Local Vertex Colouring Graph Neural Networks

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

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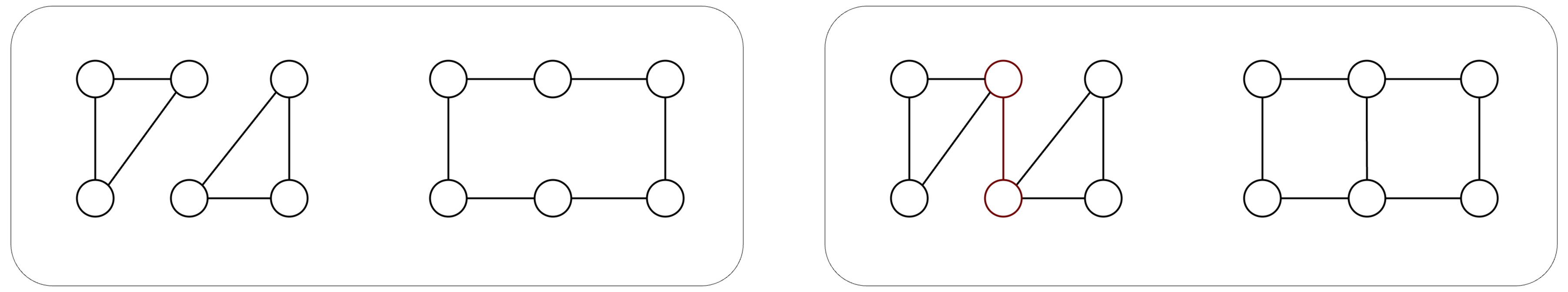
Introduction

- Can GNNs be made more powerful than 1-WL?
- Can we design GNNs to solve graph problems that MPNNs cannot, e.g. graph biconnectivity?

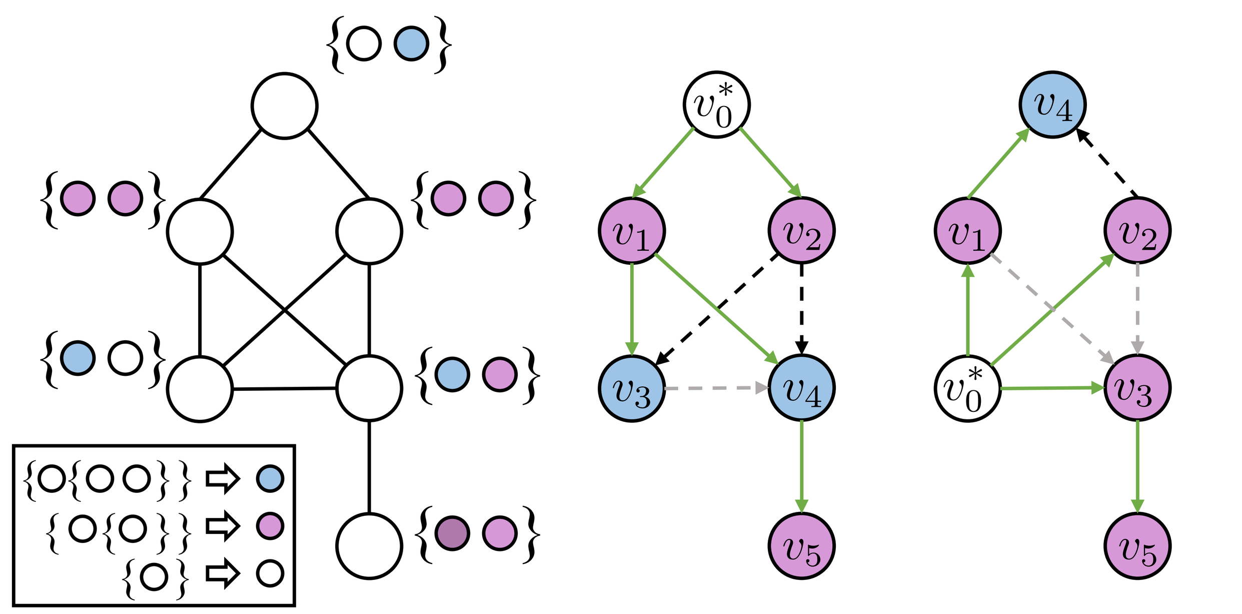


(a) Indistinguishable by 1-WL (b) Graph biconnectivity

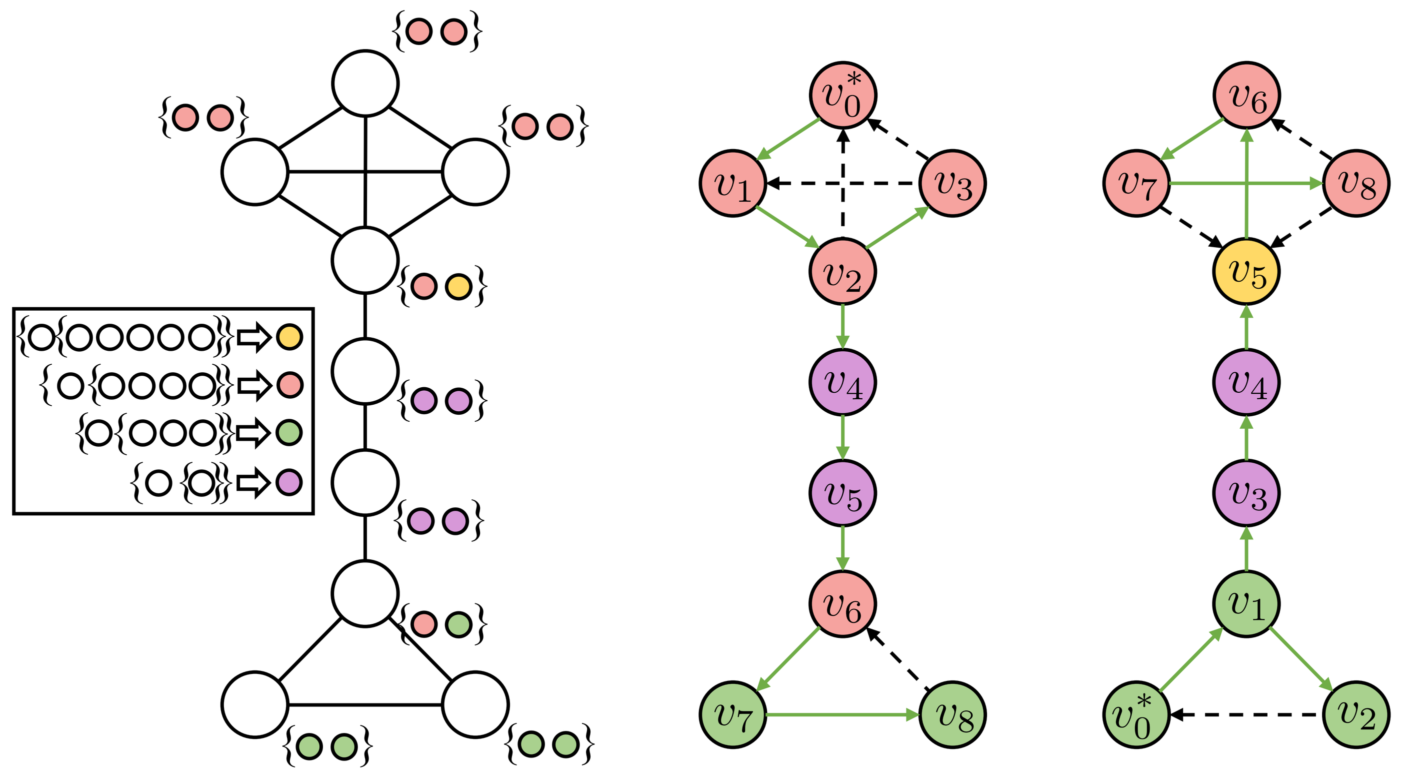
Search-based Vertex Colouring

We colour vertices based on tree edges and back edges from *graph search*.

Breadth-first Colouring (*BFC*):



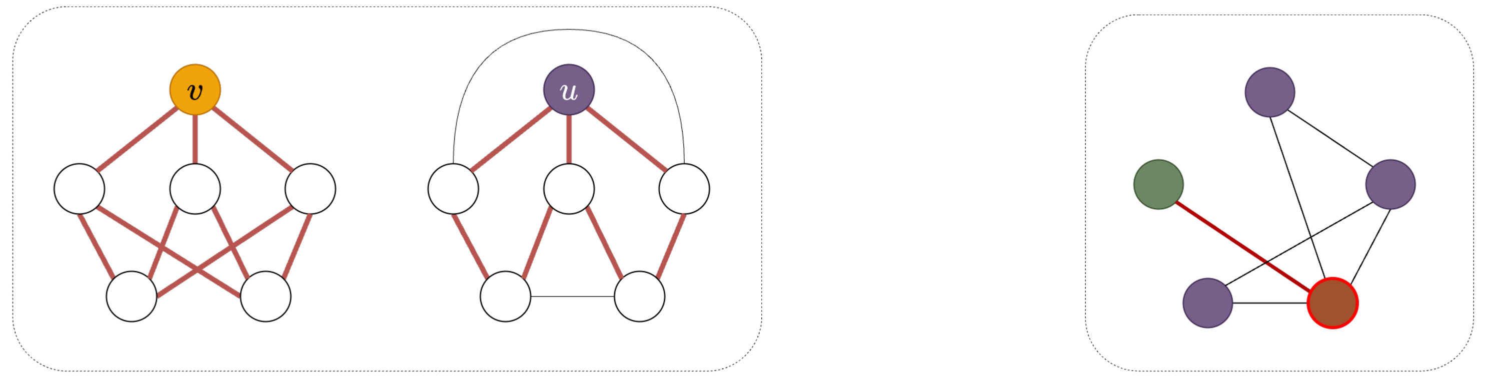
Depth-first Colouring (*DFC*):



Main Results

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

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



(a) Ego Shortest-Path Graph (ESPG) (b) Cut vertex and edge

Expressivity

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

Theorem: BFC-δ + 1 is strictly more expressive BFC-δ.

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

Lemma: DFC-1 is more expressive than 1-WL.

Theorem: The expressivity of DFC-δ is more incomparable with 3-WL.

(a) 1-WL ✗, BFC-1 ✗, BFC-2 ✓, DFC-1 ✓ (b) 1-WL ✗, BFC-2 ✗, BFC-3 ✓, DFC-1 ✗, DFC-2 ✓

Search Guided Graph Neural Network

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

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

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

Vertex Classification

	Computers	Photo	CiteSeer	Cora	Pubmed	Wisconsin	Cornell	Texas	Chameleon	Squirrel
MLP	82.9±0.4	84.7±0.3	76.6±0.9	77.0±1.0	85.9±0.2	85.3±3.6	90.8±1.6	91.5±1.1	46.9±1.5	31.0±1.2
GCN	83.3±0.3	88.3±0.7	79.9±0.7	87.1±1.0	86.7±0.3	59.8±7.0	65.9±4.4	77.4±3.3	59.6±2.2	46.8±0.9
GCN+JK†	-	-	74.5±1.8	85.8±0.9	88.4±0.5	74.3±6.4	74.3±6.4	64.6±8.7	63.4±2.0	40.5±1.6
GAT	83.3±0.4	90.9±0.7	**80.5**±0.7	88.0±0.8	87.0±0.2	55.3±8.7	78.2±3.0	80.8±2.1	63.1±1.9	44.5±0.9
APPNP	85.3±0.4	88.5±0.3	80.5±0.7	88.1±0.7	88.1±0.3	-	**91.8**±2.0	91.0±1.6	51.8±1.8	34.7±0.6
ChevNet	87.5±0.4	93.8±0.3	79.1±0.8	86.7±0.8	88.0±0.3	82.6±4.6	83.9±2.1	86.2±2.5	59.3±1.3	40.6±0.4
GPRGNN	86.9±0.3	93.9±0.3	80.1±0.8	88.6±0.7	88.5±0.3	-	91.4±1.8	93.0±1.3	67.3±1.1	50.2±1.9
BernNet	87.6±0.4	93.6±0.4	80.1±0.8	88.5	88.5±1.0	-	-	-	-	-
H_2GCN†	-	-	77.1±1.6	87.8±1.4	89.6±0.3	86.7±4.7	82.2±4.8	84.5±6.8	59.4±2.0	37.9±2.0
SGN-BF	90.7	**96.1**±0.2	78.0±1.0	88.7±0.1	**90.2**±3.5	**91.2**±1.0	89.5±2.7	88.7±4.3	**72.8**±0.2	**59.0**±0.3
SGN-DF	**90.9**±0.4	95.2±0.8	79.7±0.7	**89.5**±0.6	89.5±0.6	84.1±3.6	83.2±5.8	86.8±5.2	56.6±3.0	47.0±1.5

Graph Classification

	D&D	NCI1	PROTEINS	ENZYMES	IMDB-BINARY
Baseline	**78.4**±4.5	69.8±2.2	75.8±3.7	65.2±6.4	70.8±5.0
DGCNN	76.6±4.3	76.4±1.7	72.9±3.5	38.9±5.7	69.2±3.0
DiffPool	75.0±3.5	76.9±1.9	73.7±3.5	59.5±5.6	68.4±3.3
ECC	72.6±4.1	76.2±1.4	72.3±3.4	29.5±8.2	67.7±2.8
GIN	75.3±2.9	80.0±1.4	73.3±4.0	59.6±4.5	71.2±3.9
GraphSAGE	72.9±2.0	76.0±1.8	73.0±4.5	58.2±6.0	68.8±4.5
E-CGMM‡	73.9±4.1	78.5±1.7	73.3±4.1	-	70.7±3.8
ICGMM‡	76.3±5.6	77.6±1.5	73.3±2.9	-	73.0±4.3
SGN-BF	76.3±3.2	78.8±2.9	74.0±3.9	64.8±7.2	71.4±7.1
SGN-DF	78.01±4.0	**81.0**±1.4	**76.1**±1.6	**66.9**±7.5	**72.3**±5.4

Model Complexity

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