Beyond Homophily in Graph Neural Networks: Current Limitations and Effective Designs

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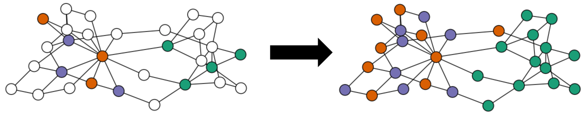
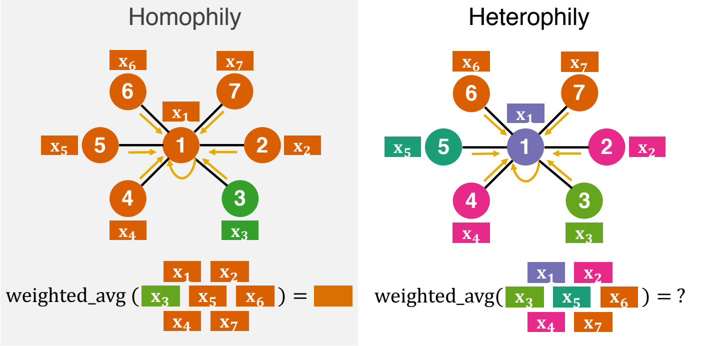
Limitations of GNNs Beyond Homophily

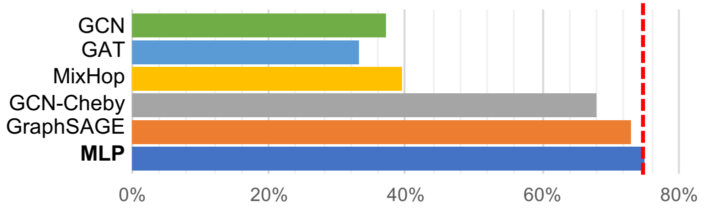
Task: semi-supervised node classification with node features



Problem: many popular GNN models (e.g. GCN) rely on assumed **homophily** and fail to generalize in **heterophily**.



Observation: In heterophily, existing methods have worse classification accuracy than graph-agnostic MLP.



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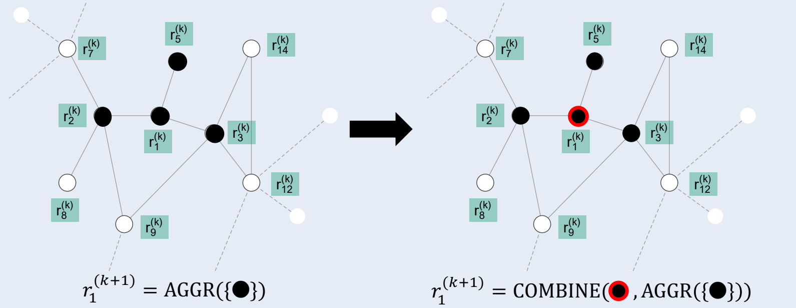
Effective Designs for GNNs in Heterophily

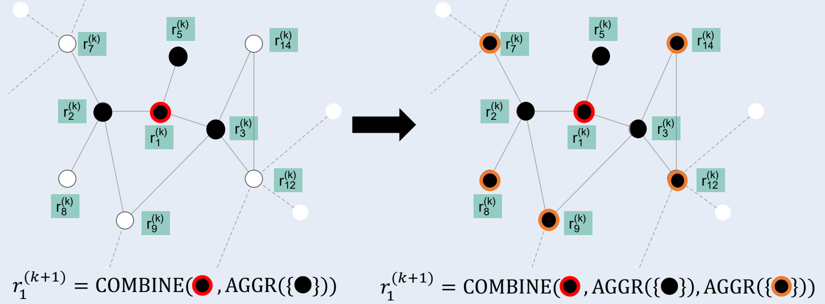
Design D1: Model the of ego- and neighbor-embeddings distinctly (per layer).

- In heterophily, neighbors may have information complementary to ego.



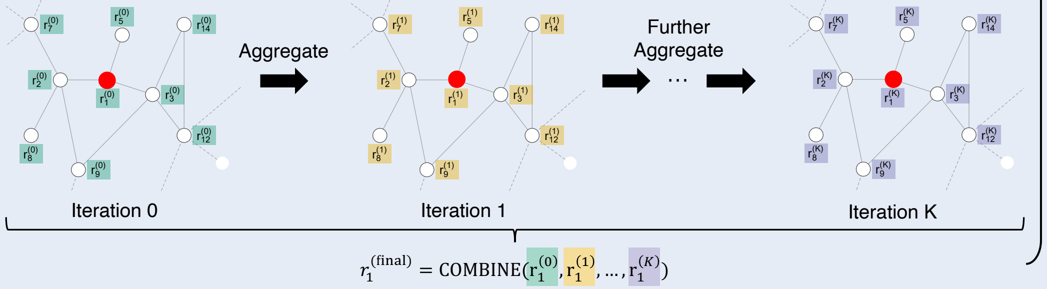
Design D2: Leverage representations of neighbors at different hops distinctly (per layer).

- Under heterophily, higher-order neighborhoods may still show homophily.



Design D3: Leverage the intermediate representations distinctly (at the final layer).

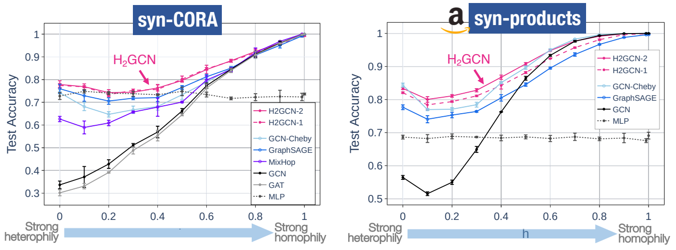
- Information with different locality contains different frequency components.



H2GCN

Empirical Analysis

Synthetic Benchmarks



Edge homophily ratio $h = \frac{\textit{intra-class edges}}{\textit{total edges}}$

- H_2GCN, our base model effectively combining all designs, has the best trend overall.
- Ablation study on H_2GCN shows effectiveness of each design, which results in up to 40% performance gain in heterophily.

Real Benchmarks

- In heterophily, models leveraging all or subsets of the designs perform significantly better than methods lacking them (e.g. GCN, GAT):
  - GraphSAGE (D1) vs. GCN: up to +23%
  - GCN-Cheby (D2) vs. GCN: up to +20%
  - GCN+JK (D3) vs. GCN: up to +14%

Method (Designs)	Average Rank Het.	Hom.	Overall
H_2GCN-1 (D1, D2, D3)	3.8	3.0	3.6
H_2GCN-2 (D1, D2, D3)	4.0	2.0	3.3
GraphSAGE (D1)	5.0	6.0	5.3
GCN-Cheby (D2)	7.0	6.3	6.8
MixHop (D2)	6.5	6.0	6.3
GraphSAGE+JK (D1, D3)	5.0	7.0	5.7
GCN-Cheby+JK (D2, D3)	3.7	7.7	5.0
GCN+JK (D3)	7.2	8.7	7.7
GCN	9.8	5.3	8.3
GAT	11.5	10.7	11.2
GEOM-GCN*	8.2	4.0	6.8
MLP	6.2	11.3	7.9

Detailed Results, Theorems & Code

GemsLab/H2GCN