Higher-order Graph Convolutional Network with Flower-Petals Laplacians on Simplicial Complexes

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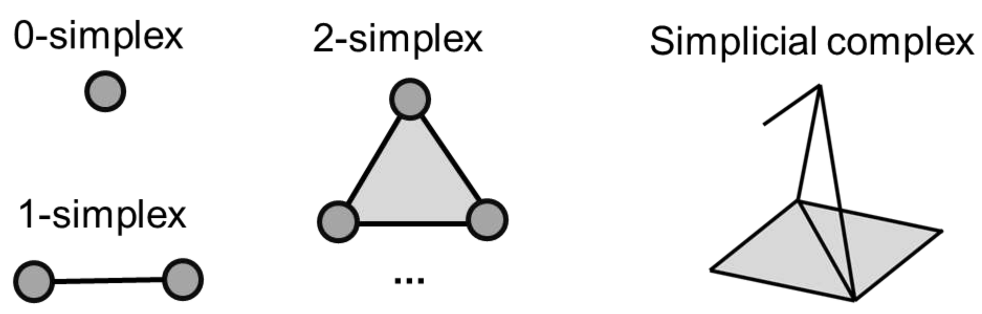
Why?

1.Pairwise networks can't capture higher-order interactions.



2. The expressiveness of classical GNNs is upper bounded by WL test.

3. Higher-order + GNN ≫ GNN

4. Existing higher-order GNNs are limited by their high **complexity** and **low flexibility**.

Method

1. Flower-petals (FP) model:

- Flower petals adjacency matrices:

$$\tilde{\mathcal{A}}_p = \frac{1}{p+1} D_{p,v}^{-1/2} \mathcal{H}_p \mathcal{H}_p^{\intercal} D_{p,v}^{-1/2}$$

- Flower petals Laplacians:

$$\mathcal{L}_p = I - \tilde{\mathcal{A}}_p$$

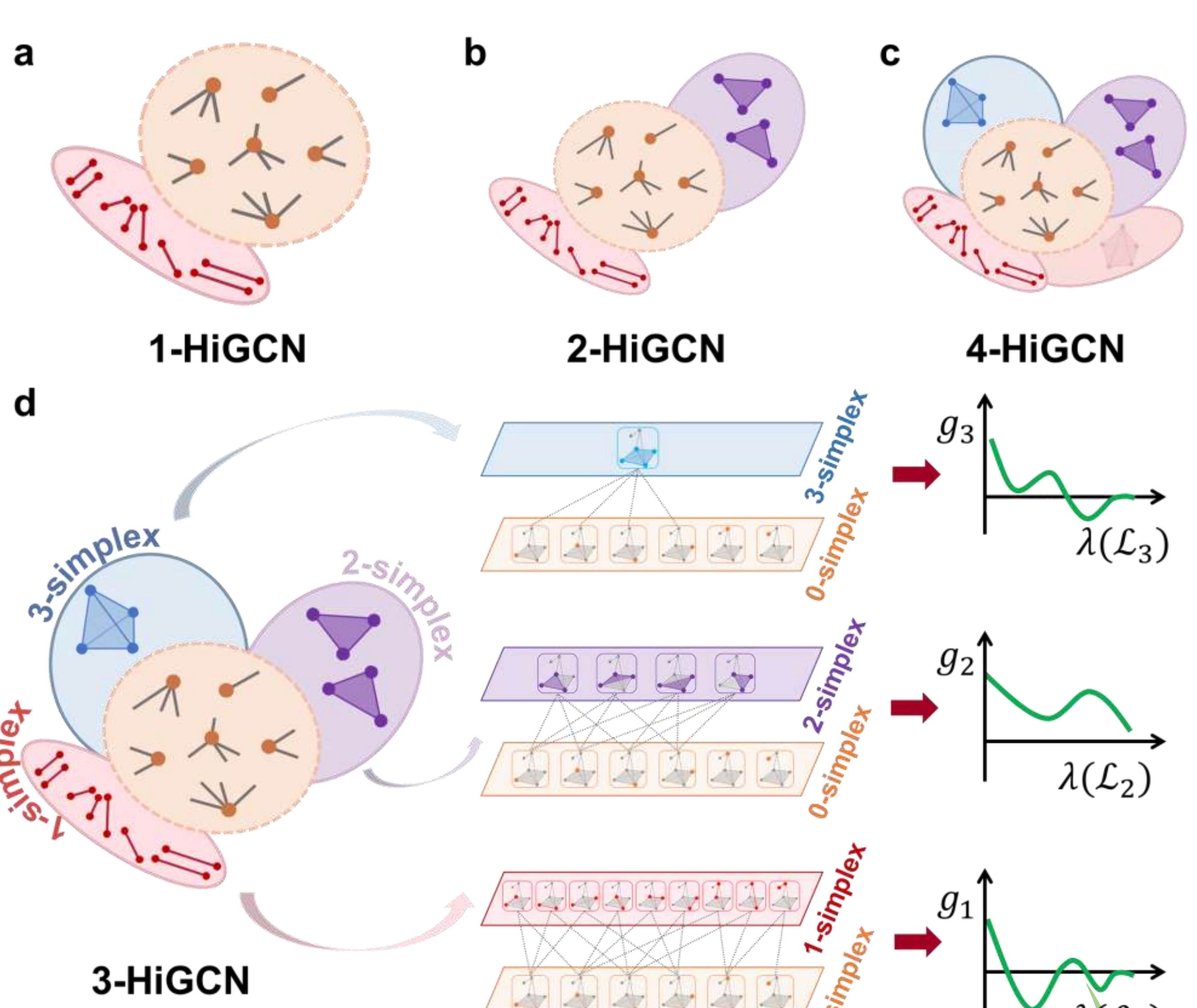
Theorem1: FP adjacency matrices $\tilde{\mathcal{A}}_p$ and FP Laplacian matrices $\mathcal{L}_p$ are both symmetric positive semidefinite.

$$\left(0 \le \lambda(\tilde{\mathcal{A}}_p),\ \lambda(\mathcal{L}_p) \le 1\right)$$

2. HiGCN Model:

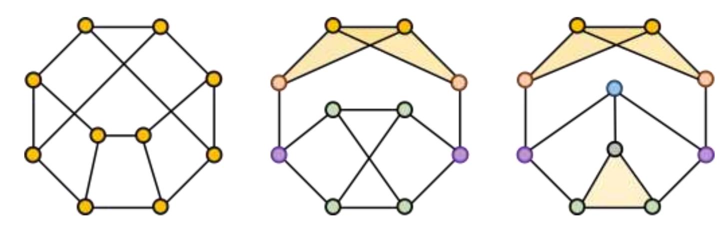
$$Y = \Big\Vert_{p=1}^{P} \left(\left(\sum_{k=0}^{K} \gamma_{p,k} \tilde{\mathcal{A}}_p^k X \Theta_p \right) W \right)$$

HiGCN is **highly-scalable**



Expressive Ability

Define the higher-order version WL test (**HWL**) and simplified higher-order WL test (**SHWL**)



Theorem2: SHWL with clique complex lifting is strictly more powerful than the WL test.

HiGCN is more expressive than traditional GCNs.

Relation to other GCNs

HiGCN generalizes pairwise graph-based GCNs, showing superiority for exploiting higher-order information.

Model	Convolution Filter	Spectral	Learnable
GCN (Kipf and Welling 2017)	$(1-\lambda)^K$	Graph Laplacian	✗
APPNP (Gasteiger, Bojchevski, and Günnemann 2019)	$\sum_{k=0}^{K} \frac{\gamma^k}{1-\gamma}(1-\lambda)^k$	Graph Laplacian	✗
GPRGNN (Chien et al. 2020)	$\sum_{k=0}^{K} \gamma_k (1-\lambda)^k$	Graph Laplacian	γ_k
ChebNet (Defferrard, Bresson, and Vandergheynst 2016)	$\sum_{k=0}^{K} \gamma_k \cos(k \arccos(1-\lambda))$	Graph Laplacian	γ_k, K
SNN (Ebli, Defferrard, and Spreemann 2020)	λ^K	Hodge Laplacian	✗
SCoNe (Roddenberry, Glaze, and Segarra 2021)	$\lambda_{down}^K, \lambda_{up}^K$	Hodge Laplacian	✗
SCNN (Yang, Isufi, and Leus 2022)	$\sum_{k=0}^{K_1} \gamma_{d,k} \lambda_{down}^k + \sum_{k=0}^{K_2} \gamma_{u,k} \lambda_{up}^k$	Hodge Laplacian	✗
BScNets (Chen, Gel, and Poor 2022)	$f(\lambda_1, \lambda_2, \cdots, \lambda_P; \theta)^K$	Block Hodge Laplacian	θ
HiGCN (Ours)	$\sum_{k=0}^{K} \gamma_{p,k} (1-\lambda_p)^k, p = 1, 2, \cdots, P$	FP Laplacian	$\gamma_{p,k}$

Experiments

Superior in node/graph classification & simplicial data imputation

SCs	Method	10%	30%	50%	70%
History	SNN	0.201±0.013	0.354±0.016	0.495±0.002	0.661±0.002
	SGAT	0.180±0.010	0.330±0.002	0.432±0.016	0.602±0.005
	SGATEF	0.200±0.002	0.340±0.017	0.454±0.021	0.633±0.012
	HiGCN	**0.258**±0.004	**0.438**±0.002	**0.579**±0.005	**0.666**±0.009
Geology	SNN	0.265±0.022	0.417±0.004	0.594±0.02	0.704±0.003
	SGAT	0.223±0.004	0.345±0.030	0.599±0.009	0.631±0.008
	SGATEF	0.230±0.002	0.369±0.018	0.615±0.031	0.682±0.012
	HiGCN	**0.463**±0.012	**0.565**±0.007	**0.644**±0.014	**0.708**±0.002
DBLP	SNN	0.222±0.021	0.348±0.008	0.496±0.005	0.668±0.003
	SGAT	0.210±0.015	0.279±0.054	0.487±0.022	0.643±0.017
	SGATEF	0.223±0.004	0.311±0.002	0.491±0.008	0.678±0.005
	HiGCN	**0.385**±0.011	**0.511**±0.004	**0.587**±0.021	**0.685**±0.002

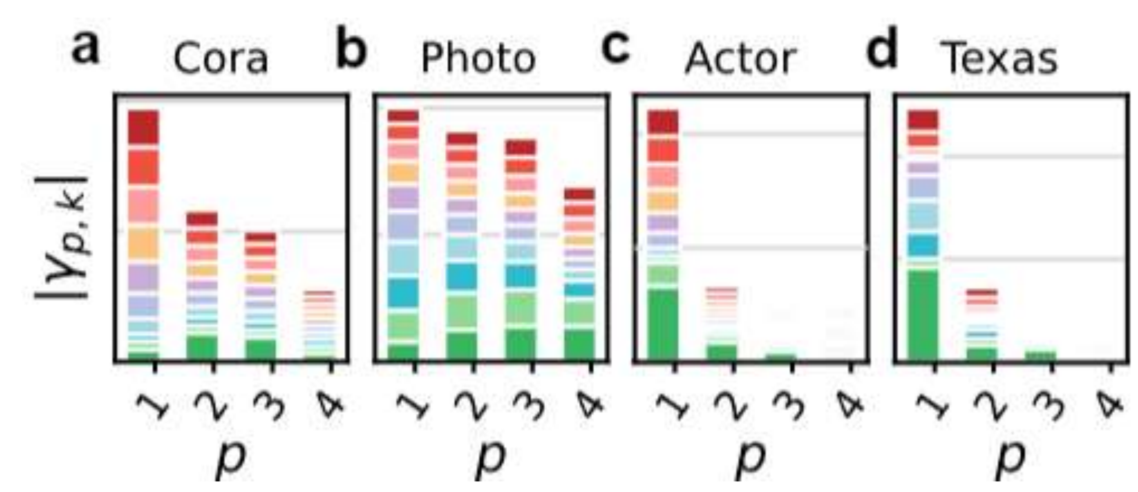
Dataset	PROTEINS	MUTAG	PTC	IMDB-B	IMDB-M
RWK	59.6±0.1	79.2±2.1	55.9±0.3	N/A	N/A
GK (k=3)	71.4±0.3	81.4±1.7	55.7±0.5	N/A	N/A
PK	73.7±0.7	76.0±2.7	59.5±2.4	N/A	N/A
WL kernel	75.0±3.1	90.4±5.7	59.9±4.3	73.8±3.9	50.9±3.8
DCNN	61.3±1.6	N/A	N/A	49.1±1.4	33.5±1.4
DGCNN	75.5±0.9	85.8±1.8	58.6±2.5	70.0±10.9	47.8±10.9
IGN	76.6±5.5	83.9±13.0	58.5±6.9	72.0±5.5	48.7±3.4
GIN	76.2±2.8	89.4±5.6	64.6±7.0	75.1±5.1	52.3±2.8
PPGNs	**77.2**±4.7	90.6±8.7	66.2±6.6	73.0±15.8	50.5±3.6
Natural GN	71.7±1.0	89.4±1.6	**66.8**±1.7	73.5±2.0	51.3±1.5
MPSN	76.7±4.6	89.8±5.5	61.8±9.1	75.6±3.2	52.4±2.9
HiGCN	77.0±4.2	**91.3**±6.4	66.2±6.9	**76.2**±5.1	**52.7**±3.5

Quantify Higher-order Strength

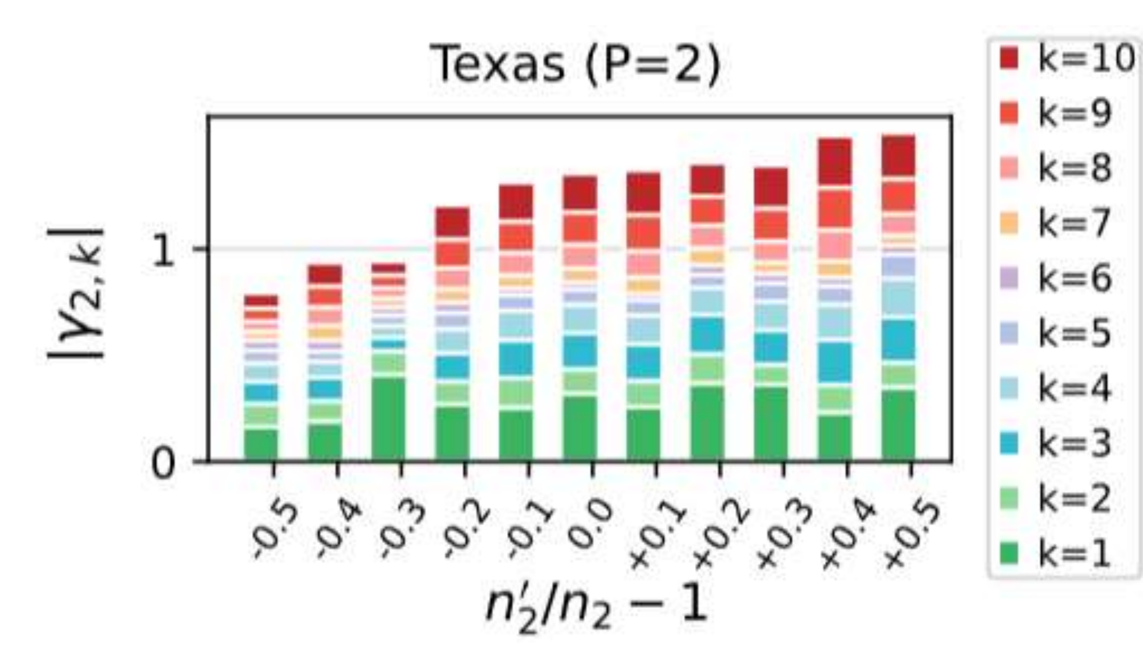
- Higher-order Strength:

$$S_p = \sum_{k=0}^{K} |\gamma_{p,k}|$$

- The higher-order strength **decreases** with the **increase** of order p.
- The decreasing phenomenon is more prominent in **heterogeneous** graphs.



- We modulate the quantity of higher-order structures as in 1k null models, observing that S_2 and HiGCN's accuracy ranking improves as the density of higher-order structures rises.



ρ_2	0	10%	20%	30%	40%	50%
MLP	91.45±1.14	91.02±0.98	91.90±0.95	91.18±1.11	91.74±0.92	91.05±0.95
GCN	75.16±0.96	64.36±1.83	64.89±2.16	64.07±1.93	62.92±2.34	64.75±2.16
GAT	78.87±0.86	79.97±1.03	78.89±1.07	78.20±1.20	77.28±1.30	77.93±1.42
ChebNet	86.08±0.96	82.10±1.52	83.08±1.09	79.21±1.55	81.34±1.48	81.41±1.34
BernNet	**93.12±0.65**	**92.10±0.95**	92.89±0.92	**92.33±1.08**	91.54±1.02	91.57±1.21
GGCN	85.81±1.72	85.95±1.42	85.51±1.67	83.84±1.70	91.15±1.02	83.95±1.73
APPNP	90.98±1.64	89.87±1.01	89.31±1.05	89.08±0.98	90.39±1.10	89.57±1.10
GPRGNN	92.95±1.30	86.10±2.76	88.16±1.13	83.05±2.05	84.69±1.77	83.54±2.72
HiGCN	92.15±0.73	91.70±1.06	**93.11±0.87**	91.64±1.14	**91.93±0.84**	**92.24±1.41**
Rank	3	2	**1**	2	**1**	**1**

Conclusion

- **New representation**

Propose a novel higher-order representation, which can easily model the interactions between different order simplices and is **highly scalable**.

- **New model**

We propose a higher-order GNN model based on this novel representation with superior expressiveness.

- **New perspective**

We quantify the strength of higher-order interactions in a **data-driven** manner.

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Complex Networks