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Investigating Hypernode Classification of Complex System Based on High-Order Graph Neural Networks

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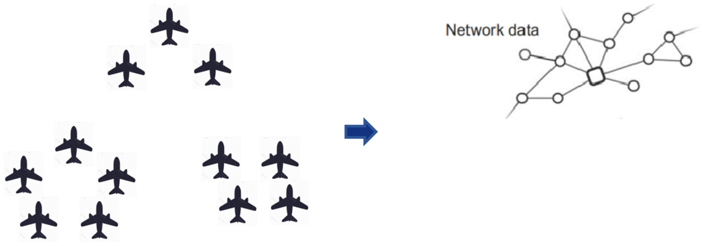
Motivations

Research of complex interactions in swarm control on networks motivates effective decision-making.

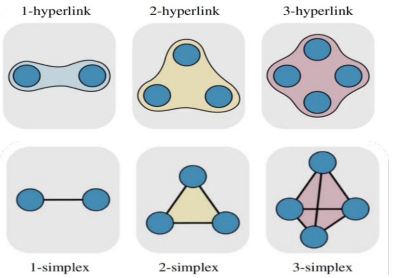
Swarm intelligence

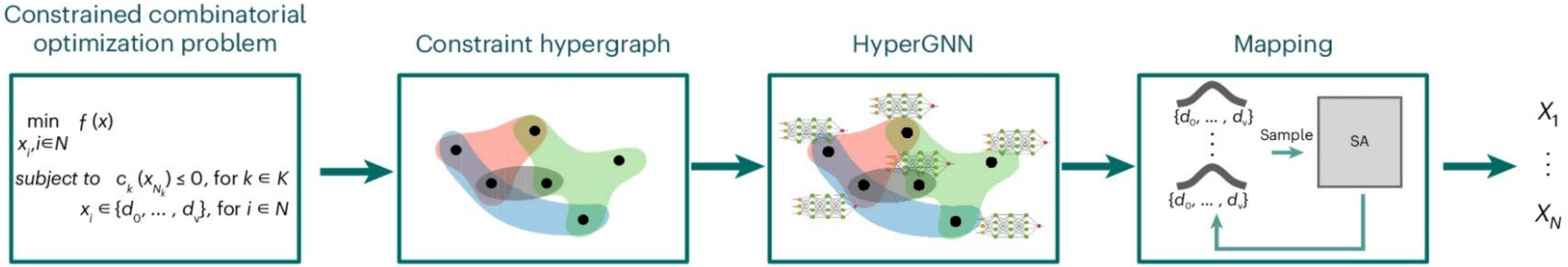
Multi-scenario decision



Formation grouping

➢ Hypergraph models High-dimensional Problems





➢ Research Difficulties

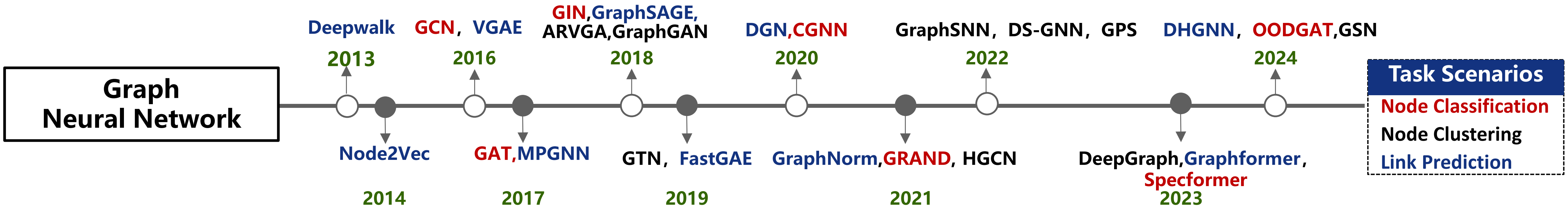
- Higher-order relations are ignored, some **unobserved labels are usually missing**
- Modeling of **high-order interactions** of different individuals **lacks explicit mathematical formulation**

Higher-order interactions, Incomplete and limited information, Hypernode labels prediction.

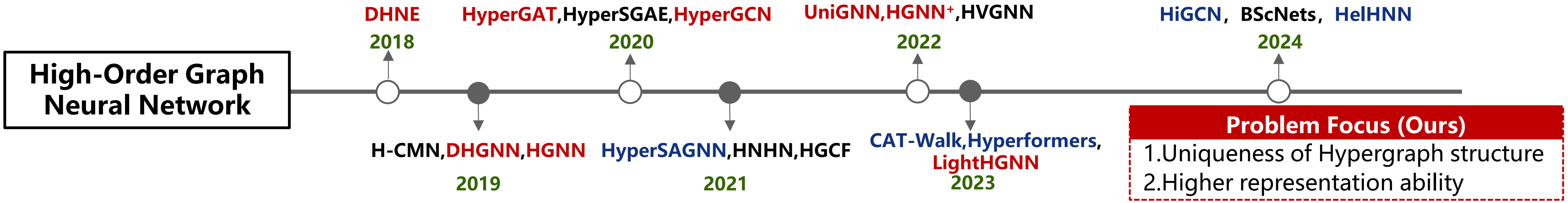
[1]Heydaribeni, N., Zhan, X., Zhang, R. et al. Distributed constrained combinatorial optimization leveraging hypergraph neural networks. Nat Mach Intell 6, 664–672 (2024).

Background and Challenges

- **Limitations: limited expressive ability**, GNNs only model binary relationships of nodes
- **Chanllenges :** GNNs fail to capture the **higher-order interactions** and influences



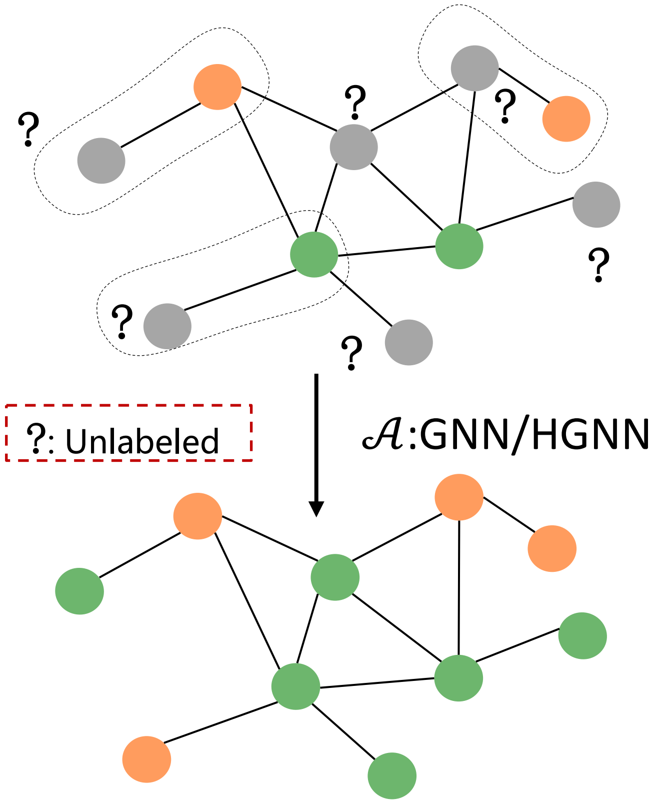
- **Limitations:** low hypernodes classification accuracy, HGNNs ignore **self-hyperedges** of nodes
- **Chanllenges:** HGNNs fail to **distinguish non-isomorphic hypergraphs** due to **poor representation**



How to fill the gap of Hypegraph Isomorphic Neural Networks in Hypernode Classification?

Problems: What is hypernode classification?

Definition 2. Hypernode classification $H(V,E)$, $V = (V_{labeled} \cup V_{unlabeled})$. $V_{unlabeled}$ is the nodes without labels, and the labels of $V_{unlabeled}$ are deduced using the labeled nodes $V_{labeled}$ in semi-supervised learning.



- 1-Graph Weisfeiler-Lehman label iteration $\mathcal{A}: G \to R^d$ (GNN)

$$\begin{cases} l_{G,u}^{(k)} = \{\{l_{G,i}^{(k)}\}\}_{i \in N(u)}, & \forall u \in V \\ l_{G,v}^{(k+1)} = \{\{l_{G,v}^{(k)}, l_{G,u}^{(k)}\}\}_{u \in N(v)}, & \forall v \in V \end{cases}$$

Neighborhood

- 1-Hypergraph Weisfeiler-Lehman label iteration $\mathcal{A}: H \to R^d$ $(HGNN)$

$$\begin{cases} l_{H,e}^{(k)} = \{\{l_{H,u}^{(k)}\}\}_{u \in e}, & \forall e \in E \\ l_{H,v}^{(k+1)} = \{\{l_{H,v}^{(k)}, l_{H,e}^{(k)}\}\}_{u \in E_v}, & \forall v \in V \end{cases}$$

High-order Interactions

Infering unlabeled nodes based on observed labels, Distinguishing non-isomorphic hypergraphs

[2] Feng, Y., Han, J., Ying, S., Gao, Y. Hypergraph isomorphism computation. IEEE Transactions on Pattern Analysis and Machine Intelligence. (2024)

Preliminaries: Hypergraph Weisfeiler-Lehman Test

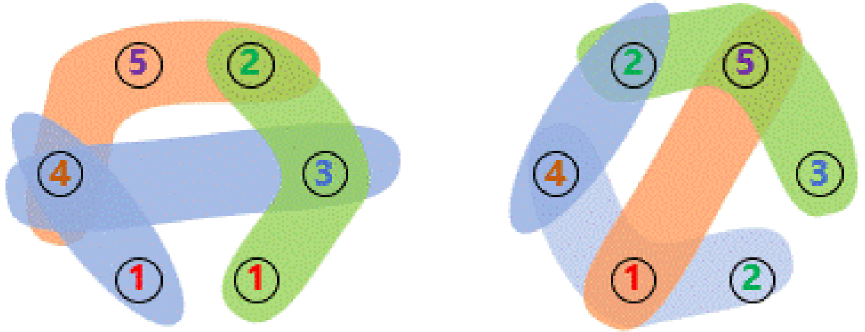
Lemma 1. (Sufficient Condition) Let $E_{H,v}$ denote the set of hyperedges of node v , $l_{H,v}^{(j)}$ and $h_{H,v}^{(j)}$ are the label and feature vector of node v in hypergraph H at iterations j , respectively. If for the iterations $0, 1, \ldots, k$,

$$\begin{cases} l_{H_1}^{(j)} = l_{H_2}^{(j)}, & \forall j \leq k \\ h_{H_1}^{(j)} = h_{H_2}^{(j)}, \forall j \leq k-1 & \end{cases}$$

then, for nodes $v_1 \in H_1$ and $v_2 \in H_2$, if $l_{H_1,v_1}^{(k)} = l_{H_2,v_2}^{(k)}$ holds, it follows that $h_{H_1,v_1}^{(k)} = h_{H_2,v_2}^{(k)}$ at iterations k.

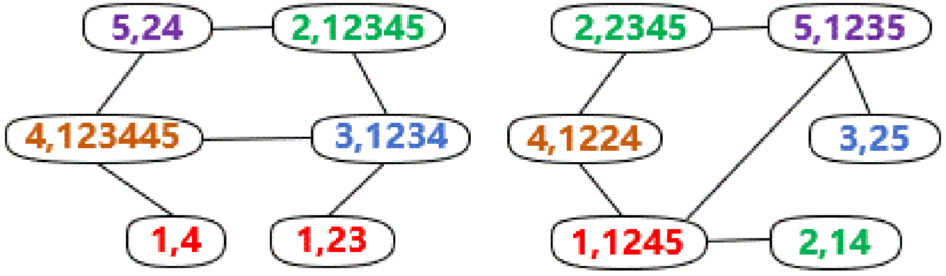
Lemma 2. (Necessary Condition) Let $\mathcal{A}: H \rightarrow R^d$ is a hypergraph neural network with k layers. If $\mathcal{A}$ maps two hypergraphs H_1 and H_2 such that $\mathcal{A}(H_1) \neq \mathcal{A}(H_1)$, then H_1 and H_2 are non-isomorphic decided by WL-test.

Step 1: Labled hypergraphs H_1 and H_2



$H_1 : l_{H_1}^{(0)}$ $H_2 : l_{H_2}^{(0)}$

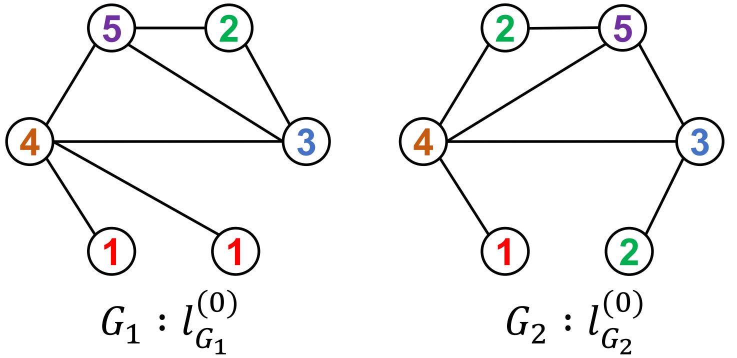
Step 2: Multiset-label upgraded by WL-test



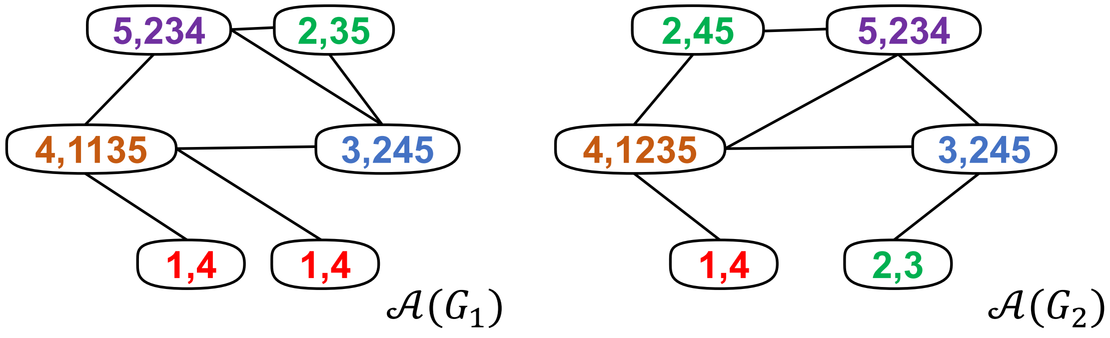
$\mathcal{A}(H_1)$ $\mathcal{A}(H_2)$

Preliminaries: Hypergraph Weisfeiler-Lehman Test

Step 1： Labled graphs G_1 and G_2



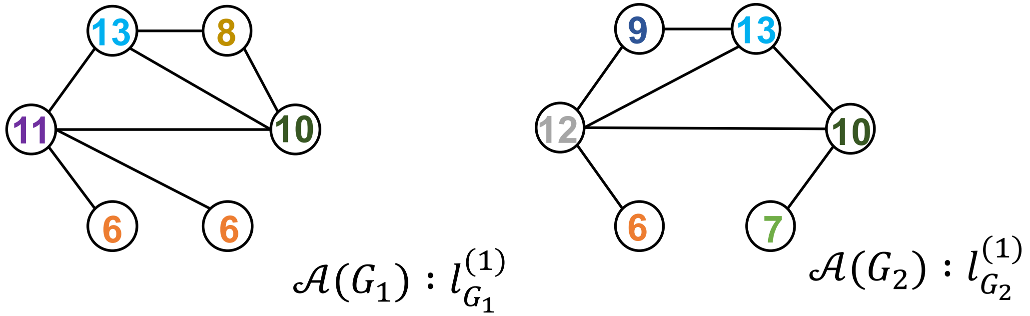
Step 2： Multiset-label upgraded by neighbors



Step 3： Label compression

1,4 → 6
2,3 → 7
2,35 → 8
2,45 → 9
3,245 → 10
4,1135 → 11
4,1235 → 12
5,234 → 13

Step 4： Relabel



$\varphi^{(1)}_{WLstree}(G_1)$ =(2,1,1,1,1, 2,0,1,0,1,1,0,1)

$\varphi^{(1)}_{WLstree}(G_2)$=(1,2,1,1,1, 1,1,0,1,0,1,1,1)

$\mathcal{A}(G_1) \neq \mathcal{A}(G_2)$ **non-isomorphic**

Multset Theory aggregates community information, members are divided into different groups

Self-Hypergraph Isomorphic networks (Our Theorem)

Theorem 1. (Equivalence) Let $\mathcal{A}: H \rightarrow R^d$ be a **hypergraph neural network** with k layers. If $\mathcal{A}$ maps H_1 and H_2 that are non-isomorphic by the **Weisfeiler-Lehman (WL) test** to different embeddings, then $\mathcal{A}$ satisfies the following conditions:

1. Iterative Aggregation and Update of Node Features:

High-order interactions information aggregation

$$h_{H,v}^{(k)} = \boldsymbol{\phi_1}\left(\left\{\left\{\left(h_{H,v}^{(k-1)}, \boldsymbol{\phi_2}\left(\left\{h_{H,u}^{(k-1)}\right\}_{u \in e}\right)\right)\right\}\right\}\right)$$

Update the labels information operations

where ϕ_1 and ϕ_2 are **injective functions.**

2. Injective Graph-Level Readout Function: The function $\mathcal{A}$ **operates injectively** on the multisets.

Self-hypergraph Isomorphic Network (SHGIN): Multi-layer Linear Perceptron (MLP) is employed to learn ϕ_1, and hyperedges aggregation models ϕ_2, defined as

$$h_{H,v}^{(k)} = \boldsymbol{MLP^{(k)}}\left((1+\epsilon^{(k)}) \cdot h_{H,v}^{(k-1)}, + \sum_{e \in \tilde{E}_v} \boldsymbol{h_{H,e}^{(k-1)}}\right)$$

where ϵ is a parameter, $\tilde{E}_v$ denotes the set of hyperedges of node v and the self-hyperedges.

Theorem and Experimental Results

- **Hypergraph Weisfeiler-Lehman Test Theorem:** distinguish the non-isonorphic hypergraphs, demonstrate the equivalent conditions between hypergraph Weisfeiler-Lehman and hypergraph neural networks
- **SHGIN Algorithm:** introduce **Multi-layer Linear Perceptron (MLP)** and **hyperedges aggregation** to model injective functions, thereby capturing higher-order interactions

Methods	Co-authorship	
	Cora	DBLP
GCN*	70.3 ± 4.75	88.2 ± 0.57
GraphSAGE*	71.8 ± 3.59	87.3 ± 0.31
GIN*	61.2 ± 2.93	76.5 ± 0.54
HGNN	59.2 ± 3.19	76.4 ± 0.39
HGNN $^{+}$	63.2 ± 2.73	77.1 ± 0.57
HyperGCN	54.5 ± 1.17	75.9 ± 0.56
HyperSAGE	68.4 ± 1.39	78.1 ± 0.42
HNHN	69.3 ± 2.13	85.1 ± 0.49
UniGCN	69.9 ± 0.55	87.5 ± 0.41
UniGCNII	68.7 ± 0.91	88.4 ± 0.78
UniGAT	71.1 ± 0.78	88.4 ± 0.57
UniSAGE	73.9 ± 1.19	88.6 ± 0.81
UniGIN	74.3 ± 1.29	88.5 ± 0.14
SHGIN(ours)	**76.6 ± 1.12** ↑	**89.1 ± 0.27** ↑

Methods	Co-citation	
	Citeseer	PubMed
GCN*	71.7 ± 0.65	77.4 ± 0.91
GraphSAGE*	70.6 ± 0.29	76.4 ± 0.75
GIN*	53.8 ± 0.37	74.7 ± 0.41
HGNN	54.7 ± 0.52	78.3 ± 0.57
HGNN $^{+}$	60.6 ± 0.47	**78.5 ± 0.30**
HyperGCN	62.7 ± 0.61	75.9 ± 0.43
HyperSAGE	69.3 ± 0.19	78.5 ± 0.61
HNHN	64.8 ± 0.35	40.7 ± 0.13
UniGCN	71.2 ± 0.47	78.1 ± 0.57
UniGCNII	68.9 ± 0.69	72.6 ± 1.03
UniGAT	70.9 ± 0.68	78.2 ± 0.48
UniSAGE	71.1 ± 0.94	78.1 ± 0.93
UniGIN	72.5 ± 0.86	77.3 ± 0.74
SHGIN(ours)	**72.7 ± 0.13** ↑	78.3 ± 0.26

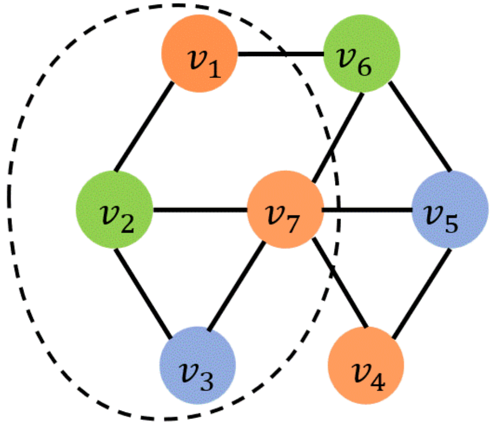
↑ Improvement

Higher hypernode classification accuracy on Co-citation and Co-authorship datasets

Contributions and Innovations

- Contribution 1. Propose self-hypergraph isomorphic network (SHGIN) to address the limitations of structural isomorphism, achieve **higher accuracy of hypernode classification** than GNN and HGNN models
- Contribution 2. Demonstrate **equivalence** between hypergraph Weisfeiler-Lehman (WL) test and hypergraph neural networks (HGNNs), and further prove **the upper bound of HGNNs' expressive ability**

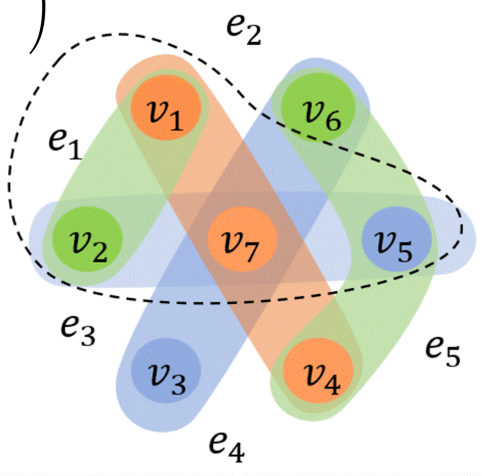
GNN Message Passing Mechanism



$$\begin{cases} h_u = \phi_2(\{x_i:\ i \in N(u)\}) \\ \tilde{x}_v = \phi_1(x_v + \{h_u\}_{u\in N(v)}) \end{cases}$$

SHGIN Message Passing Mechanism(Ours)

$$h_{H,v}^{(k)} = \boldsymbol{MLP}^{(k)}\left((1+\epsilon^{(k)})\cdot h_{H,v}^{(k-1)}, + \sum_{e\in\tilde{E}_v} \boldsymbol{h}_{H,e}^{(k-1)}\right)$$



- **Theory Innovations**

1. Explicit mathematical formulation

2. Distinguishing non-isomorphic hypergraph structure

equivalent conditions

3. Maximum theoretical Upper bound of Hypergraph neural network

Conclusions and Expectations

To investigate high-order interactions in complex systems, we propose **Self-Hypergraph Isomorphic Neural Network (SHGIN) :**

- Present an **explicit mathematical formulation of high-order interactions,** and define the **equivalent conditions** for hypergraph neural networks to the Weisfeiler-Lehman Test.
- SHGIN algorithm outperforms graph neural network (GNN) and hypergraph neural network (HGNN) models. **Average accuracy of improvement was 1.83%** on Co-authorship datasets.
- Future expectations: **Evolution** of high-order interactions in dynamic hypergraph, **Node Importance Estimation** on heterogeneous hypergraphs

➢ References

[1] Heydaribeni, N., Zhan, X., Zhang, R. et al. Distributed constrained combinatorial optimization leveraging hypergraph neural networks. Nat Mach Intell 6, 664–672 (2024).
[2] Feng, Y., Han, J., Ying, S., Gao, Y. Hypergraph isomorphism computation. IEEE Transactions on Pattern Analysis and Machine Intelligence. (2024)
[3] Bouritsas, G., Frasca, F., Zafeiriou, S., Bronstein, M. M. . Improving graph neural network expressivity via subgraph isomorphism counting. IEEE Transactions on Pattern Analysis and Machine Intelligence(Vol. 45, No. 01, pp. 657-668).(2022).

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Thanks For Attention

Changsha, China

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