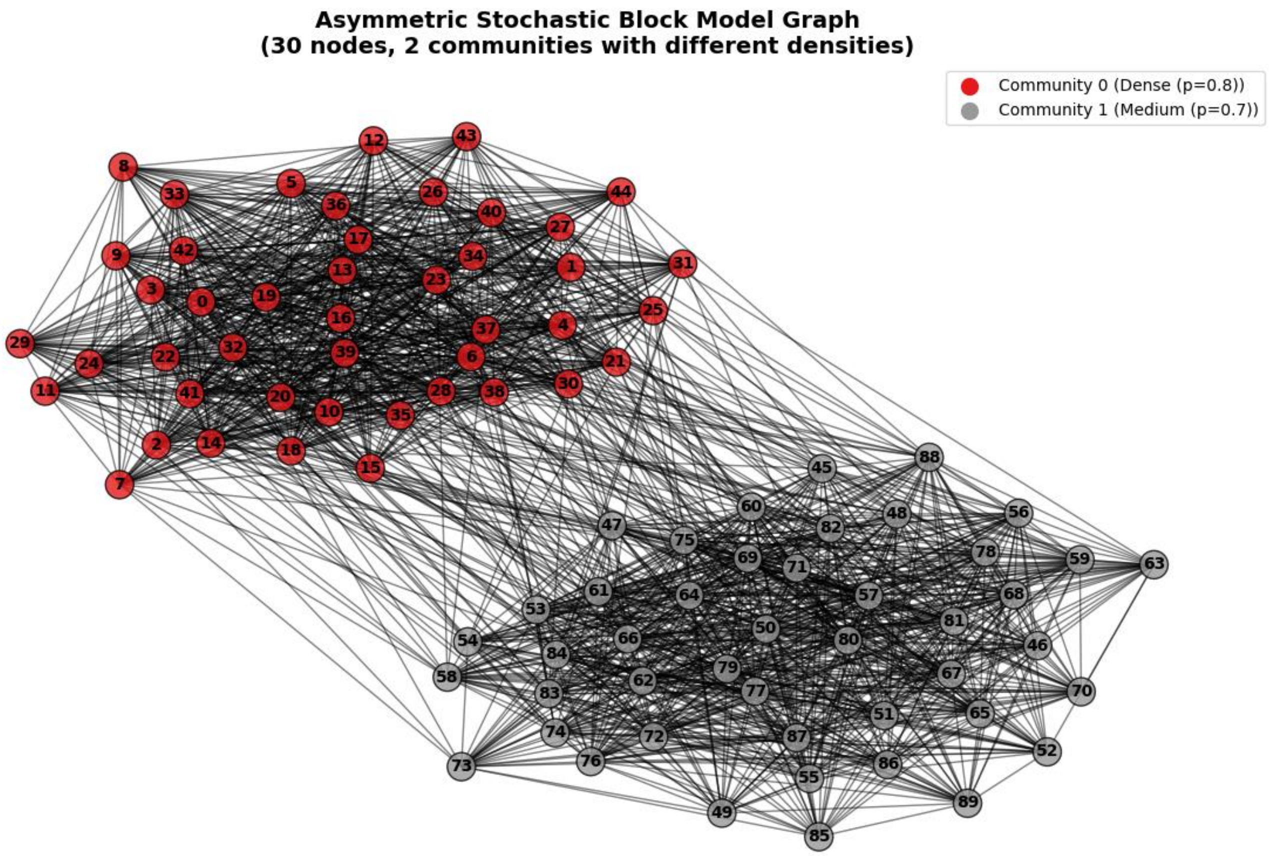
Higher-Order Learning with Graph Neural Networks via Hypergraph Encodings

Raphael Pellegrin*, Lukas Fesser*, Melanie Weber

Advances in Neural Information Processing Systems (NeurIPS 2025)

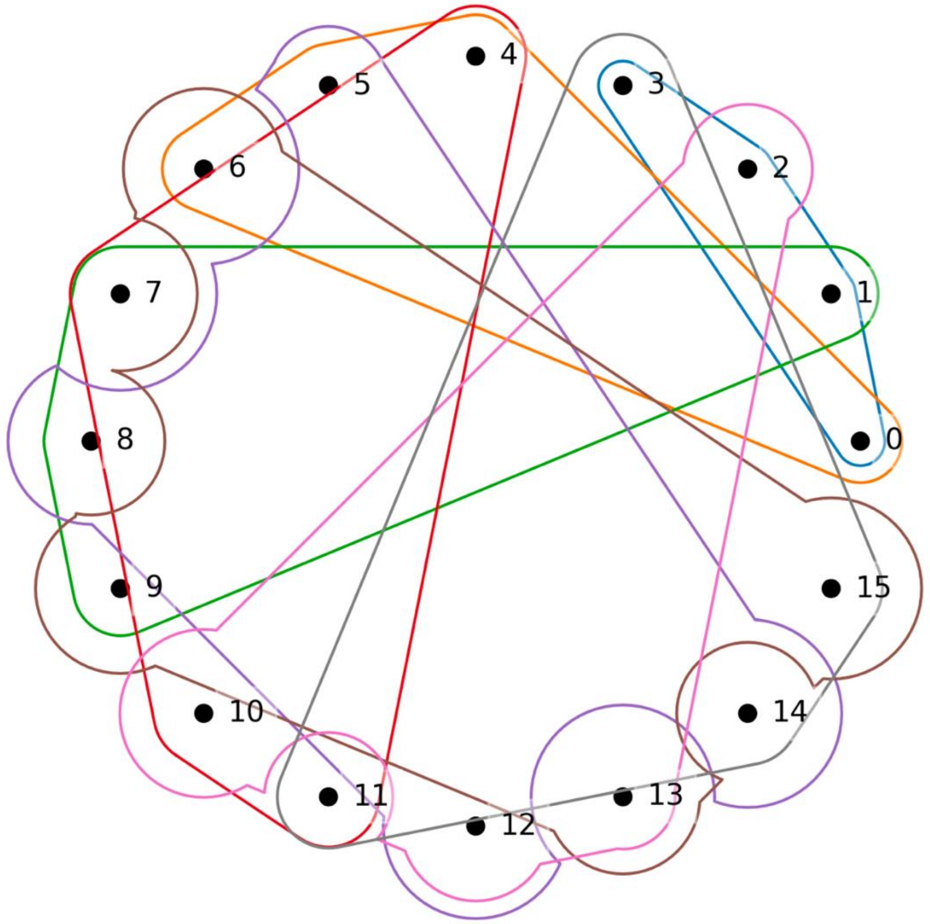
Graphs

Edges in a graph represent pairwise relations



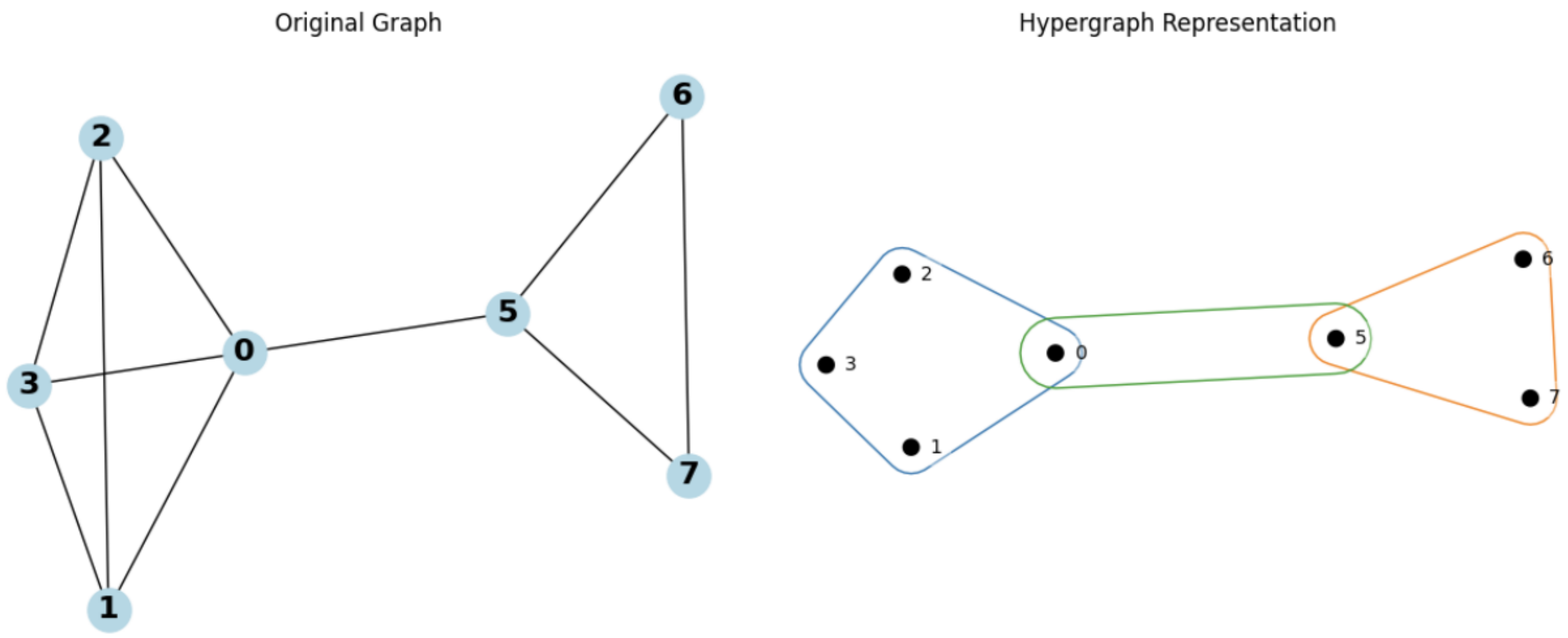
Hypergraphs

Hyperedges can connect any number of nodes



Topological Architectures

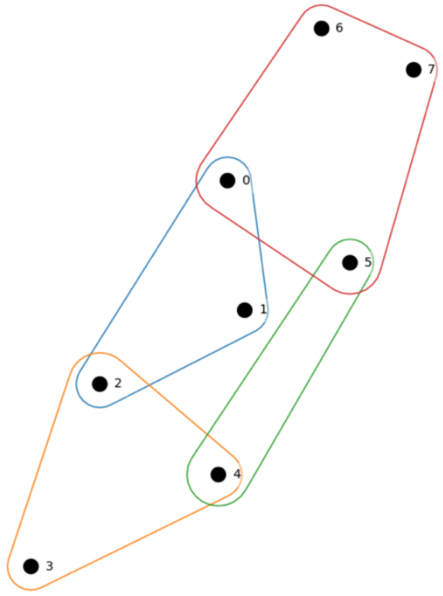
Parametrizing higher-order relations via hypergraphs (lifting)



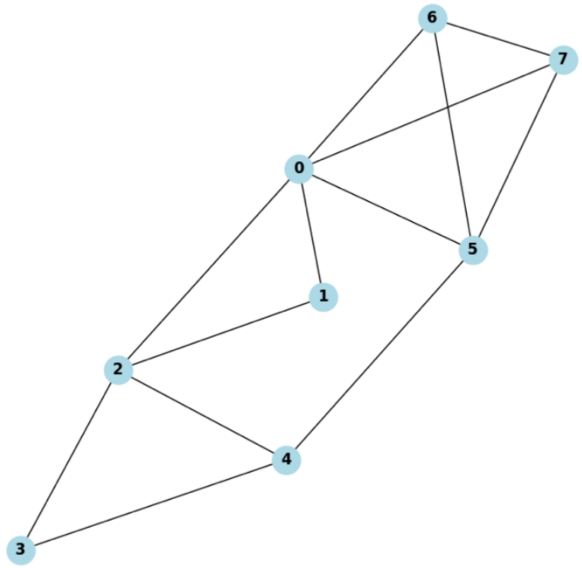
Topological Architectures

Parametrizing hypergraphs as graphs (clique expansion)

Original Hypergraph



Clique Expansion



Topological Architectures

GNNs vs HNNs

To leverage hypergraph parametrizations in relational learning, we can define message-passing on hypergraphs. Is this the solution?

Graph Neural Networks (GNN)

$$x_v^{l+1} = \phi_l\Big(\bigoplus_{p \in \mathcal{N}_v \cup \{v\}} \psi_l\left(x_p^l\right)\Big)$$

Hypergraph Neural Networks (HNN)

$$\begin{aligned} h_e^{l+1} &= \phi_1\left(\left\{x_j^l\right\}_{j \in e}\right) \\ \tilde{x}_i^{l+1} &= \phi_2\left(x_i^l, \left\{h_e^{l+1}\right\}_{e \in E_i}\right) \end{aligned}$$

HNNs are two-phase schemes: Messages are passed from nodes to hyperedges and then back to nodes (Huang and Yang, 2021).

Topological Characterizations

GNN on clique expansion outperforms HNN

Model (Encodings)	citeseer-CC (↑)	cora-CA (↑)	cora-CC (↑)	pubmed-CC (↑)	DBLP (↑)
GCN (No Encoding)	69.28 ± 0.28	76.51 ± 0.82	75.43 ± 0.26	84.66 ± 0.49	75.66 ± 0.81
GCN (HCP-FRC)	$\mathbf{71.03 \pm 0.51}$	78.43 ± 0.76	$\mathbf{76.61 \pm 0.31}$	84.78 ± 0.57	76.49 ± 0.90
GCN (HCP-ORC)	70.89 ± 0.54	79.25 ± 0.81	76.09 ± 0.70	85.12 ± 0.61	76.57 ± 0.85
GCN (EE H-19-RWPE)	69.63 ± 0.71	76.84 ± 0.69	75.92 ± 0.28	86.24 ± 0.63	76.18 ± 0.88
GCN (EN H-19-RWPE)	68.85 ± 0.91	77.19 ± 0.64	75.33 ± 0.35	$\mathbf{86.53 \pm 0.61}$	76.76 ± 0.84
GCN (Hodge H-20-LAPE)	69.61 ± 0.45	$\mathbf{79.61 \pm 0.85}$	75.62 ± 0.31	86.06 ± 0.52	$\mathbf{77.48 \pm 0.93}$
GCN (Norm. H-20-LAPE)	69.13 ± 0.77	78.13 ± 0.79	76.18 ± 0.29	85.78 ± 0.55	76.92 ± 0.88
UniGCN (No Encoding)	63.36 ± 1.76	75.72 ± 1.16	71.10 ± 1.37	75.32 ± 1.09	71.05 ± 1.40
UniGCN (HCP-FRC)	61.20 ± 1.83	74.64 ± 1.45	68.98 ± 1.59	67.37 ± 1.73	71.02 ± 1.43
UniGCN (HCP-ORC)	61.81 ± 1.70	75.03 ± 1.33	70.42 ± 1.17	71.64 ± 1.52	70.69 ± 1.62
UniGCN (EE H-19-RWPEE)	63.29 ± 1.52	75.34 ± 1.28	71.13 ± 1.24	74.61 ± 1.18	71.21 ± 1.53
UniGCN (EN H-19-RWPEE)	63.09 ± 1.62	75.30 ± 1.37	71.21 ± 1.34	74.61 ± 1.09	71.26 ± 1.47
UniGCN (Hodge H-20-LAPE)	63.46 ± 1.58	75.64 ± 1.37	71.31 ± 1.19	75.37 ± 1.01	70.71 ± 1.61
UniGCN (Norm. H-20-LAPE)	63.41 ± 1.61	75.55 ± 1.48	71.20 ± 1.24	75.30 ± 1.01	71.10 ± 1.33

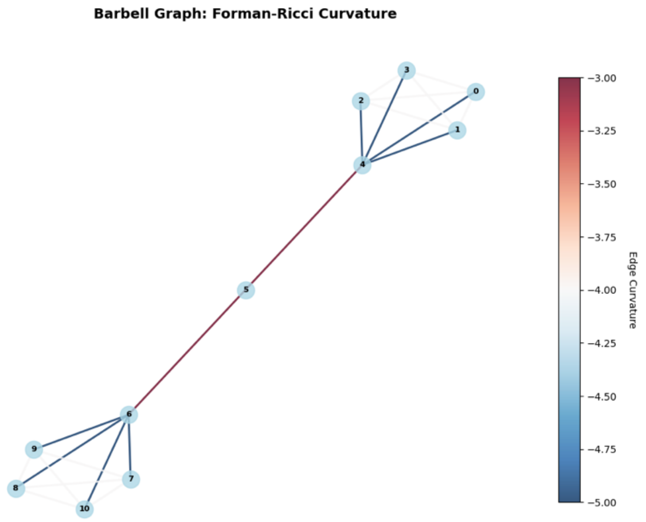
Enhancing Representational Power of GNNs

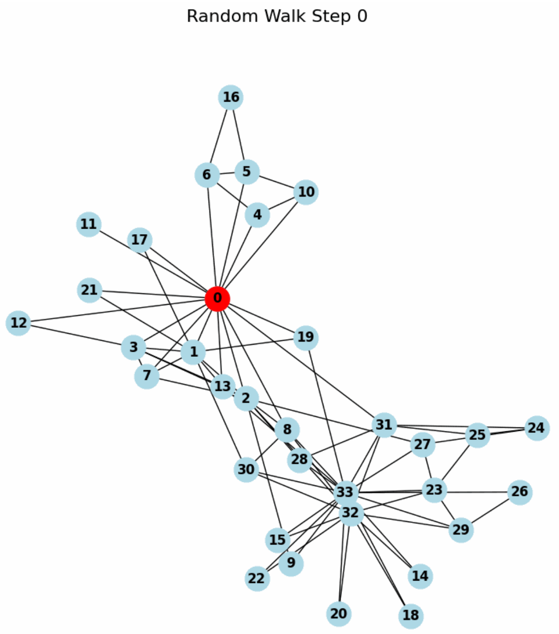
Can we endow GNNs with additional structure? Yes!

Data Augmentation: Encodings computed at the graph level

Structural (SE) and Positional (PE) encodings endow GNNs with information that it cannot learn on its own.

- Graph Laplacian
- Substructure counts
- Node degrees
- Discrete curvature
- Random walks statistics





Hypergraph-level Encodings

H-Encodings are more expressive than G-Encodings

How to best leverage higher-order relational information?
Augment graph with structural information, computed at the hypergraph-level.

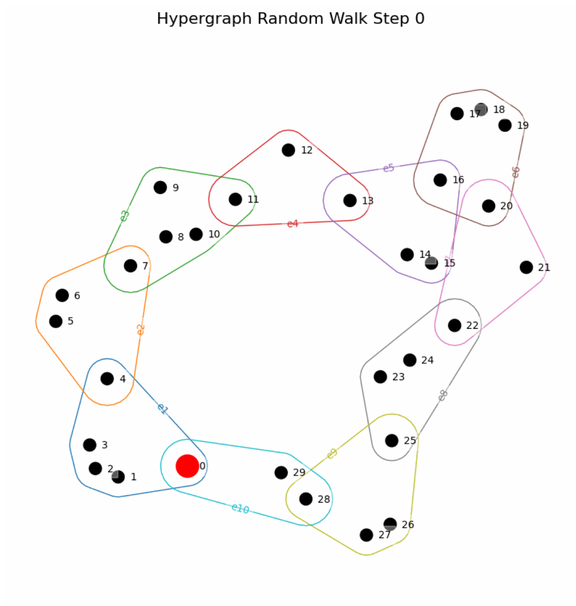
1. **Eigenvectors of the Hodge Laplacian (H-LAPE)**

$$H_0 = B_1^T B_1$$

$$H_1 = B_1 B_1^T.$$

$$(B_1)_{i,j} = \begin{cases} 1 \text{ if } i \prec j \\ 0 \text{ otherwise} \end{cases} \in \mathbb{R}^{V \times E}$$

2. **Hypergraph curvature (H-LCP)**
3. **Hyper-degree profiles (H-LDP)**
4. **Hypergraph random walk statistics (H-RWPE)**



Hypergraph-level Encodings

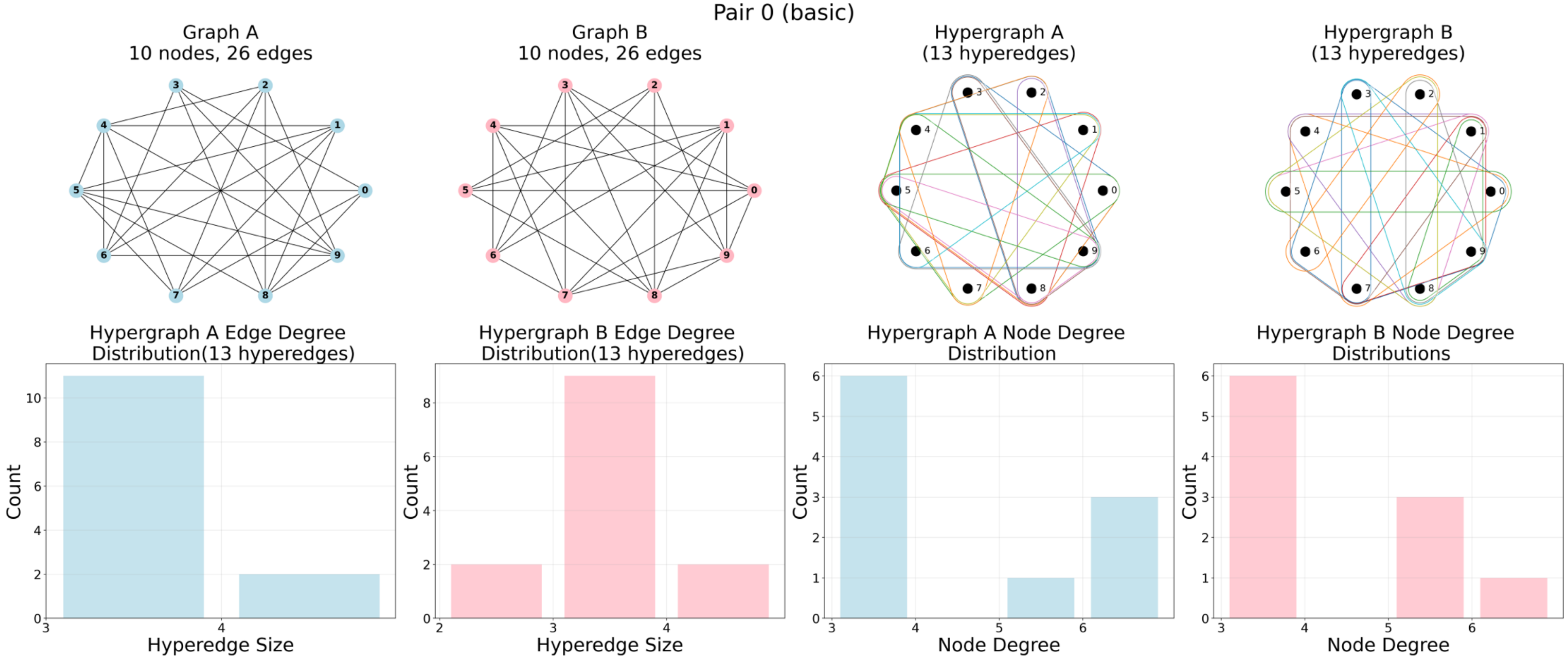
H-Encodings provide additional boost to GNNs compared to G-Encodings

Model (Encodings)	Collab (↑)	Imdb (↑)	Reddit (↑)
GCN (No Encoding)	61.94 ± 1.27	48.10 ± 1.02	67.87 ± 1.38
GCN (LCP-FRC)	68.36 ± 1.13	63.42 ± 1.47	79.53 ± 1.62
GCN (LCP-ORC)	70.48 ± 0.97	67.93 ± 1.55	80.75 ± 1.54
GCN (19-RWPE)	49.63 ± 2.38	50.41 ± 1.26	78.93 ± 1.60
GCN (20-LAPE)	58.33 ± 1.64	48.82 ± 1.31	77.26 ± 1.58
GCN (HCP-FRC)	$\mathbf{72.03 \pm 0.51}$	64.64 ± 0.88	82.09 ± 0.58
GCN (HCP-ORC)	70.82 ± 0.68	66.16 ± 0.75	80.35 ± 0.72
GCN (EE H-19-RWPE)	69.63 ± 0.71	$\mathbf{73.96 \pm 0.65}$	82.79 ± 0.62
GCN (EN H-19-RWPE)	68.85 ± 0.91	73.84 ± 0.48	$\mathbf{83.30 \pm 0.79}$
GCN (Hodge H-20-LAPE)	69.61 ± 0.45	71.38 ± 0.75	79.46 ± 0.82
GCN (Norm. H-20-LAPE)	69.13 ± 0.77	71.05 ± 0.82	80.08 ± 0.67

GNN with G-Encodings
vs. H-Encodings

Hypergraph-level Encodings

H-Encodings are more expressive than G-Encodings



Thank you!

https://arxiv.org/abs/2502.09570