5$

Model	EXP ↓
GIN	600
3-WL	**0**
pathNN	**0**
PAIN	**0**



1-PATH-WL with $\ell=4$

← Ablation study on CSL

ℓ	1 Layer 0-PAIN	1 Layer 1-PAIN	1 Layer 2-PAIN	2 Layers 0-PAIN	2 Layers 1-PAIN	2 Layers 2-PAIN
2	12 ± 4	20 ± 0	20 ± 0	12 ± 4	64 ± 8	70 ± 9
3	18 ± 4	40 ± 0	50 ± 0	20 ± 0	47 ± 6	64 ± 4
4	29 ± 5	54 ± 5	90 ± 0	32 ± 3	64 ± 5	90 ± 0
5	50 ± 0	59 ± 1	100 ± 0	46 ± 5	67 ± 2	100 ± 0
6	50 ± 0	90 ± 0	100 ± 0	46 ± 5	90 ± 0	100 ± 0

Additionally, we perform experiments on the molecule datasets **ZINC** and **OGBG-MOLHIV**, outperforming standard message-passing GNNs.

WHAT'S NEXT?

Hopefully some exciting things, such as identifiying graph classes where we can **upper bound** the path length or number of paths, providing **tighter bounds** for expressivity, and investigating **long-range interactions**.