

NoisyGL: A Comprehensive Benchmark for Graph Neural Networks under Label Noise

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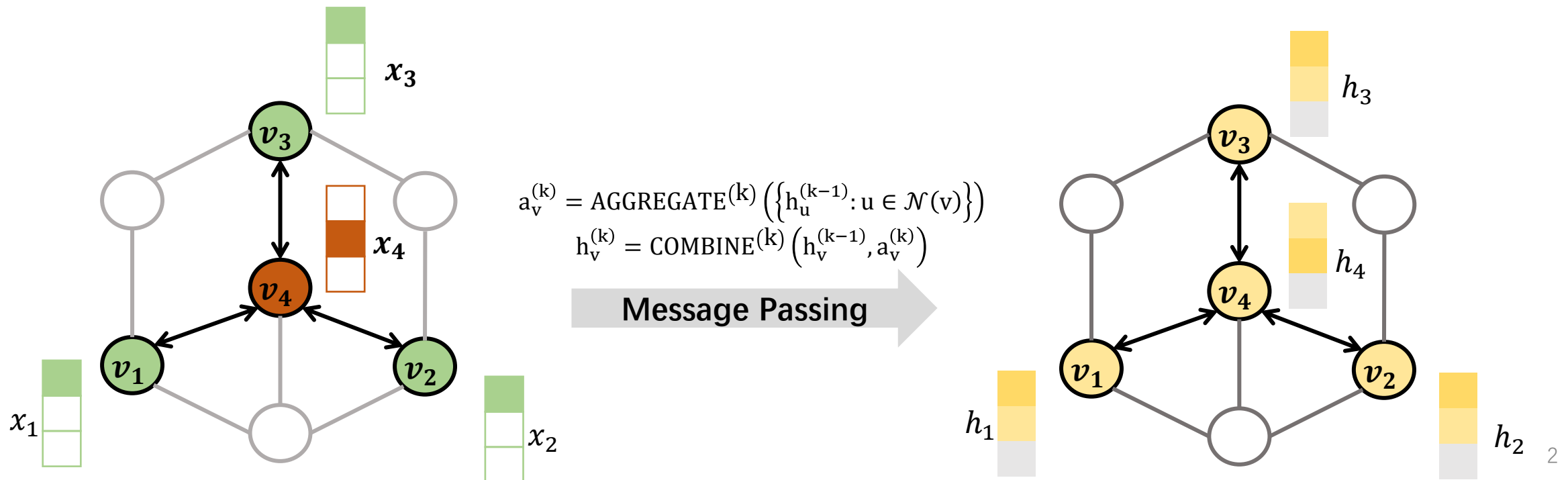
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Background

Graph Neural Networks

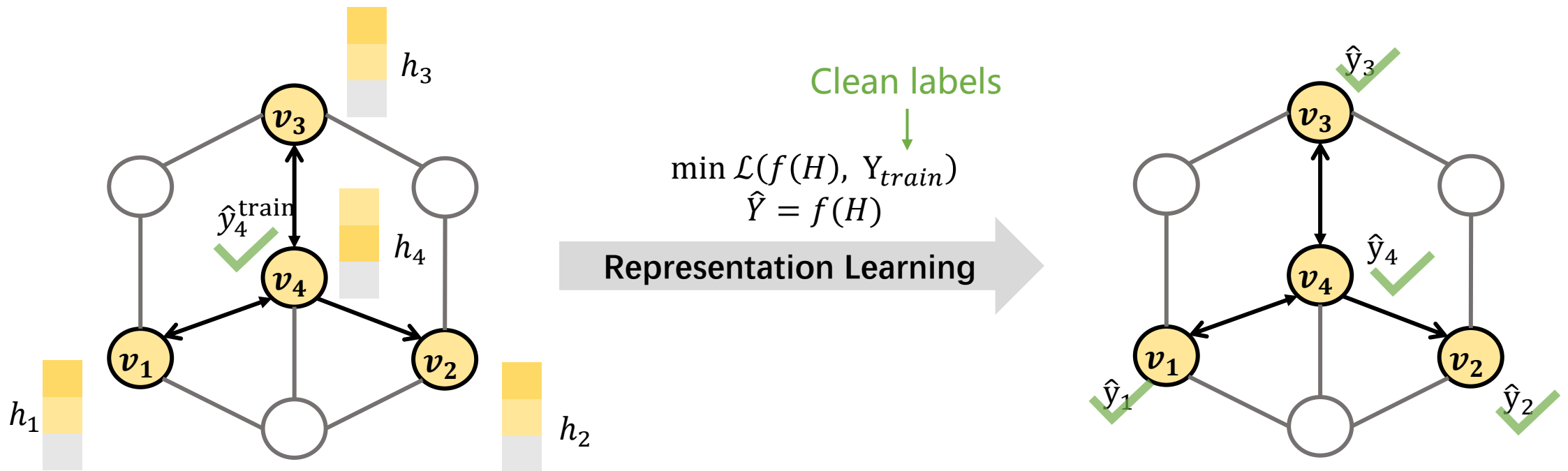
- Graph Neural Networks (GNNs) demonstrate strong potential in node classification tasks through the **message-passing** mechanism.
- The **message-passing** mechanism aggregates information from neighboring nodes, resulting in **similar (homophily) representations** for adjacent nodes.



Background

Graph Neural Networks

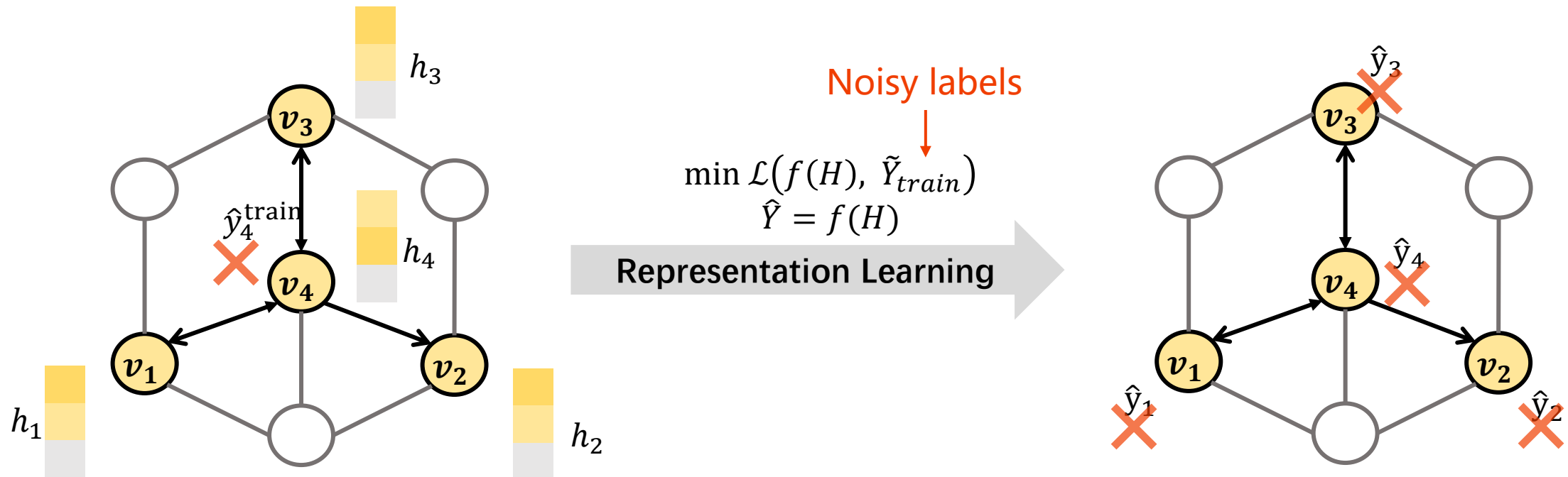
- Using **semi-supervised** learning to develop homophily node representations, GNNs can effectively generalize patterns from labeled training nodes to neighboring unlabeled nodes.
- Thus, GNNs can **perform well** on node-level tasks **with relatively few labels**.



Background

Graph Neural Networks

- However, if the **training labels are incorrect**, it can cause the unlabeled nodes with similar representations in the neighborhood to **be incorrectly learned together**.
- Therefore, node classification tasks using **GNNs rely on high-quality node labels**.



Background

Graph Label Noise

- Graphs are inherently abstract high-dimensional data that are **difficult for humans to understand**, and labeling methods cannot be universally applied to different graph data.
- According to Li et al.^[1], at least 6.91% of labels in the PubMed dataset are incorrect.

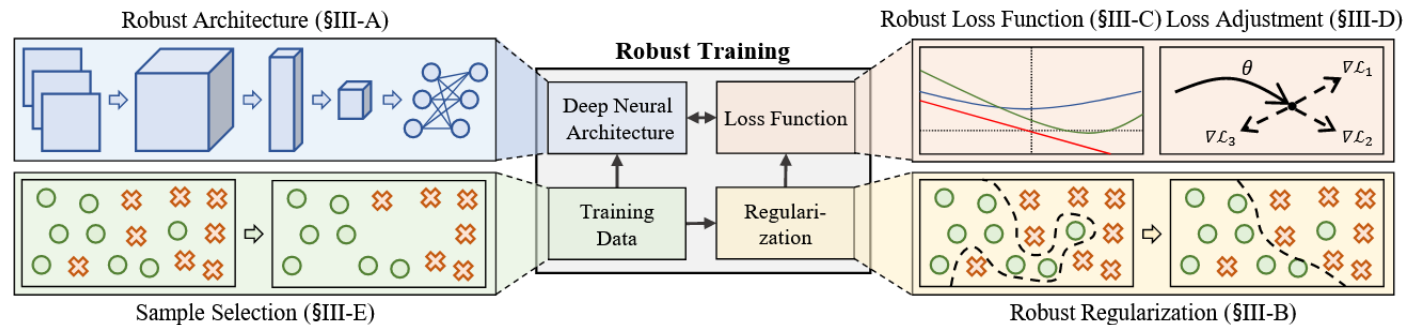
PubMed		Cora	
<p>Severe hypoglycemia in IDDM children</p> <p>Abstract: The incidence of severe hypoglycemia was determined in a 1-yr prospective study of 350 insulin-dependent diabetic (IDDM) children. There were no significant differences in mean glycosylated hemoglobin, age, and duration of disease between the patients who had severe hypoglycemia and those who did not...</p> <p>Original label: Type 2 Diabetes Corrected label: Type 1 Diabetes</p>	<p>Autoimmunity to two forms of glutamate decarboxylase in insulin-dependent diabetes mellitus</p> <p>Abstract: insulin-dependent diabetes mellitus (IDDM) is thought to result from the autoimmune destruction of the insulin-producing beta cells of the pancreas. Years before IDDM symptoms appear, we can detect autoantibodies to one or both forms of glutamate decarboxylase (GAD65 and GAD67), synthesized from their respective...</p> <p>Original label: Type 2 Diabetes Corrected label: Type 1 Diabetes</p>	<p>Beyond Independence: Conditions for the Optimality of the Simple Bayesian Classifier</p> <p>Abstract: The simple Bayesian classifier (SBC) is commonly thought to assume that attributes are independent given the class, but this is apparently contradicted by the surprisingly good performance it exhibits in many domains that contain clear attribute dependences. No explanation for this has been proposed so far. In this paper we show that...</p> <p>Original label: Case-Based Corrected label: Probabilistic Methods</p>	<p>MLC: A Machine Learning Library in C</p> <p>Abstract: We present MLC++, a library of C++ classes and tools for supervised Machine Learning. While MLC++ provides general learning algorithms that can be used by end users, the main objective is to provide researchers and experts with a wide variety of tools that can accelerate algorithm development, increase software reliability...</p> <p>Original label: Theory Corrected label: Probabilistic Methods</p>

[1] Li, Yuwen, Miao Xiong, and Bryan Hooi. "Graphcleaner: Detecting mislabelled samples in popular graph learning benchmarks." International Conference on Machine Learning. PMLR, 2023.

Background

Challenges when dealing with graph label noise

- To address this challenge, an intuitive solution is to draw on the success of previous Learning with Label Noise (LLN)^[2] strategies and apply them to GNNs.



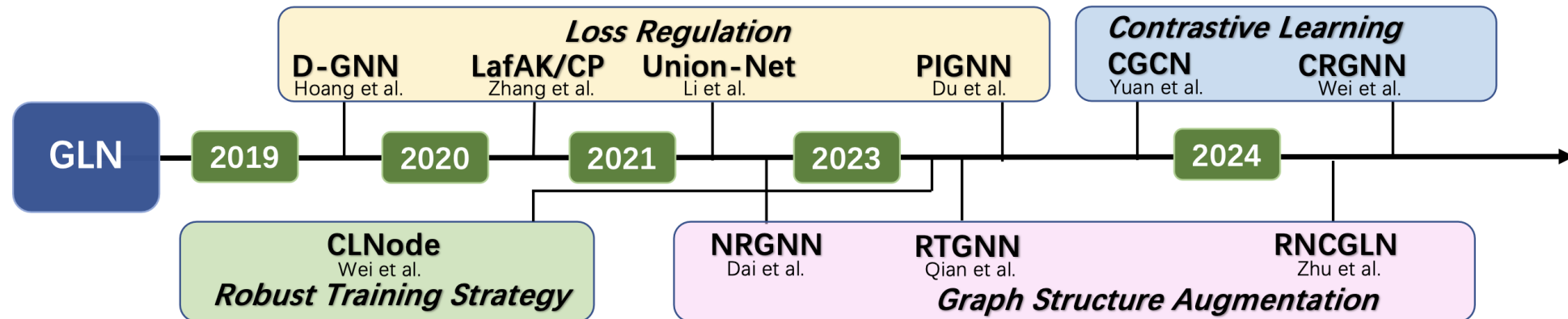
- However, these approaches are not always applicable to graph learning tasks due to:
 1. Non-i.i.d nature of graph data.
 2. Sparse labeling of graph data
 3. Message-passing mechanism of GNNs.

[2] Song H, Kim M, Park D, et al. Learning from noisy labels with deep neural networks: A survey[J]. IEEE transactions on neural networks and learning systems, 2022, 34(11): 8135-8153.

Background

GNN with Label Noise

- To achieve robust graph learning, researchers have proposed a series of GNN with Label Noise (GLN) methods.
- However, these works use different experimental settings in their benchmarks (Dataset selection, Data splitting strategy, Noise type, Noise rate, etc.)



NoisyGL-Introduction

NoisyGL: A Comprehensive Benchmark for Graph Neural Networks under Label Noise

- We introduce NoisyGL: A comprehensive benchmark for graph neural networks under label noise.
- NoisyGL enables **fair comparisons** and **detailed analyses** of GLN methods on noisy labeled graph data across **various datasets**, with **unified experimental settings** and interface.
- Our benchmark has uncovered several important **insights**, and we believe these findings will be **highly beneficial for future studies**.

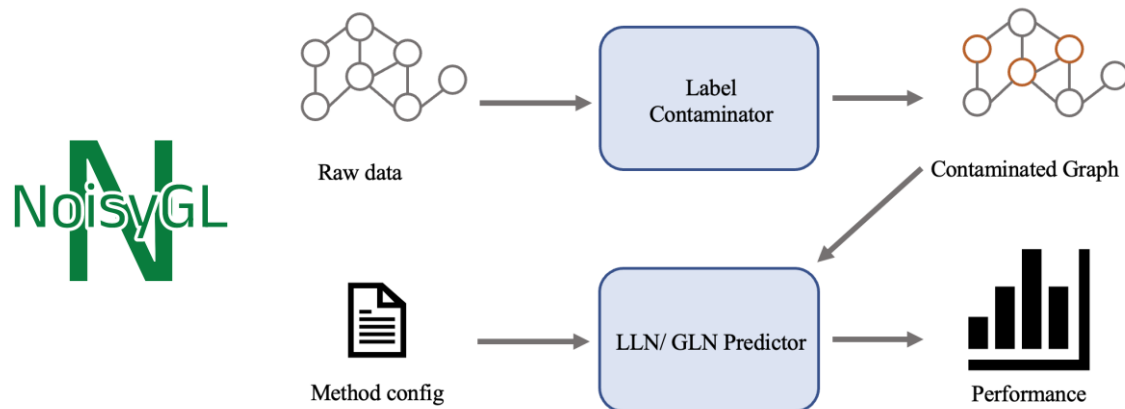


Table A7: Overview of the datasets used in this study.

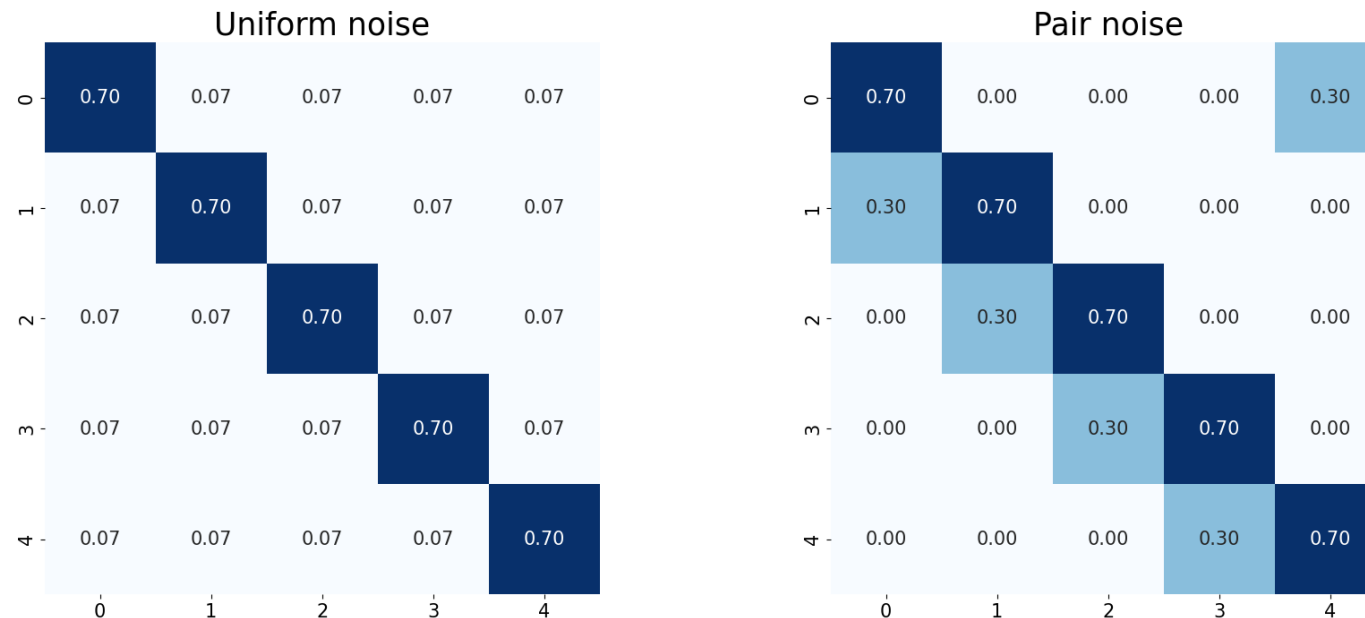
Dataset	# Nodes	# Edges	# Feat.	# Classes	# Homophily	Avg. # degree
Cora	2,708	5,278	1,433	7	0.81	3.90
Citeseer	3,327	4,552	3,703	6	0.74	2.74
Pubmed	19,717	44,324	500	3	0.80	4.50
Amazon-Computers	13,752	491,722	767	10	0.78	35.76
Amazon-Photos	7,650	238,162	745	8	0.83	31.13
DBLP	17,716	105,734	1,639	4	0.83	5.97
BlogCatalog	5,196	343,486	8,189	6	0.40	66.11
Flickr	7575	239738	12047	9	0.24	63.30

NoisyGL-Introduction

NoisyGL: A Comprehensive Benchmark for Graph Neural Networks under Label Noise

We mainly consider two types of label noise that were most commonly used:

- **Pair Noise:** Labels only flip to their corresponding pair class.
- **Uniform Noise:** Labels flip to any class with equal probability.



NoisyGL-Research Questions

Research Questions:

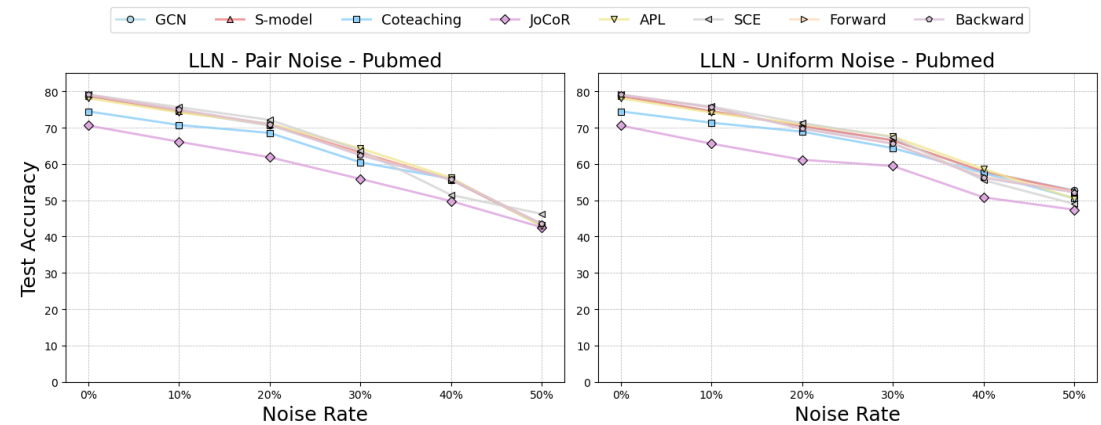
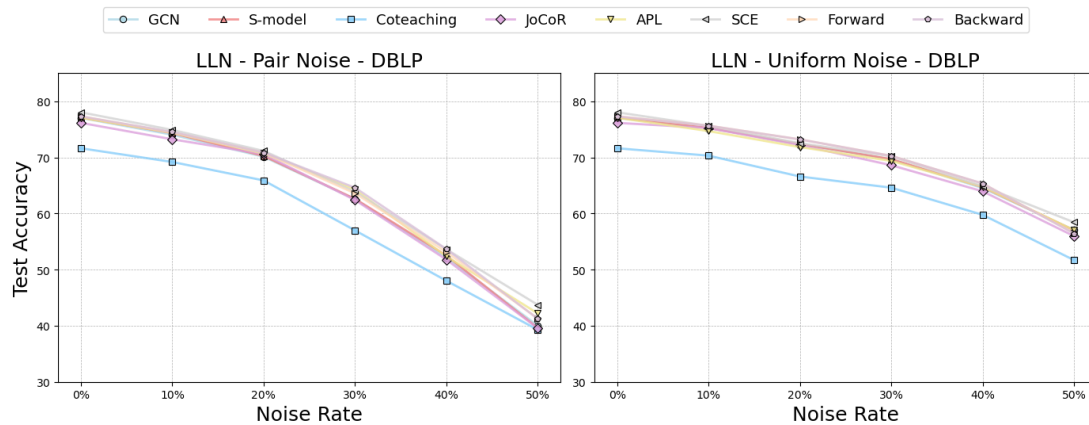
In this study, we aim to answer the following research questions:

- RQ1: Can LLN methods be applied directly to graph learning tasks?
- RQ2: How much progress has been made by existing GLN methods?
- RQ3: Are existing GLN methods computationally efficient?
- RQ4: Are existing GLN methods sensitive to noise rate?
- RQ5: Are existing GLN methods robust to different types of label noise?
- RQ6: Good or bad? Revisiting the role of graph structure in label noise.

NoisyGL-Findings

Finding 1: Most LLN methods do not significantly improve GNN robustness to label noise.

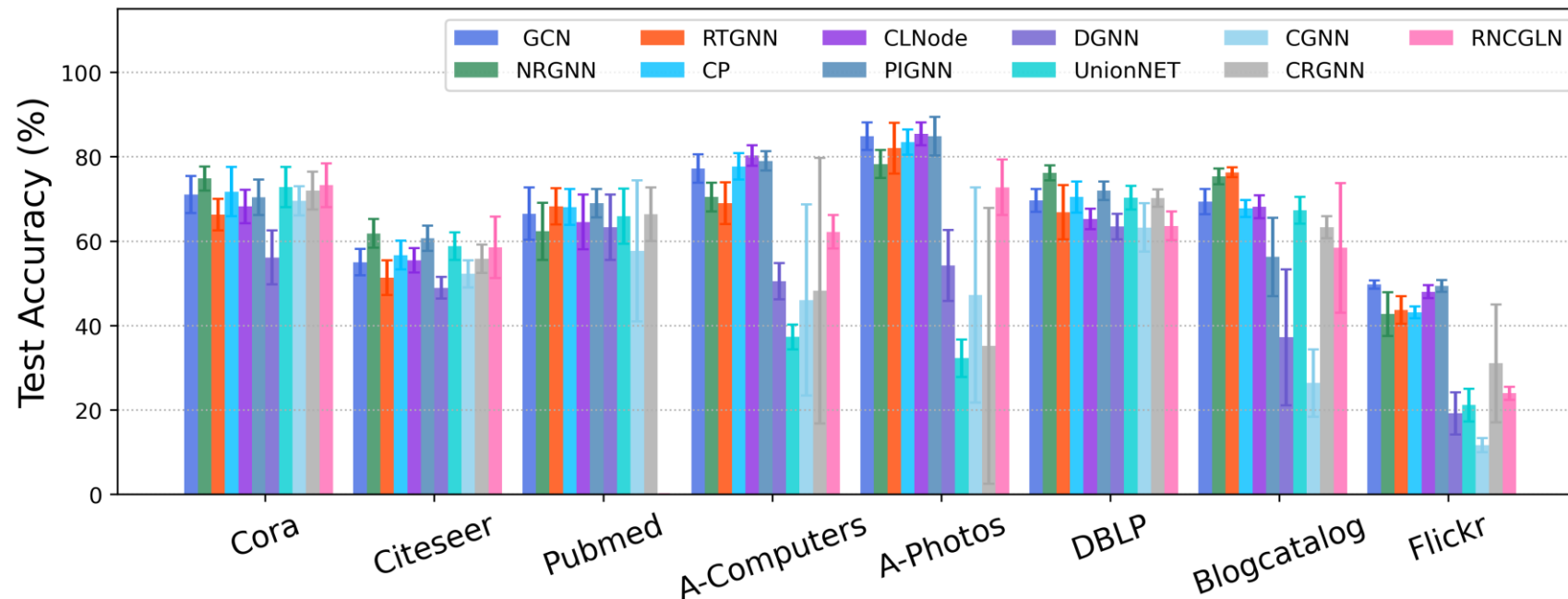
- Most of the selected LLN methods do not substantially improve the performance of the GNN backbone under label noise.



NoisyGL-Findings

Finding 2: Existing GLN methods can alleviate the negative impact of label noise in specific applicable scenarios.

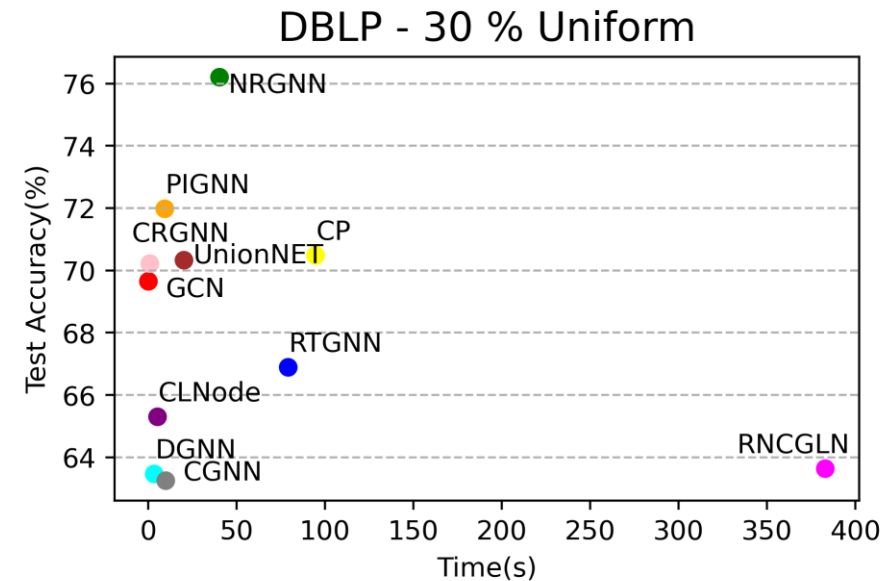
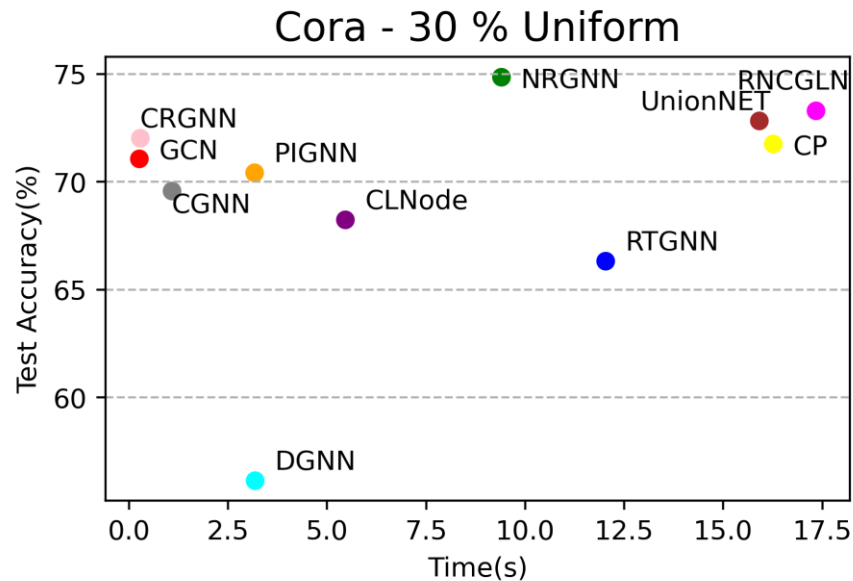
- In most circumstances, **GLN methods are more robust to label noise** than the baseline method. However, **none of them consistently perform well** across all datasets, especially on highly **heterophilous graph**.



NoisyGL-Findings

Finding 3: Some GLN methods are computationally inefficient.

- Some GLN methods take more time to converge.
- For instance, RNCGLN is the slowest, taking 66.8 times longer than GCN on the Cora dataset and an astounding 2945.8 times longer on the DBLP dataset.



NoisyGL-Findings

Finding 4: Pair noise is more harmful to graph learning.

- In our experiments, we consistently observed that **pair noise poses the most significant threat** to the generalization ability of models.
- Our empirical study shows that pair noise has the greatest impact, leading the model to overfit the mislabeled classes.

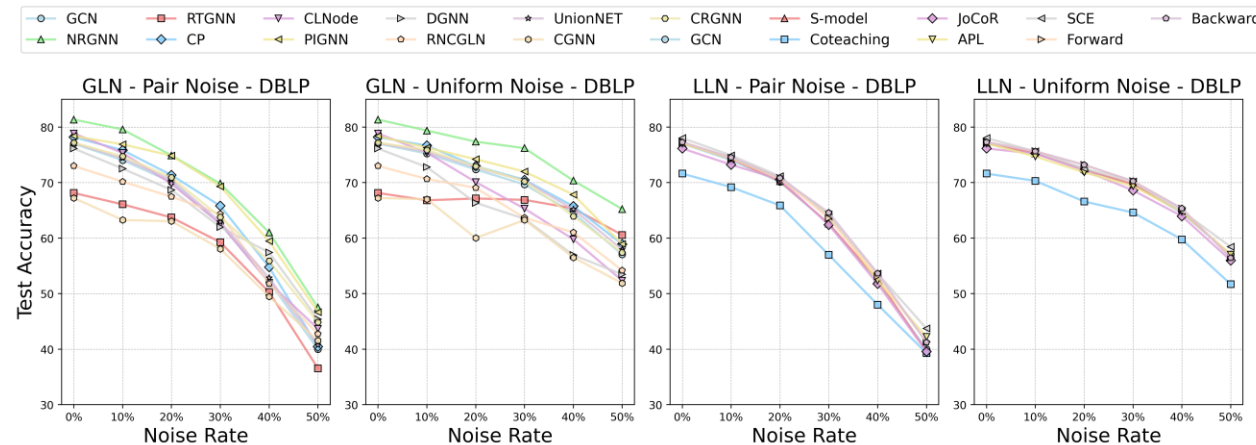


Table 1: Misleading train accuracy of GCN under pair and uniform noise (10 Runs)

Noise type / Dataset (Avg. # Degree)	Cora (3.90)	Citeseer (2.74)	Pubmed (4.50)	A-Computers (35.76)	Blogcatalog (66.11)
50% Pair noise	92.86 ± 6.63	99.00 ± 2.23	91.23 ± 9.38	69.63 ± 12.93	71.67 ± 8.84
50% Uniform noise	76.41 ± 6.52	96.36 ± 4.02	90.24 ± 18.34	22.05 ± 7.28	32.53 ± 12.61

NoisyGL-Findings

Finding 4: Pair noise is more harmful to graph learning.

- **Intuitively:** Pair noise flips labels to the pair class, which can be more misleading than uniform noise.
- **Formally:** A simplified GCN with ridge regression has the following closed-form solution^[3]:

$$\hat{Y} = A^k X \left((A^k X)^T (A^k X) + \lambda I \right)^{-1} (A^k X)^T Y_t = P Y_t$$

- Introducing label noise is equivalent to multiplying the prediction by a transition matrix: $\hat{Y}_{ptb} = P Y_t Q$
- The difference in prediction results trained under clean and noisy labels:

$$\Delta Y = \|\hat{Y} - \hat{Y}_{ptb}\|_2 = \|P Y_t - P Y_t Q\|_2 = \|P Y_t (I - Q)\|_2$$

- The upper bound of prediction error can be expressed as:

$$\Delta Y \leq \|P\|_2 \cdot \|Y_t\|_2 \cdot \|I - Q\|_2$$

[3] Zhang, Mengmei, et al. "Adversarial label-flipping attack and defense for graph neural networks." 2020 IEEE International Conference on Data Mining (ICDM). IEEE, 2020.

NoisyGL-Findings

Finding 4: Pair noise is more harmful to graph learning.

- The upper bound of prediction error can be expressed as:

$$\Delta Y \leq \|P\|_2 \cdot \|Y_t\|_2 \cdot \|I - Q\|_2,$$

- where $\|P\|_2 \cdot \|Y_t\|_2$ are fixed values and are independent of the noise model.
- Let the noise rate be ϵ , for Uniform noise and Pair noise, $\|I - Q\|_2$ has different values:

$$\|I - Q_{uniform}\| = \sqrt{c\epsilon^2 + c(c-1)\left(-\frac{\epsilon}{c-1}\right)^2} = \epsilon\sqrt{c + \frac{c}{c-1}}$$

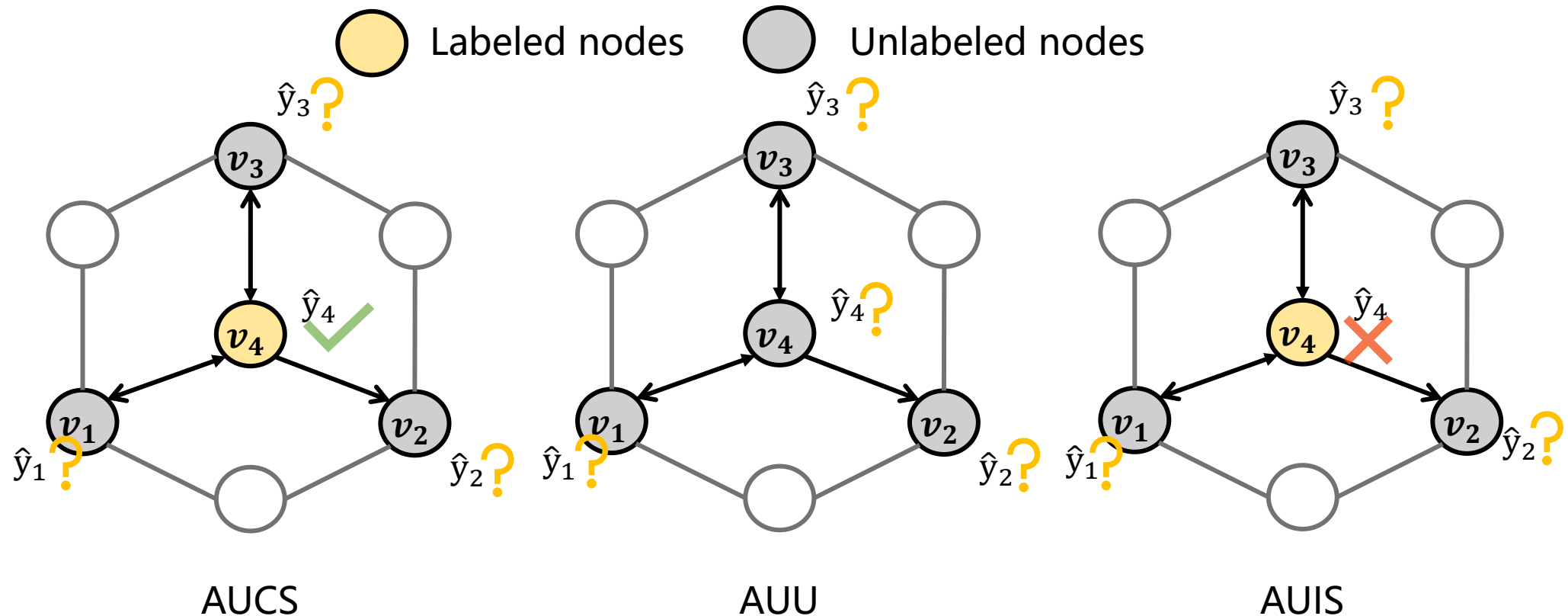
$$\|I - Q_{pair}\| = \sqrt{c\epsilon^2 + c\epsilon^2} = \sqrt{2c\epsilon^2} = \epsilon\sqrt{2c}$$

- In multi-class node classification tasks, where $c \geq 2$, we have $\|I - Q_{uniform}\| \leq \|I - Q_{pair}\|$.
- This proves that **the upper bound of the prediction error caused by pair noise is greater** than uniform noise, indicating that **pair noise is more disruptive**.

NoisyGL-Findings

Finding 5: Label noise can Propagate through graph topology.

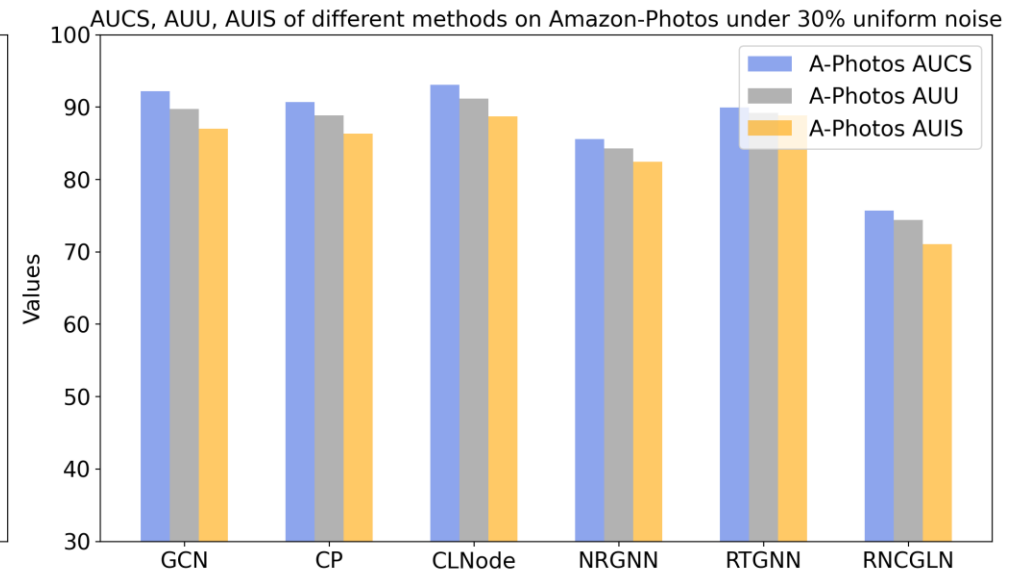
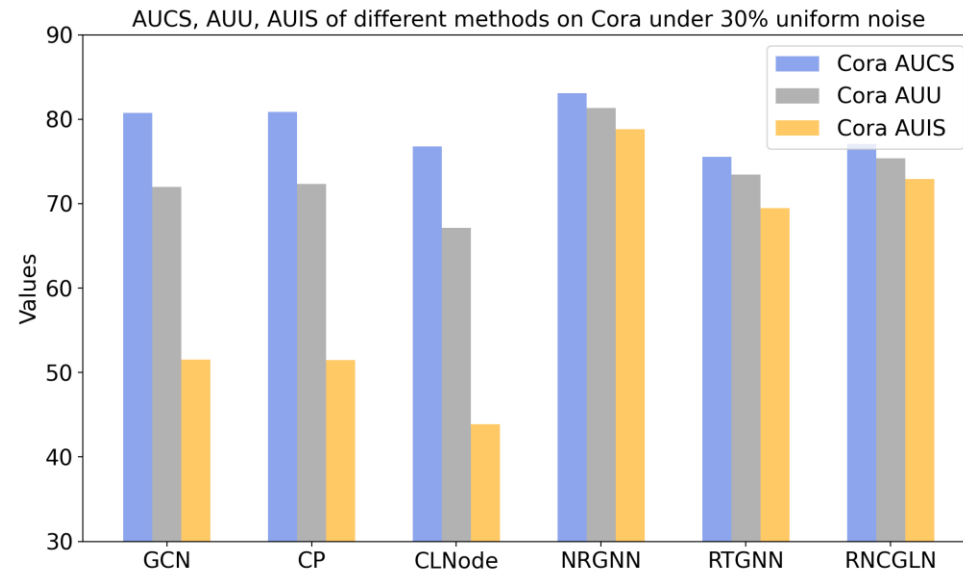
- **AUCS**, **AUU**, and **AUIS** represent the probability of **correctly classifying an unlabeled node** (test node) under three conditions: the presence of **correctly labeled neighboring nodes**, **no labeled neighboring nodes**, and the presence of **incorrectly labeled neighboring nodes**, respectively.



NoisyGL-Findings

Finding 5: Label noise can Propagate through graph topology.

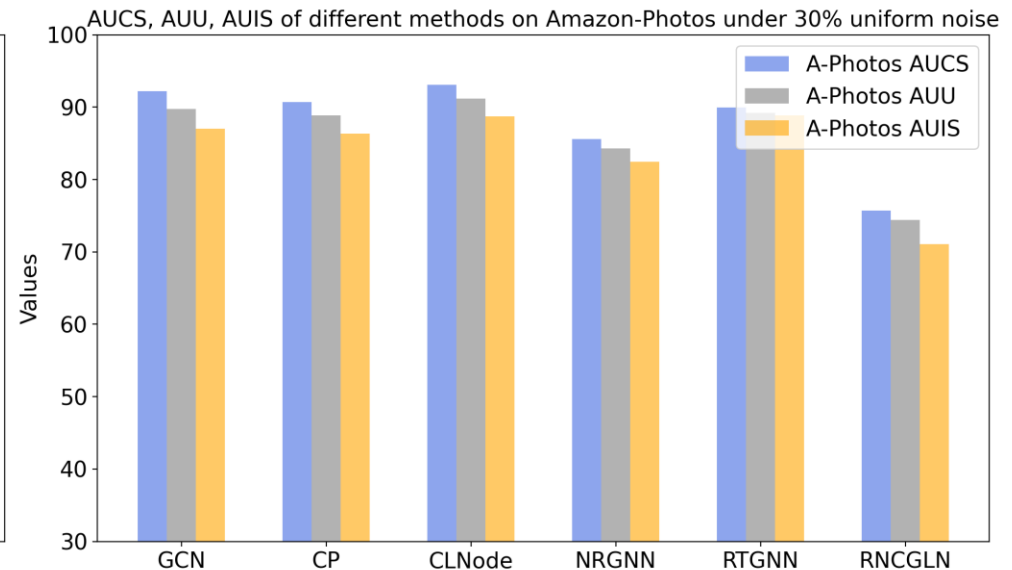
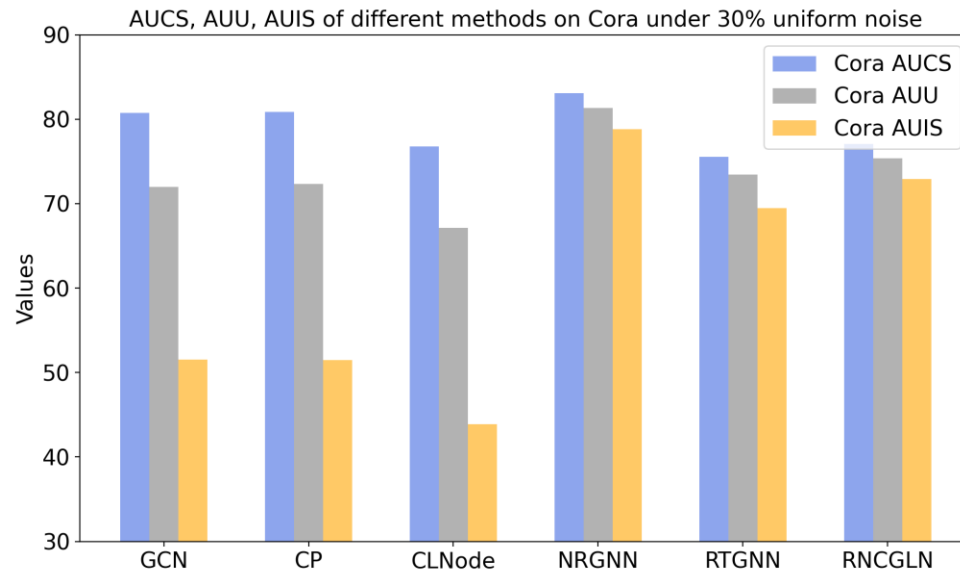
- Experimental results show that the classification accuracy of unlabeled data significantly decreases when there are incorrectly labeled nodes in the neighborhood.



NoisyGL-Findings

Finding 6: Sparse graphs are more vulnerable to the propagation effect of label noise.

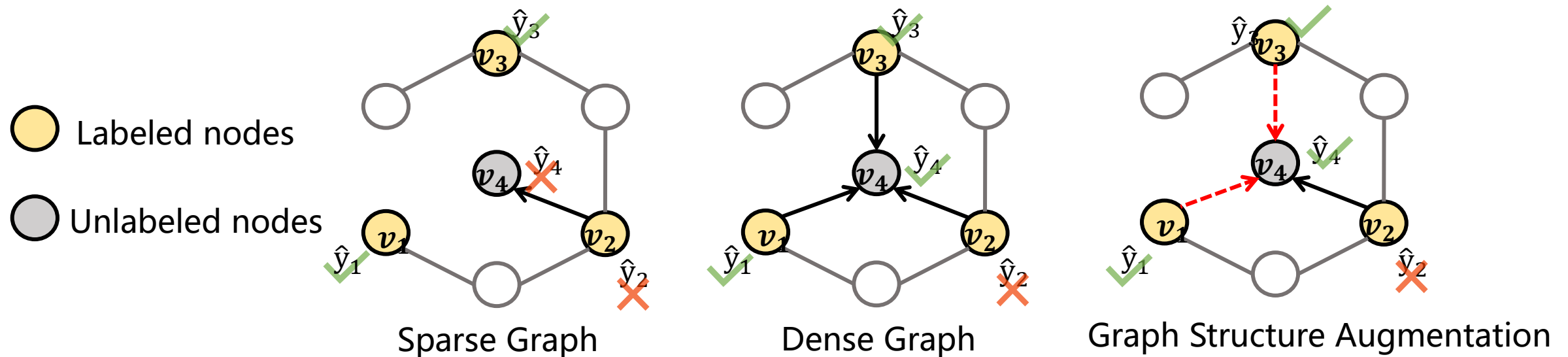
- **The propagation of label noise is more apparent in sparse graphs (e.g. Cora) and less noticeable in dense graphs (e.g. A-Photos). This probably because nodes in dense graphs can receive more supervision from the neighboring nodes.**



NoisyGL-Findings

Finding 6: Sparse graphs are more vulnerable to the propagation effect of label noise.

- **Graph Structure Augmentation** methods (NRGNN, RTGNN, RNCGLN) can mitigate the propagation of label noise in sparse graphs.
- The **up-sampling process** in these methods introduces more edges, providing additional supervision for unlabeled nodes.



NoisyGL-Future directions

Designing widely applicable GLN approaches

- There is no existing GLN method applicable for all scenarios, **especially for highly heterophilous graphs**. Therefore, it is necessary to develop GLN methods that are broadly applicable to various types of data.

Designing GLN approaches for various graph learning tasks

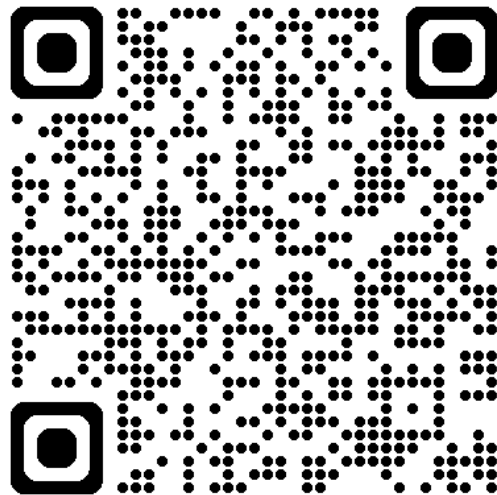
- Previous studies on GLN have predominantly focused on node classification tasks. Hence, designing GLN methods for more graph learning tasks (e.g. link prediction, graph classification) is crucial .

Considering other types of label noise in graph learning

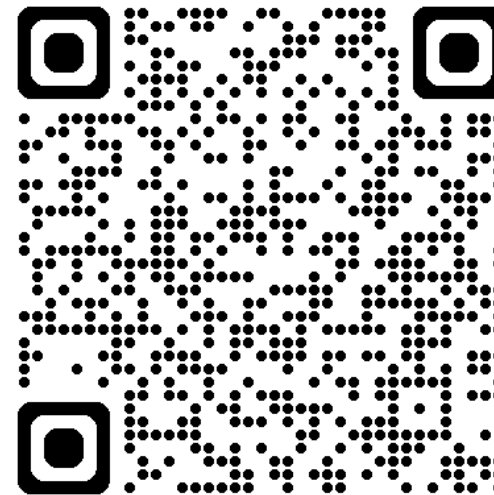
- Current GLN methods assume that labels are affected by i.i.d. label noise. However, the non-i.i.d. Graph data, may also have non-i.i.d. label noise. Therefore, it is necessary to redesign noise models and GLN schemes under new assumptions.

NoisyGL

Paper



Code



Thank you for listening!