# $\mathscr{N}$-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

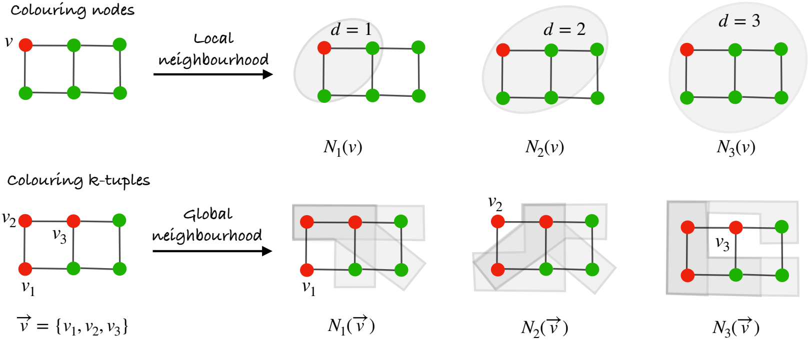
$k$-Weisfeiler-Lehman (k-WL) hierarchy is a theoretical framework for graph isormorphism tests

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

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

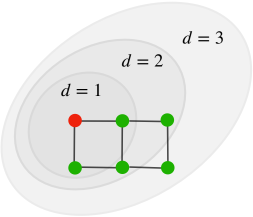
**Question:**

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

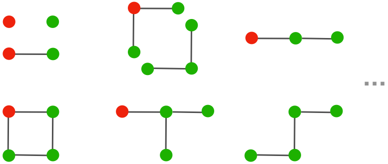

Colouring nodes
v
Local
neighbourhood
d = 1
d = 2
d = 3
N1(v)
N2(v)
N3(v)
Colouring k-tuples
v2
v3
v1
Global
neighbourhood
v1
v2
v3
v = {v1, v2, v3}
N1(v)
N2(v)
N3(v)

# Our $\mathcal{N}$-WL Hierarchy

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



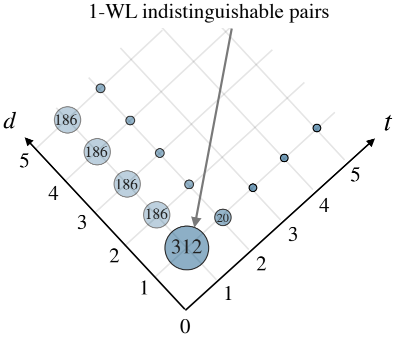

$d$-hop neighbourhoods



$t$-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 $\mathscr{N}$-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

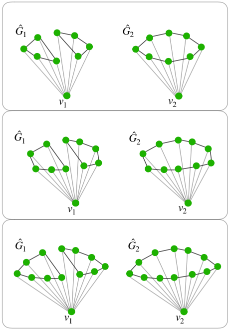
Induced connected subgraphs remain the same expressive power – *Surprising but can be proved*

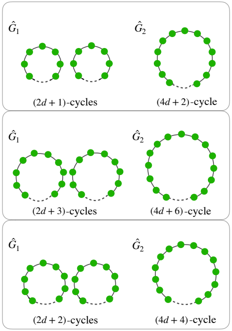
**Theorem:** (Equivalence) $\mathscr{N}^{c}(t,d)$-WL $\equiv$ $\mathscr{N}(t,d)$-WL

**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.



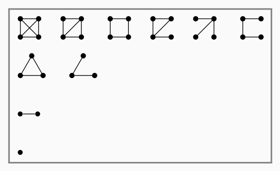



# Main Ideas in Proofs (2)

**Theorem:**
**(Equivalence)**

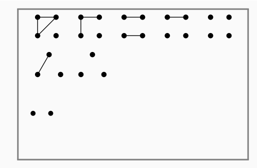
$$\mathscr{N}^c(t,d)\text{-WL} \equiv \mathscr{N}(t,d)\text{-WL}$$

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



subgraph counts

implies
$\longrightarrow$



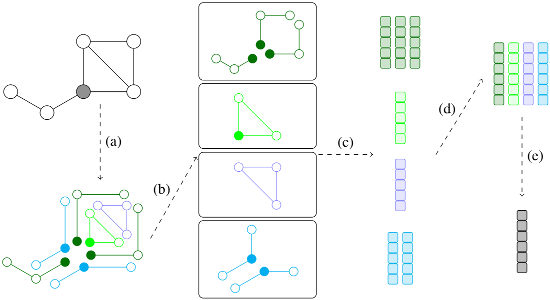
subgraph counts

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

| | $k$-WL | $\delta$-$k$-LWL | $(k,s)$-LWL | $(k,c)(\leq)$-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 | $n \times k$ | $a \times k$ | $a \times k$ | $n \times q$ | $\binom{a^d}{t}$ | subset$(\sum_{q=1}^{t}\binom{a^d}{q}, 1)$ |
| ΔColoured objects | $k$-tuples | $k$-tuples | $k$-tuples | $\leq k$-sets | nodes | nodes |
| ΔNeighbour objects | $k$-tuples | $k$-tuples | $k$-tuples | [illegible] | $t$-sets | $\leq t$-sets |
| Sparsity -awareness | ✗ | ✓ | ✓ | | ✗ | ✓ |

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

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




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

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