Homomorphism Expressivity of Spectral Invariant Graph Neural Networks

Jingchu Gai [1] Yiheng Du [1] Bohang Zhang[1] Haggai Maron [2,3]
Liwei Wang [1]
[1]Peking University [2]Technion [3]NVIDIA Research
gaijingchu@stu.pku.edu.cn, zhangbohang@pku.edu.cn,
duyiheng@stu.pku.edu.cn
hmaron@nvidia.com, wanglw@pku.edu.cn

April 18, 2025

Overview

Outline

Background: Graph Spectral

- Eigen-decomposition of graph G:

$$\mathbf{M}_G = \sum_{k=1}^{k} \lambda_{M,k}^{G} \mathbf{P}_{M,k}^{G}, \quad \mathbf{M}_G \in \{\mathbf{A}, \mathbf{L}, \widehat{\mathbf{A}}, \widehat{\mathbf{L}}\}$$

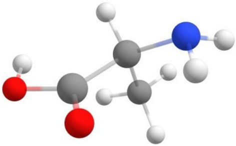
  M can be either a standard or normalized adjacency matrix, or a standard or normalized Laplacian matrix.
- Spectral Information: eigenvalue $\{\lambda_{M,k}^{G}\}_{k=1}^{m}$ and projection matrix to eigenspaces $\{\mathbf{P}_{M,k}^{G}\}_{k=1}^{m}$.

Background: Application of Graph Spectral

- Theoretical and graph theory: How much information of graph does spectral information
  - Widely known conjecture [9, 6]: If two graphs are cospectral (have same eigenvalues), are they isomorphic?
- Application and machine learning:
  - Spectral encodes information regarding connectivity.
  - Related to practical applications such as molecular property prediction.
  - Adopted in the design of neural networks

Background: Graph Neural Network

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



- To develop GNNs that more effectively encode spectral information, recent research in graph learning has incorporated spectral information into their design, leading to what we call spectral GNNs.

Questions and Motivations

- GNN based on spectral:
  - Basisnet [8]
  - SPE [7]
  - Spectral Invariant GNN (Spectral-IGN) [10]
  - GCN, ChebNet
- Questions:
  - Incorporating spectral information into the design of GNNs increases computational cost. Does this enhance the expressive power of GNNs?
  - What is the relationship between the expressive power of GNNs based on spectral information and other GNNs?
  - How do spectral GNNs compare to other mainstream GNN architectures?
  - What are the key properties of spectral GNNs (e.g., subgraph counting capabilities)?

Outline

Spectral Invariant GNN

- Spectral Invariant GNN : A variation of 1-WL that incorporates spectral information, also the most widely studied spectral-based GNN.

$$\chi_G^{\mathsf{Spec},(d+1)}(u) = \mathsf{hash}\left(\chi_G^{\mathsf{Spec},(d)}(u), \{\!\{(\chi_G^{\mathsf{Spec},(d)}(v), \mathcal{P}(u,v)) | v \in V_G\}\!\}\right) \quad \text{for } u \in V_G, d \in N_+,$$

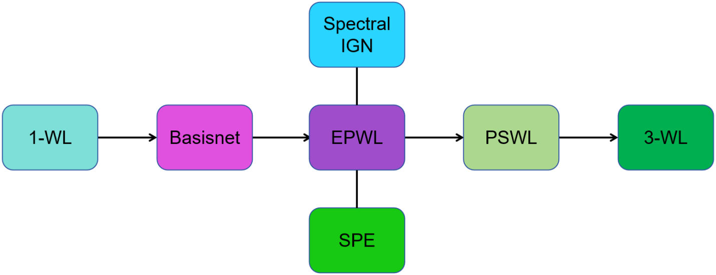
$$\mathcal{P}(u,v) := \{\!\{(\lambda, \boldsymbol{P}_\lambda(u,v)) | \lambda \in \Lambda\}\!\} \quad \text{for } u, v \in V_G.$$

$\mathbf{A} = \sum_\lambda \mathbf{P}_\lambda$ is the eigen-decomposition of adjacency matrix $\mathbf{A}$.

Previous Result: Expressive Power of Spectral GNNs

Theorem

- *Spectral IGN is as expressive as EPWL in distinguishing non-isomorphic graphs.*
- *SPE is as expressive as EPWL.*
- *Basisnet is strictly weaker than EPWL.*
- *EPWL is strictly stronger than 1-WL, and is strictly weaker than PSWL. Thus. EPWL is strictly weaker than 3-WL.*



Result and Limitation

- Conclusion:
  - A fine-grained expressiveness hierarchy among different architectures.
  - Spectral IGN essentially unifies all prior spectral invariant architectures, in that they are either strictly less expressive or equivalent to Spectral IGN.
- Limitation:
  - How to compare Spectral IGN with other main stream GNNs?
  - Other properties of Spectral IGN? (e.g. subgraph count)
  - Open problem of [2]—expressive power of Spectral IGN with finite iterations:
    For any d, is the expressive power of $\chi_G^{\mathrm{Spec},(d+1)}$ strictly stronger than $\chi_G^{\mathrm{Spec},(d)}$? (i.e. does the iteration of spectral IGN converges in finite number of iterations?)
- **A more fine-grained analysis is required !**

Outline

Homomorphic Expressivity of Spectral GNN

BEYOND WEISFEILER-LEHMAN: A QUANTITATIVE FRAMEWORK FOR GNN EXPRESSIVENESS

Bohang Zhang[1*†] **Jingchu Gai**[1*] **Yiheng Du**[1] **Qiwei Ye**[2] **Di He**[1] **Liwei Wang**[1]
[1]Peking University [2]Beijing Academy of Artificial Intelligence
zhangbohang@pku.edu.cn, {gaijingchu,duyiheng}@stu.pku.edu.cn
qwye@baai.ac.cn, {dihe,wanglw}@pku.edu.cn

- **Introduce tools of discrete geometry and algebraic graph theory to the analysis of GNNs' expressive power.**

Homomorphic Expressivity of GNN

Definition (Homomorphism)

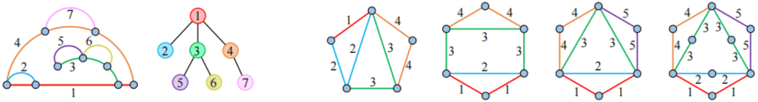
Given two graphs $F = (V_F, E_F)$ and $G = (V_G, E_G)$, a homomorphism from F to G is a mapping $f\colon V_F \to V_G$ that preserves edges, i.e. $\{f(u), f(v)\} \in E_G$ for all $\{u, v\} \in E_F$.

Definition (Homomorphic Expressivity)

The homomorphism expressivity of a GNN model M, denoted as $\mathcal{F}^M$, is a family of 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 maximum, i.e., for any graph $F \notin \mathcal{F}^M$, there exists a pair graphs G, H such that $\chi_G^M(G) = \chi_H^M(H)$ and $\hom(F, G) \neq \hom(F, H)$.

Homomorphic Expressivity of Main Stream GNNs



(a) Illustration of NED (b) Endpoint-shared/strong/almost-strong/general NED

Theorem

The homomorphism expressivity of main stream GNNs are presented as follows:

- ***MPNN***: $\mathcal{F}^{\mathsf{MP}} = \{F : F \text{ is a forest}\}$;
- ***Subgraph GNN***: $\mathcal{F}^{\mathsf{Sub}} = \{F : F \text{ has an endpoint-shared NED}\}$;
- ***Local 2-GNN***: $\mathcal{F}^{\mathsf{L}} = \{F : F \text{ has a strong NED}\}$;
- ***Local 2-FGNN***: $\mathcal{F}^{\mathsf{LF}} = \{F : F \text{ has a almost-strong NED}\}$;
- ***2-FGNN***: $\mathcal{F}^{\mathsf{LF}} = \{F : F \text{ is a subgraph a series-parallel graph}\}$.

Homomorphic Expressivity of Spectral GNN

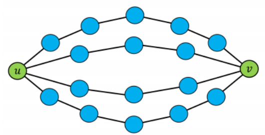
Definition (Parallel Edge)

A graph G is called a *parallel edge* if there exist two different vertices $u, v \in V_G$ such that the edge set E_G can be partitioned into a sequence of simple paths $P_1, \ldots, P_m$, where all paths share endpoints (u, v). We refer to (u, v) as the endpoints of G.

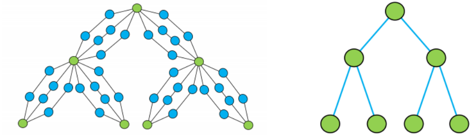
Definition (Parallel Tree)

A graph F is called a *parallel tree* if there exists a tree T such that F can be obtained from T by replacing each edge $(u, v) \in E_T$ with a parallel edge that has endpoints (u, v). We refer to T as the *parallel tree skeleton* of the graph F. Given a parallel tree F, the *parallel tree depth* of F is defined as the minimum depth of any parallel tree skeleton of F.

Homomorphic Expressivity of Spectral GNN



(a) A parallel edge with endpoints (u, v)



(b) An example of parallel tree and its tree skeleton

Theorem (Homomorphism Expressivity)

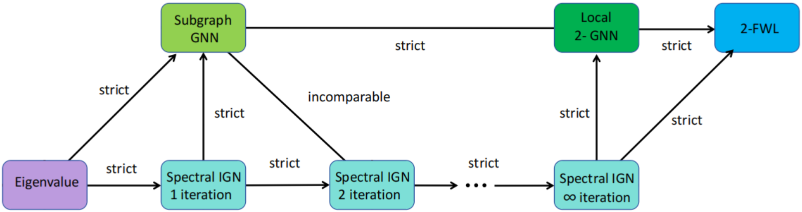
For any $d \in \mathbb{N}$, the homomorphism expressivity of spectral invariant GNNs with d iterations exists and can be characterized as follows:

$$\mathcal{F}^{\text{Spec},(d)} = \{F \mid F \text{ has parallel tree depth at most } d\}.$$

Theorem (Subgraph Counting Power)

$\forall d \in \mathbb{N}$, spectral IGNs with d iterations can subgraph count graph F iff all the homomorphic images of F lies in $\mathcal{F}^{\text{Spec},(d)}$.

Implication of Homomorphic Expressivity



- **Hierarchy:** A hierarchy of spectral IGN and other mainstream GNNs.
- **Subgraph Count:** Extending the results of previous works [3, 1, 5].
  1. Spectral invariant GNNs can subgraph-count all cycles up to 7 vertices within 2 iterations.
  2. The above upper bound is tight: spectral invariant GNNs with only 1 iteration (i.e., Fürer's weak spectral invariant) cannot subgraph-count 7-cycle.
  3. Spectral invariant GNNs with 1 iteration suffice to subgraph-count all cycles up to 6 vertices.

Extension: Higher Order Spectral

- **Higher Order Spectral GNN:**
  The homomorphism expressivity of k-order spectral invariant GNNs is the set of all graphs that admit a parallel k-order strong NED.
- **Higher Order Symmetric Power:**

Theorem

The Local 2k-GNN can encode the symmetric k-th power. Specifically, for given graphs G and H, if G and H have the same representation under Local 2k-GNN, then $G^{\{k\}}$ and $H^{\{k\}}$ have the same representation under the spectral invariant GNNs.

Outline

Experiment

Table 1: Experimental results on homomorphism counting, real-world tasks and substructure count.

Task / Model	Homomorphism Count					ZINC		Substructure Count					
						Subset	Full						
MPNN	.300	.261	.276	.233	.341	.138 ± .006	.030 ± .002	.358	.208	.188	.146	.261	.205
Spectral Invariant GNN	.045	.046	.053	.048	.303	.103 ± .006	.028 ± .003	.072	.072	.089	.089	.060	.099
Subgraph GNN	.011	.013	.010	.015	.260	.110 ± .007	.028 ± .002	.010	.020	.024	.046	.007	.027
Local 2-GNN	.008	.006	.008	.008	.112	.069 ± .001	.024 ± .002	.008	.011	.017	.034	.007	.016

- **Homomorphism Count.** GNN models perform well in homomorphism counting when the substructure is captured by the model's homomorphism expressivity.
- **Subgraph Count.** GNN models perform well in subgraph counting when the substructure's homomorphic images are within the model's homomorphism expressivity.
- **Real-World Task.** We evaluate our GNN models on the ZINC-subset and ZINC-full datasets [4].

References I

[1] Vikraman Arvind, Frank Fuhlbrück, Johannes Köbler, and Oleg Verbitsky. On weisfeiler-leman invariance: Subgraph counts and related graph properties. *Journal of Computer and System Sciences*, 113:42–59, 2020.

[2] Vikraman Arvind, Frank Fuhlbrück, Johannes Köbler, and Oleg Verbitsky. On a hierarchy of spectral invariants for graphs. In *41st International Symposium on Theoretical Aspects of Computer Science (STACS 2024)*. Schloss Dagstuhl–Leibniz-Zentrum für Informatik, 2024.

[3] Dragos Cvetkovic, Dragoš M Cvetković, Peter Rowlinson, and Slobodan Simic. *Eigenspaces of graphs*. Cambridge University Press, 1997.

References II

[4] Vijay Prakash Dwivedi, Chaitanya K Joshi, Thomas Laurent, Yoshua Bengio, and Xavier Bresson. Benchmarking graph neural networks. *arXiv preprint arXiv:2003.00982*, 2020.

[5] Martin Fürer. On the combinatorial power of the weisfeiler-lehman algorithm. In *International Conference on Algorithms and Complexity*, pages 260–271. Springer, 2017.

[6] Willem H Haemers and Edward Spence. Enumeration of cospectral graphs. *European Journal of Combinatorics*, 25(2):199–211, 2004.

[7] Yinan Huang, William Lu, Joshua Robinson, Yu Yang, Muhan Zhang, Stefanie Jegelka, and Pan Li. On the stability of expressive positional encodings for graph neural networks. *arXiv preprint arXiv:2310.02579*, 2023.

References III

[8] Derek Lim, Joshua Robinson, Lingxiao Zhao, Tess Smidt, Suvrit Sra, Haggai Maron, and Stefanie Jegelka. Sign and basis invariant networks for spectral graph representation learning. *arXiv preprint arXiv:2202.13013*, 2022.

[9] Edwin R Van Dam and Willem H Haemers. Which graphs are determined by their spectrum? *Linear Algebra and its applications*, 373:241–272, 2003.

[10] Bohang Zhang, Lingxiao Zhao, and Haggai Maron. On the expressive power of spectral invariant graph neural networks. *arXiv preprint arXiv:2406.04336*, 2024.