# Beyond Weisfeiler-Lehman: A Quantitative Framework for GNN Expressiveness

Bohang Zhang*, Jingchu Gai*, Yiheng Du, Qiwei Ye, Di He, Liwei Wang

Peking University

July 21, 2024

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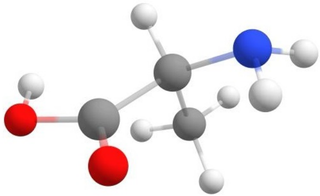
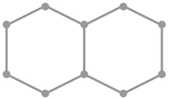
# Introduction

- Graph neural networks (GNNs) have become the dominant approach for learning graph-structured data.



# The Expressive Power of GNNs

- Are GNNs able to learn a general function on graphs?

$f\Big($  $\Big) = y$

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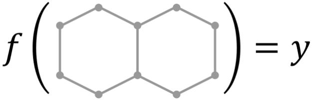
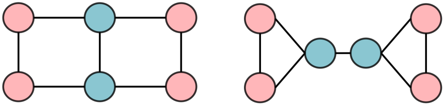


- No! Standard message-passing GNNs (MPNNs) cannot output different representations for the following two graphs.

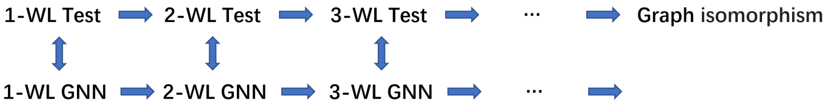


# Central Question

How can we quantify & improve the expressive power of GNNs?

# How to Quantify & Improve the Expressive Power

- Prior approach 1: graph isomorphism
  - Standard MPNNs are as expressive as the 1-dimensional Weisfeiler-Lehman test in distinguishing non-isomorphic graphs [Morris et al., 2019, Xu et al., 2019].
  - Improvements: higher-order GNNs



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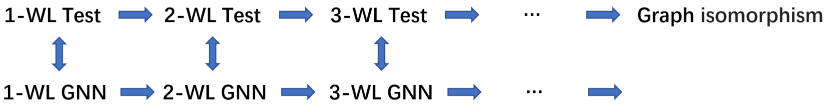
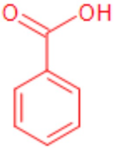
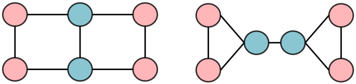



- Drawbacks:
  - Not practical: severe computation/memory costs
  - Coarse and qualitative
  - Unclear about *necessity* for real-world tasks

# How to Quantify/Improve the Expressive Power

- Prior approach 2: substructure-based GNNs:
  - Standard MPNNs cannot encode structural information, such as counting cycles or cliques in a graph.
  - Method: preprocess substructures and use them to design more expressive GNNs.



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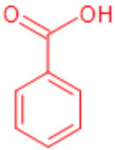


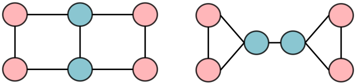

- Drawbacks: Heuristic, not principled, only reflects restricted aspects of expressivity.

# Our Goal: A Universal Expressivity Framework

Can we develop a new framework to study the expressive power of GNNs in a quantitative, systematic, and practical way?

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# Our Idea

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- What structural information can a GNN model "encode"?
- Given a GNN model $M$, the family of substructures $M$ can "encode", denoted as $\mathcal{F}^M$, can naturally be viewed as a measure of expressivity.
- By identifying $\mathcal{F}^M$ for each model $M$, the expressive power of different models can be quantitatively compared via set inclusion relation and set difference.

# Key Idea

- How to define the notion of “encodability”?

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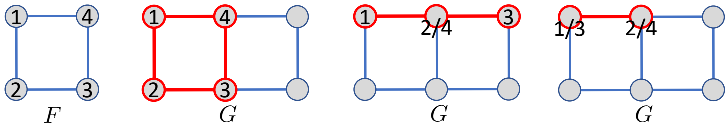
- How to define the notion of "encodability"?
- We focus on a fundamental concept called homomorphism.
- Given two graphs $F$ and $G$, a homomorphism from $F$ to $G$ is a mapping $f: V_F \to V_G$ that preserves local structures:
  - Vertex labels: $\ell_F(u) = \ell_G(f(u))$ for all $u \in V_F$.
  - Edge relations: $\{f(u), f(v)\} \in E_G$ for all $\{u, v\} \in E_F$;



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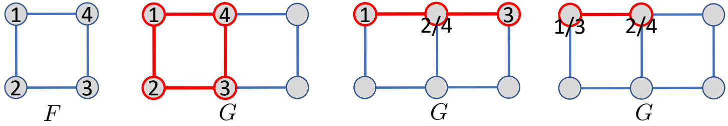
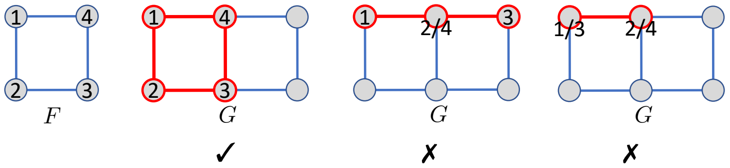



- A GNN can encode substructure $F$ in terms of homomorphism if for any input graph $G$, the computed graph representation of $G$ can count the number of homomorphisms from $F$ to $G$ (denoted $\hom(F, G)$).

# Discussions with Subgraph Counting

- A homomorphism is called injective if it maps different vertices in $F$ to different vertices in $G$.



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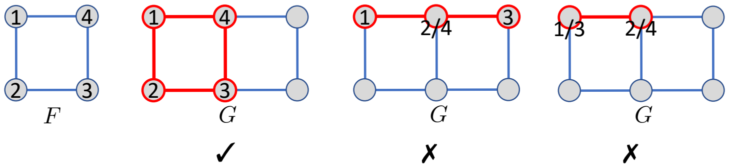


- Injective homomorphism preserves full graph structures (corresponding to subgraph counting $\mathrm{sub}(F, G)$).
- Why using homomorphism counting instead of subgraph counting?
  - Homomorphism counting is more fundamental.
  - It aligns more with GNNs: the aggregation in GNN layers only encodes local structure.

# Homomorphism Is Complete

**Theorem** [Lovász, 1967]

Any graph $G$ can be uniquely determined (up to isomorphism) by the homomorphism counts $\hom(F, G)$ of all graphs $F$.

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Any graph $G$ can be uniquely determined (up to isomorphism) by the homomorphism counts $\hom(F, G)$ of all graphs $F$.

- Question: can homomorphism count completely determine the graph representation for general GNNs?
- Conjecture: the graph representation of $G$ computed by a GNN model can be determined by the homomorphism counts $\hom(F, G)$ of a smaller set of graphs $F$.

# Formal Definition

- Given GNN model $M$ and graph $G$, denote by $\chi_G^M(G)$ the graph representation of $G$ computed by model $M$.

## Definition (homomorphism expressivity)

The homomorphism expressivity of a GNN model $M$, denoted by $\mathcal{F}^M$, is a family of (labeled) graphs satisfying the following conditions:

1. For any two graphs $G, H$, $\chi_G^M(G) = \chi_H^M(H)$ iff $\hom(F, G) = \hom(F, H)$ for all $F \in \mathcal{F}^M$;
2. $\mathcal{F}^M$ is maximal, i.e., for any graph $F \notin \mathcal{F}^M$, there exists a pair of graphs $G, H$ such that $\chi_G^M(G) = \chi_H^M(H)$ and $\hom(F, G) \neq \hom(F, H)$.

- Remark: Due to the "iff" term, the existence of homomorphism expressivity is non-trivial for general GNNs.

# Homomorphism Expressivity Is Complete and Quantitative

- Homomorphism expressivity is much finer than the WL hirarchy and more insightful than the graph isomorphism test:
  - Given two models $M_1$ and $M_2$, $\mathcal{F}^{M_1} \subset \mathcal{F}^{M_2}$
    $\iff$ for any graphs $G, H$, $\chi_G^{M_2}(G) = \chi_H^{M_2}(H)$ implies $\chi_G^{M_1}(G) = \chi_H^{M_1}(H)$
    $\iff$ $M_2$ is more expressive than $M_1$ in distinguishing non-isomorphism graphs
  - $\mathcal{F}^{M_1} \subsetneq \mathcal{F}^{M_2}$ iff $M_2$ is **strictly** more expressive than $M_1$ in distinguishing non-isomorphism graphs.

# Case Study: Message-passing GNNs

- Let's begin with the simplest MPNN:
  - Maintain a color $\chi_G^{\mathsf{MP}}(u)$ for each vertex $u \in V_G$;
  - Initially, the color depends on the vertex label, i.e., $\chi_G^{\mathsf{MP},(0)}(u) = \ell_G(u)$.
  - In each iteration:

$$\chi_G^{\mathsf{MP},(t+1)}(u) = \mathsf{hash}\left(\chi_G^{\mathsf{MP},(t)}(u), \{\!\{\chi_G^{\mathsf{MP},(t)}(v) : v \in N_G(u)\}\!\}\right).$$

  - Denote by $\chi_G^{\mathsf{MP}}(u)$ the stable color of $u$.
  - Graph representation: $\chi_G^{\mathsf{MP}}(G) = \{\!\{\chi_G^{\mathsf{MP}}(u) : u \in V_G\}\!\}$.

# Case Study: Message-passing GNNs

- How can we derive the homomorphism expressivity for MPNNs?

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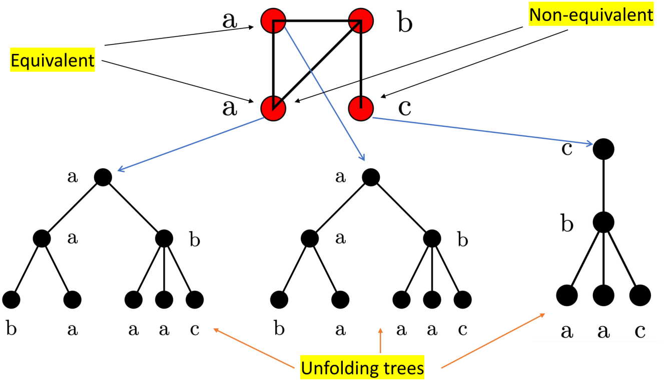
- How can we derive the homomorphism expressivity for MPNNs?
- Intuition: the computed node feature of an MPNN can be fully determined by the structure of the unfolding tree.



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- This shows $\chi_G^{\mathsf{MP}}(u)$ contains $\hom(F^w, G^u)$ for all rooted trees $F^w$.

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- Since $\hom(F, G) = \sum_{u \in V_G} \hom(F^w, G^u)$, the graph representation $\chi_G^{\mathsf{MP}}(G)$ encodes $\hom(F, G)$ for all trees $F$.

# Case Study: Message-passing GNNs

- This shows $\chi_G^{\mathsf{MP}}(u)$ contains $\hom(F^w, G^u)$ for all rooted trees $F^w$.
- Since $\hom(F, G) = \sum_{u \in V_G} \hom(F^w, G^u)$, the graph representation $\chi_G^{\mathsf{MP}}(G)$ encodes $\hom(F, G)$ for all trees $F$.
- A more involved analysis can show the other two directions:
  - $\hom(F, G)$ for all trees $F$ determines $\chi_G^{\mathsf{MP}}(G)$ [Dvořák, 2010, Dell et al., 2018].
  - $\mathcal{F}^{\mathsf{MP}}$ does not contain any graph that contains cycles [Roberson, 2022].

**Theorem**

$\mathcal{F}^{\mathsf{MP}} = \{F : F \text{ is a forest}\}$.

# More Advanced GNN Models

- Subgraph GNN [Qian et al., 2022, Bevilacqua et al., 2022]:
  - Treat a graph $G$ as a set of subgraphs $\{\!\{G^u : u \in V_G\}\!\}$, each obtained from $G$ by marking a special vertex $u \in V_G$.
  - Maintain a color $\chi_G^{\mathsf{Sub}}(u, v)$ for each vertex $v$ in graph $G^u$;
  - Initially, $\chi_G^{\mathsf{Sub},(0)}(u, v) = (\ell_G(v), \mathbb{I}[u = v])$;
  - It then runs MPNNs independently on each graph $G^u$:

$$\chi_G^{\mathsf{Sub},(t+1)}(u, v) = \mathsf{hash}\left(\chi_G^{\mathsf{Sub},(t)}(u, v), \{\!\{\chi_G^{\mathsf{Sub},(t)}(u, w) : w \in N_G(v)\}\!\}\right).$$

  - Denote by $\chi_G^{\mathsf{Sub}}(u, v)$ the stable color of $(u, v)$.
  - Node feature of $u$: $\chi_G^{\mathsf{Sub}}(u) := \mathsf{hash}\left(\{\!\{\chi_G^{\mathsf{Sub}}(u, v) : v \in V_G\}\!\}\right)$;
  - Graph representation: $\chi_G^{\mathsf{Sub}}(G) = \{\!\{\chi_G^{\mathsf{Sub}}(u) : u \in V_G\}\!\}$.

# More Advanced GNN Models

- Local 2-GNN [Morris et al., 2020]:
  - Initial color: $\chi_G^{\mathsf{L},(0)}(u,v) = (\ell_G(u), \ell_G(v), \mathbb{I}[u=v], \mathbb{I}[\{u,v\} \in E_G]);$
  - Aggregation rule:

$$\chi_G^{\mathsf{L},(t+1)}(u,v) = \mathsf{hash}\left(\chi_G^{\mathsf{L},(t)}(u,v), \{\!\{\chi_G^{\mathsf{L},(t)}(w,v) : w \in N_G(u)\}\!\}, \{\!\{\chi_G^{\mathsf{L},(t)}(u,w) : w \in N_G(v)\}\!\}\right).$$

- Folklore-type GNNs:
  - 2-FGNN [Maron et al., 2019]:

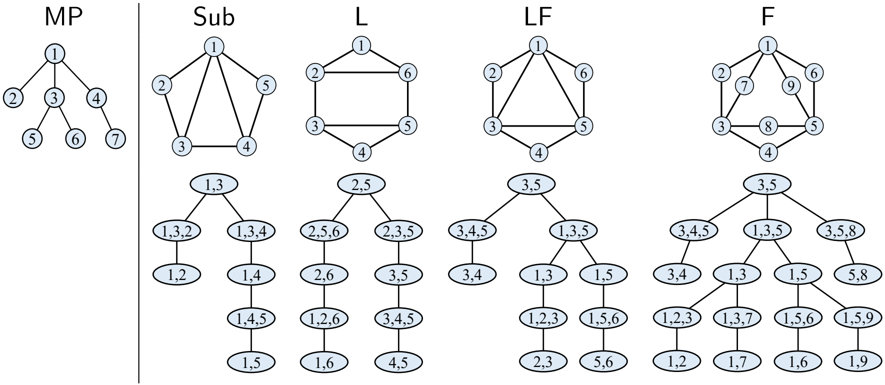
$$\chi_G^{\mathsf{F},(t+1)}(u,v) = \mathsf{hash}\left(\chi_G^{\mathsf{F},(t)}(u,v), \{\!\{(\chi_G^{\mathsf{F},(t)}(w,v), \chi_G^{\mathsf{F},(t)}(u,w)) : w \in V_G\}\!\}\right).$$

  - Local 2-FGNN [Zhang et al., 2023]:

$$\chi_G^{\mathsf{LF},(t+1)}(u,v) = \mathsf{hash}\left(\chi_G^{\mathsf{LF},(t)}(u,v), \{\!\{(\chi_G^{\mathsf{LF},(t)}(w,v), \chi_G^{\mathsf{LF},(t)}(u,w)) : w \in N_G(u) \cup N_G(v)\}\!\}\right).$$

# Unfolding Tree and Tree Decomposition

- In general, if a substructure $F$ can be counted by a GNN model, $F$ should admit a tree decomposition that aligns with the structure of the GNN's unfolding tree.



# Characterization using Nested Ear Decomposition

## Definition

Given a graph $G$, a NED $\mathcal{P}$ is a partition of the edge set $E_G$ into a *sequence* of simple paths $P_1, \cdots, P_m$ (called ears), such that:

- Any two ears $P_i$ and $P_j$ $(1 \le i < j \le c)$ do not intersect, where $c$ is the number of connected components of $G$.
- For each ear $P_j$ $(j > c)$, there is an ear $P_i$ $(1 \le i < j)$ such that one or two endpoints of $P_j$ lie in ear $P_i$ (we say $P_j$ is *nested* on $P_i$). Moreover, except for the endpoints lying in ear $P_i$, no other vertices in $P_j$ are in any previous ear $P_k$ for $1 \le k < j$. If both endpoints of $P_j$ lie in $P_i$, the subpath in $P_i$ that shares the endpoints of $P_j$ is called the *nested interval* of $P_j$ in $P_i$, denoted as $I(P_j) \subset P_i$. If only one endpoint lies in $P_i$, define $I(P_j) = \emptyset$.
- For all ears $P_j$, $P_k$ $(c < j < k \le m)$, either $I(P_j) \cap I(P_k) = \emptyset$ or $I(P_j) \subset I(P_k)$.

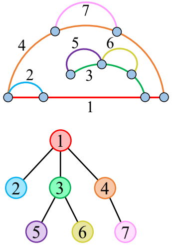
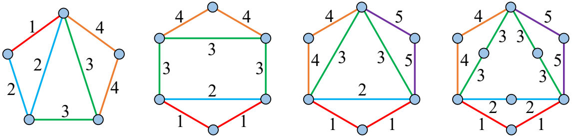



Illustration of NED

# NED Variants




(a) Endpoint-shared/strong/almost-strong/general NED

- Endpoint-shared NED: a NED is called endpoint-shared if all ears with non-empty nested intervals share a common endpoint.
- Strong NED: a NED is called strong if for any two children $P_j$, $P_k$ $(j < k)$ nested on the same parent ear, we have $I(P_j) \subset I(P_k)$.
- Almost-strong NED: a NED is called almost-strong if for any children $P_j$, $P_k$ $(j < k)$ nested on the same parent ear and $|I(P_j)| > 1$ , we have $I(P_j) \subset I(P_k)$.

# Main Results

## Theorem

*For all GNN models $M$ above, the graph family $\mathcal{F}^M$ exists. Moreover, each $\mathcal{F}^M$ can be separately described below:*

- ***MPNN***: $\mathcal{F}^{\mathsf{MP}} = \{F : F \text{ is a forest}\}$;
- ***Subgraph GNN***: $\mathcal{F}^{\mathsf{Sub}} = \{F : \exists u \in V_F \text{ s.t. } F \backslash \{u\} \text{ is a forest}\} = \{F : F \text{ has an endpoint-shared NED}\}$;
- ***Local 2-GNN***: $\mathcal{F}^{\mathsf{L}} = \{F : F \text{ has a strong NED}\}$;
- ***Local 2-FGNN***: $\mathcal{F}^{\mathsf{LF}} = \{F : F \text{ has an almost-strong NED}\}$;
- ***2-FGNN***: $\mathcal{F}^{\mathsf{F}} = \{F : F \text{ has a NED}\}$.

- Proofs are based on: (i) algebraic graph theory [Dell et al., 2018]; (ii) CFI construction [Cai et al., 1992, Fürer, 2001]; (iii) pebble game [Cai et al., 1992, Zhang et al., 2023].

# Extending to Node/Edge-Level Expressivity

## Definition

The node-level homomorphism expressivity of a GNN model $M$, denoted by $\mathcal{F}_{\mathsf{n}}^{M}$, is a family of connected *rooted* graphs satisfying the following conditions:

1. For any connected graphs $G, H$ and vertices $u \in V_G$, $v \in V_H$, $\chi_G^M(u) = \chi_H^M(v)$ *iff* $\hom(F^w, G^u) = \hom(F^w, H^v)$ for all $F^w \in \mathcal{F}_{\mathsf{n}}^{M}$;
2. For any connected rooted graph $F^w \notin \mathcal{F}_{\mathsf{n}}^{M}$, there exists a pair of connected graphs $G, H$ and vertices $u \in V_G$, $v \in V_H$ such that $\chi_G^M(u) = \chi_H^M(v)$ and $\hom(F^w, G^u) \neq \hom(F^w, H^v)$.

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- What about edge-level expressivity?

# Extending to Node/Edge-Level Expressivity

## Theorem

*For all model $M$ above, $\mathcal{F}_{\mathsf{n}}^{M}$ and $\mathcal{F}_{\mathsf{e}}^{M}$ (except MPNN) exist. Moreover,*

- ***MPNN**: $\mathcal{F}_{\mathsf{n}}^{\mathsf{MP}} = \{F^w : F \text{ is a tree}\}$;*
- ***Subgraph GNN**:*
  $\mathcal{F}_{\mathsf{n}}^{\mathsf{Sub}} = \{F^w : F \text{ has a NED with shared endpoint } w\} = \{F^w : F \backslash \{w\} \text{ is a forest}\}$,
  $\mathcal{F}_{\mathsf{e}}^{\mathsf{Sub}} = \{F^{wx} : F \text{ has a NED with shared endpoint } w\} = \{F^{wx} : F \backslash \{w\} \text{ is a forest}\}$;
- ***2-FGNN**: $\mathcal{F}_{\mathsf{n}}^{\mathsf{F}} = \{F^w : F \text{ has a NED where } w \text{ is an endpoint of the first ear}\}$,*
  $\mathcal{F}_{\mathsf{e}}^{\mathsf{F}} = \{F^{wx} : F \text{ has a NED where } w \text{ and } x \text{ are endpoints of the first ear}\}$.

*The cases of Local 2-GNN and Local 2-FGNN are similar to 2-FGNN by replacing "NED" with "strong NED" and "almost-strong NED", respectively.*

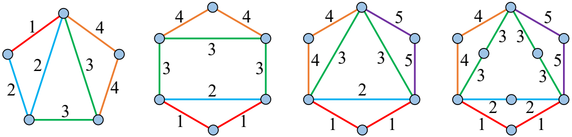
# Index

# Quantitative Expressivity Comparison

- Given two models $M_1$ and $M_2$
  - $\mathcal{F}^{M_1} \subset \mathcal{F}^{M_2}$
    iff $M_2$ is more expressive than $M_1$ in distinguishing non-isomorphism graphs
  - $\mathcal{F}^{M_1} \subsetneq \mathcal{F}^{M_2}$
    iff $M_2$ is **strictly** more expressive than $M_1$ in distinguishing non-isomorphism graphs

## Example

The expressive power of the following GNN models strictly increases in order (in terms of distinguishing non-isomorphic graphs): MPNN, Subgraph GNN, Local 2-GNN, Local 2-FGNN, and 2-FGNN. $\mathcal{F}^{\mathsf{MP}} \subsetneq \mathcal{F}^{\mathsf{Sub}} \subsetneq \mathcal{F}^{\mathsf{L}} \subsetneq \mathcal{F}^{\mathsf{LF}} \subsetneq \mathcal{F}^{\mathsf{F}}$.



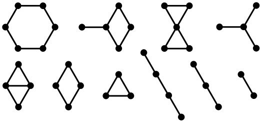
(a) Endpoint-shared/strong/almost-strong/general NED

# Subgraph Counting Power

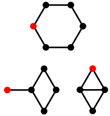
- Denote by Spasm$(F)$ the set of homomorphism images of $F$.

**Theorem**

For any GNN model $M$ such that their homomorphism expressivity $\mathcal{F}^M$ exists, $M$ can subgraph-count $F$ *iff* Spasm$(F) \subset \mathcal{F}^M$.



(a) Spasm$^{\not\cong}(C_6)$ has 10 graphs.



(b) Rooted $C_6$

**Example: Cycle/Path Counting Power**

| Model \ Structure | Cycle $C_n$ | Cycle $C_n^u$ | Cycle $C_n^{uv}$ | Path $P_n$ | Path $P_n^w$ | Path $P_n^{wx}$ |
|---|---|---|---|---|---|---|
| MPNN | None | None | None | $n \le 3$ | $n \le 3$ | $n \le 3$ |
| Subgraph GNN | $n \le 7$ | $n \le 4$ | $n \le 4$ | $n \le 7$ | $n \le 4$ | $n \le 4$ |
| Local 2-GNN<br>Local 2-FGNN<br>2-FGNN | $n \le 7$ | | | $n \le 7$ | | |

# More Extensions & Implications

- Homomorphism expressivity for higher-order GNNs
- Node/edge-level homomorphism expressivity and subgraph counting
- Related to polynomial expressivity [Puny et al., 2023]

# Experiments

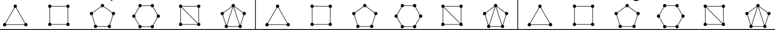
Table 1: Experimental results on homomorphism counting. Red/blue nodes indicate marked vertices.

| Model \ Task | Graph-level | | | Node-level | | Edge-level | | |
|---|---|---|---|---|---|---|---|---|
| MPNN | .300 | .233 | .254 | .505 | .478 | - | - | - |
| Subgraph GNN | .011 | .015 | .012 | .004 | .058 | .003 | .058 | .048 |
| Local 2-GNN | .008 | .008 | .010 | .003 | .004 | .005 | .006 | .008 |
| Local 2-FGNN | .003 | .005 | .004 | .005 | .005 | .007 | .007 | .008 |

Table 2: Experimental results on ZINC and Alchemy datasets.

| Model \ Task | ZINC Subset | ZINC Full | Alchemy |
|---|---|---|---|
| MPNN | $.138 \pm .006$ | $.030 \pm .002$ | $.122 \pm .002$ |
| Subgraph GNN | $.110 \pm .007$ | $.028 \pm .002$ | $.116 \pm .001$ |
| Local 2-GNN | $.069 \pm .001$ | $.024 \pm .002$ | $.114 \pm .001$ |
| Local 2-FGNN | $.064 \pm .002$ | $.023 \pm .001$ | $.111 \pm .001$ |

Table 3: Experimental results on the (Chordal) Cycle Counting task.



| Model \ Task | Graph-level | | | | | | Node-level | | | | | | Edge-level | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| MPNN | .358 | .208 | .188 | .146 | .261 | .205 | .600 | .413 | .300 | .207 | .318 | .237 | - | - | - | - | - | - |
| Subgraph GNN | .010 | .020 | .024 | .046 | .007 | .027 | .003 | .005 | .092 | .082 | .050 | .073 | .001 | .003 | .090 | .096 | .038 | .065 |
| Local 2-GNN | .008 | .011 | .017 | .034 | .007 | .016 | .002 | .005 | .010 | .023 | .004 | .015 | .001 | .005 | .010 | .019 | .005 | .014 |
| Local 2-FGNN | .003 | .004 | .010 | .020 | .003 | .010 | .004 | .006 | .012 | .021 | .004 | .014 | .003 | .006 | .012 | .022 | .005 | .012 |

# Conclusion

- We propose a new framework for systematically and quantitatively studying the expressive power of GNN architectures.
- Through the lens of homomorphism expressivity, we give exact descriptions of the graph family each model can encode in terms of homomorphism counting.
- Homomorphism expressivity framework stands as a valuable toolbox to unify the landscape between different subareas in the GNN community, providing deep insights into a number of prior works and answering their open problems.

# Thank You!

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