The Expressive Power of Graph Neural Networks from Three Perspectives

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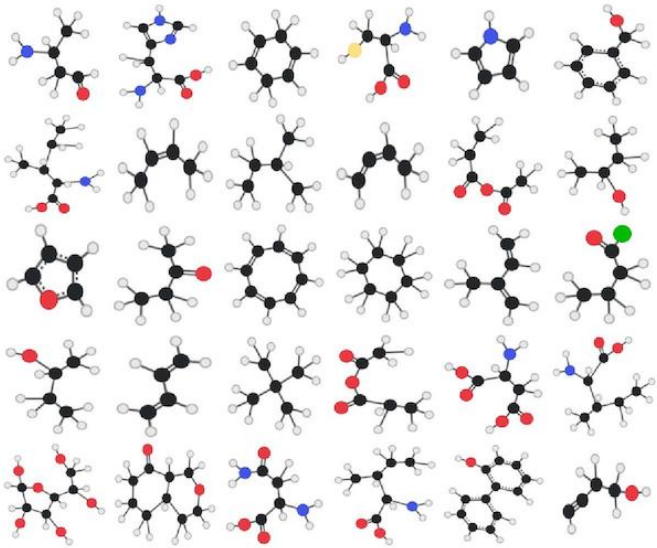
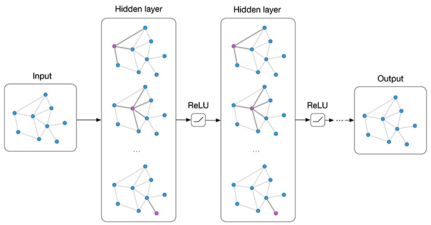
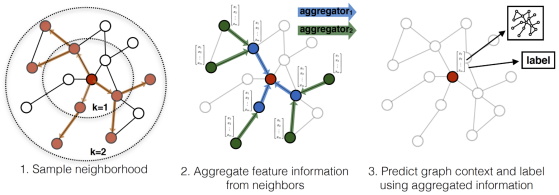
- molecular chemistry
- social networks
- knowledge graphs
- particle physics
- combinatorial optimization

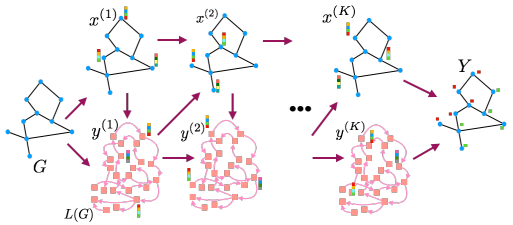


[1]

[1] https://github.com/chemplexity/molecules







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Advantages of (many) GNN architectures:

- Built-in permutation-invariance
- Efficiency of computation
- Can be applied to graphs of different sizes

Question: Have we sacrificed expressive power to gain such advantages? How should we study the expressive power of GNNs?

[2] Kipf and Welling (2016); Hamilton et al. (2017); Chen et al. (2019a)

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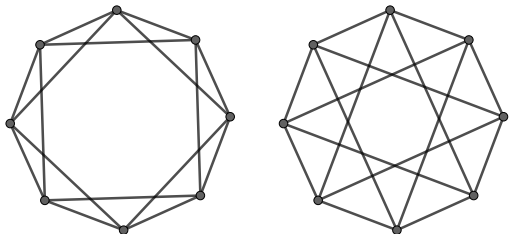
Question: Can GNNs distinguish any pair of non-isomorphic graphs?

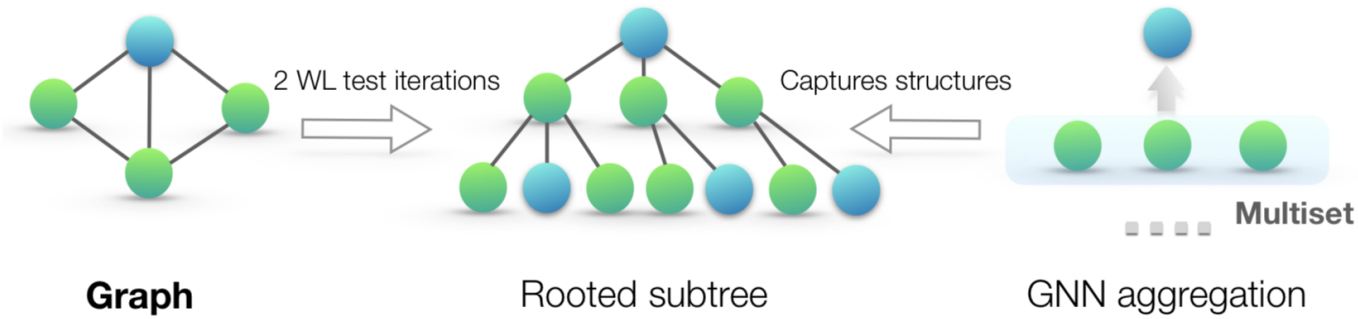
Answer: No, for GNNs based upon message-passing. For example,



Theorem (Xu et al. (2018); Morris et al. (2019))

If two graphs cannot be distinguished by the WL test, then they cannot be distinguished by any GNN based on message-passing.

WL test compares the rooted subtree substructures of the graphs.



[3]

Xu et al. (2018) and Morris et al. (2019) also propose GNN models that are as powerful as the WL test.

[3] Xu et al. (2018)

Problems:

- WL can distinguish almost all pairs of non-isomorphic graphs (Babai et al., 1980).

  Does this mean that the existing GNNs are already powerful enough?

- Is graph isomorphism testing necessarily relevant to real-world tasks on graph datasets?

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GNNs Represent Functions on Graphs

A GNN architecture defines a family of functions on graphs.

Training a GNN for a graph-level prediction task
$\approx$ fitting an underlying target function.

Question: Can certain families of graph neural networks approximate "arbitrary" functions on graphs?

Let $\mathcal{G}$ be a finite space of graphs, and $\mathcal{F}$ a set of functions $\mathcal{G} \to \mathbb{R}$.

Definition

We say $\mathcal{F}$ is **universally approximating** if $\forall$ function $g : \mathcal{G} \to \mathbb{R}$ and $\forall \epsilon > 0$, $\exists f \in \mathcal{F}$ such that $\sup_{G \in \mathcal{G}} |g(G) - f(G)| < \epsilon$.

Definition

We say $\mathcal{F}$ is **GISO-discriminating** if $\forall G_1, G_2 \in \mathcal{G}$ that are not isomorphic, $\exists f \in \mathcal{F}$ such that $f(G_1) \neq f(G_2)$.

Proposition (Chen et al. (2019b, 2020))

- *If $\mathcal{F}$ is universally approximating on $\mathcal{G}$, then it is also GISO-discriminating on $\mathcal{G}$;*
- *If $\mathcal{F}$ is GISO-discriminating on $\mathcal{G}$, then $\mathcal{F}^{+1}$ is universally approximating on $\mathcal{G}$.*

$\mathcal{F}^{+1}$ consists of functions in $\mathcal{F}$ augmented with one extra layer.

Corollary

GNNs based on message-passing are not universally approximating.

Remaining question: What functions can and cannot GNNs approximate, and how to understand them intuitively?

We want a criterion for the expressive power of GNNs that is:

- Intuitive and concrete
- Relevant for applications
- Helpful in guiding the search for more powerful GNNs

Some other interesting perspectives: Turing universality (Loukas, 2019); ability to decide several graph properties (Garg et al., 2020)

Our answer: **substructure counting**.

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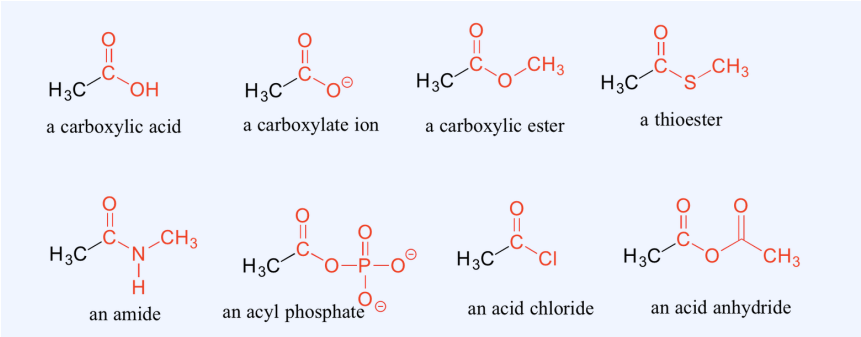
Why is Substructure Counting Relevant?

- For example, functional groups in organic chemistry[4]

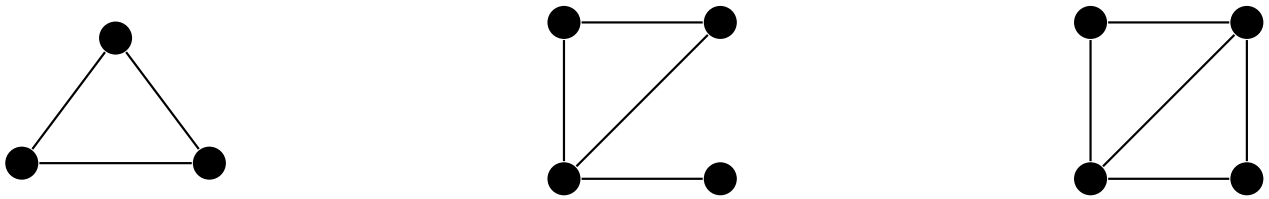


- Computational biology and social network studies
- Generating molecular fingerprints, computing molecular similarities, computing graph kernels...
- Interpreting GNNs' predictions via substructures (Ying et al., 2019)

[4] https://chem.libretexts.org/Courses/Sacramento_City_College

Given two graphs $G_A = (V_A, E_A)$ and $G_B = (V_B, E_B)$:

- G_A is a **subgraph** of G_B if $V_A \subseteq V_B$ and $E_A \subseteq E_B$.
- G_A is an **induced subgraph** of G_B if $V_A \subseteq V_B$ and $E_A = E_B \cap (V_A \times V_A)$.



Can be similarly defined for graphs with node and edge attributes.

Subgraph-count and induced-subgraph-count

Let G be a graph, and $G^{[\mathrm{P}]}$ be a pattern we are interested in counting.

The **subgraph-count** of $G^{[\mathrm{P}]}$ in G, denoted by $\mathrm{C}_S(G; G^{[\mathrm{P}]})$, is the number of *subgraphs* of G that are isomorphic to $G^{[\mathrm{P}]}$.

The **induced-subgraph-count** of $G^{[\mathrm{P}]}$ in G, denoted by $\mathrm{C}_I(G; G^{[\mathrm{P}]})$, is the number of *induced subgraphs* of G that are isomorphic to $G^{[\mathrm{P}]}$.

What does it mean for GNNs to count substructures?

Say $\mathcal{F}$ is a family of GNNs, $G^{[\mathrm{P}]}$ is a given pattern.

- Defined via function approximation

  Can $\mathcal{F}$ approximate $\mathrm{C}_S(\cdot; G^{[\mathrm{P}]})$ or $\mathrm{C}_I(\cdot; G^{[\mathrm{P}]})$ as functions on the graph space arbitrarily well?

- Defined via graph isomorphism testing

  Given any two graphs, $G^{[1]}$ and $G^{[2]}$ with different (induced-)subgraph-counts of a pattern $G^{[\mathrm{P}]}$, can we always find a function in $\mathcal{F}$ that distinguishes them?

Equivalence between the two definitions above. ✓

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Initially, set $h_i^{(0)} = x_i$ for each node $i \in V$.

For $t \in \{0, ..., T-1\}$,

$$m_i^{(t+1)} = \sum_{\mathcal{N}(i)} M_t(h_i^{(t)}, h_j^{(t)}, e_{i,j})$$

$$h_i^{(t+1)} = U_t(h_i^{(t)}, m_i^{(t+1)})$$

Finally,

$$\hat{y} = R(\{h_i^{(T)} : i \in V\}),$$

Trainable parameters in each M_t, U_t and R.

Question: For what patterns can MPNNs perform (induced-)subgraph-count?

Answer completely determined by the size of the pattern, assuming that the pattern of interest is connected.

- Pattern with 1 node
  (i.e., to count the number of nodes with a given node feature x^*)

  Can be solved by an MPNN with 0 hidden layer and

$$R(\{h_i^{(0)} : i \in V\}) = \sum_{i \in V} \mathbb{1}(h_i^{(0)} = x^*)$$

- Pattern with 2 nodes
  (i.e. to count the number of edges with a given edge feature e^*)

  Can be solved by an MPNN with 1 hidden layer and

$$M_0(h_i^{(0)}, h_j^{(0)}, e_{i,j}) = \mathbb{1}(e_{i,j} = e^*)$$
$$U_0(h_i^{(0)}, m_i^{(1)}) = m_i^{(1)}$$
$$R(\{h_i^{(1)} : i \in V\}) = \frac{1}{2} \sum_{i \in V} h_i^{(1)}$$

- What about patterns consisting of 3 nodes or more?

Theorem (Chen et al. (2020))

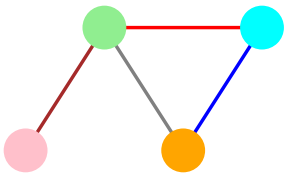
MPNNs **cannot** *perform* **induced-subgraph-count** *of any connected pattern consisting of 3 or more nodes.*

Proof strategy:

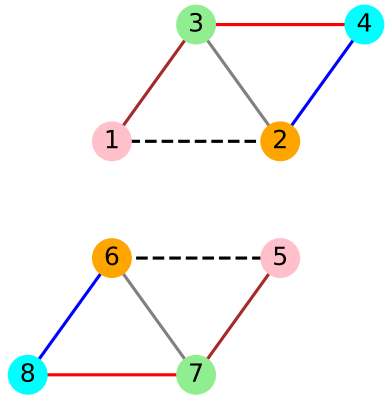
Construct a pair of graphs that have the different induced-subgraph-counts but cannot be distinguished by any MPNN.

Counter-example pair of graphs

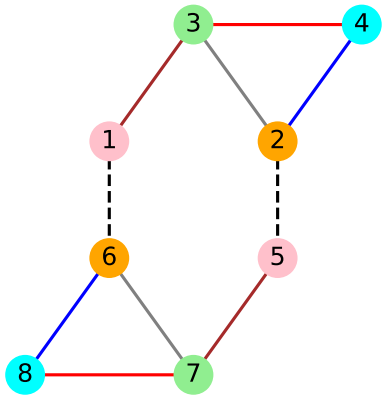
For example,



$G^{[P]}$



$G^{[1]}$



$G^{[2]}$

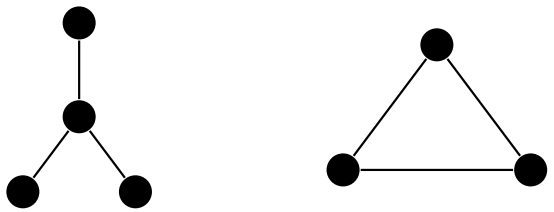
On one hand, $\mathsf{C}_I(G^{[1]}; G^{[P]}) = 0$ whereas $\mathsf{C}_I(G^{[2]}; G^{[P]}) = 2$.

On the other hand, no MPNN can distinguish $G^{[1]}$ from $G^{[2]}$.

For subgraph-count, we have the following positive result:

Theorem (5, Chen et al. (2020))

2-WL and MPNNs **can** *perform* **subgraph-count** *of star-shaped patterns.*



This is an extension of a result in Arvind et al. (2018) on WL to the cases that include node and edge features.

GNNs based on higher-order message-passing have been proposed, achieving k-WL-level of power for $k > 1$ (Morris et al., 2019).

Theorem (7, Chen et al. (2020))

k-WL, at initialization, **can** *perform both* **induced-subgraph-count** *and* **subgraph-count** *of patterns consisting of at most k nodes.*

Theorem (9, Chen et al. (2020))

Running T iterations of k-WL **cannot** *perform* **induced-subgraph-count** *of any path pattern of $(k+1)2^T$ or more nodes.*

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Definition (Maron et al. (2018, 2019b))

A kth-order Invariant Graph Network (k-IGN) is a function $F : \mathbb{R}^{n^k \times d_0} \to \mathbb{R}$ that can be decomposed in the following way:

$$F = m \circ h \circ L^{(T)} \circ \sigma \circ \cdots \circ \sigma \circ L^{(1)},$$

where each $L^{(t)}$ is a linear equivariant layer from $\mathbb{R}^{n^k \times d_{t-1}}$ to $\mathbb{R}^{n^k \times d_t}$, σ is a pointwise activation function, h is a linear invariant layer from $\mathbb{R}^{n^k \times d_T}$ to $\mathbb{R}$, and m is an MLP.

Theorem (Maron et al. (2019a))

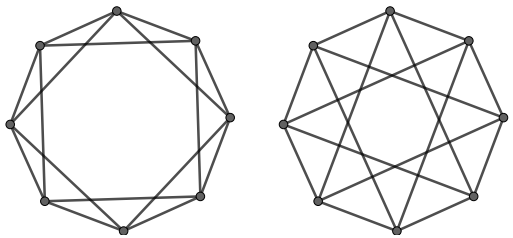
k-IGNs are no less powerful than k-WL.

Theorem (Maron et al. (2019b))

For graphs whose sizes are bounded above, k-IGNs are universally approximating if k is large enough.

Theorem (7, Chen et al. (2019b))

2-IGNs cannot distinguish between non-isomorphic regular graphs with the same degree.



Theorem (11, Chen et al. (2020))

If two graphs cannot be distinguished by 2-WL, then they cannot be distinguished by any 2-IGN.

Corollary

2-IGNs are exactly as powerful as 2-WL.

Corollary

2-IGNs **cannot** *perform* **induced-subgraph-count** *of any connected pattern consisting of 3 or more nodes.*

Corollary

2-IGNs **can** *perform* **subgraph-count** *of star-shaped patterns.*

Corollary

k-IGNs, at initialization, **can** *perform both* **induced-subgraph-count** *and containment-count of patterns consisting of at most k nodes.*

Two tasks:

- induced-subgraph-count of triangles
- subgraph-count of 3-stars

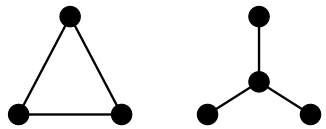


Figure 1: Triangles and 3-stars.

Table 1: Test MSE of different models divided by the variance of ground-truth counts.

	Erdős-Renyi				Random Regular			
	Triangle (M)		3-Star (C)		Triangle (M)		3-Star (C)	
	top 1	top 3	top 1	top 3	top 1	top 3	top 1	top 3
LRP-1-4	1.56E-4	2.49E-4	2.17E-5	5.23E-5	2.47E-4	3.83E-4	1.88E-6	2.81E-6
2-IGN	9.83E-2	9.85E-1	5.40E-4	5.12E-2	2.62E-1	5.96E-1	1.19E-2	3.28E-1
GIN	1.23E-1	1.25E-1	1.62E-4	3.44E-4	4.70E-1	4.74E-1	3.73E-4	4.65E-4
GCN	6.78E-1	8.27E-1	4.36E-1	4.55E-1	1.82	2.05	2.63	2.80
sGNN	9.25E-2	1.13E-1	2.36E-3	7.73E-3	3.92E-1	4.43E-1	2.37E-2	1.41E-1

Observation: To count small (induced)-subgraphs, we only need to look at local neighborhoods.

Definition

An **egonet** of depth l centered at a node i is the induced subgraph consisting of i and all nodes within distance l from it.

Idea: Apply a very expressive (and perhaps expensive) model to each egonet, and then aggregate over all egonets.

Relational Pooling (RP) (Murphy et al., 2019)

One can obtain a *permutation-invariant* function by summing or averaging a *non-permutation-invariant* function over all permutations:

$$f_{\mathrm{RP}}(G) = \sum_{\pi \in S_n} \bar{f}(\pi \circ \boldsymbol{B}(G))$$

This can achieve universal approximation of permutation-invariant functions.

Drawback: Computational complexity is $O(n!)$.

But not as big of an issue if we only apply them to local neighborhoods.

Depth-l LRP (applying RP to every egonet of depth l):

$$f_{\mathrm{LRP}}^{l}(G) = \sum_{i \in V} \sum_{\pi \in S_{n_{i,l}}} \bar{f}\left(\pi \circ \boldsymbol{B}_{i,l}^{[\mathrm{ego}]}\right)$$

Further reducing complexity with size-k cropping and BFS permutations:

$$f_{\mathrm{LRP}}^{l}(G) = \sum_{i \in V} \sum_{\pi \in S_{n_{i,l}}^{\mathrm{BFS}}} \bar{f}\left(C_k(\pi \circ \boldsymbol{B}_{i,l}^{[\mathrm{ego}]})\right)$$

Can also apply LRP iteratively, which yields *Deep LRP*.

Table 2: Results on ogbg-molhiv (measured by ROCAUC)

Model	Training	Validation	**Testing**
Deep LRP-1-4	89.81±2.90	81.31±0.88	76.87±1.80
Deep LRP-1-4 (ES)	87.56±2.11	82.09±1.16	**77.19±1.40**
GIN†	88.64±2.54	82.32±0.90	75.58±1.40
GIN + VN†	92.73±3.80	84.79±0.68	77.07±1.49
GCN†	88.54±2.19	82.04±1.41	76.06±0.97
GCN + VN†	90.07±4.69	83.84±0.91	75.99±1.19
GAT ‡	-	-	72.9±1.8
GraphSAGE ‡	-	-	74.4±0.7

Table 3: Performances on QM9 (measured by MAE)

Target	DTNN	MPNN	123-gnn	Powerful-IGN	Deep LRP-1-4
μ	0.244	0.358	0.476	0.231	0.399
α	0.95	0.89	0.27	0.382	0.337
ϵ_{homo}	0.00388	0.00541	0.00337	0.00276	0.00287
ϵ_{lumo}	0.00512	0.00623	0.00351	0.00287	0.00309
Δ_ϵ	0.0112	0.0066	0.0048	0.00406	**0.00396**
$\langle R^2 \rangle$	17	28.5	22.9	16.07	20.4
ZPVE	0.00172	0.00216	0.00019	0.00064	0.00067
U_0	2.43	2.05	0.0427	0.234	0.590
U	2.43	2	0.111	0.234	0.588
H	2.43	2.02	0.0419	0.229	0.587
G	2.43	2.02	0.0469	0.238	0.591
C_v	0.27	0.42	0.0944	0.184	0.149
Loss	0.1014	0.1108	0.0657	0.0512	0.0641

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Three perspectives on the power of GNNs:

- Graph isomorphism testing
- Approximation of permutation-invariant functions
- **Substructure counting**

Case studies on MPNNs and k-IGNs

Proposing LRP for substructure counting and real tasks

Future directions:

- Other GNN architectures
- Explaining real-world tasks with substructure counting (Ying et al., 2019)

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Thanks!



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