

Generate or Re-Weight? A Mutual-Guidance Method for Class-Imbalanced Graphs

Zhongying Zhao, Gen Liu, Qi Meng, Chao Li*, Qingtian Zeng*

College of Computer Science and Engineering, Shandong University of Science and Technology,
Qingdao 266590, China

zzysuin@163.com, lg97@sdust.edu.cn, mengqi@sdust.edu.cn, lichao@sdust.edu.cn, qtzeng@163.com

Abstract

Class imbalance is a widespread problem in graph-structured data. The existing studies tailored for class-imbalanced graphs are typically categorized into generative and re-weighting methods. However, the former merely focuses on quantity balance rather than learning balance. The latter performs the fine-tuning in a majority-minority paradigm, overlooking the authentic-generative one. In fact, their collaboration is capable of relieving respective limitations. To this end, we propose a **Mutual-Guidance** method for class-imbalanced graphs, namely **GraphMuGu**. Specifically, we first design an uncertainty-aware method to quantify the number of synthesized samples for each category. Furthermore, we devise a similarity-aware method to re-weight the importance of the authentic and generative samples. To the best of our knowledge, the proposed GraphMuGu is the first try to incorporate the generative and re-weighting methods into a unified framework. The experimental results on five class-imbalanced datasets demonstrate the superiority of the proposed method. The source codes are available at <https://github.com/ZZY-GraphMiningLab/GraphMuGu>.

1 Introduction

Graph Neural Networks (GNNs) have demonstrated impressive success across a range of graph analyzing tasks, including fraud detection, transportation analysis, disease diagnosis, and so on [Zhang *et al.*, 2024; Rahmani *et al.*, 2023; Sun *et al.*, 2020]. Their remarkable performance is typically under the assumption of class balance, i.e., samples across various categories are unbiased in quantity [Ju *et al.*, 2024]. However, the above assumption barely holds, as the class imbalance exists inherently in real-world scenarios [Dou *et al.*, 2020; Liu *et al.*, 2021]. It refers to a few classes holding enormous labeled nodes (i.e., majority class), while most classes contain limited labeled nodes (i.e., minority class). For instance, in fake account detection, the majority of users are benign, while only a few of them are bots. Analogously, in financial

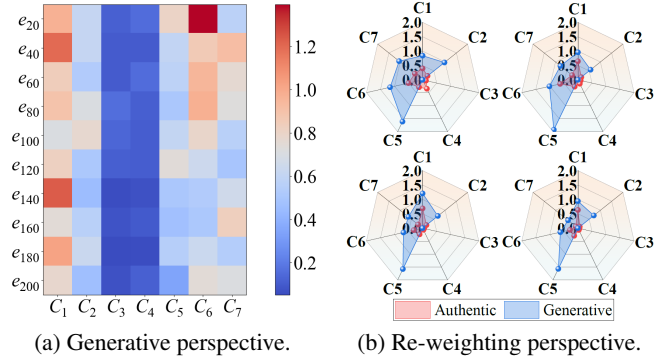


Figure 1: The exploration of potential problems in generative and re-weighting perspectives on Cora-LT dataset.

fraud detection, the quantity of compliant users far exceeds that of fraudsters. Once trapped in the problem of class imbalance, the GNN-based models over-fit the majority classes and under-represent the minority ones.

The studies tailored for the class-imbalanced graphs are categorized into generative and re-weighting methods. The former intends to synthesize new samples for minority classes, thereby balancing the distribution of samples across various categories. For example, GraphSMOTE first extends the existing over-sampling methods to graph-structured data [Zhao *et al.*, 2021]. GraphSHA explores the subspace squeeze issue of minority classes and enlarges the decision boundaries of minority classes by synthesizing harder minority samples [Li *et al.*, 2023]. The latter aims to fine-tune the weight of each sample, thus compelling the model to focus on minority ones. For instance, ReNode provides a unified perspective on analyzing the quantity and topology imbalance jointly by taking into account the node influence shift [Chen *et al.*, 2021]. TAM adjusts margins node-wisely according to the extent of deviation from connectivity patterns [Song *et al.*, 2022]. However, both generative and re-weighting methods only adhere to their standpoints and ignore potential collaboration. To this end, we revisit the generative and re-weighting methods to explore the underlying problems with an empirical study in Figure 1. It tells us two inspiring observations.

(1) **Generative Perspective.** The generative methods focus on synthesizing samples for each category until matching

*Corresponding Authors.

the majority. Thus, a question arises: Does the generated equal quantity balance the learning ability of the model for each category? To answer this question, we plot the mean loss of each category in Figure 1 (a). It can be observed that even if the number of samples in each category is balanced, the model still exhibits differences in its learning ability. This observation demonstrates that generative methods still lack the supervision to quantify the number of synthesized samples for each category.

(2) **Re-weighting Perspective.** The re-weighting methods are designed to increase the significance of minority samples, thereby compelling the model to allocate greater attention to these instances. In general, the authentic and generative samples are treated equally. Nevertheless, can the model learn them impartially? Analogously, we visualize the mean loss of authentic and generative samples for each category, respectively. The results are shown in Figure 1 (b). It can be seen that the model generalizes well on the authentic samples but struggles with the generative ones. This phenomenon indicates that it is essential to re-weight the authentic and generative samples to balance the concern of the model.

To this end, we propose a Mutual-Guidance method for the class-imbalanced graphs. To the best of our knowledge, it is the first try to incorporate the generative and re-weighting method into a unified framework. Specifically, we present an uncertainty-aware method to quantify the number of synthesized samples for each category. It first measures the mean loss of samples for each category to identify the uncertainty of the model. Then, it leverages the uncertainty to quantify the number of synthesized samples for each category adaptively. Furthermore, we devise a similarity-aware method to re-weight the importance of the authentic and generative samples. It summarizes the pacesetter feature by averaging the features of labeled samples belonging to the same category. Subsequently, it re-weights the generative samples by evaluating the similarity of their features and the corresponding pacesetter features. We conduct experiments under two imbalanced settings on five datasets. The experimental results demonstrate that our method outperforms ten competitive methods.

The main contributions of this work are as follows.

- We propose a mutual-guidance method for class-imbalanced graphs. It is the first try to incorporate the generative and re-weighting method into a unified framework.
- We design an uncertainty-aware method to quantify the number of synthesized samples for each category.
- We devise a similarity-aware method to re-weight the importance of the authentic and generative samples.
- We conduct extensive experiments on five class-imbalance datasets to verify the effectiveness of the proposed method.

2 Related Work

2.1 Graph Neural Networks

Graph Neural Networks are deep learning models designed to learn and reason directly on graph-structured data [Wu *et al.*, 2020].

They can be categorized into Spectral Graph Neural Networks and Spatial Graph Neural Networks based on their implementation manners. Spectral Graph Neural Networks aim to define the graph convolution through spectral graph theory and the convolution operation. Bruna *et al.* first formalized the definition of spectral graph convolution and emphasized its high computational complexity [Bruna *et al.*, 2014]. To this end, Defferrard *et al.* introduced the k -order Chebyshev polynomial to approximate the graph convolution kernel [Defferrard *et al.*, 2016]. Kipf *et al.* advanced it by leveraging the limited 1-order Chebyshev polynomial and re-normalization technique, giving rise to Graph Convolutional Networks (GCN) [Kipf and Welling, 2017]. Spatial Graph Neural Networks incorporate structural and node feature information by defining neighborhood aggregation functions. Gilmer *et al.* proposed the Message Passing Neural Network (MPNN), a general framework for spatial graph convolution [Gilmer *et al.*, 2017]. Veličković *et al.* presented the Graph Attention Network (GAT), which defines the aggregation function using a learnable attention mechanism [Veličković *et al.*, 2018]. Hamilton *et al.* introduced GraphSAGE, a model that leverages neighbor sampling and a variety of aggregation functions to explore the fusion of neighboring information [Hamilton *et al.*, 2017]. Furthermore, researchers also investigated some interesting techniques for GNNs, such as graph transformer [Yun *et al.*, 2019], graph diffusion [Li *et al.*, 2024], graph foundation model [Mao *et al.*, 2024], etc.

2.2 Class-Imbalance Problem

Class imbalance is a ubiquitous challenge in graph representation learning [Liu *et al.*, 2023]. The existing countermeasures can be classified into generative and re-weighting methods. The former is devoted to synthesizing minority samples to balance the training set. For example, Zhao *et al.* extended the over-sampling methods for i.i.d data to the graph [Zhao *et al.*, 2021]. They utilized the feature extractor to construct an intermediate embedding space, then proceeded to train an edge estimator and the GNN-based classifier on top of that. Park *et al.* proposed GraphENS to relieve the neighbor memorization problem encountered by existing generative methods [Park *et al.*, 2021]. It synthesizes an ego network for minor classes with neighbor sampling and saliency-based node mixing. Li *et al.* explored the problem of squeezed minority [Li *et al.*, 2023]. Hence, they presented GraphSHA, which synthesizes harder samples to avoid invading the spaces of neighbor classes. The re-weighting methods intend to tilt the training focus towards minority samples. For instance, Cui *et al.* leveraged the number of effective samples among each class to re-weight the classes [Cui *et al.*, 2019]. Wang *et al.* introduced a class prototype-driven training paradigm to balance the loss between majority and minority classes [Wang *et al.*, 2022]. Park *et al.* explored the decision boundary in class-imbalance scenarios and presented a novel influence-balance loss to solve the overfitting problem of majority classes. Song *et al.* proposed a topology-aware loss to re-weight margins node-wisely according to the extent of deviation from connectivity patterns [Song *et al.*, 2022]. In addition, researchers also explored contrastive-based methods to mitigate the class imbalance on graphs [Zeng *et al.*, 2023].

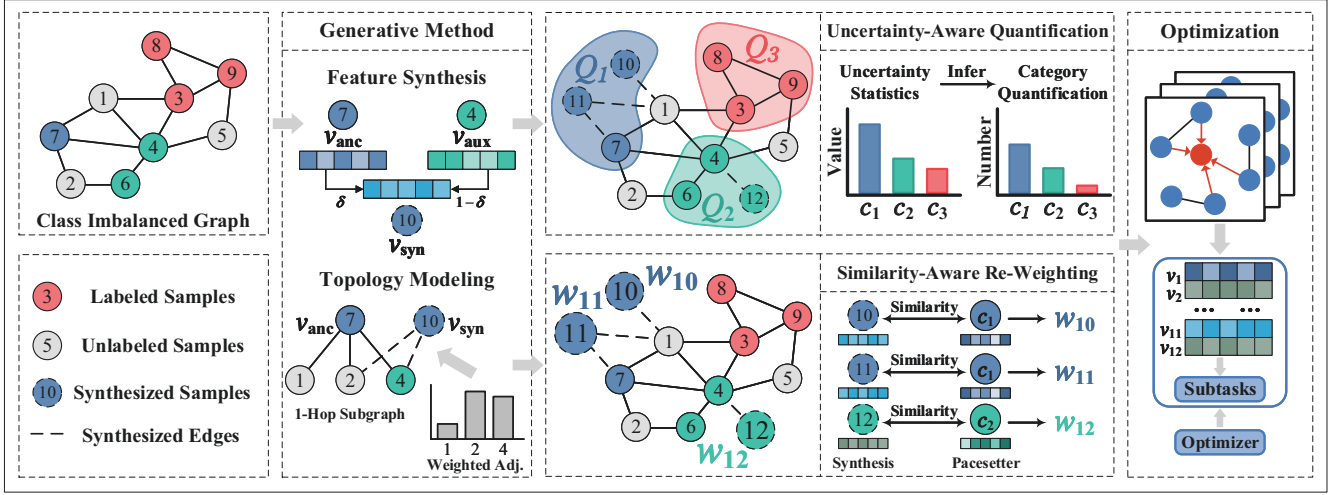


Figure 2: The overall framework of the proposed GraphMuGu.

3 Proposed Method

3.1 Preliminaries

In this section, we first define the attributed graph and imbalance ratio. Then, we formulate the Graph Neural Networks. Finally, we clarify the task of node classification.

Definition 1. Attributed Graph. Suppose $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{X})$ is an attributed graph, where $\mathcal{V} = \{v_1, v_2, \dots, v_n\}$ is the set of nodes and $\mathcal{E} = \{e_1, e_2, \dots, e_m\}$ is the set of edges. $\mathbf{X} \in \mathbb{R}^{|\mathcal{V}| \times d}$ is the feature matrix, where d represents the dimension of node features. $\mathbf{A} \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{V}|}$ is the adjacency matrix, where $A_{ij} = 1$ indicates that there is an edge between v_i and v_j , otherwise, $A_{ij} = 0$.

Definition 2. Imbalance Ratio. Suppose the potential categories are in $\mathcal{C} = \{c_1, c_2, \dots, c_l\}$, where the class with the most samples is denoted as c_{max} and the class with the least samples is abbreviated as c_{min} . Then, the imbalance ratio ρ is defined in Eqn. (1).

$$\rho = \frac{|c_{max}|}{|c_{min}|}. \quad (1)$$

Definition 3. Graph Neural Networks. The message-passing paradigm of GNNs can be summarized as aggregate-update, which are specified in Eqn. (2) and Eqn. (3).

$$\mathbf{a}_i^{(l)} = \text{AGGREGATE}^{(l)}(\mathbf{h}_j^{(l-1)}, \forall v_j \in \mathcal{N}_i), \quad (2)$$

$$\mathbf{h}_i^{(l)} = \text{UPDATE}^{(l)}(\mathbf{h}_i^{(l-1)}, \mathbf{a}_i^{(l)}), \quad (3)$$

where \mathbf{a}_i^l is the aggregation of neighboring features at the l -th layer, \mathcal{N}_i is the set of neighbors of v_i , and \mathbf{h}_i^l is the embedding of v_i at the l -th layer which is updated on \mathbf{h}_i^{l-1} and \mathbf{a}_i^l .

Problem. Node Classification. An attributed graph is denoted as $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{X})$. \mathcal{V}^L is the set of labeled nodes and \mathcal{V}^U is the set of unlabeled nodes, where $|\mathcal{V}^L| \ll |\mathcal{V}^U|$. The goal of node classification is to train a model that takes feature matrix \mathbf{X} and adjacency matrix \mathbf{A} as input and predicts the labels of unlabeled nodes by learning and optimizing the function $f(\mathbf{X}, \mathbf{A}) \rightarrow \hat{\mathcal{Y}}$.

3.2 Framework

In this section, we propose a mutual-guidance method for class-imbalanced graphs, as illustrated in Figure 2. It mainly consists of two modules: (i) Uncertainty-Aware Quantification and (ii) Similarity-Aware Re-Weighting. In particular, it first schemes the synthetic paradigm of generated samples. Then, it focuses on their quantitative and weighting problems. Specifically, it evaluates the loss distribution to assess the uncertainty of the model across various classes and adjusts the number of samples generated for each class accordingly. Furthermore, it summarizes the pacesetter features by averaging the features of labeled samples in the same category. Subsequently, it measures the similarity of synthesized sample features and their corresponding class-wise pacesetter features. Afterward, it fine-tunes the weights of each synthesized sample. Finally, the GNN-based models are trained on the graph balanced from the perspectives of generative and re-weighting. The implementation details are elaborated in the subsequent sections.

3.3 Synthetic Paradigm of Generative Sample

To synthesize a minority node, it first identifies an anchor node (i.e., v_{anc}) and an auxiliary node (i.e., v_{aux}). The anchor node is sampled from the minority class. Note that, to enlarge the decision boundary of the minority, it refers to the hardness-aware sampling strategy [Li et al., 2023]. Specifically, the hardness is measured in Eqn. (4).

$$\mathcal{H}_i = 1 - \frac{\exp(\mathbf{Z}_{i, \hat{y}_i} / \tau)}{\sum_{j=1}^{|\mathcal{C}|} \exp(\mathbf{Z}_{i, j} / \tau)}, \quad (4)$$

where \mathcal{H}_i is the hardness of node v_i , \mathbf{Z}_i is the logits of v_i , and τ is the temperature.

Then, it samples the minority anchor node v_{anc} from the hardness-based multinomial distribution. In identifying the auxiliary node v_{aux} , the category of v_{aux} is sampled from the classification probability of the anchor node. Afterward,

within the nodes belonging to c_{aux} , the auxiliary node is sampled from the multinomial with their confidence in c_{anc} as the probability.

Let the feature of v_{anc} and v_{aux} be abbreviated as \mathbf{X}_{anc} and \mathbf{X}_{aux} , respectively. The feature of the synthesized node is mixed up according to Eqn (5).

$$\mathbf{X}_{syn} = \delta \mathbf{X}_{anc} + (1 - \delta) \mathbf{X}_{aux}, \quad (5)$$

where \mathbf{X}_{syn} is the feature of synthesized node and $\delta \in [0, 1]$ is the hyper-parameter that controls the relative importance of \mathbf{X}_{anc} and \mathbf{X}_{aux} .

In modeling the topology of the synthesized node, it first identifies the degree of the synthesized node by sampling from the degree distribution of the entire graph as formulated in Eqn. (6) and Eqn. (7).

$$\mathcal{P}_{Dg}(k) = \frac{\sum_{v \in \mathcal{V}} \mathbb{I}_{\{d(v)=k\}}}{|\mathcal{V}|}, \quad (6)$$

$$k_{syn} \sim \mathcal{P}_{Dg}(k), \quad (7)$$

where $\mathcal{P}_{Dg}(k)$ is the probability of a node occupying degree k , $\mathbb{I}_{\{\cdot\}}$ is an indicator function, and k_{syn} is the degree of v_{syn} .

Then, it connects v_{syn} to the nodes within the 1-hop subgraph of v_{anc} , as they tend to share the same label with v_{anc} according to graph homophily. However, the 1-hop subgraph of v_{anc} may contain fewer nodes than the sampled degree of v_{syn} . Furthermore, neighbor sampling from the unweighted graph ignores the topological information. Thus, it leverages graph diffusion to construct a normalized weighted graph as specified in Eqn. (8).

$$\bar{\mathbf{S}} = \mathbf{D}^{-1} \sum_{r=0}^{\infty} \theta_r \mathbf{T}^r, \quad (8)$$

where $\bar{\mathbf{S}} \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{V}|}$ is the normalized diffusion matrix, $\theta_r = \alpha(1 - \alpha)^r$, α is a hyper-parameter, $\mathbf{T} = \mathbf{A}\mathbf{D}^{-1}$, and \mathbf{D} is the diagonal matrix.

To reduce the computational cost, it only retains the top- K elements in each column of $\bar{\mathbf{S}}$ and sets the remaining elements to 0, sparsifying the normalized diffusion matrix. The sparsified diffusion matrix is denoted as $\tilde{\mathbf{S}}$. Finally, it leverages $\tilde{\mathbf{S}}_{anc}$ to sample the neighbors of v_{syn} .

In summary, the synthesized node is defined in Eqn. (9).

$$\begin{cases} \mathbf{X}_{syn} = \delta \mathbf{X}_{anc} + (1 - \delta) \mathbf{X}_{aux} \\ \mathcal{N}_{syn} \sim \tilde{\mathbf{S}}_{anc} \\ \mathcal{Y}_{syn} = \mathcal{Y}_{anc} \end{cases}, \quad (9)$$

where \mathbf{X}_{syn} , \mathcal{N}_{syn} , and \mathcal{Y}_{syn} represent the feature, neighbor distribution, and class label of the synthesized sample, respectively.

3.4 Uncertainty-Aware Sample Quantification

The existing generative methods typically synthesize samples for each category until matching the majority. However, empirical studies have revealed that an equal number of training samples across various categories does not ensure balanced model learning. Hence, we propose an uncertainty-aware sample method to adaptively quantify the numbers of the synthesized samples for each category.

As we all know, the uncertainty of the model can be naturally reflected by training loss. Thus, it first measures the uncertainty for each category as specified in Eqn. (10) and Eqn. (11).

$$\mathcal{L}_{c_i} = - \sum_{u \in \{v \in \{\mathcal{V}^L \cup \mathcal{V}^S\} | y_v = i\}} y_u \log \hat{y}_u, \quad (10)$$

$$\mathcal{U}_{c_i} = \frac{\mathcal{L}_{c_i}}{|\{v \in \{\mathcal{V}^L \cup \mathcal{V}^S\} | y_v = i\}|}, \quad (11)$$

where \mathcal{V}^L is the set of labeled nodes, \mathcal{V}^S indicates the set of synthesized nodes, y is the ground truth label, \hat{y} is the prediction, \mathcal{L}_{c_i} represents the total loss of category c_i , and \mathcal{U}_{c_i} indicates the uncertainty of model for category c_i .

Then, it schemes a flexible sample generation strategy. In contrast to existing methods that synthesize samples for each category until matching the majority, it exclusively focuses on synthesizing samples for categories whose sample count is less than the average one across all categories.

Specifically, it evaluates the class-wise average sample quantity by Eqn. (12).

$$\bar{\mathcal{Q}} = \frac{|\mathcal{V}^L|}{|\mathcal{C}|}, \quad (12)$$

where $\bar{\mathcal{Q}}$ is the class-wise average sample quantity and $|\mathcal{C}|$ indicates the number of categories.

Afterward, it quantifies the numbers of synthesized samples for each category by Eqn. (13) and Eqn. (14).

$$\mathcal{U}'_{c_i} = \frac{\mathcal{U}_{c_i}}{\sum_{i=1}^{|\mathcal{C}|} \mathcal{U}_{c_i}}, \quad (13)$$

$$\mathcal{Q}_{c_i} = \begin{cases} \beta \mathcal{U}'_{c_i} \bar{\mathcal{Q}}, & |\{v \in \mathcal{V}^L | y_v = i\}| < \bar{\mathcal{Q}} \\ 0, & |\{v \in \mathcal{V}^L | y_v = i\}| \geq \bar{\mathcal{Q}} \end{cases}, \quad (14)$$

where \mathcal{U}'_{c_i} is the normalized uncertainty, \mathcal{Q}_{c_i} is the number of synthesized samples for category c_i , β is the scale factor.

In summary, the uncertainty-aware quantification method adaptively identifies the numbers of the synthesized samples for each category from the perspective of the model, realizing the transition from “quantity balance” to “learning balance”. Furthermore, it reduces the computational cost and avoids the noise introduced by excessive synthesized samples.

3.5 Similarity-Aware Sample Re-Weighting

The existing re-weighting methods aim to fine-tune the focus of the model on majority and minority. Nevertheless, the difference in learning difficulty between authentic and synthesized samples still troubles the model. Thus, we devise a similarity-aware method to re-weight the importance of synthesized samples.

As empirical studies have proven, the model generalizes well on the authentic samples but struggles with the synthesized ones. Therefore, it measures the difference between authentic and synthesized samples by similarity and emphasizes the focus of the model on the latter accordingly.

Specifically, it first evaluates the average feature of the labeled samples within the same class and denotes it as “pacesetter” in Eqn. (15).

$$\mathbf{X}_{pac}^{c_i} = \frac{\sum_{\{v \in \mathcal{V}^L | y_v = i\}} \mathbf{X}_v}{|\{v \in \mathcal{V}^L | y_v = i\}|}, \quad (15)$$

where $\mathbf{X}_{pac}^{c_i}$ is the pacesetter of class c_i .

Subsequently, it identifies the weights by calculating the cosine similarity of the synthesized sample and its corresponding pacesetter as formulated in Eqn. (16).

$$\mathcal{W}_{u \in \{v \in \mathcal{V}^S | y_v = i\}} = (\mathcal{R}(\sigma(\frac{\mathbf{X}_u \mathbf{X}_{pac}^{c_i}}{\|\mathbf{X}_u\| \cdot \|\mathbf{X}_{pac}^{c_i}\|})))^\gamma, \quad (16)$$

where \mathcal{V}^S is the set of synthesized samples, $\mathbf{X}_{pac}^{c_i}$ is the pacesetter for category c_i , $\|\cdot\|$ is the Euclidean norm, γ is the gain factor, $\sigma(\cdot)$ is the sigmoid function, and $\mathcal{R}(\cdot)$ is the reciprocal operation.

To sum up, the similarity-aware re-weighting method fine-tunes the importance of each synthesized sample, achieving the switch of the re-weighting paradigm from “majority-minority” to “authentic-generative”. Moreover, it improves the generalization ability of the model and relieves the risk of overfitting.

3.6 Optimization

The synthesized samples are inserted into the class-imbalanced graph, steering the graph towards class balance. Finally, the GNNs are trained on the class-balance graph by optimizing the objective as formulated in Eqn. (17).

$$\mathcal{L} = - \sum_{v \in \mathcal{V}^L} y_v \log \hat{y}_v - \sum_{u \in \mathcal{V}^S} \mathcal{W}_u y_u \log \hat{y}_u, \quad (17)$$

where \mathcal{L} is the final optimization objective.

3.7 Algorithm and Complexity Analysis

The main procedures of our proposed GraphMuGu are summarized in Algorithm 1. The complexity of identifying the anchor and auxiliary nodes is $\mathcal{O}(|\mathcal{V}^L|^2)$. For feature synthesis, the complexity is $\mathcal{O}(|\mathcal{V}^L|d)$. For topology modeling, the corresponding complexity is $\mathcal{O}(\frac{|\mathcal{V}^L|}{|\mathcal{V}|}|\mathcal{E}|)$. For our proposed uncertainty-aware sample quantification, the time complexity of measuring the uncertainty is $\mathcal{O}(|\mathcal{V}^L| + |\mathcal{V}^S|)$. For our proposed similarity-aware sample re-weighting, the time complexity of evaluating the pacesetter is $\mathcal{O}(|\mathcal{V}^L|)$, and that of measuring weights is $\mathcal{O}(|\mathcal{V}^S|)$. In general, the additional complexity introduced by our method is $\mathcal{O}(2(|\mathcal{V}^L| + |\mathcal{V}^S|))$, which enables its generalization to the large-scale graph.

4 Experiments

In this section, we conduct experiments to verify the effectiveness of our proposed method. We first introduce the datasets and baselines used in the experiments. Then, we elaborate on the implementation details. Finally, we conduct a comprehensive and in-depth analysis of the experimental results. We aim to answer the following four **Research Questions**.

Algorithm 1 The Proposed GraphMuGu Method

Input: Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{X})$, adjacency matrix \mathbf{A} , labeled node set \mathcal{V}^L with their labels \mathcal{Y}^L , unlabeled node set \mathcal{V}^U , potential categories \mathcal{C} , GNN-based model f_θ .
Output: f_θ trained on the class-balance graph.

- 1: Calculate $\tilde{\mathcal{S}}$ via graph diffusion and sparsification;
- 2: Calculate degree distribution \mathcal{P}_{Dg} via Eqn. (6);
- 3: Calculate pacesetter \mathbf{X}_{pac} according to Eqn. (15);
- 4: **while** not converge **do**
- 5: Calculate uncertainty \mathcal{U}_{c_i} according to Eqn. (11);
- 6: Calculate uncertainty-aware synthesized sample quantification \mathcal{Q}_{c_i} via Eqn. (14);
- 7: Calculate node hardness according to Eqn. (4);
- 8: Sample anchor node v_{anc} based on hardness;
- 9: Identify auxiliary node v_{aux} based on classification probability of anchor node;
- 10: Mix feature of the synthesized node by Eqn. (5);
- 11: Model topology of synthesized node $\mathcal{N}_{syn} \sim \tilde{\mathcal{S}}_{anc}$;
- 12: Calculate the weight of the synthesized node according to Eqn. (16);
- 13: Insert the synthesized nodes to \mathcal{G} and train f_θ on the class-balanced graph by optimizing Eqn. (17);
- 14: **end while**
- 15: **return** Optimized GNN model f_θ .

- **RQ1:** How does the proposed method perform on long-tailed and step imbalance issues?
- **RQ2:** How does each proposed module contribute to the performance?
- **RQ3:** How do the hyper-parameters take effect on the performance?
- **RQ4:** How does each proposed module work to benefit the model?

4.1 Datasets and Baselines

We evaluate the effectiveness of our proposed GraphMuGu on five widely-used datasets, including three citation datasets (Cora, Citeseer, and Pubmed) and two co-purchase datasets (Amazon-Photo and Amazon-Computers). The details of datasets are summarized in Table 1.

We compare the proposed GraphMuGu with ten competitive methods for class imbalance. They are classified into two categories, including loss modifying methods (Re-weight [Japkowicz and Stephen, 2002], PC Softmax [Hong *et al.*, 2021], CB Loss [Cui *et al.*, 2019], Focal Loss [Lin *et al.*,

Datasets	Nodes	Features	Edges	Classes
Cora	2,708	1,433	5,429	7
Citeseer	3,327	3,703	4,732	6
Pubmed	19,717	500	44,338	3
Amazon-Photo	7,650	745	238,126	8
Amazon-Computers	13,752	767	245,861	10

Table 1: The brief description of datasets.

	Dataset	Cora-LT			Citeseer-LT			Pubmed-LT		
	$\rho=100$	Acc.	bAcc.	F1	Acc.	bAcc.	F1	Acc.	bAcc.	F1
GCN	Vanilla	72.32±0.48	59.63±0.72	59.23±0.86	51.47±0.45	44.57±0.51	37.91±0.60	51.53±0.86	42.13±0.45	34.63±0.77
	Re-weight	78.38±0.13	72.69±0.35	71.57±0.33	63.52±0.23	56.83±0.25	55.17±0.13	77.15±0.18	72.41±0.12	72.03±0.17
	PC Softmax	77.39±0.17	72.02±0.32	71.54±0.38	62.19±0.43	<u>59.17±0.32</u>	58.38±0.31	74.40±0.66	72.67±0.47	71.85±0.57
	CB Loss	77.92±0.23	72.65±0.28	73.23±0.28	61.49±0.55	55.27±0.58	53.53±0.69	76.82±0.27	72.17±0.25	72.95±0.24
	Focal Loss	78.47±0.21	73.15±0.27	73.42±0.20	59.76±0.32	53.45±0.39	51.82±0.43	76.32±0.21	71.57±0.38	71.87±0.39
	ReNode	78.72±0.19	72.97±0.17	74.03±0.18	62.33±0.30	55.53±0.29	53.78±0.25	75.97±0.11	70.75±0.15	71.44±0.19
	TAM	77.33±0.25	72.19±0.27	72.37±0.29	63.45±0.36	56.82±0.31	55.87±0.41	78.02±0.18	72.65±0.22	72.81±0.33
	Upsample	75.55±0.12	66.88±0.14	68.39±0.31	55.14±0.11	48.47±0.15	45.23±0.21	71.31±0.09	64.01±0.11	64.51±0.10
	GraphSMOTE	75.46±0.41	68.93±0.52	70.47±0.53	56.34±0.25	50.10±0.28	47.86±0.33	74.51±0.11	69.51±0.13	71.07±0.15
	GraphENS	76.12±0.27	71.26±0.38	70.87±0.48	63.11±0.32	56.75±0.32	55.52±0.47	77.27±0.15	71.82±0.23	72.77±0.18
GAT	GraphSHA	79.54±0.29	74.21±0.42	75.09±0.31	64.39±0.45	58.88±0.36	59.02±0.30	79.58±0.17	74.47±0.15	75.08±0.20
	GraphMuGu	80.88±0.42	75.59±0.39	75.79±0.36	65.79±0.35	59.83±0.41	59.78±0.37	<u>79.05±0.23</u>	74.52±0.17	75.12±0.22
	Vanilla	67.72±0.55	54.25±0.86	55.32±0.77	49.25±0.21	42.47±0.19	35.85±0.28	47.65±1.15	40.01±1.08	29.75±1.68
	Re-weight	77.62±0.25	72.15±0.47	72.81±0.52	61.87±0.49	55.45±0.66	53.79±0.74	74.12±0.37	69.45±0.89	69.35±0.66
	PC Softmax	68.72±0.71	64.25±0.76	64.15±0.76	56.74±1.45	56.37±1.22	55.38±1.52	76.76±0.38	73.29±0.17	73.18±0.28
	CB Loss	77.32±0.30	72.02±0.66	72.89±0.45	61.64±0.55	55.19±0.57	53.66±0.58	74.64±0.30	69.76±0.58	70.57±0.53
	Focal Loss	77.85±0.13	72.57±0.22	73.12±0.29	59.73±0.38	53.48±0.30	52.26±0.36	74.12±0.21	70.32±0.35	70.69±0.25
	ReNode	78.02±0.22	71.77±0.35	73.49±0.38	60.82±0.37	54.02±0.34	51.92±0.43	74.14±0.27	69.08±0.38	69.53±0.47
	TAM	77.74±0.23	72.88±0.32	73.07±0.39	64.04±0.33	57.49±0.51	56.31±0.37	78.13±0.19	71.83±0.27	73.14±0.20
	Upsample	72.66±0.31	62.37±0.35	64.99±0.29	53.46±0.28	46.98±0.21	43.15±0.47	67.69±0.87	57.37±0.61	54.87±0.92
GraphSAGE	GraphSMOTE	74.61±0.27	67.73±0.35	69.12±0.38	57.42±0.28	51.35±0.33	49.46±0.55	74.08±0.31	69.13±0.40	70.53±0.45
	GraphENS	77.18±0.26	72.05±0.37	72.15±0.43	61.95±0.38	55.89±0.31	54.32±0.43	76.67±0.18	70.29±0.23	71.38±0.29
	GraphSHA	78.86±0.24	74.18±0.28	75.19±0.23	63.87±0.46	58.15±0.37	57.52±0.40	78.36±0.24	73.75±0.25	74.46±0.23
	GraphMuGu	80.69±0.46	74.85±0.38	75.81±0.29	65.17±0.36	60.47±0.29	60.08±0.36	78.62±0.32	<u>73.49±0.26</u>	<u>73.87±0.33</u>
	Vanilla	73.33±0.12	61.85±0.15	63.29±0.14	47.85±0.23	41.88±0.29	36.86±0.35	58.76±0.11	47.86±0.08	42.56±0.15
	Re-weight	76.85±0.14	68.65±0.38	70.29±0.33	57.32±0.56	50.82±0.48	49.23±0.52	65.87±0.46	59.64±0.86	58.72±0.94
	PC Softmax	76.85±0.29	73.55±0.34	73.38±0.19	58.37±0.24	56.14±0.13	56.52±0.22	71.86±0.17	73.85±0.20	70.35±0.18
	CB Loss	77.15±0.30	70.37±0.39	71.29±0.32	57.65±0.38	51.27±0.37	48.76±0.42	67.75±0.33	60.62±0.49	61.76±0.53
	Focal Loss	77.19±0.19	69.82±0.25	70.73±0.28	57.09±0.65	50.65±0.69	48.48±0.73	70.52±0.39	65.56±0.37	66.28±0.46
	ReNode	77.15±0.26	69.28±0.27	71.18±0.23	57.75±0.54	51.36±0.49	49.08±0.45	67.37±0.53	60.54±0.76	60.72±0.65
GraphSAGE	TAM	77.18±0.31	71.22±0.36	71.19±0.49	62.88±0.23	56.41±0.35	54.57±0.25	78.22±0.33	72.81±0.73	73.68±0.69
	Upsample	73.76±0.18	63.39±0.27	65.65±0.19	50.38±0.18	44.29±0.15	41.49±0.24	64.27±0.09	54.67±0.15	53.42±0.17
	GraphSMOTE	74.29±0.22	66.18±0.38	67.82±0.45	52.75±0.66	47.05±0.63	44.27±0.62	65.19±0.37	56.89±0.52	56.88±0.59
	GraphENS	76.71±0.25	70.16±0.24	70.39±0.37	62.65±0.39	56.18±0.36	54.19±0.38	77.68±0.17	72.67±0.24	73.29±0.19
	GraphSHA	78.75±0.22	73.15±0.38	74.29±0.35	63.78±0.35	58.37±0.36	58.09±0.45	78.27±0.27	74.25±0.39	74.81±0.23
	GraphMuGu	79.77±0.23	74.24±0.18	74.66±0.27	65.20±0.33	59.66±0.28	58.86±0.23	78.62±0.33	74.53±0.36	75.02±0.31

Table 2: The experimental results (\pm std) on long-tailed class-imbalance settings. The reported results are the mean values of 10 runs, where the best result is highlighted in **bold**, and the runner-up is highlighted in underline.

2017], ReNode [Chen *et al.*, 2021], and TAM [Song *et al.*, 2022]) and generative methods (Upsample, GraphSMOTE [Zhao *et al.*, 2021], GraphENS [Park *et al.*, 2021], and GraphSHA [Li *et al.*, 2023]).

4.2 Experimental Setup and Configurations

We leverage various GNNs (i.e., GCN [Kipf and Welling, 2017], GAT [Veličković *et al.*, 2018], and GraphSAGE [Hamilton *et al.*, 2017]) as the backbones. All of them are set to a 2-layer pattern. The number of multi-head is set to 8 for GAT. The dimension of the hidden layer is set to 64. Specifically, for our proposed GraphMuGu, α is set to 0.05 to measure the diffusion matrix, K is set to 128 to sparsify the diffusion matrix, and δ is sampled from $\beta(1, 100)$. We perform the long-tailed class-imbalance experiments on the citation datasets and set the imbalance ratio $\rho = 100$. The step class-imbalance experiments are implemented on the co-purchase datasets with an imbalance ratio $\rho = 20$. We refer to the reference [Li *et al.*, 2023] to construct the class-imbalance datasets. For evaluation, we adopt Accuracy (Acc.), balanced Accuracy (bAcc.), and macro F1 score (F1) as the metrics.

	Dataset	Amazon-Photot-ST			Amazon-Computers-ST		
	$\rho=20$	Acc.	bAcc.	F1	Acc.	bAcc.	F1
GraphSAGE	Vanilla	59.26±1.38	59.93±1.27	47.12±1.95	63.72±0.09	46.98±0.08	30.12±0.18
	Re-weight	84.82±0.25	87.56±0.27	82.86±0.18	83.55±0.37	87.96±0.29	<u>77.76±0.42</u>
	PC Softmax	86.19±0.15	86.97±0.18	83.52±0.11	81.39±0.19	80.55±0.54	72.35±0.51
	CB Loss	83.12±0.22	85.65±0.27	80.53±0.33	83.76±0.21	87.34±0.17	77.18±0.20
	Focal Loss	82.53±0.47	85.55±0.39	79.10±0.56	82.56±0.45	86.98±0.28	76.54±0.20
	ReNode	84.76±0.17	86.49±0.29	81.96±0.23	81.27±0.35	87.49±0.27	76.79±0.54
	TAM	87.69±0.11	89.24±0.18	85.75±0.22	80.37±0.53	86.84±0.27	77.09±0.43
	Upsample	82.56±0.39	84.57±0.17	79.56±0.27	83.16±0.35	87.13±0.17	77.23±0.38
	GraphSMOTE	80.26±0.24	84.59±0.32	79.14±0.39	83.52±0.27	88.26±0.23	76.13±0.33
	GraphENS	88.12±0.18	<u>90.32±0.12</u>	86.43±0.22	83.27±0.31	88.47±0.16	76.71±0.40
GraphSAGE	GraphSHA	88.93±0.27	90.22±0.21	87.01±0.19	84.03±0.35	89.27±0.26	77.55±0.66
	GraphMuGu	89.77±0.23	90.99±0.18	88.72±0.15	85.12±0.22	89.96±0.20	78.88±0.37

Table 3: The experimental results (\pm std) on co-purchase datasets in step class-imbalance settings.

4.3 Experimental Results and Analyses (RQ1)

The experimental results of long-tailed class-imbalance and step class-imbalance settings are shown in Table 2 and Table 3, respectively. The key observations are summarized as follows. 1) The proposed method achieves superior performance compared to the competitive methods (i.e., loss modifying methods and generative methods), demonstrating its

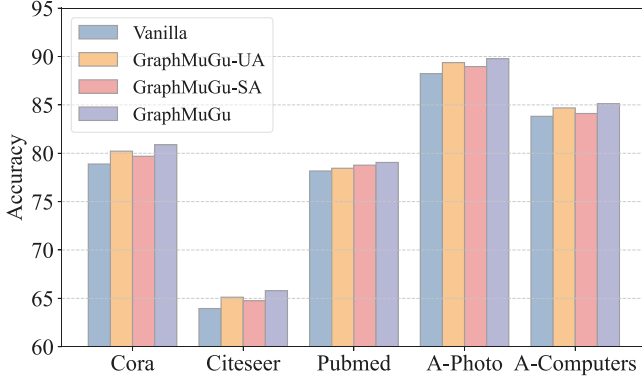


Figure 3: The experimental results of ablation studies.

effectiveness in addressing the class-imbalance issues among graph data. 2) The proposed GraphMuGu performs well on both the long-tailed and step class-imbalance settings, exhibiting the outstanding versatility of our method. 3) The proposed method yields a consistent improvement of performance across various datasets, proving the generalization ability of our proposed GraphMuGu.

4.4 Ablation Studies (RQ2)

In this section, we conduct ablation studies to verify the contribution of each component in the proposed GraphMuGu. We remove similarity-aware re-weighting and abbreviate the variant as GraphMuGu-UA. Analogously, we remove uncertainty-aware quantification and denote the variant as GraphMuGu-SA. We leverage GCN as the backbone and show the results in Figure 3. It can be observed that both uncertainty-aware quantification and similarity-aware re-weighting lead to significant improvement in performance. Furthermore, uncertainty-aware quantification performs well on datasets with more categories, and similarity-aware re-weighting exhibits significant performance on datasets with more samples.

4.5 Hyper-Parameter Sensitivity Analysis (RQ3)

In this section, we investigate the performance of the method under various hyper-parameter settings. β controls total number of generated samples and γ controls the gain of weights. We leverage GCN as the backbone and exhibit the results in

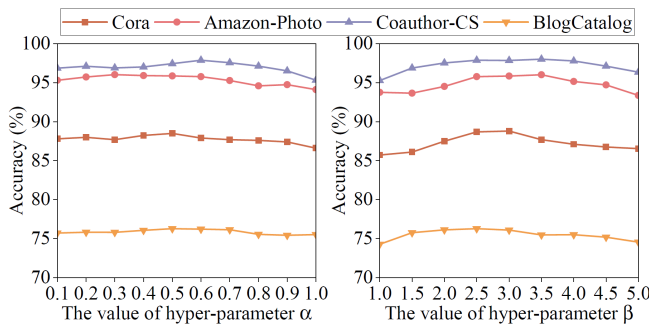


Figure 4: The experimental results of hyper-parameter analysis.

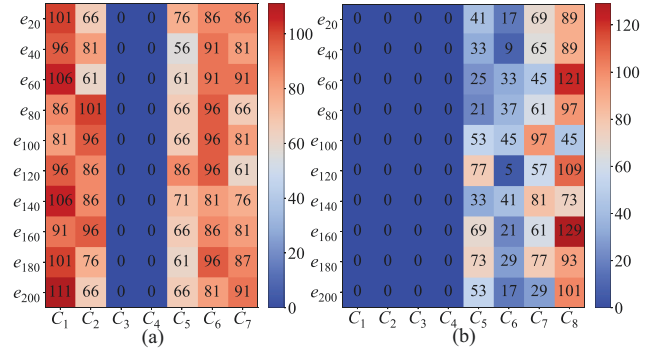


Figure 5: The number of synthesized samples for each category on (a) Cora and (b) Amazon-Photo datasets.

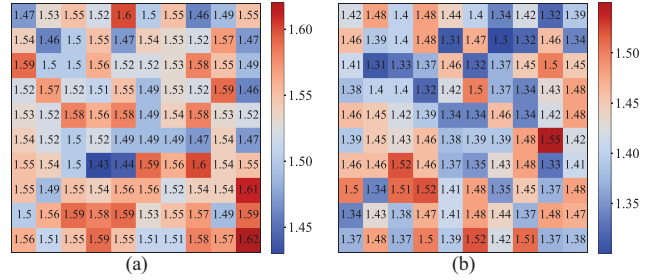


Figure 6: The weights of 100 randomly selected synthesized samples on (a) Cora and (b) Amazon-Photo datasets.

Figure 4. It can be seen that the model achieves the optimal results when β approximates the number of minority classes. The excessive value of β leads to the risk of noise, decreasing the performance of the model. In addition, the excessive value of γ results in insufficient learning of authentic samples, impairing the effectiveness of the model.

4.6 Visualization (RQ4)

In this section, we visualize the quantity of synthesized samples for each category and the weights of synthesized samples. We leverage GCN as the backbone and perform the experiments on Cora and Amazon-Photo datasets. The results are shown in Figure 5 and Figure 6. It can be seen that uncertainty-aware quantification and similarity-aware re-weighting balance the model training by adaptively fine-tuning the number and importance of synthesized samples.

5 Conclusion

In this paper, we incorporate the generative and re-weighting methods into a unified framework to relieve the class-imbalance problem on the graphs. It quantifies the uncertainty to identify the number of synthesized samples for each category. Furthermore, it measures similarity to re-weight the importance of the generative samples. Experimental results on five datasets demonstrate the effectiveness of our proposed method.

Acknowledgments

This research is supported by the National Key R&D Program of China (Grant No. 2022ZD0119501), the National Natural Science Foundation of China (Grant No. 62472263, 62072288, 52374221), the Taishan Scholar Program of Shandong Province, Shandong Youth Innovation Team, the Natural Science Foundation of Shandong Province (Grant No. ZR2024MF034, ZR2022MF268).

References

- [Bruna *et al.*, 2014] Joan Bruna, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. Spectral Networks and Deep Locally Connected Networks on Graphs. In *International Conference on Learning Representations*, pages 1–14, 2014.
- [Chen *et al.*, 2021] Deli Chen, Yankai Lin, Guangxiang Zhao, Xuancheng Ren, Peng Li, Jie Zhou, and Xu Sun. Topology-Imbalance Learning for Semi-Supervised Node Classification. *Advances in Neural Information Processing Systems*, 34:29885–29897, 2021.
- [Cui *et al.*, 2019] Yin Cui, Menglin Jia, Tsung-Yi Lin, Yang Song, and Serge Belongie. Class-Balanced Loss Based on Effective Number of Samples. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 9268–9277, 2019.
- [Defferrard *et al.*, 2016] Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering. *Advances in Neural Information Processing Systems*, 29:1–9, 2016.
- [Dou *et al.*, 2020] Yingdong Dou, Zhiwei Liu, Li Sun, Yutong Deng, Hao Peng, and Philip S Yu. Enhancing Graph Neural Network-Based Fraud Detectors against Camouflaged fraudsters. In *Proceedings of the 29th ACM International Conference on Information and Knowledge Management*, pages 315–324, 2020.
- [Gilmer *et al.*, 2017] Justin Gilmer, Samuel S Schoenholz, Patrick F Riley, Oriol Vinyals, and George E Dahl. Neural message passing for quantum chemistry. In *International Conference on Machine Learning*, pages 1263–1272, 2017.
- [Hamilton *et al.*, 2017] Will Hamilton, Zhitao Ying, and Jure Leskovec. Inductive Representation Learning on Large Graphs. *Advances in Neural Information Processing Systems*, 30:1–11, 2017.
- [Hong *et al.*, 2021] Youngkyu Hong, Seungju Han, Kwanghee Choi, Seokjun Seo, Beomsu Kim, and Buru Chang. Disentangling Label Distribution for Long-Tailed Visual Recognition. In *Proceedings of The IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 6626–6636, 2021.
- [Japkowicz and Stephen, 2002] Nathalie Japkowicz and Shaju Stephen. The Class Imbalance Problem: A Systematic Study. *Intelligent Data Analysis*, 6(5):429–449, 2002.
- [Ju *et al.*, 2024] Wei Ju, Siyu Yi, Yifan Wang, Zhiping Xiao, Zhengyang Mao, Hourun Li, Yiyang Gu, Yifang Qin, Nan Yin, Senzhang Wang, et al. A Survey of Graph Neural Networks in Real World: Imbalance, Noise, Privacy and OOD Challenges. *CoRR*, pages 1–20, 2024.
- [Kipf and Welling, 2017] Thomas N Kipf and Max Welling. Semi-Supervised Classification with Graph Convolutional Networks. In *International Conference on Learning Representations*, pages 1–14, 2017.
- [Li *et al.*, 2023] Wenzhi Li, Changdong Wang, Hui Xiong, and Jianhuang Lai. GraphSHA: Synthesizing Harder Samples for Class-Imbalanced Node Classification. In *Proceedings of the 29th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, pages 1328–1340, 2023.
- [Li *et al.*, 2024] Yibo Li, Xiao Wang, Hongrui Liu, and Chuan Shi. A Generalized Neural Diffusion Framework on Graphs. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 38, pages 8707–8715, 2024.
- [Lin *et al.*, 2017] Tsung-Yi Lin, Priya Goyal, Ross Girshick, Kaiming He, and Piotr Dollár. Focal Loss for Dense Object Detection. In *Proceedings of The IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 2980–2988, 2017.
- [Liu *et al.*, 2021] Yang Liu, Xiang Ao, Zidi Qin, Jianfeng Chi, Jinghua Feng, Hao Yang, and Qing He. Pick and Choose: A GNN-Based Imbalanced Learning Approach for Fraud Detection. In *Proceedings of the Web Conference*, pages 3168–3177, 2021.
- [Liu *et al.*, 2023] Zemin Liu, Yuan Li, Nan Chen, Qian Wang, Bryan Hooi, and Bingsheng He. A Survey of Imbalanced Learning on Graphs: Problems, Techniques, and Future Directions. *CoRR*, pages 1–27, 2023.
- [Mao *et al.*, 2024] Haitao Mao, Zhikai Chen, Wenzhuo Tang, Jianan Zhao, Yao Ma, Tong Zhao, Neil Shah, Mikhail Galkin, and Jiliang Tang. Position: Graph Foundation Models Are Already Here. In *International Conference on Machine Learning*, pages 1–23, 2024.
- [Park *et al.*, 2021] Joonhyung Park, Jaeyun Song, and Eunho Yang. GraphENS: Neighbor-Aware Ego Network Synthesis for Class-Imbalanced Node Classification. In *International Conference on Learning Representations*, 2021.
- [Rahmani *et al.*, 2023] Saeed Rahmani, Asiye Baghbani, Nizar Bouguila, and Zachary Patterson. Graph Neural Networks for Intelligent Transportation Systems: A Survey. *IEEE Transactions on Intelligent Transportation Systems*, 24(8):8846–8885, 2023.
- [Song *et al.*, 2022] Jaeyun Song, Joonhyung Park, and Eunho Yang. TAM: Topology-Aware Margin Loss for Class-Imbalanced Node Classification. In *International Conference on Machine Learning*, pages 20369–20383, 2022.
- [Sun *et al.*, 2020] Zhenchao Sun, Hongzhi Yin, Hongxu Chen, Tong Chen, Lizhen Cui, and Fan Yang. Disease Prediction via Graph Neural Networks. *IEEE Journal of Biomedical and Health Informatics*, 25(3):818–826, 2020.

- [Veličković *et al.*, 2018] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. Graph Attention Networks. In *International Conference on Learning Representations*, pages 1–12, 2018.
- [Wang *et al.*, 2022] Yu Wang, Charu Aggarwal, and Tyler Derr. Distance-Wise Prototypical Graph Neural Network for Imbalanced Node Classification. In *Proceedings of the International Workshop on Mining and Learning with Graphs*, pages 1–10, 2022.
- [Wu *et al.*, 2020] Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and S Yu Philip. A Comprehensive Survey on Graph Neural Networks. *IEEE Transactions on Neural Networks and Learning Systems*, 32(1):4–24, 2020.
- [Yun *et al.*, 2019] Seongjun Yun, Minbyul Jeong, Raehyun Kim, Jaewoo Kang, and Hyunwoo J Kim. Graph Transformer Networks. *Advances in Neural Information Processing Systems*, 32:1–11, 2019.
- [Zeng *et al.*, 2023] Liang Zeng, Lanqing Li, Ziqi Gao, Peilin Zhao, and Jian Li. ImGCL: Revisiting Graph Contrastive Learning on Imbalanced Node Classification. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 37, pages 11138–11146, 2023.
- [Zhang *et al.*, 2024] Jinghui Zhang, Zhengjia Xu, Dingyang Lv, Zhan Shi, Dian Shen, Jiahui Jin, and Fang Dong. DiG-In-GNN: Discriminative Feature Guided GNN-Based Fraud Detector against Inconsistencies in Multi-Relation Fraud Graph. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 38, pages 9323–9331, 2024.
- [Zhao *et al.*, 2021] Tianxiang Zhao, Xiang Zhang, and Suhang Wang. GraphSMOTE: Imbalanced Node Classification on Graphs with Graph Neural Networks. In *Proceedings of the 14th ACM International Conference on Web Search and Data Mining*, pages 833–841, 2021.