The Expressive Power of Pooling in Graph Neural Networks

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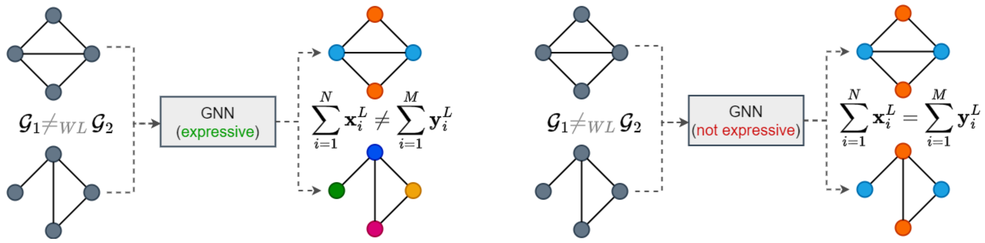
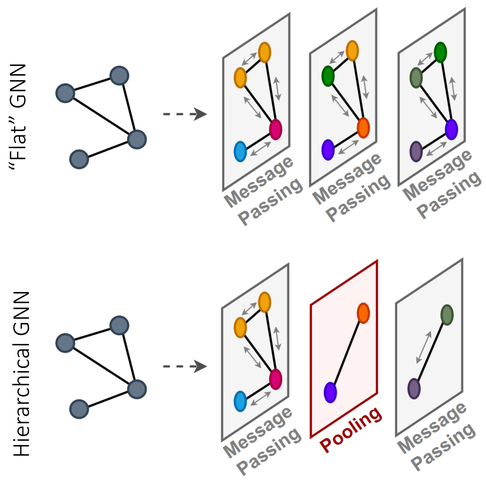
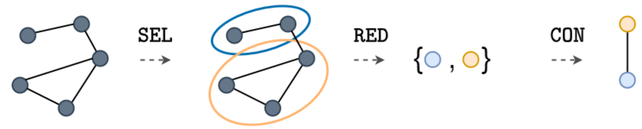
Motivation



- GNN expressiveness ↔ distinguish non-isomorphic graphs ↔ WL test.
- Expressivity studied only in flat GNNs.
- How to study expressiveness in hierarchical GNNs?

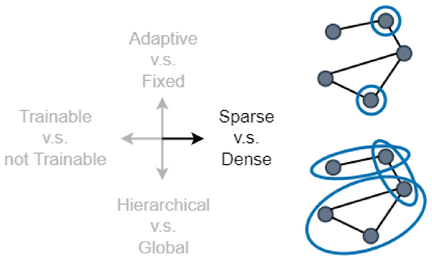


Graph Pooling



Select Reduce Connect (SRC) framework [1]

Taxonomy of pooling operators

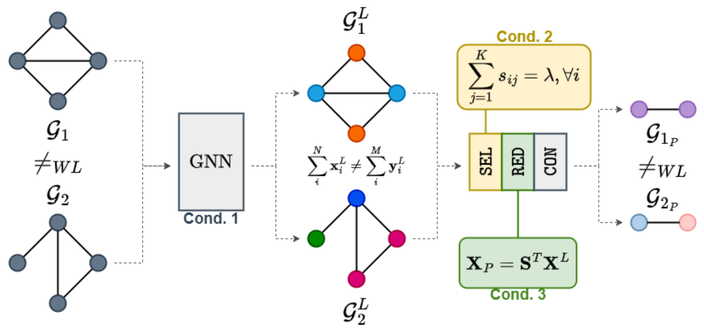


Conditions for Expressiveness

Let $\mathcal{G}_1 \neq_{WL} \mathcal{G}_2$, $X^L \in \mathbb{R}^{N \times F}$ and $Y^L \in \mathbb{R}^{M \times F}$ be the node features obtained after L MP layers and $\mathcal{G}_{1_p} = POOL(\mathcal{G}_1^L)$ and $\mathcal{G}_{2_p} = POOL(\mathcal{G}_2^L)$.
If the following conditions hold:

1. $\sum_i^N x_i^L \neq \sum_i^M y_i^L$;
2. For each node i, the memberships generated by SEL satisfy $\sum_{j=1}^K s_{ij} = \lambda,\ \lambda > 0$;
3. The function RED is of type $RED: (X^L, S) \mapsto X_P = S^T X^L$;

$\mathcal{G}_{1_p}$ and $\mathcal{G}_{2_p}$ will have different nodes features.



Expressiveness of Existing Pooling Operators

Dense-Expressive

- ✓ DiffPool (Ying et al., 2018)
- ✓ MinCut (Bianchi et al., 2020)
- ✓ DMoN (Tsitsulin et al., 2020)

Supernodes

SEL: $\mathbf{S} = \begin{bmatrix} 0.3 & 0.2 & 0.5 \\ 0.1 & 0.1 & 0.8 \\ 0.4 & 0.5 & 0.1 \\ 0.3 & 0.6 & 0.1 \end{bmatrix}$ Nodes

RED: $\mathbf{X}_p = \mathbf{S}^T \mathbf{X}^L$

Sparse-Expressive

- ✓ Graclus (Dhillon et al., 2007)
- ✓ ECPool (Diehl et al., 2019)
- ✓ k-MIS (Bacciu et al., 2023)

SEL: $\mathbf{S} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$

RED: $\mathbf{X}_p = \mathbf{S}^T \mathbf{X}^L$

Sparse-NonExpressive

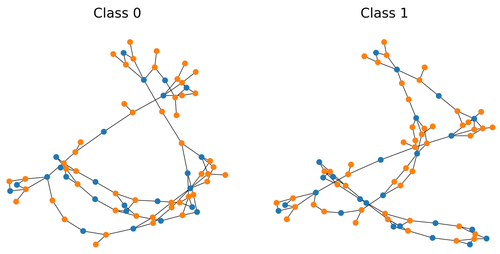
- × Top-k (Gao et al., 2019)
- × SAGPool (Lee et al., 2019)
- × ASAPool (Ranjan et al., 2020)
- × PanPool (Ma et al., 2020)

SEL: $\mathbf{S} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$

RED: $\mathbf{X}_p = \mathbf{X}^L \odot \sigma(\mathbf{y}))_t$

Empirical Analysis

1. New dataset: EXPWL1



Contains pairs of non-isomorphic 1-WL distinguishable graphs.

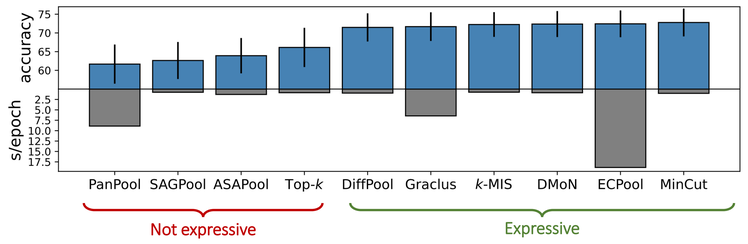
Allows to empirically evaluate the expressive power of *any* GNN.

Pooling	s/epoch	GIN layers	Pool Ratio	Test Acc	Expressive
No-pool	0.33s	3	–	99.3±0.3	✓
DiffPool	0.69s	2+1	0.1	97.0±2.4	✓
DMoN	0.75s	2+1	0.1	99.0±0.7	✓
MinCut	0.72s	2+1	0.1	98.8±0.4	✓
ECPool	20.71s	2+1	0.2	100.0±0.0	✓
Graclus	1.00s	2+1	0.1	99.9±0.1	✓
k-**MIS**	1.17s	2+1	0.1	99.9±0.1	✓
Top-k	0.47s	2+1	0.1	67.9±13.9	✗
PanPool	3.82s	2+1	0.1	63.2±7.7	✗
ASAPool	1.11s	1+1	0.1	83.5±2.5	✗
SAGPool	0.59s	1+1	0.1	79.5±9.6	✗
Rand-dense	0.41s	2+1	0.1	91.7±1.3	✓
Cmp-Graclus	8.08s	2+1	0.1	91.9±1.2	✓
Rand-sparse	0.47s	2+1	0.1	62.8±1.8	✗

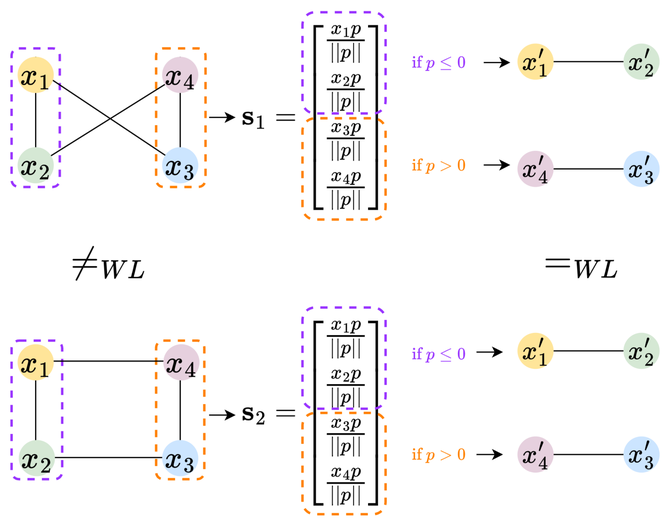
2. Expressiveness in practice

GNNs with expressive operators perform better on average on 13 benchmark datasets.

Dense operators are expressive and fast in modern deep learning pipelines.



Example of failure of Top-k. Assume $x_1 \leq x_2 \leq x_3 \leq x_4$



[1] Grattarola et al. "Understanding Pooling in Graph Neural Networks", 2022.