Block Modeling-Guided Graph Convolutional Neural Networks

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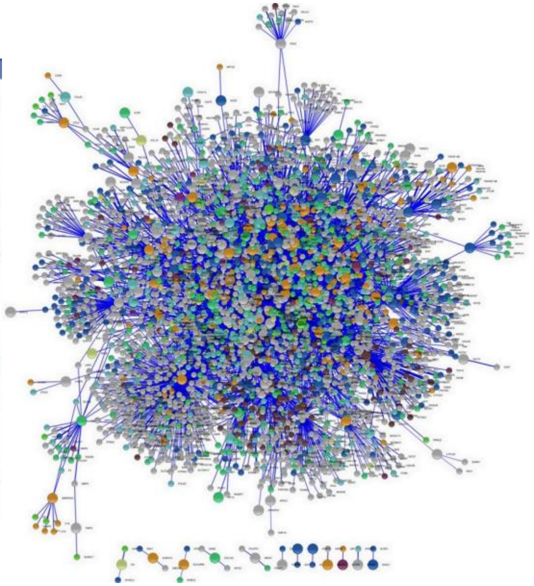
Outline

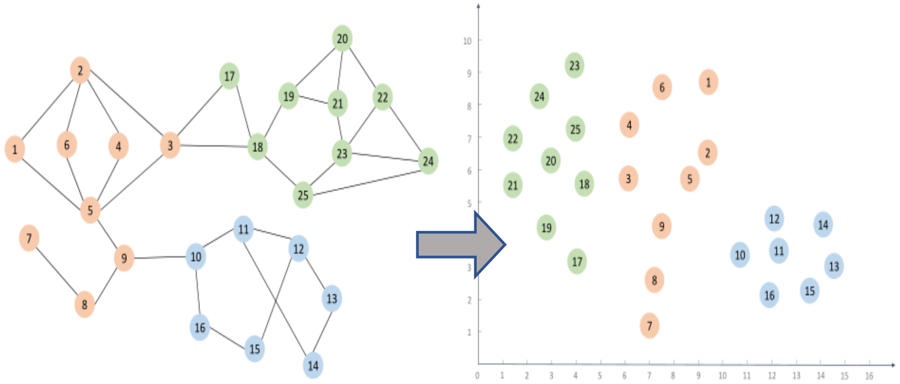
- Motivation
- Method
- Experiments
- Conclusion

Network Representation Learning

social network



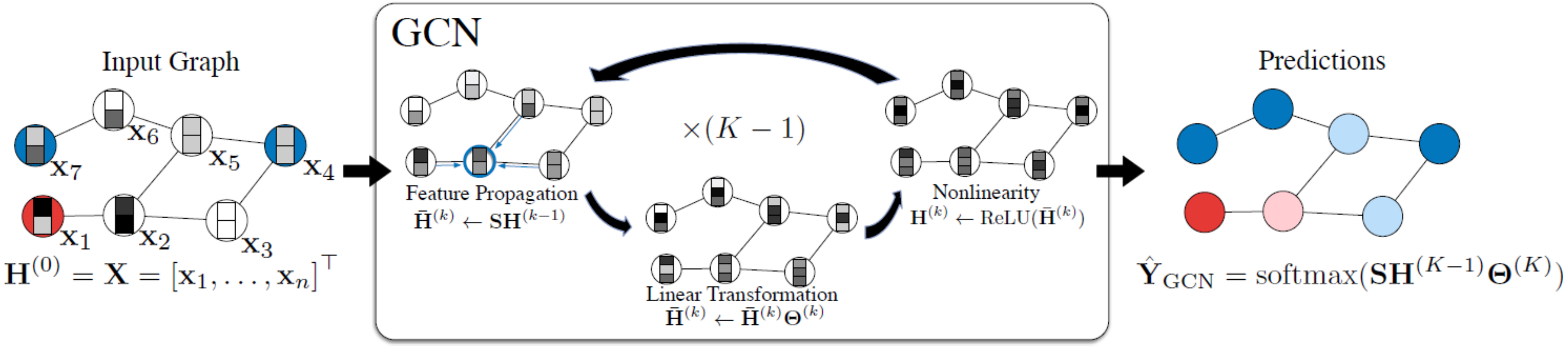
biology network



network representation learning

Graph Convolutional Networks

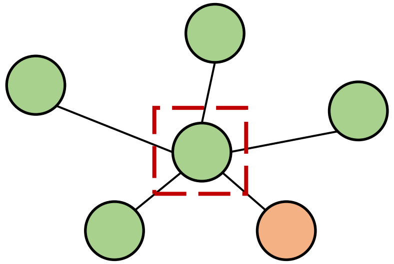
- **Essence**: propagate node attributes in neighbors guided by graph structure.
- **Goal**: encode nodes to embedding space by preserving network structure and properties.



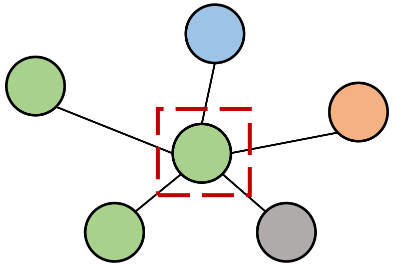
[1] T. N. Kipf and M. Welling. Semi-supervised classification with graph convolutional networks. ICLR, 2017.
[2] Wu F, Souza A, Zhang T, et al. Simplifying graph convolutional networks. PMLR, 2019.

Is GCN Universal?

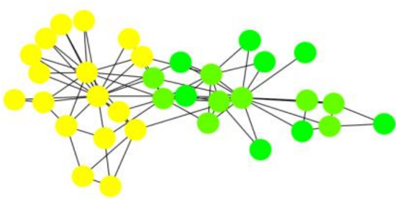
- **Question**: Can neighbor information represent a node?



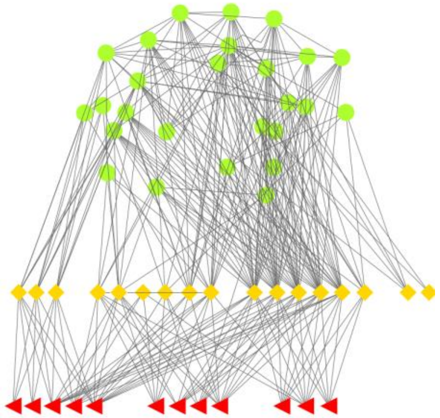
✓ GCN work



✗ GCN **NOT** work



homophily network



heterophily network

- **Homophily Assumption**: GCN only works on homophily networks.

most connections happen among
nodes in the same or similar classes

Existing Related Work

- **Aggregating higher-order neighbors**:
  - H_2GCN [Zhu *et al.*, 2020]
  - MixHop [Abu-El-Haija *et al.*, 2019]
  - …
- **Passing signed messages**:
  - GGCN [Yan *et al.*, 2021]
  - GPR-GNN [Chien *et al.*, 2019]
  - …

⚠ damage network topology

⚠ fail to define optimal aggregating mechanism

A BETTER WAY

automatically learn corresponding aggregation rules for neighbors of different classes

Homophily Ratio & Block Matrix

- **Homophily Ratio**: measure the overall homophily level in a network.

$$h = \frac{1}{|\mathcal{V}|} \sum_{v_i \in \mathcal{V}} \frac{|\{v_j | v_j \in \mathcal{N}_i, Y_j = Y_i\}|}{|\mathcal{N}_i|}$$

- **Block Matrix**: measure the connected possibility of nodes in any two classes.

$$H = (Y^T A \boxed{Y}) \oslash (Y^T A E)$$

Challenge 1: how to derive the block matrix in GCN without all known labels.

Challenge 2: how to design aggregation mechanism based on block matrix.

block matrix depicts the heterophilic property of the network in heterophilic situations.

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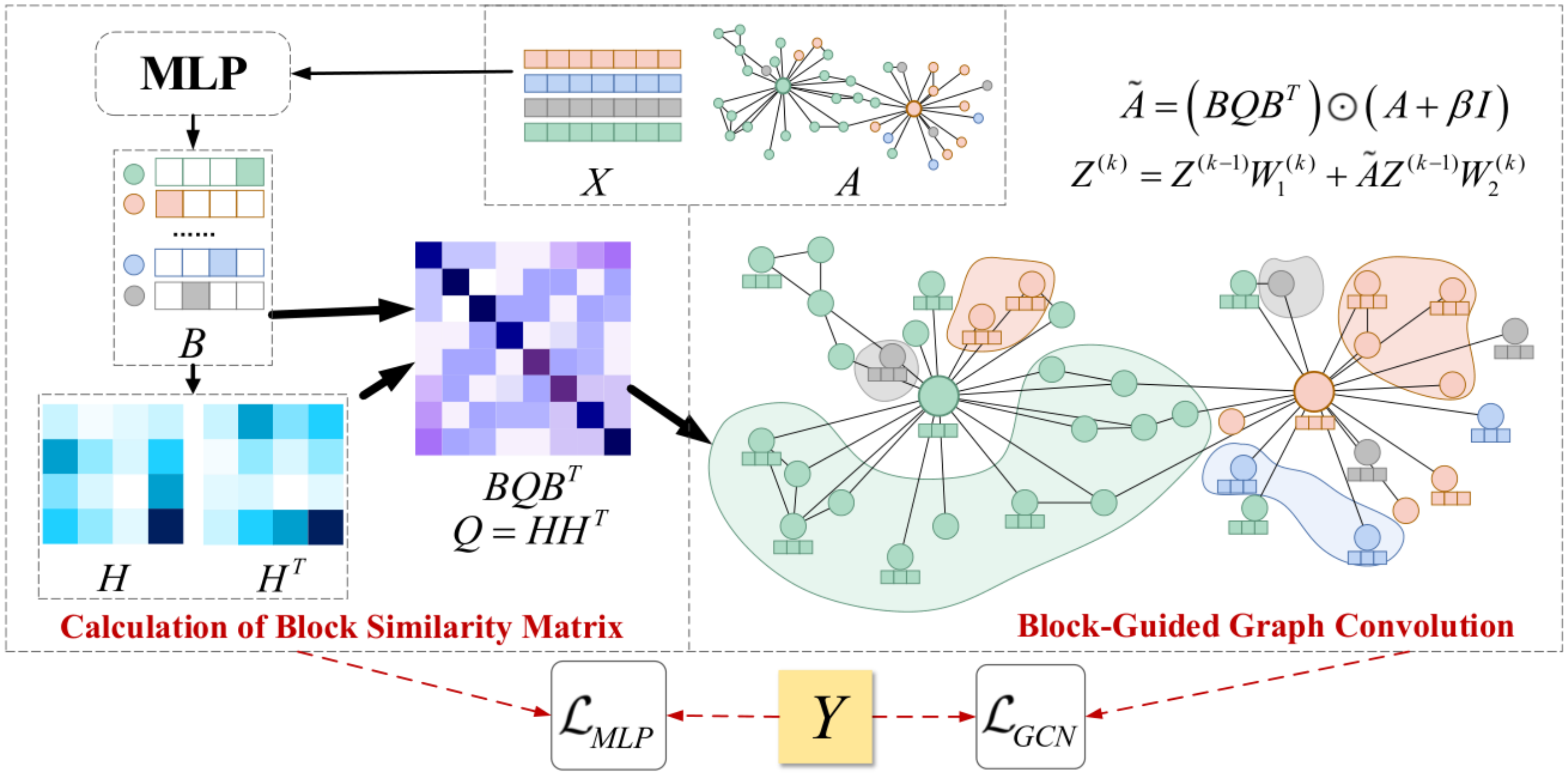
Overview – BM-GCN



Block Similarity Matrix

1) Pre-train MLP for soft labels

$$\bar{B} = \sigma\left(\mathrm{MLP}\left(X\right)\right)$$

$$B = \mathrm{softmax}\left(\bar{B}\right)$$

$$\mathcal{L}_{MLP} = \sum\nolimits_{v_i \in \mathcal{T}_{\mathcal{V}}} f\left(B_i, Y_i\right)$$

- obtain predicted soft labels via node attributes
- train MLP in a semi-supervised way

2) Calculate block matrix H

$$Y_s = \{Y_i, B_j | \forall v_i \in \mathcal{T}_{\mathcal{V}}, \forall v_j \notin \mathcal{T}_{\mathcal{V}}\}$$

$$H = \left(Y_s^T A Y_s\right) \oslash \left(Y_s^T A E\right)$$

- make full use of existing known labels
- H depicts the connecting pattern between classes

3) Calculate block similarity matrix Q

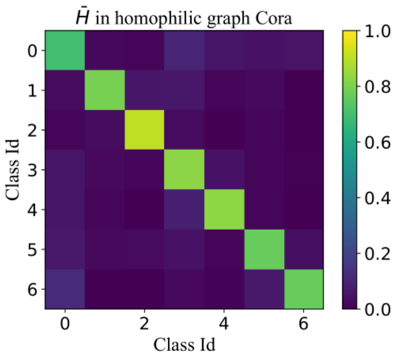
$$Q = HH^T$$

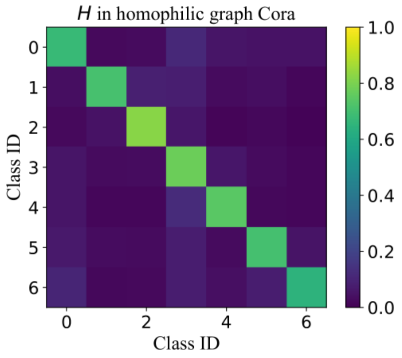
$$\mathrm{Diag}\left(Q\right) \leftarrow \alpha \cdot \mathrm{Diag}\left(Q\right)$$

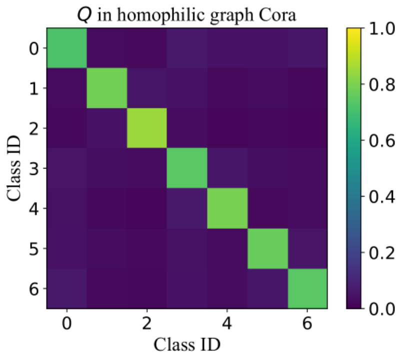
- Q depicts the similarity of connecting patterns between classes
- The more similar the two classes, the greater the value of the corresponding element in Q

Illustration on Why Block Modeling Effective

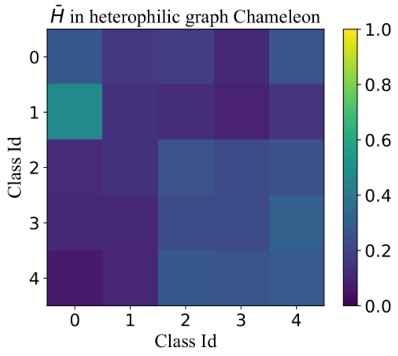
Homophilic Cora

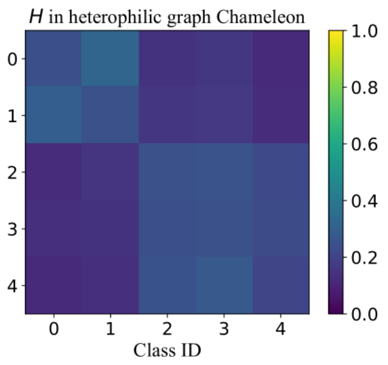


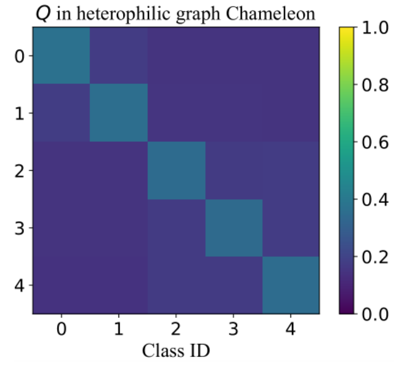




Heterophilic Chameleon







Block-Guided Graph Convolution Process

Soft label vector B_i: $\boxed{B_i^1 \mid B_i^2 \mid B_i^3 \mid B_i^4}$ The probability that v_i belongs to 2-th class

Soft label vector B_j: $\boxed{B_j^1 \mid B_j^2 \mid B_j^3 \mid B_j^4}$ The probability that v_j belongs to 3-th class

$B_i^2 B_j^3 \longrightarrow$ The probability that (v_i, v_j) belongs to (2-3) class-combination

$$Q = \begin{bmatrix} \; & \; & \; & \; \\ \; & \; & Q_{2,3} & \; \\ \; & \; & \; & \; \\ \; & \; & \; & \; \\ \; & \; & \; & \; \end{bmatrix}$$

Information propagating ratio between 2-th class and 3-th class

$Q_{2,3} B_i^2 B_j^3 \longrightarrow$ Under the (2-3) class-combination,
How many message should be propagated between v_i and v_j

$$\omega_{ij} = \sum_{r=1}^{c} \sum_{t=1}^{c} q_{r,t} b_i^r b_j^t \longrightarrow$$

Consider all kinds of class-combinations,
information propagating ratio between v_i and v_j

Block-Guided Graph Convolution Process

Information propagating ratio for two nodes

$$\omega_{ij} = \sum_{r=1}^{c}\sum_{t=1}^{c} q_{r,t} b_i^r b_j^t$$

Information propagating ratio for all node pairs (in the form of matrix)

$$\Omega = BQB^T$$

A refined topology matrix based on Ω

$$A' = \Omega \odot (A + \beta I)$$

New graph convolutional layer

$$Z^{(k)} = Z^{(k-1)} W_1^{(k)} + \tilde{A} Z^{(k-1)} W_2^{(k)}$$

Semi-supervised Model Optimization (with fine-tuning MLP)

$$\mathcal{L}_{final} = \lambda \mathcal{L}_{GCN} + (1-\lambda)\,\mathcal{L}_{MLP} \quad , \quad \mathcal{L}_{GCN} = \sum_{v_i \in \mathcal{T}_{\mathcal{V}}} f\left(Z_i, Y_i\right)$$

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Experiments

- ## Datasets

Heterophilic Networks: texas, squirrel, chameleon

Homophilic Networks: cora, pubmed, citeseer

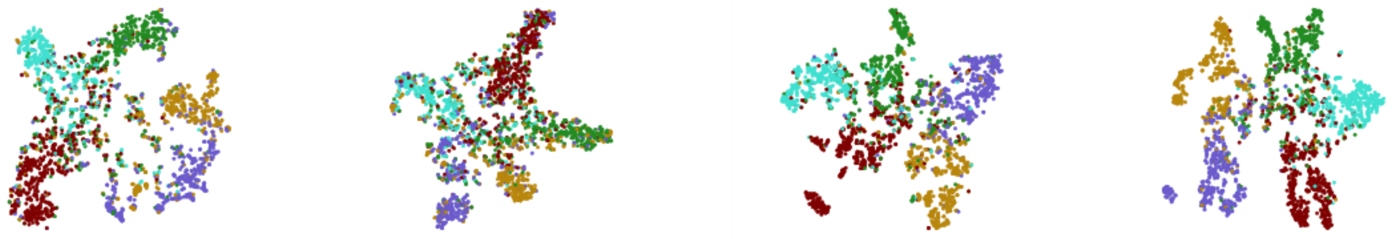
Datasets	$\|\mathcal{V}\|$	$\|\mathcal{E}\|$	c	d	h
texas	183	295	5	1703	0.11
squirrel	5,201	198,493	5	2,089	0.22
chameleon	2,277	31,421	5	2.325	0.23
cora	3,327	4,676	7	3,703	0.74
pubmed	19,717	44,327	6	500	0.80
citeseer	2,708	5,278	3	1,433	0.81

- ## Node Classification

Method/ Accuracy (%)	**heterophilic graphs**			**homophilic graphs**		
	Texas $h = 0.09$	**Squirrel** $h = 0.23$	**Chameleon** $h = 0.22$	**Cora** $h = 0.81$	**Citeseer** $h = 0.74$	**Pubmed** $h = 0.8$
MLP	82.70±6.19	33.35±1.24	48.20±2.63	74.14±1.40	69.58±2.31	86.38±0.61
GCN	55.41±3.47	44.07±1.95	67.04±2.23	86.48±1.12	72.67±1.99	87.39±0.68
H2GCN	82.16±8.21	28.91±1.78	51.58±1.51	87.69±1.37	75.95±2.18	88.78±0.53
GPR-GNN	84.59±4.37	29.45±1.27	**69.78±1.97**	86.70±1.03	75.12±1.98	87.38±0.63
CPGNN-MLP	77.09±4.22	28.65±1.50	52.63±1.79	85.23±1.71	74.29±2.41	86.83±0.78
CPGNN-Cheby	77.03±5.83	30.95±1.24	54.05±4.67	86.82±1.11	75.42±1.85	89.08±0.67
BM-GCN(Ours)	**85.13±4.64**	**51.41±1.10**	69.58±2.90	**87.99±1.29**	**76.13±1.92**	**90.25±0.75**

Experiments

Visualization



(a) H2GCN (b) CPGNN (c) GPR-GNN (d) BM-GCN

Figure 3: Visualization results on Chameleon dataset. Different colors correspond to different ground truth classes.

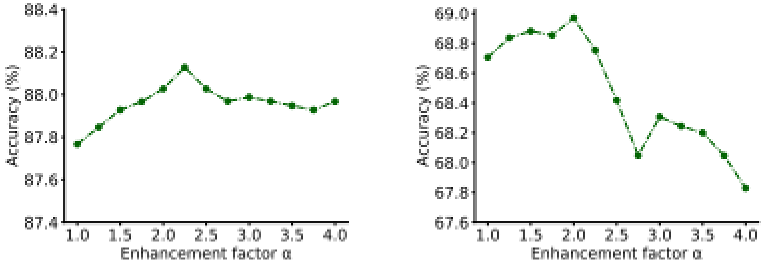
Parameter Analysis

Datasets/ Accuracy (%)	The number of graph convolutional layers k					
	1	2	3	4	5	6
Cora	81.27	86.92	87.99	87.30	60.10	40.16
Chameleon	58.71	67.74	69.58	65.00	49.28	34.69

Table 4: Node classification accuracy of BM-GCN with graph convolutional layers k varying from 1 to 6.

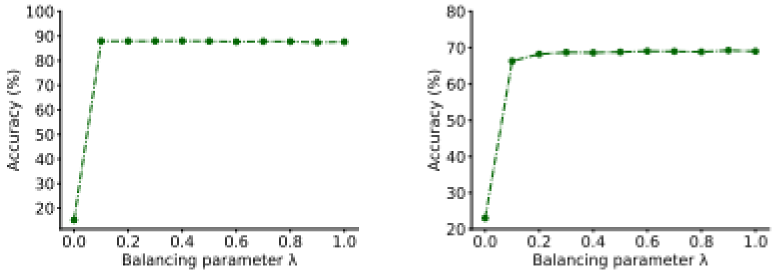
Experiments

◆ **Parameter Analysis**



(a) Cora (b) Chameleon

Figure 4: Parameter analysis of enhancement factor α in Q on Cora and Chameleon datasets. We report the average node classification accuracy over 10 random splits.



(a) Cora (b) Chameleon

Figure 5: Parameter analysis of loss balancing parameter λ on Cora and Chameleon datasets. We report the average node classification accuracy over 10 random splits.

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Conclusion

- Propose a new framework to make GCN applicable to both homophilic and heterophilic networks.
- Introduce block modeling technology to solve the problem of Homophily Assumption.
- Propose a novel design of block similarity matrix to enable block modeling technology to guide GCN to achieve classified aggregation.

Thanks

Data & Code: https://github.com/hedongxiao-tju/BM-GCN