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

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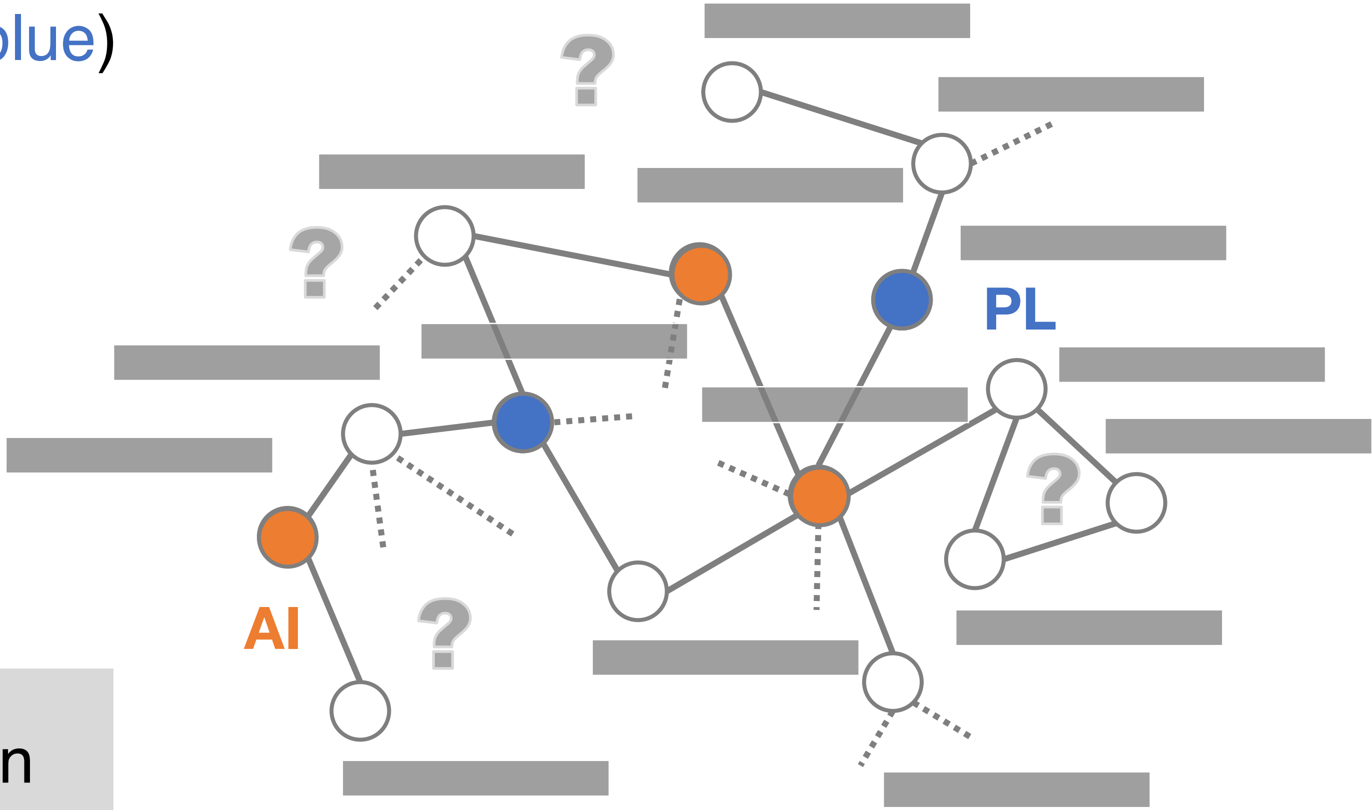
Semi-supervised Node Classification

- **Given** a graph $\mathcal{G} = (V, E)$ with adjacency matrix $\mathbf{A}$;
  feature vector $\mathbf{x}$ for each node;
  a few labeled nodes (orange/blue)
- **Find** the class label for each of the remaining nodes.

Graph Neural Networks (GNNs) are effective and widely-adopted approaches for this problem.

However, many existing GNNs relies on the homophily assumption in the network.

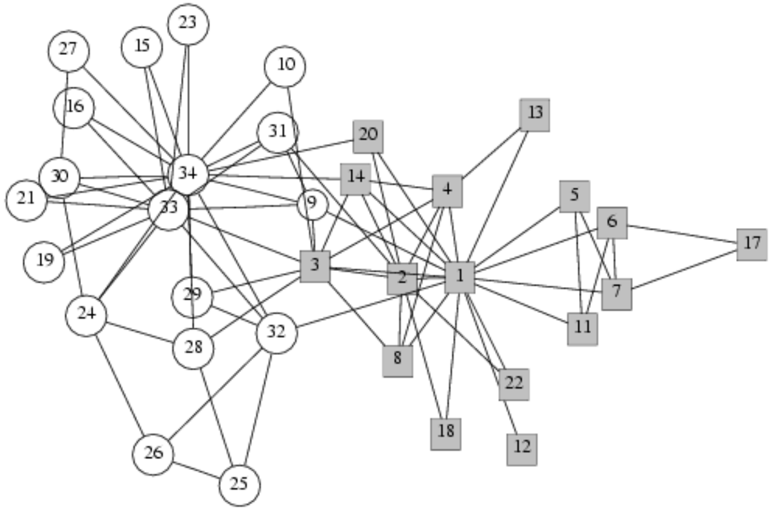


Graphs: Homophily and the Beyond

Homophily

"Birds of a feather, flock together"
Majority of linked nodes are similar

- Social Networks (wrt. political beliefs, age)
- Citation Networks (wrt. research area)

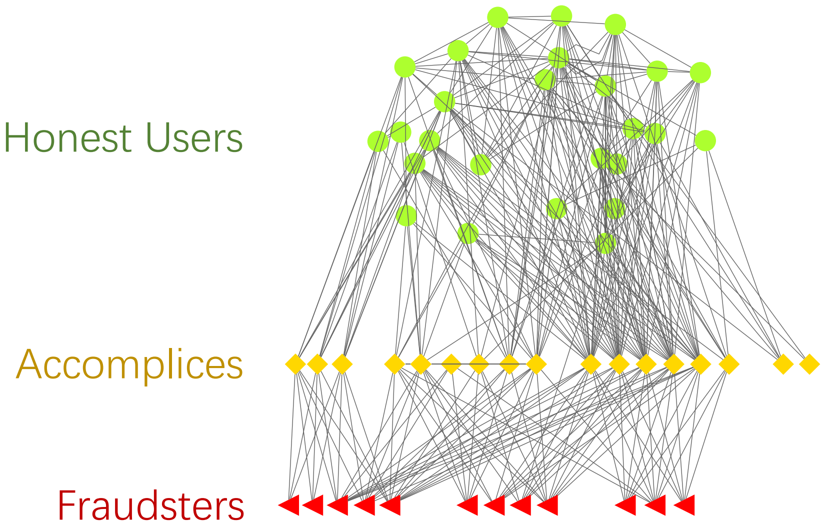


Zachary's Karate Club

Heterophily

"Opposites Attract"
Majority of linked nodes are different

- Friend network (e.g., talkative / silent friends)
- Protein structures (wrt. amino acid types)
- E-commerce (wrt. fraudsters / accomplices)



Auction Network

Largely Overlooked

[Newman *Networks18*, Newman *04*, Lee+ *arXiv18*, Chau+ *ECML/PKDD06*]

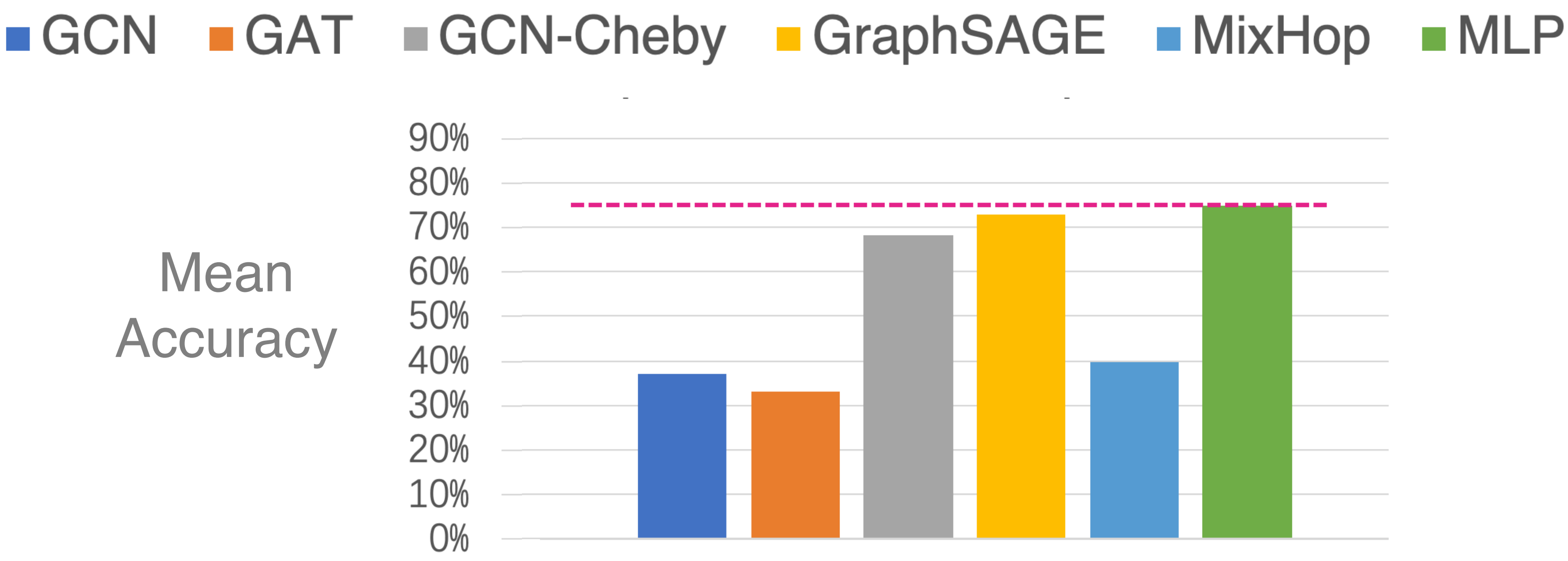
Our Contributions

We reveal current limitations of GNNs in **heterophily**.

We identify **key design choices** that boost learning in heterophily, without sacrificing in homophily, and analyze them theoretically.

We conduct **extensive empirical evaluation** across the full spectrum of low-to-high homophily, which confirms the effectiveness of the designs.

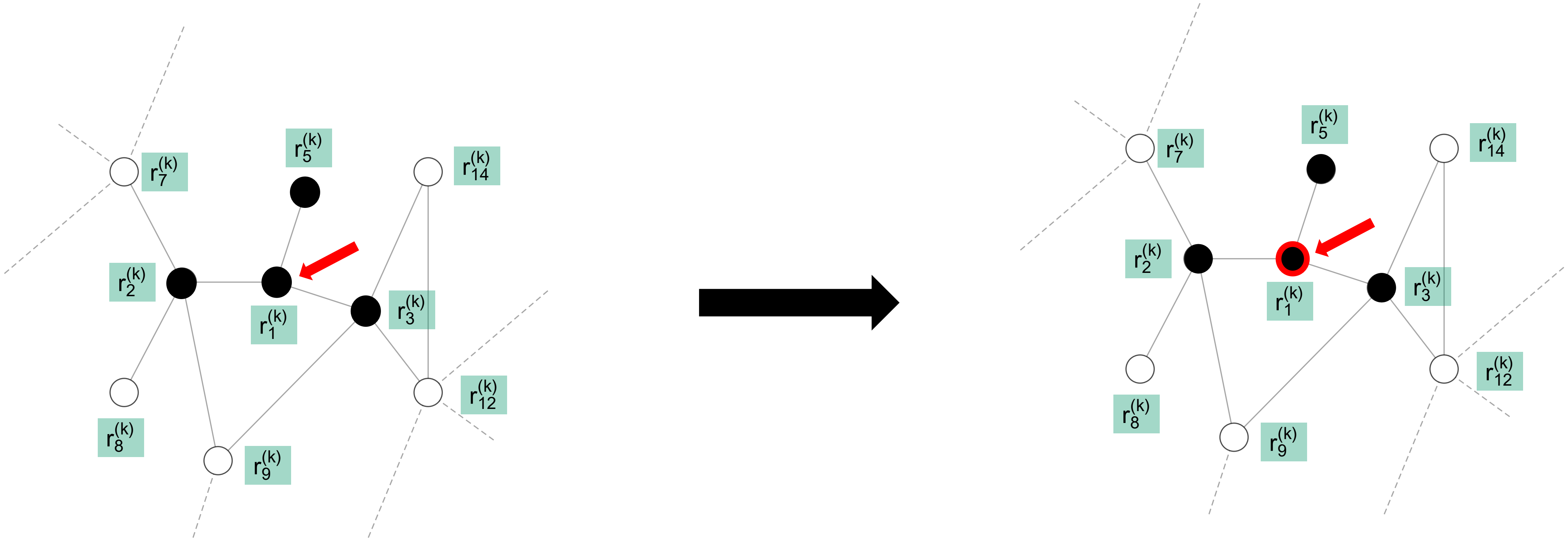
Current Limitations of GNNs in Heterophily



Under heterophily, all existing methods fail to perform better than Multilayer Perceptron (MLP), which is graph agnostic.

Designs for Boosting Learning in Heterophily

- (D1) Ego- and Neighbor-embedding Separation;

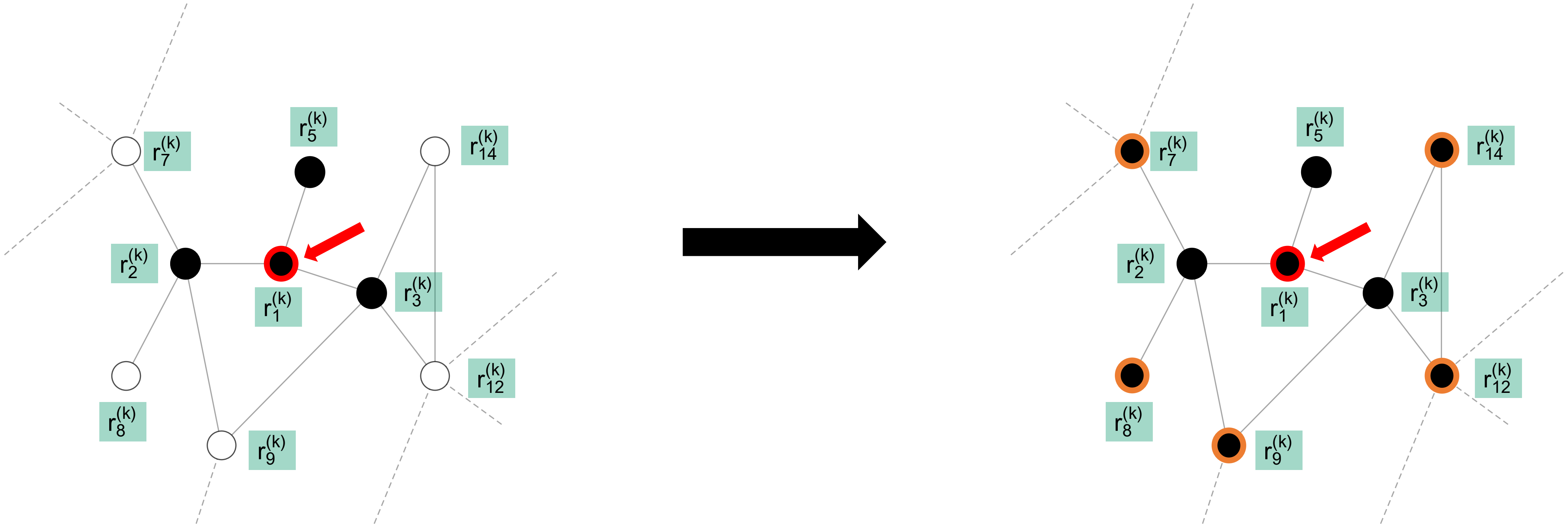


$r_1^{(k+1)} = \mathrm{AGGR}(\{\bullet\})$

$r_1^{(k+1)} = \mathrm{COMBINE}(\bullet, \mathrm{AGGR}(\{\bullet\}))$

Designs for Boosting Learning in Heterophily

- (D1) Ego- and Neighbor-embedding Separation;
- (D2) Higher-order Neighborhoods;

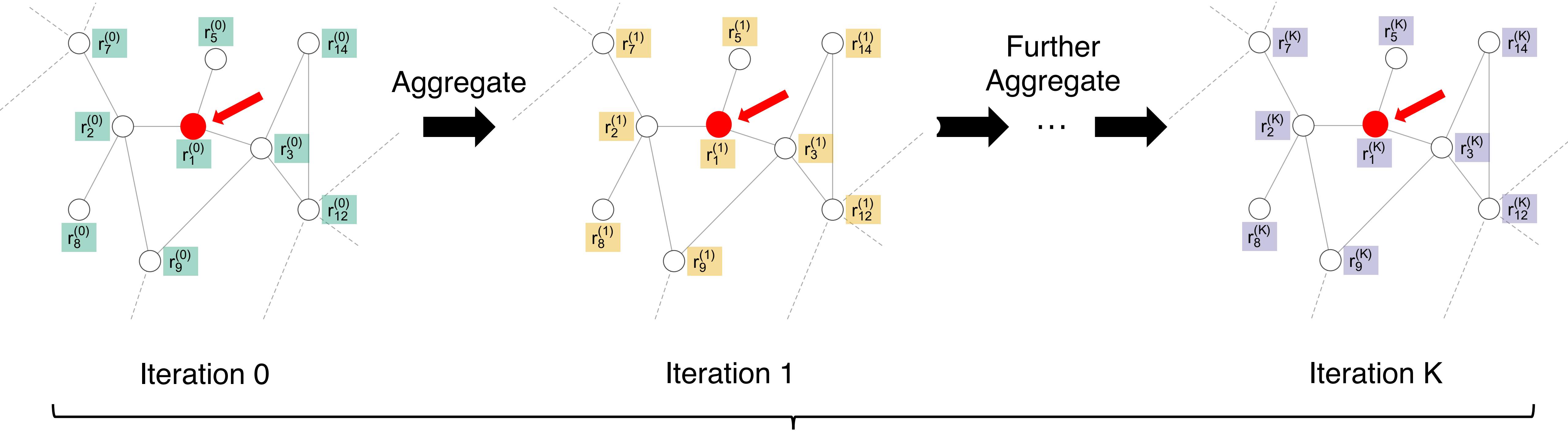


$r_1^{(k+1)} = \mathrm{COMBINE}(\bullet, \mathrm{AGGR}(\{\bullet\}))$

$r_1^{(k+1)} = \mathrm{COMBINE}(\bullet, \mathrm{AGGR}(\{\bullet\}), \mathrm{AGGR}(\{\bullet\}))$

Designs for Boosting Learning in Heterophily

- (D1) Ego- and Neighbor-embedding Separation;
- (D2) Higher-order Neighborhoods;
- (D3) Combination of Intermediate Representations.



$$r_1^{(\text{final})} = \text{COMBINE}(\mathrm{r}_1^{(0)}, \mathrm{r}_1^{(1)}, \ldots, \mathrm{r}_1^{(K)})$$

Designs for Boosting Learning in Heterophily

- (D1) Ego- and Neighbor-embedding Separation;
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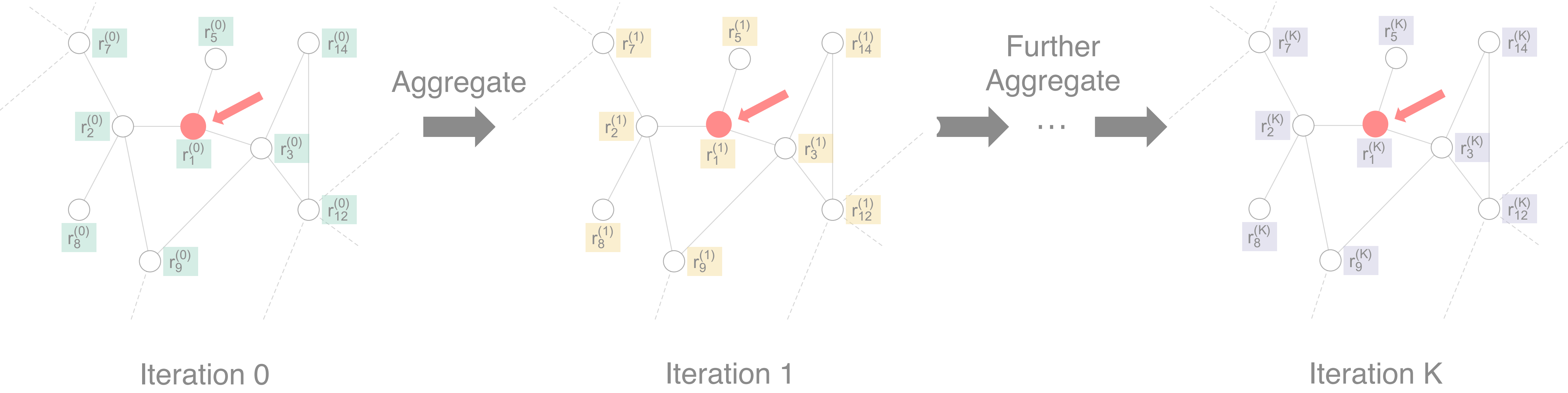
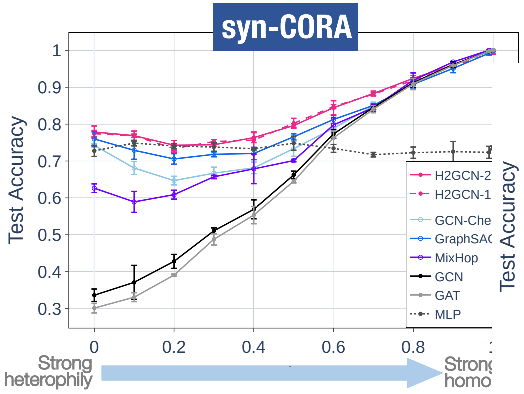
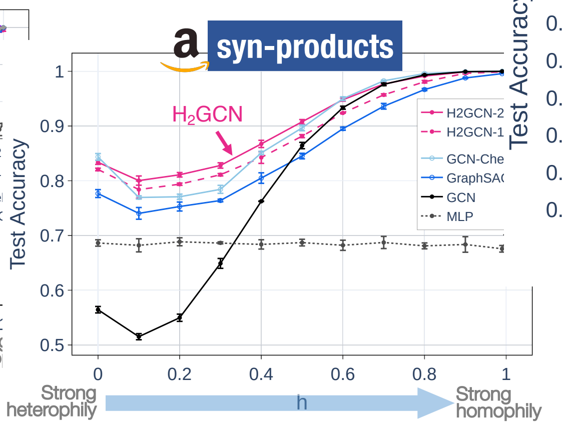
} H_2GCN

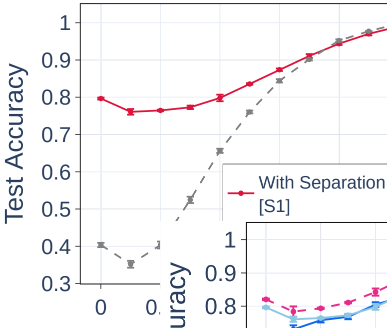


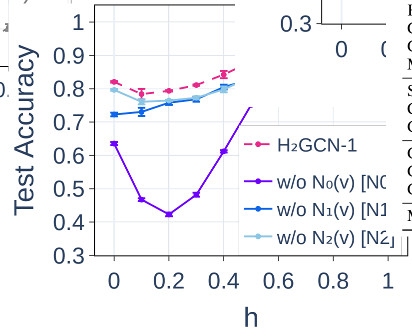
$$r_1^{(\text{final})} = \text{COMBINE}(r_1^{(0)}, r_1^{(1)}, \ldots, r_1^{(K)})$$

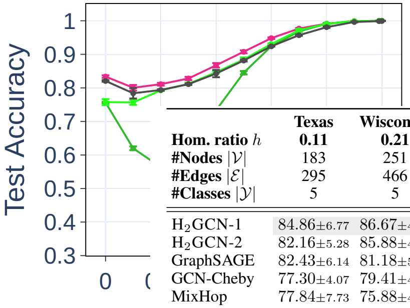
Empirical Evaluation of Identified Designs











	Texas	Wisconsin	Actor	Squirrel	Chameleon	Cornell	Cora Full	Citeseer	Pubmed	Cora
Hom. ratio h	**0.11**	**0.21**	**0.22**	**0.22**	**0.23**	**0.3**	**0.57**	**0.74**	**0.8**	**0.81**
#Nodes $\lvert\mathcal{V}\rvert$	183	251	7,600	5,201	2,277	183	19,793	3,327	19,717	2,708
#Edges $\lvert\mathcal{E}\rvert$	295	466	26,752	198,493	31,421	280	63,421	4,676	44,327	5,278
#Classes $\lvert\mathcal{Y}\rvert$	5	5	5	5	5	5	70	7	3	6
H_2GCN-1	84.86±6.77	86.67±4.69	35.86±1.03	36.42±1.89	57.11±1.58	82.16±4.80	68.13±0.49	77.07±1.64	89.40±0.34	86.92±1.37
H_2GCN-2	82.16±5.28	85.88±4.22	35.62±1.30	37.90±2.02	59.39±1.98	82.16±6.00	69.05±0.37	76.88±1.77	89.59±0.33	87.81±1.35
GraphSAGE	82.43±6.14	81.18±5.56	34.23±0.99	41.61±0.74	58.73±1.68	75.95±5.01	65.14±0.75	76.04±1.30	88.45±0.50	86.90±1.04
GCN-Cheby	77.30±4.07	79.41±4.46	34.11±1.09	43.86±1.64	55.24±2.76	74.32±7.46	67.41±0.69	75.82±1.53	88.72±0.55	86.76±0.95
MixHop	77.84±7.73	75.88±4.90	32.22±2.34	43.80±1.48	60.50±2.53	73.51±6.34	65.59±0.34	76.26±1.33	85.31±0.61	87.61±0.85
SAGE+JK	83.78±2.21	81.96±4.96	34.28±1.01	40.85±1.29	58.11±1.97	75.68±4.03	65.31±0.58	76.05±1.37	88.34±0.62	85.96±0.83
Cheby+JK	78.38±6.37	82.55±4.57	35.14±1.37	45.03±1.73	63.79±2.27	74.59±7.87	66.87±0.29	74.98±1.18	89.07±0.30	85.49±1.27
GCN+JK	66.49±6.64	74.31±6.43	34.18±0.85	40.45±1.61	63.42±2.00	64.59±8.68	66.72±0.61	74.51±1.75	88.41±0.45	85.79±0.92
GCN	59.46±5.25	59.80±6.99	30.26±0.79	36.89±1.34	59.82±2.58	57.03±4.67	68.39±0.32	76.68±1.64	87.38±0.66	87.28±1.26
GAT	58.38±4.45	55.29±8.71	26.28±1.73	30.62±2.11	54.69±1.95	58.92±3.32	59.81±0.92	75.46±1.72	84.68±0.44	82.68±1.80
GEOM-GCN*	67.57	64.12	31.63	38.14	60.90	60.81	N/A	77.99	90.05	85.27
MLP	81.89±4.78	85.29±3.61	35.76±0.98	29.68±1.81	46.36±2.52	81.08±6.37	58.76±0.50	72.41±2.18	86.65±0.35	74.75±2.22

- In synthetic graphs with heterophily, the identified designs help H_2GCN perform up to 40% better in accuracy compared to the variants without them.
- In real graphs with heterophily, methods with our identified designs perform up to 27% better compared to vanilla GCN.
- Under homophily, methods with our identified designs remain competitive.

Thank you!

We reveal current limitations of GNNs in **heterophily**.

We identify **key design choices** that boost learning in heterophily, without sacrificing in homophily, and analyze them theoretically.

Extensive empirical evaluation across the full spectrum of low-to-high homophily confirms the effectiveness of the designs.

Join our poster presentation at NeurIPS 2020 for more details!

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