$\mathscr{N}$-WL: A New Hierarchy of Expressivity for Graph Neural Networks

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k-Weisfeiler-Lehman (k-WL) hierarchy is a theoretical framework for graph isormorphism tests

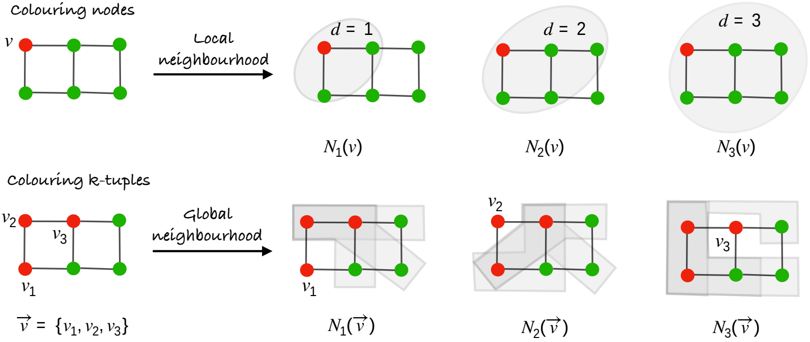
, ! but not practically useful when k 3!

- GIN 1-WL [Xu et al., 2019]
- Many expressive GNNs go beyond 1-WL

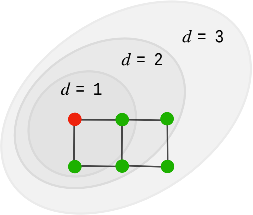
Question:

Is k-WL hierarchy a good yardstick for measuring expressivity of GNNs?

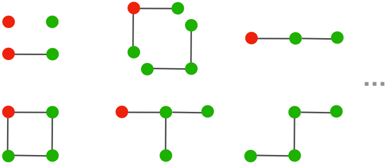
GNNs vs k-WL


Colouring nodes
v
Local
neighbourhood
d = 1
d = 2
d = 3
N1(v)
N2(v)
N3(v)
Colouring k-tuples
v2
v3
v1
Global
neighbourhood
v1
v2
v3
v⃗ = {v1, v2, v3}
N1(v⃗)
N2(v⃗)
N3(v⃗)

$\mathscr{N}$-WL hierarchy computes node coloring via t-order induced subgraphs within d-hop neighbourhoods.



d-hop neighbourhoods

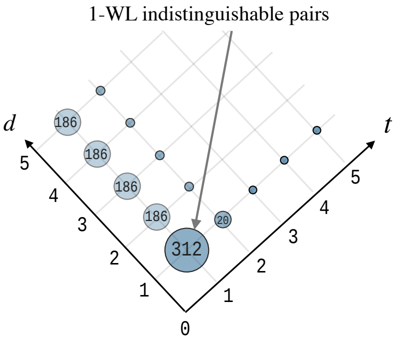


t-order induced subgraphs

A graph isomorphism test on 312 pairs of simple graphs of 8 vertices:

None-or-all: none by 1-WL but all by 3-WL

Progressive: varying with d and t by $\mathcal{N}$-WL



Increasing the order of induced subgraphs, the expressive power increases

Not surprising

Theorem: (Weak Hierarchy) $\mathscr{N}\ (t;d)$-WL ($\mathscr{N}\ (t+1;d)$-WL

Increasing the hops of neighbourhood, the expressive power may decrease

Surprising but can be xed

Theorem: (Strong Hierarchy)

$\mathscr{N}(t;d)$-WL ($\mathscr{N}(t+1;d)$-WL

$\mathscr{N}(t;d)$-WL ($\mathscr{N}(t;d+1)$-WL

Induced connected subgraphs remain the same expressive power

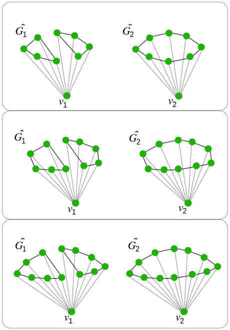
Surprising but can be proved

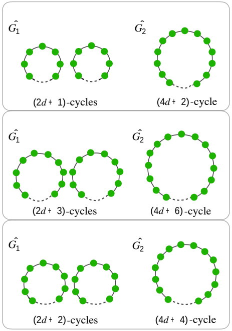
Theorem: (Equivalence) $\mathscr{N}^c(t;d)$-WL $\mathscr{N}(t;d)$-WL

Theorem:
(Strong Hierarchy)

$\mathcal{N}(t;d)$-WL ($\mathcal{N}(t+1;d)$-WL
$\mathcal{N}(t;d)$-WL ($\mathcal{N}(t;d+1)$-WL

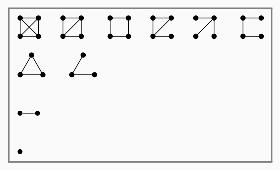
We prove strictness of hierarchies by constructing counterexample graphs.





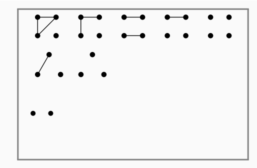
Theorem:
(Equivalence) $\mathscr{N}^c(t;d)$-WL $\mathscr{N}(t;d)$-WL

Our proof is based on Kocay's Vertex Theorem [Kocay, 1982].



subgraph counts

implies
!



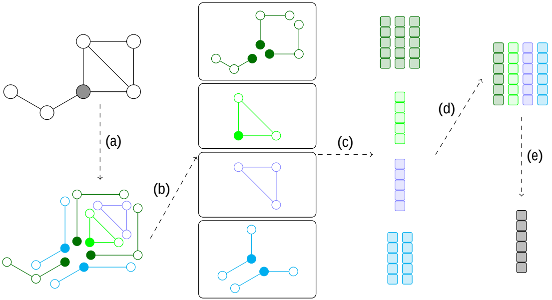
subgraph counts

k-WL Hierarchy vs $\mathcal{N}$-WL Hierarchy

	k-WL	-k-LWL	$(k;s)$-LWL	$(k;c)(\ )$-SETWL	$\mathcal{N}(t;d)$-WL	$\mathcal{N}^c(t;d)$-WL
#Coloured objects	n^k	n^k	subset$(n^k; s)$	subset$(\sum_{q=1}^{k} \binom{n}{q}; c)$	n	n
#Neighbour objects	$n \quad k$	$a \quad k$	$a \quad k$	$n \quad q$	$\binom{a^d}{t}$	subset$(\sum_{q=1}^{t} \binom{a^d}{q}; 1)$
ΔColoured objects	k-tuples	k-tuples	k-tuples	k-sets	nodes	nodes
ΔNeighbour objects	k-tuples	k-tuples	k-tuples	[illegible]	t-sets	t-sets
Sparsity -awareness	✗	✓	✓		✗	✓

Theorem: 1-WL $\quad \mathcal{N}(1;1)$-WL $\quad \mathcal{N}^c(1;1)$-WL

Graph Neighbourhood Neural Network (G3N) instantiates the ideas of $\mathscr{N}$-WL algorithms for graph learning.



$$h_u^{(l+1)} = \textsc{Combine}\left(h_u^{(l)}, \textsc{Agg}^N_{(i,j)\in I_t \times J_d}\left(\textsc{Agg}^T_{S \in S_u^{(l)}(i,j)}\ \textsc{Pool}(S)\right)\right)$$

References I

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In *Combinatorial Mathematics IX*, pages 89–114. Springer.

Xu, K., Hu, W., Leskovec, J., and Jegelka, S. (2019).
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Thank You