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

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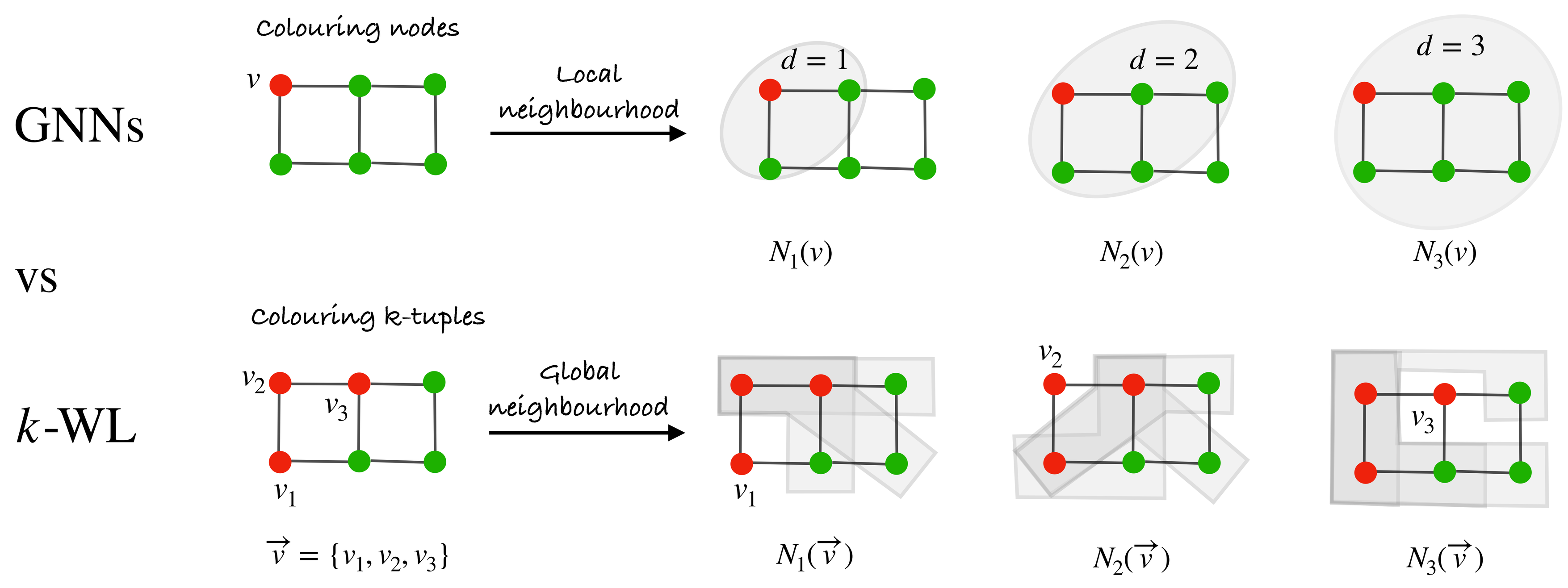
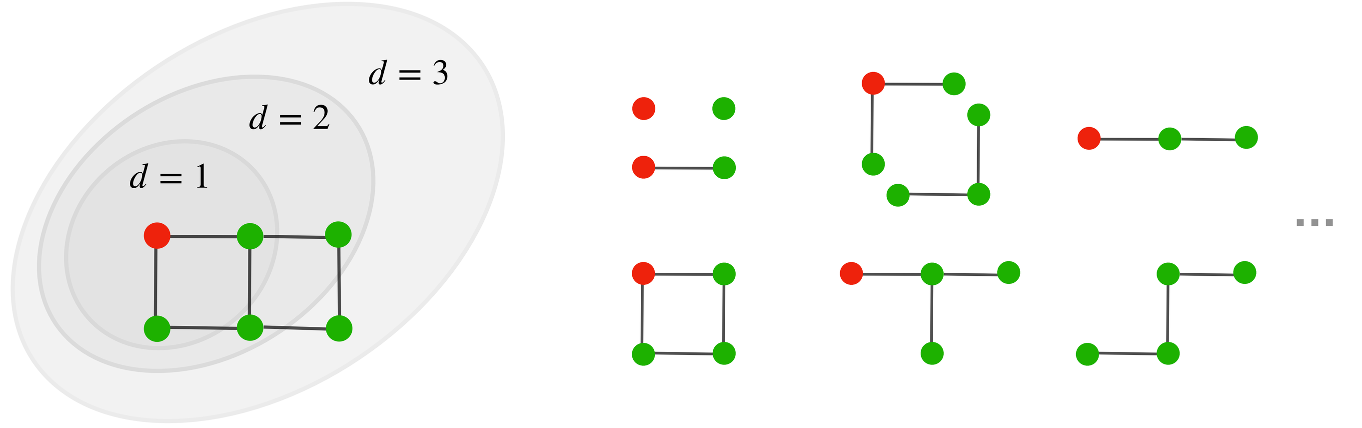
Introduction

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



Neighbourhood WL Hierarchy

Neighbourhood WL ($\mathcal{N}$-WL) hierarchy colours nodes via t-order induced subgraphs within d-hop neighbourhoods:

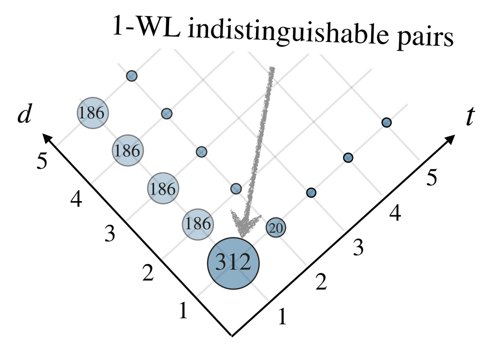


d-hop neighbourhoods *t-order induced subgraphs*

A Simple Experiment

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



Main Results

- Increasing the order of induced subgraphs, the expressive power increases:

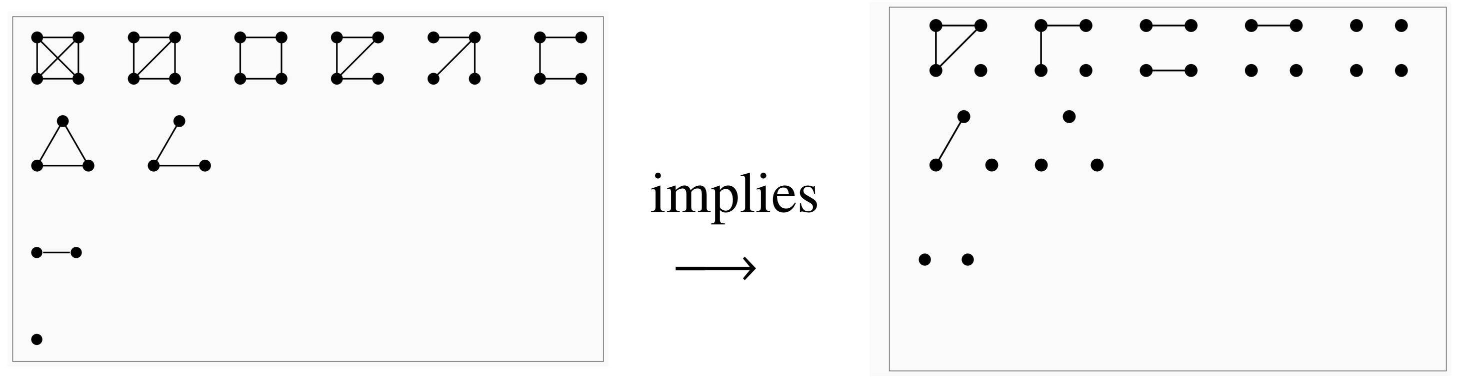
Theorem (Weak Hierarchy) $\mathcal{N}^-(t, d)\text{-WL} \subsetneq \mathcal{N}^-(t+1, d)\text{-WL}$

- Increasing the hops of neighbourhoods, the expressive power may decrease:

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

- Induced connected subgraphs remain the same expressive power:

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



Subgraph counts $\longrightarrow$ Subgraph counts

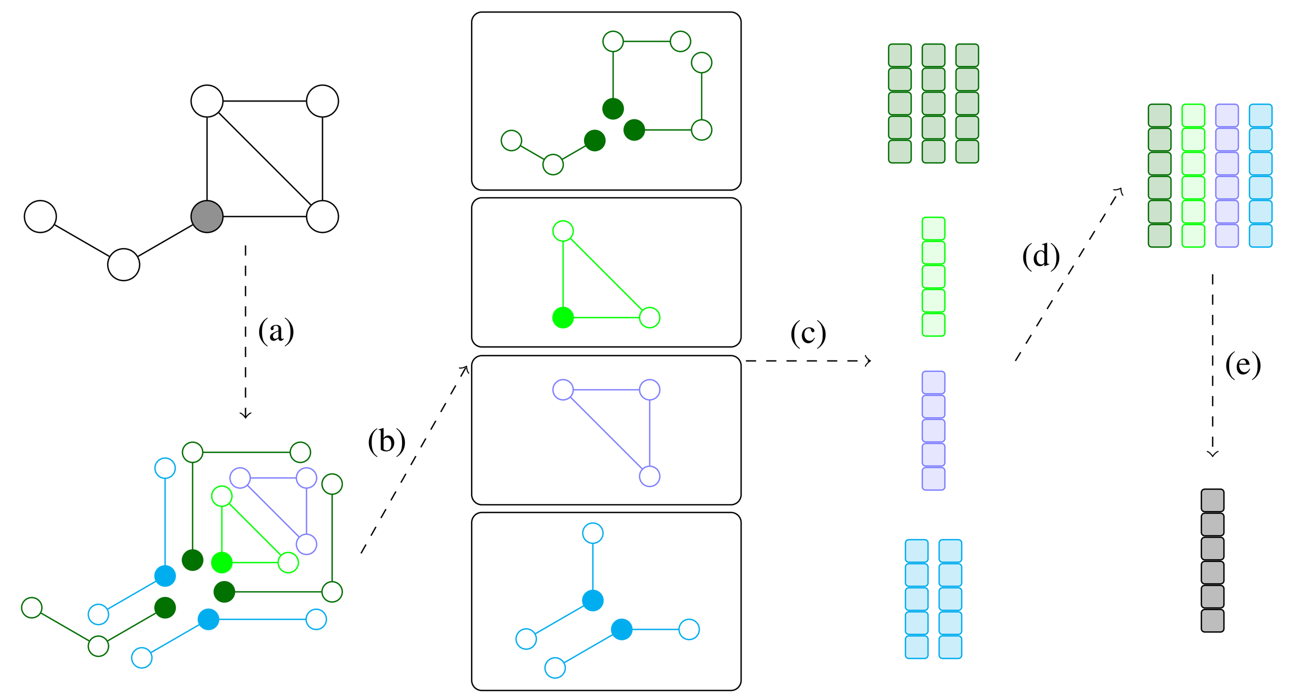
k-WL vs $\mathcal{N}$-WL

	k-WL	δ-k-LWL	(k, s)-LWL	$(k, c)(\le)$-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	$\le k$-sets	nodes	nodes
ΔNeighbour objects	k-tuples	k-tuples	k-tuples	$\le k$-sets	t-sets	$\le t$-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

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



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

- Graph classification

Model	ZINC (no edge features)	ZINC (edge features)
GCN	$0.459_{\pm 0.006}$	$0.321_{\pm 0.009}$
PPGN	$0.407_{\pm 0.028}$	-
GIN	$0.387_{\pm 0.015}$	$0.163_{\pm 0.004}$
PNA	$0.320_{\pm 0.032}$	$0.188_{\pm 0.004}$
DGN	$0.219_{\pm 0.010}$	$0.168_{\pm 0.003}$
DEEP LRP*	$0.223_{\pm 0.008}$	-
GSN*	$0.140_{\pm 0.006}$	$0.115_{\pm 0.012}$
CIN*	$\mathbf{0.115}_{\pm 0.003}$	$\mathbf{0.079}_{\pm 0.006}$
G3N-(2,3)	$\mathbf{0.165}_{\pm 0.018}$	$\mathbf{0.128}_{\pm 0.015}$

Model	MolHIV (test)	MolHIV (validation)
GCN	$0.7606_{\pm 0.0097}$	$0.8204_{\pm 0.0141}$
GIN	$0.7558_{\pm 0.0140}$	$0.8232_{\pm 0.0090}$
GraphSNN	$0.7851_{\pm 0.0170}$	$0.8359_{\pm 0.0096}$
PNA	$0.7905_{\pm 0.0132}$	-
DGN	$\mathbf{0.7970}_{\pm 0.0097}$	-
DEEP LRP*	$0.7687_{\pm 0.0180}$	$0.8131_{\pm 0.0088}$
GSN*	$0.7799_{\pm 0.0100}$	$\mathbf{0.8658}_{\pm 0.0084}$
CIN*	$\mathbf{0.8094}_{\pm 0.0057}$	-
G3N-(2,3)	$0.7900_{\pm 0.0134}$	$\mathbf{0.8359}_{\pm 0.0061}$

- Runtime analysis