Data Augmentation for Graph Neural Networks

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Backgrounds on Data Augmentation

- Why data augmentation is important for machine learning?
  - Provides more training data.
  - Reduce overfitting.
  - Improves generalization.

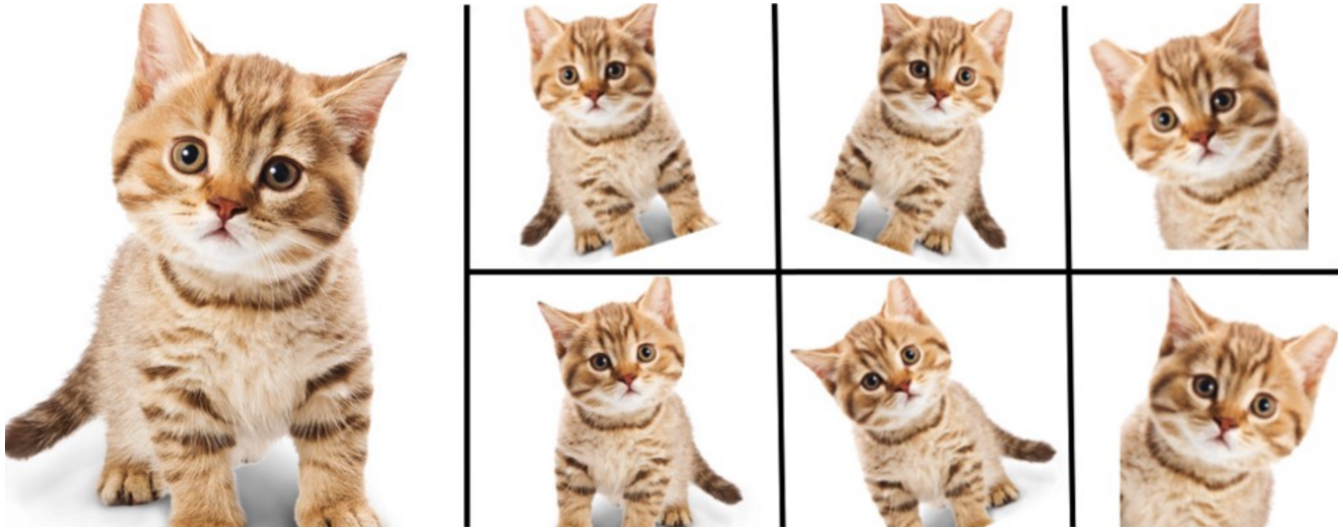

Image sources: https://www.kdnuggets.com/2018/05/data-augmentation-deep-learning-limited-data.html

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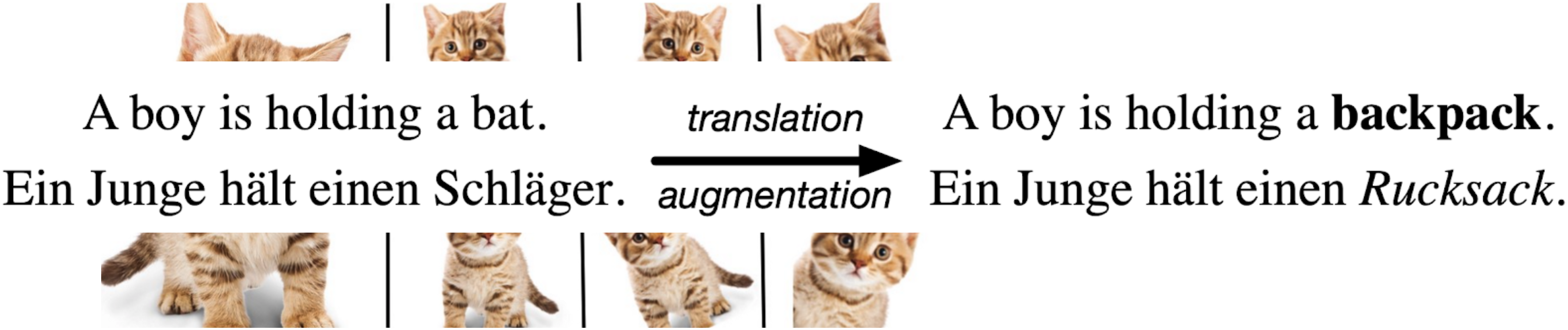
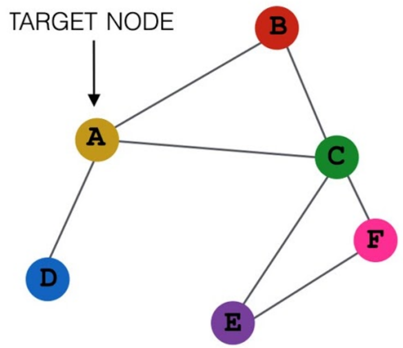


Background on Graph Neural Networks

- Given: graph $G = (V, E)$, node features $\mathbf{x}_v \in \mathbb{R}^m, \forall v \in V$.
- Learn: low dimensional node representations $\mathbf{z}_v \in \mathbb{R}^d, \forall v \in V$.

- Neighborhood aggregation: generate node representations based on local neighborhoods.



INPUT GRAPH

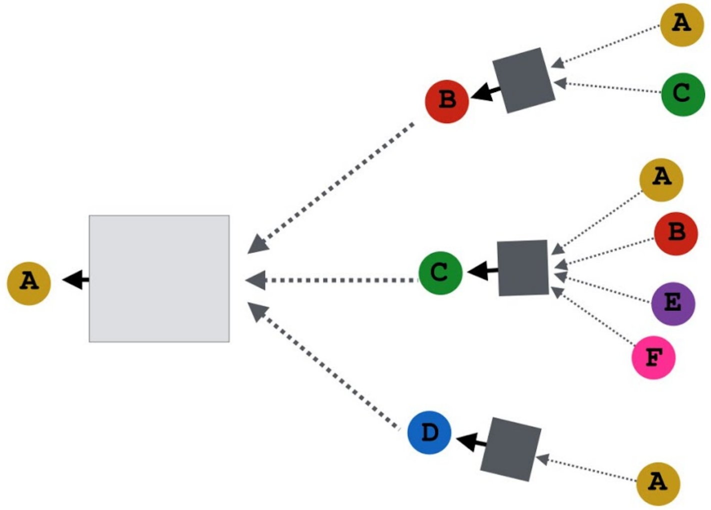


Image sources: Ying, Rex, et al. "Graph convolutional neural networks for web-scale recommender systems." Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 2018.

Data Augmentation for GNNs

- **Goal:** use graph data augmentation to improve the performance of GNNs on the task of node classification.

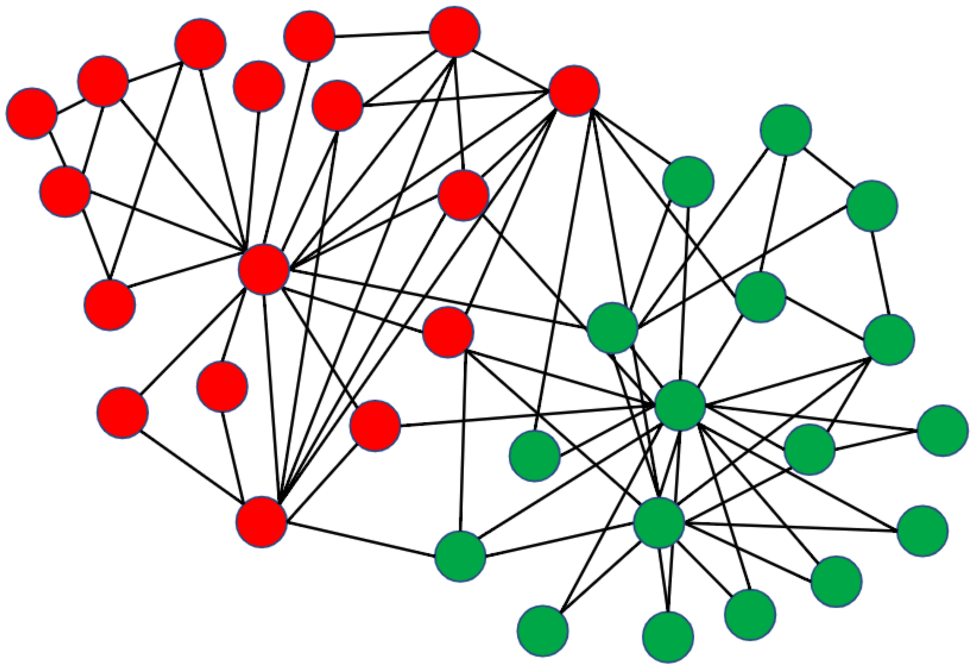
- **Challenges:**
  - There's no direct analogs of traditional data augmentation operations (flipping, rotating, blurring, etc.) on graphs.
  - Very limited operations exist for perturbing graphs.
    - Any manipulation would affect the whole graph (dataset).
    - Adding/removing edges are the best strategy available.
    - But *which* edges to add/remove?

Manipulating Edges to Augment Graph Data

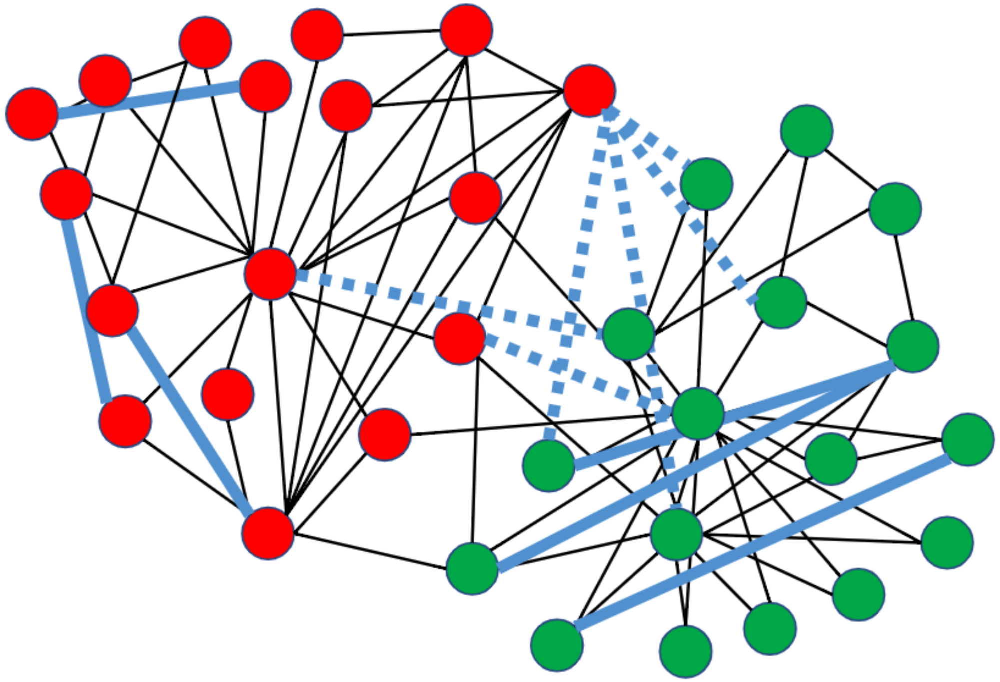
- For node classification task,
  - There could be noise edges generated by spammers, anomalies, adversarial attacks, etc.

- Adding(removing) intra(inter)-class edges improves node classification performance.

Zackary's Karate Club (ZKC) Graph

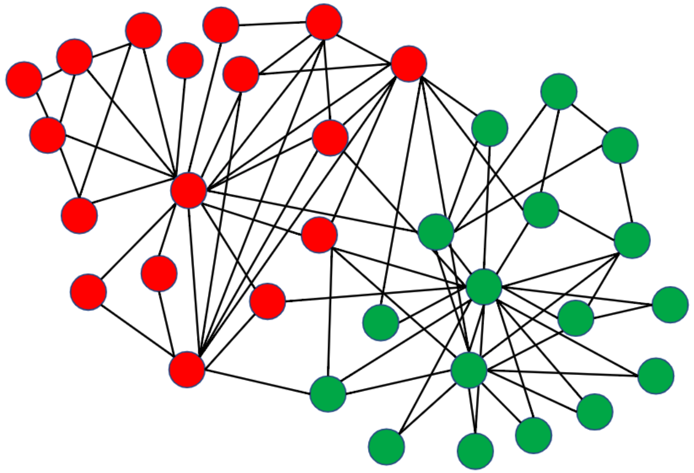


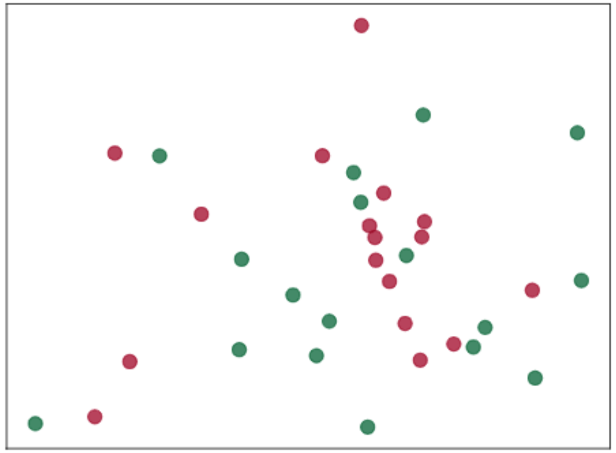
Original graph.
GCN Performance: 92.4



Omniscient modified graph.
GCN Performance: 98.6

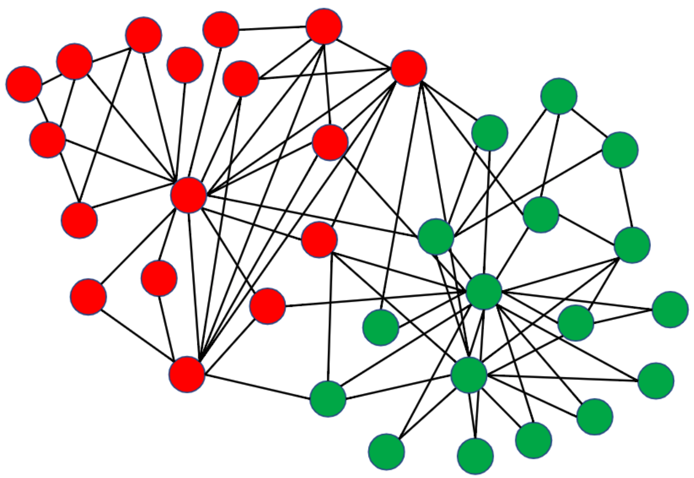
Random Initialized Features of ZKC Graph

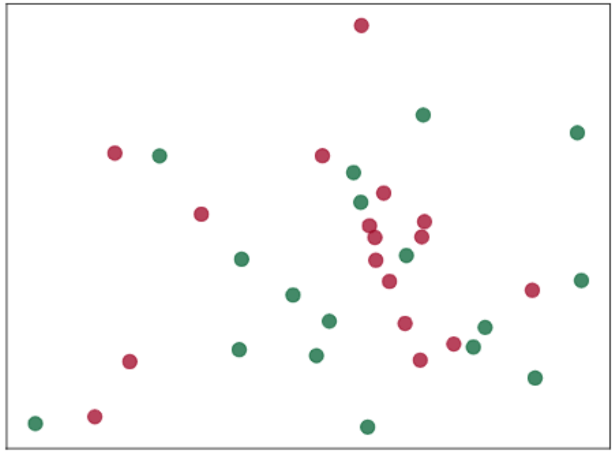




Random initialized features

Embeddings of ZKC Graph after GCN Layer





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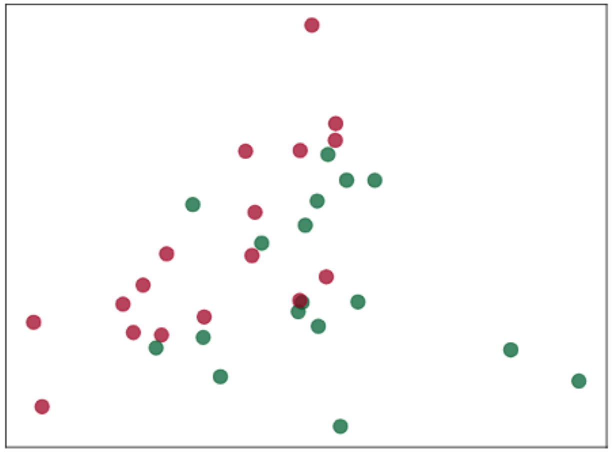

Original Graph

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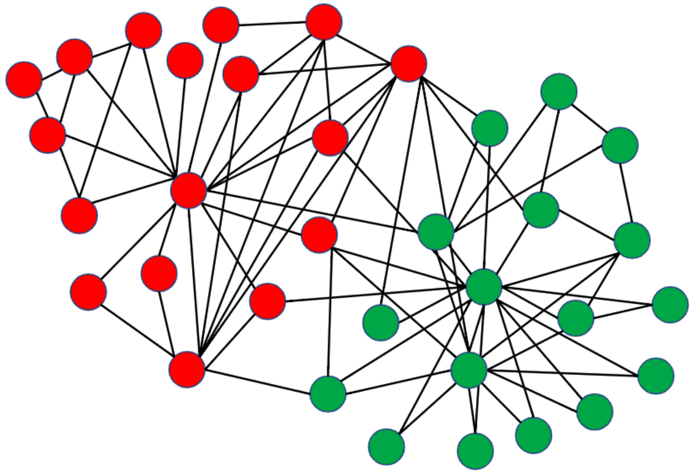

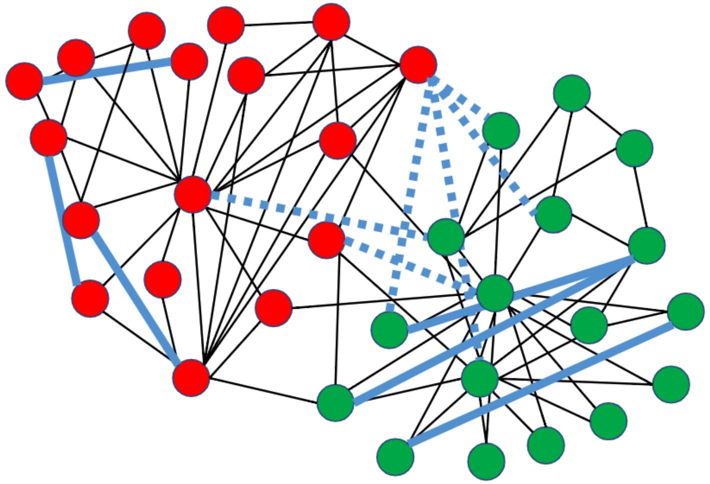

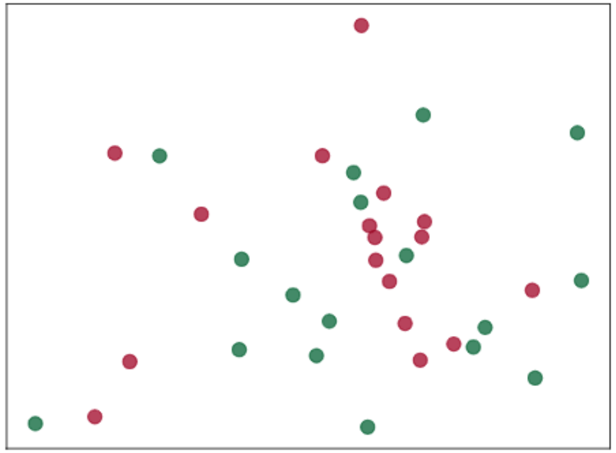

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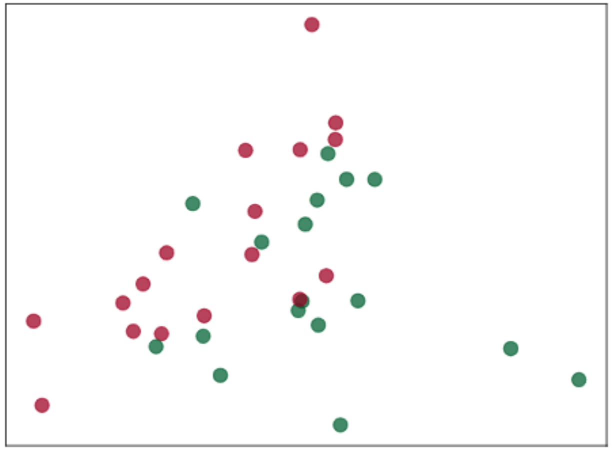
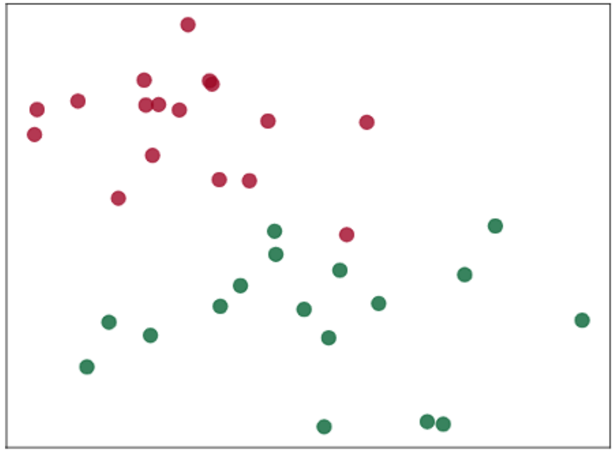
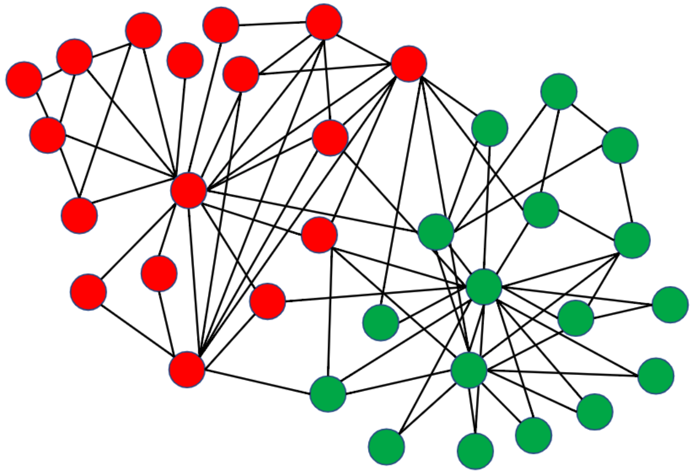


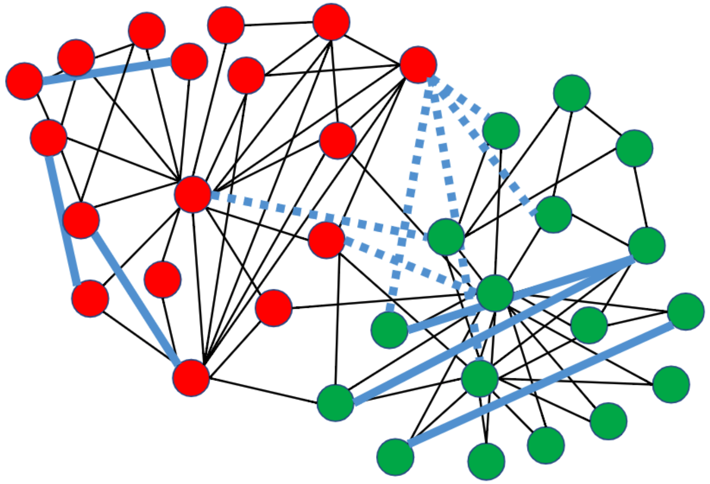
Original Graph

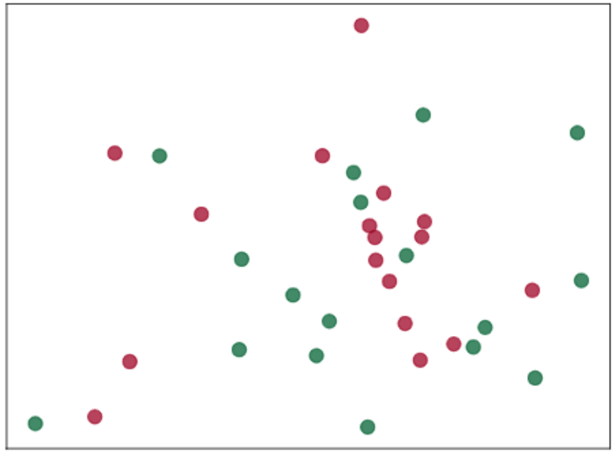


Modified Graph

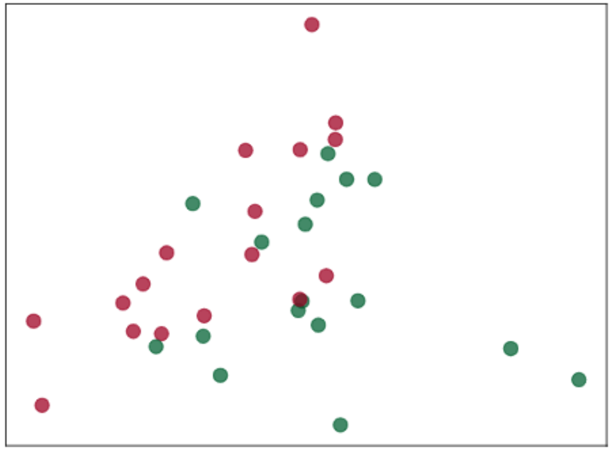
Embeddings of ZKC Graph after GCN Layer



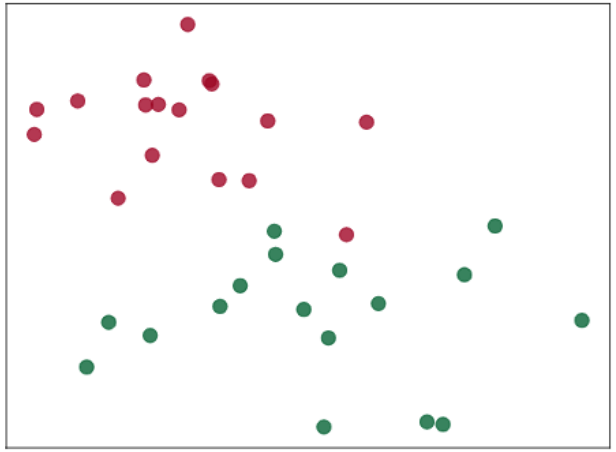




Random initialized features



Original Graph



Modified Graph

Ideal Graph

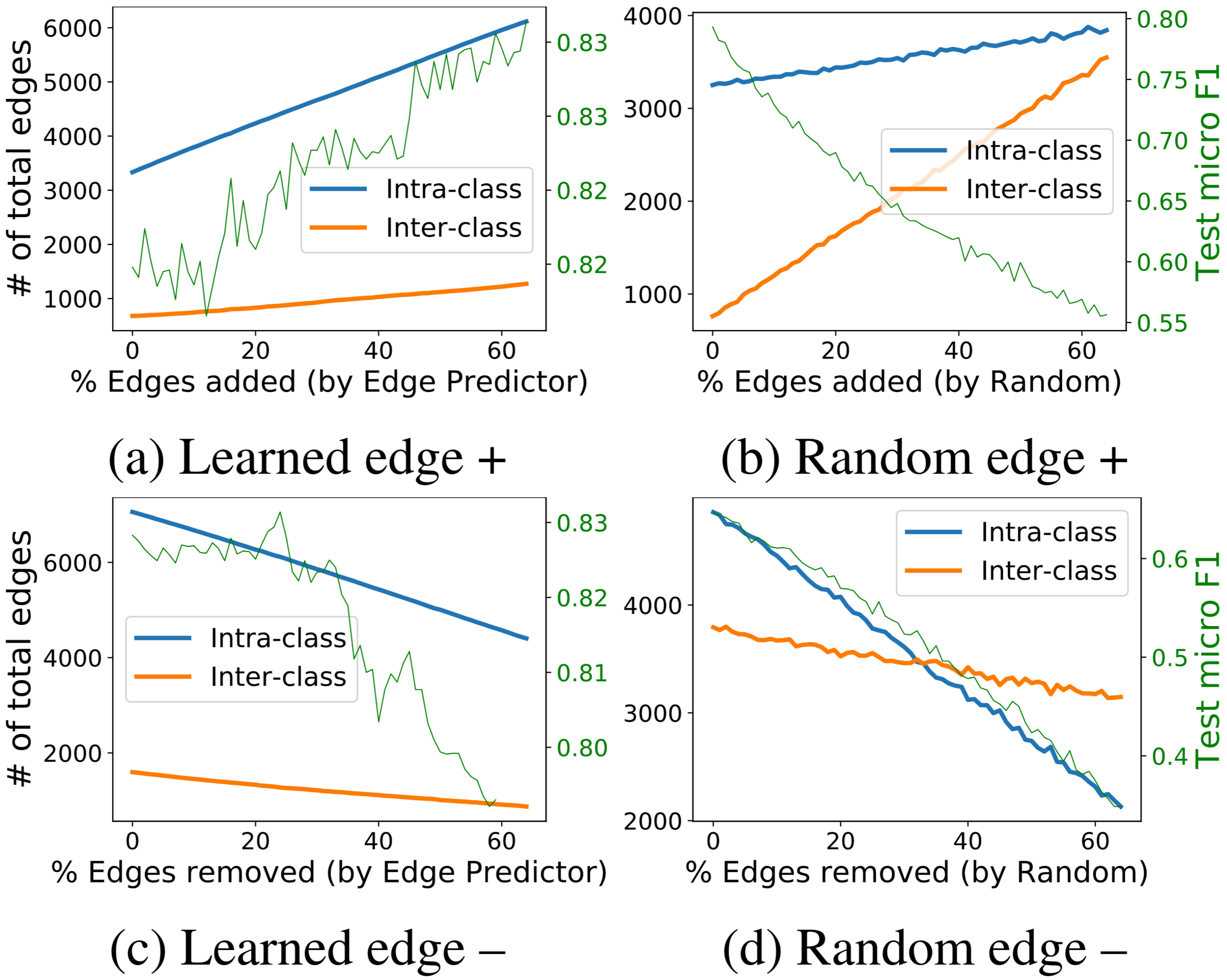
Evaluating on Modified or Original Graph

- How traditional data augmentation methods in CV works:
  - Generate augmented data variants for each data object.
  - Train model with both original and augmented data.

- On graphs: augmentation results with a new graph.
  - Training & inference on different graphs → train-test gap.
  - For real-life social networks that are consistently growing/changing, ability of inferencing with original graph is preferred.

GAug-M

1. Use an edge predictor to predict edge probabilities for all node pairs.
2. Based on the edge probabilities, deterministically add (remove) new (existing) edges to create a modified graph.



(a) Learned edge +
(b) Random edge +
(c) Learned edge –
(d) Random edge –

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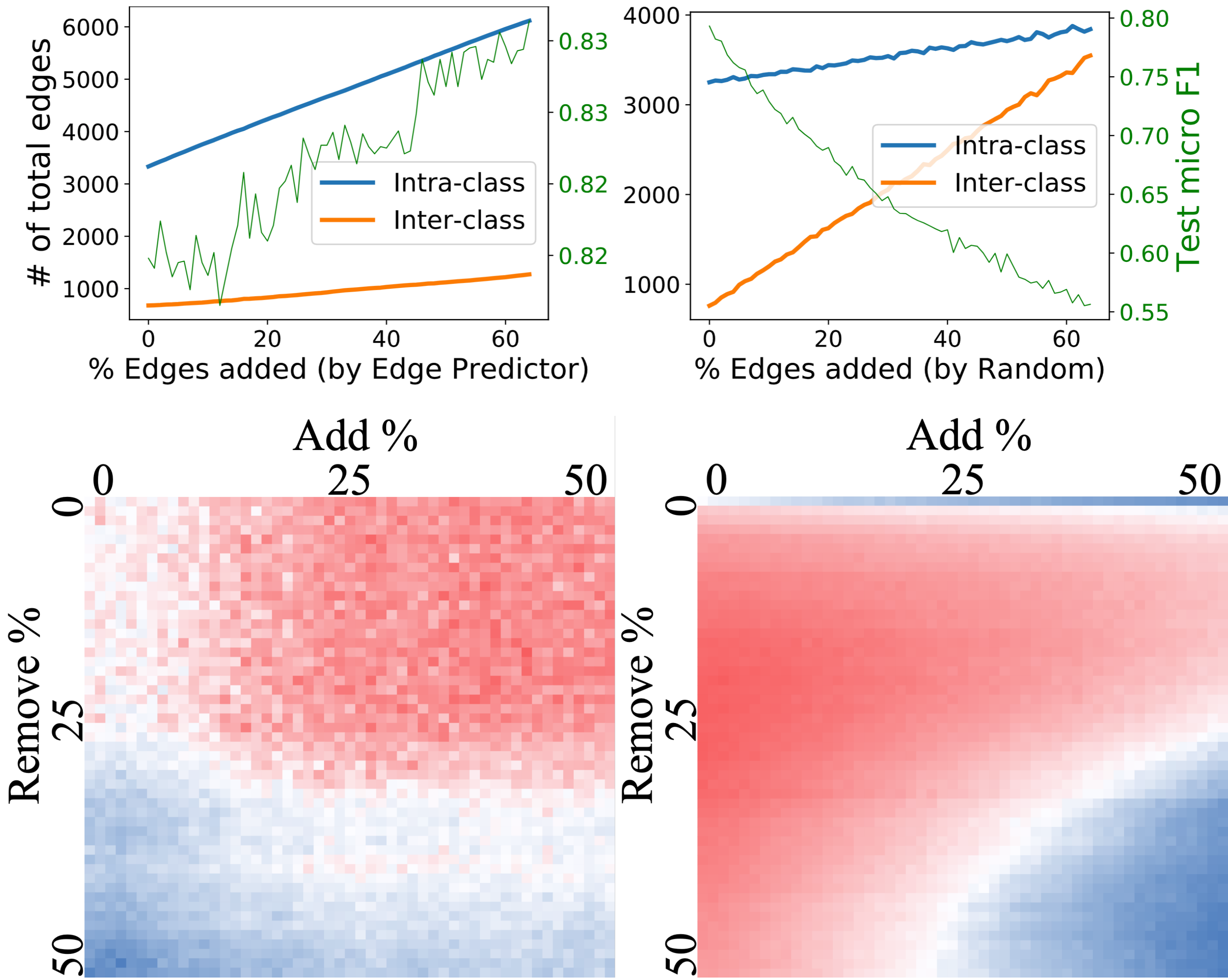
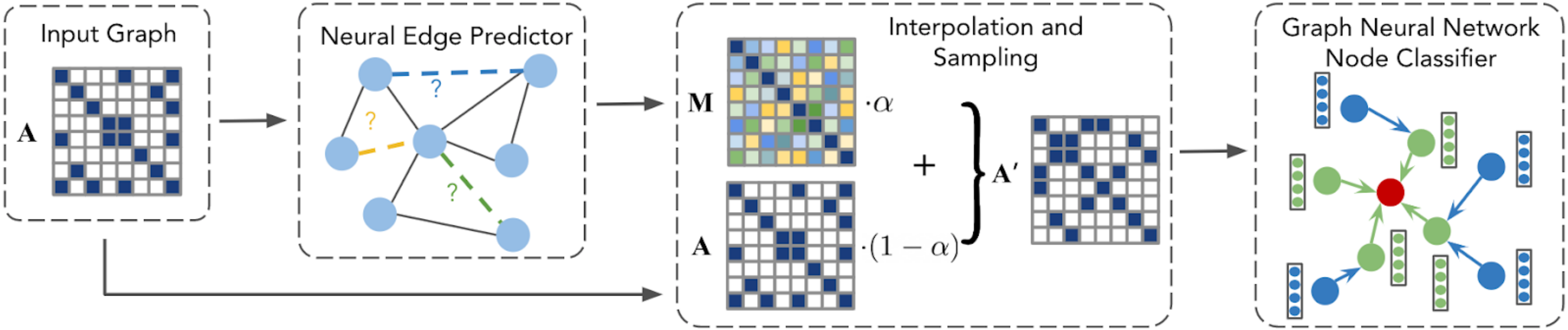


GAug-O for Evaluating on Original Graph



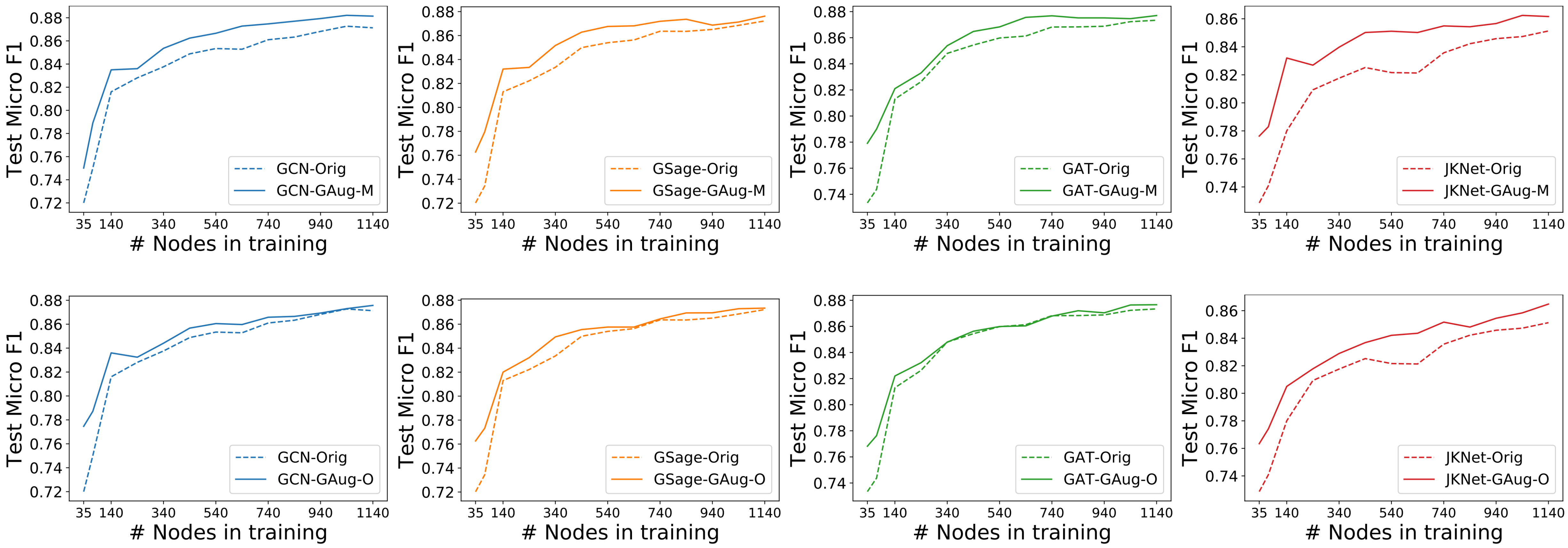
$$\mathbf{A}'_{ij} = \left\lfloor \frac{1}{1+e^{-(\log \mathbf{P}_{ij}+G)/\tau}} + \frac{1}{2} \right\rfloor, \quad \text{where} \quad \mathbf{P}_{ij} = \alpha \mathbf{M}_{ij} + (1-\alpha)\mathbf{A}_{ij}$$

$$\mathcal{L} = \mathcal{L}_{nc} + \beta \mathcal{L}_{ep}, \quad \text{where} \quad \mathcal{L}_{nc} = CE(\hat{\mathbf{y}}, \mathbf{y}) \;\; \text{and} \;\; \mathcal{L}_{ep} = BCE(\sigma(f_{ep}(\mathbf{A}, \mathbf{X})), \mathbf{A})$$

Results

GNN Arch.	Method	Cora	Citeseer	PPI	BlogC	Flickr	Air-USA
GCN	Original	81.6±0.7	71.6±0.4	43.4±0.2	75.0±0.4	61.2±0.4	56.0±0.8
	+AdaEdge	81.9±0.7	72.8±0.7	43.6±0.2	75.3±0.3	61.2±0.5	57.2±0.8
	+GAug-M	83.5±0.4	72.3±0.4	43.5±0.2	**77.6±0.4**	**68.2±0.7**	61.2±0.5
	+DropEdge	82.0±0.8	71.8±0.2	43.5±0.2	75.4±0.3	61.4±0.7	56.9±0.6
	+GAug-O	**83.6±0.5**	**73.3±1.1**	**46.6±0.3**	75.9±0.2	62.2±0.3	**61.4±0.9**
GSAGE	Original	81.3±0.5	70.6±0.5	40.4±0.9	73.4±0.4	57.4±0.5	57.0±0.7
	+AdaEdge	81.5±0.6	71.3±0.8	41.6±0.8	73.6±0.4	57.7±0.7	57.1±0.5
	+GAug-M	**83.2±0.4**	71.2±0.4	41.1±1.0	**77.0±0.4**	**65.2±0.4**	**60.1±0.5**
	+DropEdge	81.6±0.5	70.8±0.5	41.1±1.0	73.8±0.4	58.4±0.7	57.1±0.5
	+GAug-O	82.0±0.5	**72.7±0.7**	**44.4±0.5**	73.9±0.4	56.3±0.6	57.1±0.7
GAT	Original	81.3±1.1	70.5±0.7	41.5±0.7	63.8±5.2	46.9±1.6	52.0±1.3
	+AdaEdge	82.0±0.6	71.1±0.8	42.6±0.9	68.2±2.4	48.2±1.0	54.5±1.9
	+GAug-M	82.1±1.0	71.5±0.5	42.8±0.9	70.8±1.0	**63.7±0.9**	**59.0±0.6**
	+DropEdge	81.9±0.6	71.0±0.5	**45.9±0.3**	70.4±2.4	50.0±1.6	52.8±1.7
	+GAug-O	**82.2±0.8**	**71.6±1.1**	44.9±0.9	**71.0±1.1**	51.9±0.5	54.6±1.1
JK-Net	Original	78.8±1.5	67.6±1.8	44.1±0.7	70.0±0.4	56.7±0.4	58.2±1.5
	+AdaEdge	80.4±1.4	68.9±1.2	44.8±0.9	70.7±0.4	57.0±0.3	59.4±1.0
	+GAug-M	**81.8±0.9**	68.2±1.4	47.4±0.6	**71.9±0.5**	**65.7±0.8**	60.2±0.6
	+DropEdge	80.4±0.7	69.4±1.1	46.3±0.2	70.9±0.4	58.5±0.7	59.1±1.1
	+GAug-O	80.5±0.9	**69.7±1.4**	**53.1±0.3**	71.0±0.6	55.7±0.5	**60.4±1.0**

Results



Test Micro F1
Nodes in training
35 140 340 540 740 940 1140
GCN-Orig
GCN-GAug-M
GSage-Orig
GSage-GAug-M
GAT-Orig
GAT-GAug-M
JKNet-Orig
JKNet-GAug-M
GCN-Orig
GCN-GAug-O
GSage-Orig
GSage-GAug-O
GAT-Orig
GAT-GAug-O
JKNet-Orig
JKNet-GAug-O

Thank you!

Any Questions?

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