Local Vertex Colouring Graph Neural Networks

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The work is partially funded by the Australian Research Council under Discovery Project DP210102273, and by Institute of Information & communications Technology Planning & Evaluation grant (No.2019-0-01906, Artificial Intelligence Graduate School Program (POSTECH)) and National Research Foundation of Korea grant (NRF-2021R1C1C1011375) by the Korean government.

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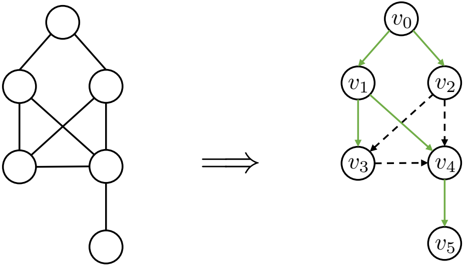
Question:

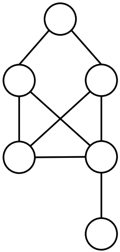
Can we develop an efficient GNN that goes beyond 1-WL and solves graph problems like biconnectivity?

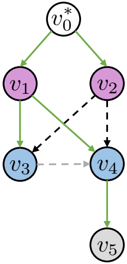
Breadth-first Search

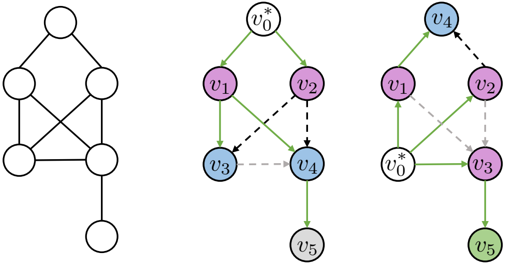


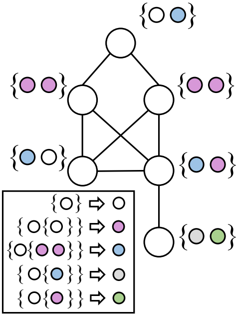
BFS Tree

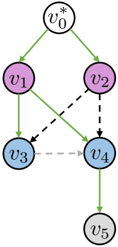
Breadth-first Colouring (BFC)

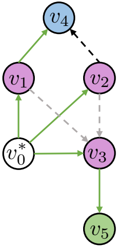


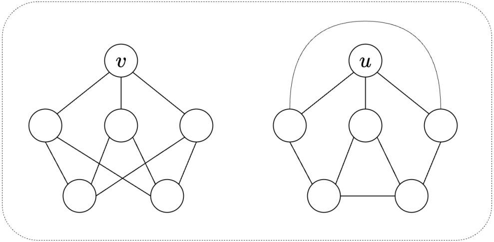



v_0^*
v_1
v_2
v_3
v_4
v_5
v_4
v_1
v_2
v_0^*
v_3
v_5

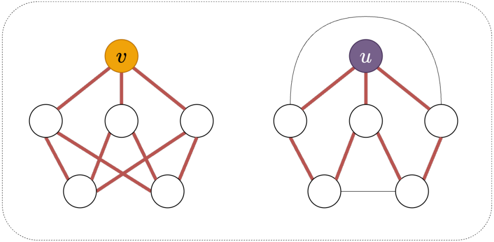



v_0^*
v_1
v_2
v_3
v_4
v_5


v_4
v_1
v_2
v_0^*
v_3
v_5



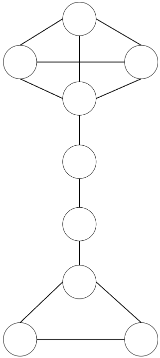
1-WL ✗



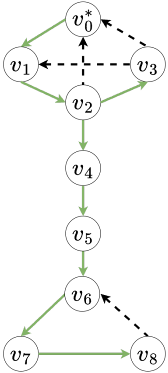
1-WL ✗

BFC ✓

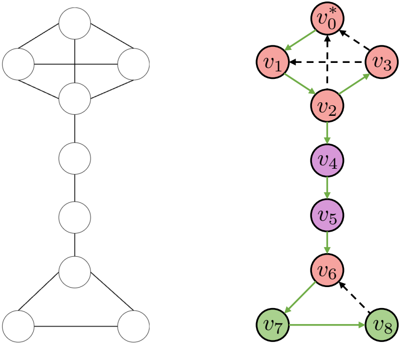
Lemma 4.2. (Informal) Under BFC, two vertices have the same colour if and only if they have the same ego shortest-path graph (ESPG).



$\Longrightarrow$



DFS Tree


v_0^*
v_1
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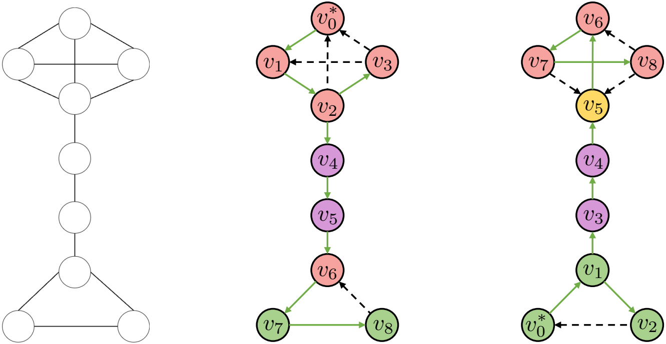
v_4
v_5
v_6
v_7
v_8


v_0^*
v_1
v_3
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v_1
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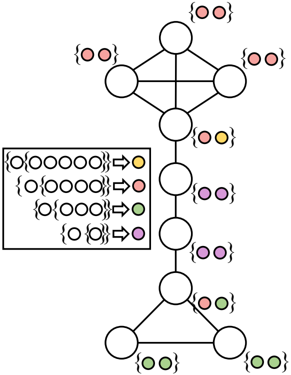
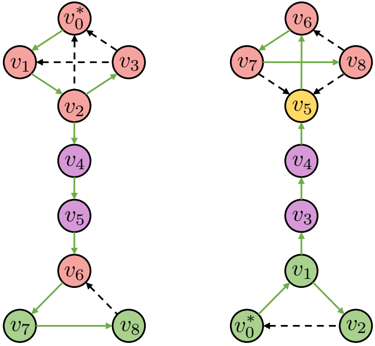
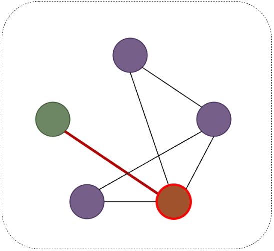
v_2





v_0^*
v_1
v_2
v_3
v_4
v_5
v_6
v_7
v_8



MPNN ✗

DFC ✓

Lemma 4.5. (Informal) DFC can solve graph biconnectivity problems, e.g. distinguishing cut vertices and edges.

Lemma 4.6. BFC-1 is equivalent to 1-WL.

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Theorem 4.3. BFC-$\delta + 1$ is strictly more expressive than BFC-δ in distinguishing non-isomorphic graphs.

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Theorem 4.3. BFC-$\delta + 1$ is strictly more expressive than BFC-δ in distinguishing non-isomorphic graphs.

Theorem 4.1. The expressivity of BFC-δ is strictly upper bounded by 3-WL.

Lemma 4.7. DFC-1 is more expressive than to 1-WL.

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Theorem 4.4. DFC-$\delta + 1$ is not necessarily more expressive than DFC-δ in distinguishing non-isomorphic graphs.

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Theorem 4.4. DFC-$\delta + 1$ is not necessarily more expressive than DFC-δ in distinguishing non-isomorphic graphs.

Theorem 4.4. The expressive powers of DFC-δ and 3-WL are incomparable.

Search Guided Graph Neural Network (SGN) inherits the ideas of local search-based vertex colouring.

$$h_u^{(l+1)} = \mathrm{MLP}\left(\left(1+\epsilon^{(l+1)}\right)\cdot h_u^{(l)} \parallel \sum_{v\in N_\delta(u)} h_{u\leftarrow v}^{(l+1)}\right)$$

where

$$h_{u\leftarrow v}^{(l+1)} = \left(h_u^{(l)} + \sum_{w\in \eta_v(u)} h_{w\leftarrow v}^{(l)}\right) W_c$$

where $\eta_v(u)$ is defined based on BFC or DFC.

	MPNN	ESAN	Graphormer-GD	3-IGN	SGN-BF	SGN-DF
Time	$\|V\|+\|E\|$	$\|V\|(\|V\|+\|E\|)$	$\|V\|^2$	$\|V\|^3$	$\|V\|d^{\delta-1}$	$\|V\|d^{2\delta}$
Space	$\|V\|$	$\|V\|^2$	$\|V\|$	$\|V\|^2$	$\|V\|d^{\delta-1}$	$\|V\|d^{2\delta}$

Thank You

https://bit.ly/3CM1DKv
Interactive Demo

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

Zhang, B., Luo, S., Wang, L., and He, D. (2023).
Rethinking the expressive power of GNNs via graph biconnectivity.
In *11th International Conference on Learning Representations, ICLR 2020, Kigali, Rwanda , May 1-5, 2023*.