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

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The work is partially funded by the Australian Research Council under Discovery Project DP210102273.

Classical k-WL Hierarchy

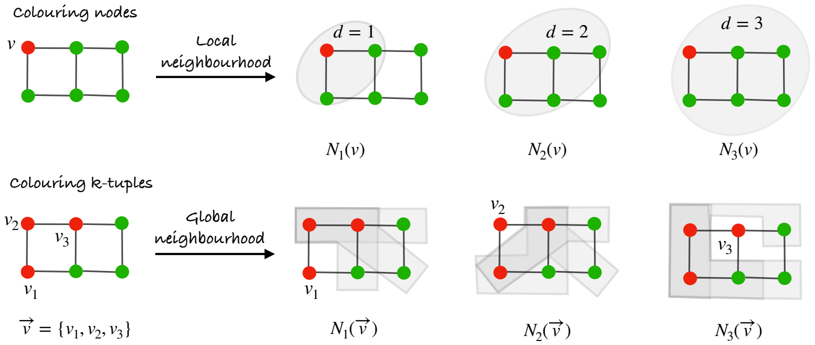
k-Weisfeiler-Lehman (k-WL) hierarchy is a theoretical framework for graph isormorphism tests

$\hookrightarrow$ but not practically useful when $k \geq 3$!

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

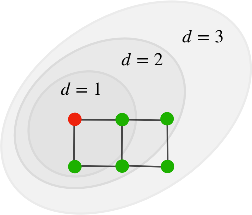
Question:

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

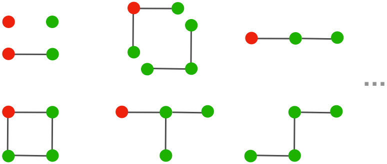

Colouring nodes
v
Local neighbourhood
$d = 1$
$d = 2$
$d = 3$
$N_1(v)$
$N_2(v)$
$N_3(v)$
Colouring k-tuples
v_2
v_3
v_1
Global neighbourhood
v_1
v_2
v_3
$\vec{v} = \{v_1, v_2, v_3\}$
$N_1(\vec{v})$
$N_2(\vec{v})$
$N_3(\vec{v})$

Our $\mathscr{N}$-WL Hierarchy

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



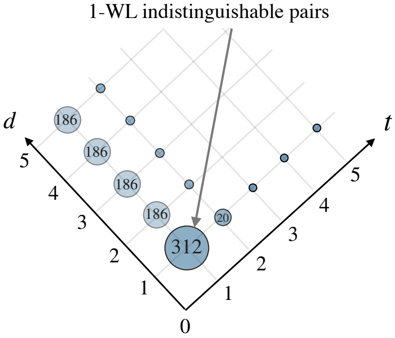
d-hop neighbourhoods



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 $\subsetneq \mathscr{N}^-(t{+}1,d)$-WL

Increasing the hops of neighbourhood, the expressive power may decrease
– *Surprising but can be fixed*

Theorem:
(Strong Hierarchy) $\mathscr{N}(t,d)$-WL $\subsetneq \mathscr{N}(t{+}1,d)$-WL
$\mathscr{N}(t,d)$-WL $\subsetneq \mathscr{N}(t,d{+}1)$-WL

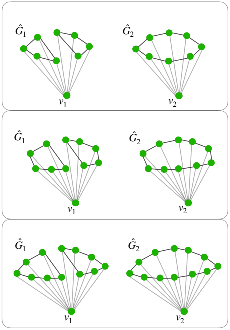
Induced connected subgraphs remain the same expressive power
– *Surprising but can be proved*

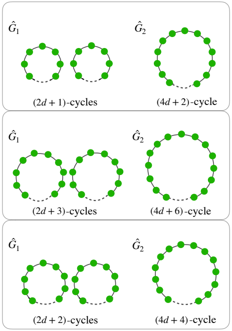
Theorem:
(Equivalence) $\mathscr{N}^c(t,d)$-WL $\equiv \mathscr{N}(t,d)$-WL

Theorem:
(Strong Hierarchy)

$$\mathcal{N}(t,d)\text{-WL} \subsetneq \mathcal{N}(t+1,d)\text{-WL}$$
$$\mathcal{N}(t,d)\text{-WL} \subsetneq \mathcal{N}(t,d+1)\text{-WL}$$

We prove strictness of hierarchies by constructing counterexample graphs.

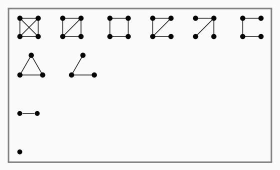




Theorem:
(Equivalence)

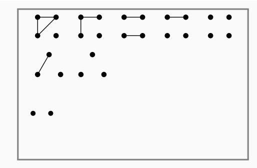
$$\mathscr{N}^c(t,d)\text{-WL} \equiv \mathscr{N}(t,d)\text{-WL}$$

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



subgraph counts

implies
$\longrightarrow$



subgraph counts

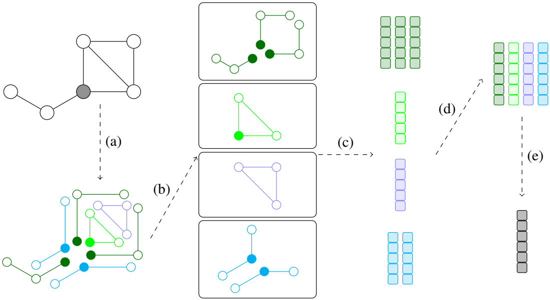
k-WL Hierarchy vs $\mathcal{N}$-WL Hierarchy

	k-WL	δ-k-LWL	(k,s)-LWL	$(k,c)(\leq)$-SETWL
#Coloured objects	n^k	n^k	$\text{subset}(n^k, s)$	$\text{subset}(\sum_{q=1}^{k}\binom{n}{q}, c)$
#Neighbour objects	$n \times k$	$a \times k$	$a \times k$	$n \times q$
ΔColoured objects	k-tuples	k-tuples	k-tuples	$\leq k$-sets
ΔNeighbour objects	k-tuples	k-tuples	k-tuples	[illegible]
Sparsity -awareness	✗	✓	✓	

$\mathcal{N}(t,d)$-WL	$\mathcal{N}^c(t,d)$-WL
n	n
$\binom{a^d}{t}$	$\text{subset}(\sum_{q=1}^{t}\binom{a^d}{q}, 1)$
nodes	nodes
t-sets	$\leq t$-sets
✗	✓

Theorem: 1-WL $\equiv \mathcal{N}(1,1)$-WL $\equiv \mathcal{N}^c(1,1)$-WL

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



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

Kocay, W. L. (1982).
Some new methods in reconstruction theory.
In *Combinatorial Mathematics IX*, pages 89–114. Springer.

Xu, K., Hu, W., Leskovec, J., and Jegelka, S. (2019).
How powerful are graph neural networks?
In *International Conference on Learning Representations (ICLR)*.

Thank You