UPL: Uncertainty-aware Pseudo-labeling for Imbalanced Transductive Node Classification

Abstract

Graph-structured datasets often suffer from class imbalance, which complicates node classification tasks. In this work, we address this issue by first providing an upper bound on population risk for imbalanced transductive node classification. We then propose a simple and novel algorithm, Uncertainty-aware Pseudo-labeling (UPL). Our approach leverages pseudo-labels assigned to unlabeled nodes to mitigate the adverse effects of imbalance on classification accuracy. Furthermore, the UPL algorithm enhances the accuracy of pseudo-labeling by reducing training noise of pseudo-labels through a novel uncertainty-aware approach. We comprehensively evaluate the UPL algorithm across various benchmark datasets, demonstrating its superior performance compared to existing state-of-the-art methods.

1 Introduction

Graphs are fundamental data structures that are universally utilized in various applications. The flexibility and expressiveness of graph representations enable us to model complex relationships and interactions within several types of data across numerous fields. From social networks, where individuals are connected by various kinds of relationships, to biological networks that represent protein interactions, graphs provide a powerful way to encapsulate the inherent complexities of many natural and human-made systems (Mohammadrezaei et al., 2018; Ying et al., 2018; Perozzi et al., 2016; Hamilton et al., 2017). In tackling the task of learning from graph data, Graph Neural Networks (GNNs) play an important role (Hamilton et al., 2017; Kipf & Welling, 2016a; Velickovic et al., 2017). GNNs leverage the rich relational information within graphs, allowing for the effective propagation of information through the network structure and the ability to generalize deep learning approaches to non-Euclidean data. However, despite their advantages, GNNs encounter significant challenges when dealing with imbalanced data in transductive scenarios where the unlabeled nodes are utilized during the training phase, a common scenario in real-world graphs (Park et al., 2022). In many graph-based applications, some classes of nodes are vastly underrepresented compared to others, leading to a problem in the learning process (Song et al., 2022; Park et al., 2022). In particular, this imbalance can result in biased models towards the majority class, which can also depend on graph structure. For instance, in social networks, minority groups might be underrepresented in friendship suggestions; rare protein interactions could be overlooked in biological networks.

The problem of imbalance in graphs thus poses unique challenges that require specialized strategies to address. Standard imbalance handling techniques, such as re-weighting and re-sampling, may work in fields such as image classification but face significant obstacles when applied to graphs. Re-weighting methods, which assign higher weights to minority nodes, do not alter the connectivity patterns of these nodes, leaving their neighborhood influences unchanged. Re-sampling strategies, intended to balance class representation, can disrupt the graph's structure, potentially altering critical message-passing pathways and affecting the semantic integrity of node classes and embedded features.

Despite these developments, balancing the enhancement of minority class representation against the integrity of majority classes remains a technical challenge due to overemphasis on minority classes which can degrade the model's ability to accurately represent more common classes (Yan et al., 2024; Song et al., 2022; Park

et al., 2022; Jervakani et al., 2024). Furthermore, the generalization error and population risk study of imbalanced node classification is overlooked. Our contributions in this work can be summarized as follows:

- **Theoretical Generalization Bound:** We derive an upper bound on population risk for imbalanced transductive node classification.

- **Uncertainty-aware Pseudo-Labeling (UPL):** We propose UPL, a novel algorithm that utilizes topology-aware uncertainty (Selective Edge Removal) and dual-threshold filtering to augment minority classes.

- **State-of-the-Art Performance:** Extensive experiments show UPL outperforms baselines on homophilic and heterophilic graphs while being faster than leading competitors like UNREAL.

2 Related works

Imbalanced Graph Classification: Due to the non-Euclidean characteristics of graph data, the imbalance problem in this type of data necessitates additional attention and specialized focus. Following the categorization of imbalance classification methodologies, we similarly categorize imbalanced graph classification models into two main groups: data-level and algorithm-level methods.

Data-level methodologies try to rebalance the learning environment by manipulating training data in feature or label spaces. Fundamental approaches such as over-sampling and under-sampling, prevalent in traditional class-imbalanced learning, require adaptation to suit the complexities inherent in graph data, characterized by intricate node dependencies and interconnections. Data-level methods could be subcategorized into data interpolation, adversarial generation, and pseudo-labeling (Ma et al., 2023). Data interpolation techniques, exemplified by SMOTE (Chawla et al., 2002) and its graph-oriented variant, GraphSMOTE (Zhao et al., 2021b), generate synthetic minority nodes by interpolating between existing node representations. Methods like GATSMOTE (Liu et al., 2022b) and GNN-CL (Li et al., 2024) enhance this process through attention mechanisms, ensuring quality edge predictions between synthetic and real nodes. Moreover, Mixup strategies, as seen in GraphMixup (Wu et al., 2022) and GraphENS (Park et al., 2022), introduce sophisticated blending techniques to combat neighbor memorization issues and prevent out-of-domain sample generation. Building upon these blending concepts, GraphSHA (Li et al., 2023a) addresses the "squeezed minority problem" by synthesizing harder minority samples. It utilizes a SemiMixup module to carefully enlarge minority decision boundaries in the latent space without deteriorating the topological subspaces of neighboring major classes.

Algorithm-level methodologies focus on refining learning algorithms to accommodate class imbalance effectively. Model refinement strategies adapt graph representation learning architectures to improve performance by incorporating class-specific adjustments and modules tailored to handle imbalance. For instance, approaches like ACS-GNN (Ma et al., 2022) and EGCN (Wang et al., 2022) modify aggregation operations within graph neural networks to prioritize minority class information, ultimately enhancing classification accuracy. Additionally, loss function engineering tries to design customized loss functions to prioritize minority class errors or encourage wider class separations, a challenging task given the connectivity properties of nodes in graphs. Recent innovations like ReNode (Chen et al., 2021) and TAM (Song et al., 2022) integrate graph topology information into loss function designs, showcasing advancements in addressing class imbalance within the graph context. Jervakani et al. (2024) proposed a KL regularization for imbalance node classification. Diverging from traditional class-rebalancing paradigms entirely, the BAT framework (Liu et al., 2023) approaches the problem through a topological augmentation lens. By leveraging model-based prediction uncertainty, BAT identifies and rectifies nodes critically influenced by ambivalent and distant message-passing, mitigating class-imbalance bias directly through dynamic structural adjustments.

Generalization Error and Node Classification: There are two different scenarios in node classification, including inductive and transductive scenarios. Inductive learning node classification involves (semi-)supervised learning on graph data samples where the test data are unseen during training. For Inductive node classification tasks, (Verma & Zhang, 2019) discussed the generalization error under node classification for GNNs via algorithm stability analysis in an inductive learning setting based on the SGD optimization algorithm. The work by Zhou & Wang (2021) extended the results in (Verma & Zhang, 2019) and found that increasing

the depth of Graph Convolutional Neural Network (GCN) enlarges its generalization error for the node classification task. In Transductive Node Classification, based on transductive Rademacher complexity, a high-probability upper bound on the generalization error of the transductive node classification task was proposed by Esser et al. (2021). The transductive modeling of node classification was studied in (Oono & Suzuki, 2020) and (Tang & Liu, 2023). (Cong et al., 2021) presented an upper bound on the generalization error of GCNs for node classification via transductive uniform stability, building on the work of (El-Yaniv & Pechyony, 2006). In contrast, our research focuses on the task of imbalanced transductive node classification and we provide an upper bound on population risk.

Uncertainty in Self-training: The integration of uncertainty estimation in GNNs has been extensively explored, particularly in self-training frameworks Wang et al. (2021); Yang et al. (2021); Zhao et al. (2021a). Early contributions, such as Li et al. (2018), introduced a simple strategy that selects the top K most confident nodes based on softmax probabilities for pseudo-labeling, expanding the labeled set iteratively. This approach was later refined by Sun et al. (2020), which employed a multi-stage self-training method, iteratively updating node labels to enhance GNN performance in sparse label settings. Extending these ideas, Yang et al. (2021) proposed a self-enhanced GNN framework that utilizes an ensemble of models to ensure consistency in pseudo-label predictions, thereby improving robustness against label noise. A common technique for uncertainty estimation in these methods is the use of entropy, as demonstrated in Cai et al. (2017); Zhang et al. (2021b), which measures prediction confidence to guide node selection. Building on this, Zhao et al. (2021a) introduced an entropy-aware self-training framework, incorporating an entropy-aggregation layer to account for graph structural information in uncertainty estimation. While traditional approaches in entropy-based uncertainty estimation, prioritize high-confidence nodes for pseudo-labeling, this practice might unintentionally reinforce distributional biases, as highlighted by Liu et al. (2022a), where over-reliance on highly certain nodes risks a distribution shift between the original labeled set and the expanded pseudo-labeled set. Furthermore, Li et al. (2023b) observed that nodes with very high confidence often contribute redundant information, limiting the diversity of the labeled dataset and potentially biased learning process. To address this concerning issue, in this work, we suggest to balance node selection across a broader confidence range to improve the performance of our model.

3 Preliminaries

Notations: We adopt the following convention for random variables and their distributions in the sequel. A random variable is denoted by an upper-case letter (e.g., Z), its space of possible values is denoted with the corresponding calligraphic letter (e.g., $\mathcal{Z}$), and an arbitrary value of this variable is denoted with the lower-case letter (e.g., z). We denote the set of integers from 1 to N by $[N] \triangleq \{1, \ldots, N\}$; the set of measures over a space $\mathcal{X}$ with finite variance is denoted $\mathcal{P}(\mathcal{X})$. For a matrix $\mathbf{X} \in \mathbb{R}^{k \times q}$, we denote the $i-$th row of the matrix by $\mathbf{X}[i,:]$. The Euclidean norm of a vector $X \in \mathbb{R}^q$ is $\|X\|_2 := (\sum_{j=1}^q x_j^2)^{1/2}$. For a matrix $\mathbf{Y} \in \mathbb{R}^{k \times q}$, we let $\|\mathbf{Y}\|_\infty := \max_{1 \leq j \leq k} \sum_{i=1}^q |\mathbf{Y}[j,i]|$ and $\|\mathbf{Y}\|_F := \sqrt{\sum_{j=1}^k \sum_{i=1}^q \mathbf{Y}^2[j,i]}$.

Information Measures: The KL divergence $\mathrm{KL}(P\|Q)$ is given by $\mathrm{KL}(P\|Q) := \int_{\mathcal{Z}} \log\left(\frac{dP}{dQ}\right) dP$. We also define the cross-entropy between P and Q, as $H(P,Q) = -\int_{\mathcal{Z}} \log\left(dP\right) dQ$.

Graph data samples: We consider transductive node classification for undirected graphs with N nodes that have no self-loops or multiple edges. Inputs to GNNs are node samples, which are comprised of their features and graph adjacency matrices. We denote the space of node feature for a node in the graph by $\mathcal{X}$. We consider the adjacency matrix $\mathbf{A} \in \mathcal{A} \subset \{0,1\}^{N \times N}$ to be fixed with maximum node degree for i-th class $\deg_i^{\max}$ and minimum node degree for i-th class $\deg_i^{\min}$. The input pair of i-th node feature with dimension k is denoted by $\mathbf{x}_i$. The GNN output (label) is denoted by $y \in \mathcal{Y}$ where $\mathcal{Y}$ is the space of labels and $|\mathcal{Y}| = k$. Define $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$. Let $\mathbf{Z}_m = \{Z_i\}_{i=1}^m \in \mathcal{Z}$ denote the training of labeled dataset, where the $i-$th node sample is $Z_i = (X_i, Y_i)$. For transductive learning in node classification, we denote $\mathbf{Z}_u = \{Z_i\}_{i=1+m}^{m+u} \in \mathcal{Z}$ as the set of unlabeled dataset. We assume that the features of nodes are i.i.d samples from the the feature space $\mathcal{X}$. We also denote the matrix of node features in the graph with $\mathbf{X} \in \mathbb{R}^{N \times k}$. We denote the learned distribution over classes as $P(\hat{\mathbf{Y}}|\mathbf{X}) := \{P(\hat{Y} = j|\mathbf{X})\}_{j=1}^k$ where $P(\hat{Y} = j|\mathbf{X}) := \frac{1}{n} \sum_{i=1}^n P(\hat{Y} = j|X_i)$ is the

prediction of model for j-th class for given node-features $\{X_i\}_{i=1}^n$. Furthermore, we define $\mathbf{P}_k := \{P_j\}_{j=1}^k$ as the target class distribution where $P_j = \frac{|m_j|}{\sum_{i=1}^k |m_i|}$ shows the probability of j-th class within the dataset.

Graph filters: Graph filters are linear functions of the adjacency matrix, $\mathbf{A}$, defined by $G_f : \mathcal{A} \mapsto \mathbb{R}^{N \times N}$ where N is the size of the graph, see in (Defferrard et al., 2016). Graph filters model the aggregation of node features in a GNN. For example, the symmetric normalized graph filter proposed by Kipf & Welling (2016b) is $G_f(\mathbf{A}) = \tilde{L} := \tilde{D}^{-1/2} \tilde{\mathbf{A}} \tilde{D}^{-1/2}$ where $\tilde{\mathbf{A}} = I + \mathbf{A}$ is the augmented adjacency matrix, $\tilde{D}$ is the degree-diagonal matrix of $\tilde{\mathbf{A}}$, and I is the identity matrix. Furthermore, $\deg_i^{\max}$ and $\deg_i^{\min}$ are the maximum and minimum degree of nodes among i-th class of the graph with the augmented adjacency matrix, $\tilde{\mathbf{A}}$. Another normalized filter, a.k.a. random walk graph filter (Xu et al., 2019), is $G_f(\mathbf{A}) = D^{-1}\mathbf{A} + I$, where D is the degree-diagonal matrix of $\mathbf{A}$. The mean-aggregator is also a well-known aggregator defined as $G_f(\mathbf{A}) = \tilde{D}^{-1}(\mathbf{A} + I)$. The sum-aggregator graph filter is defined by $G_f(\mathbf{A}) = (\mathbf{A} + I)$.

Loss function: With $\mathcal{Y}$ the label space, the loss function $\ell : \mathbb{R} \times \mathcal{Y} \to \mathbb{R}$ is denoted as $\ell(\widehat{y}, y)$, where $\widehat{y}$ is defined as the output of model, e.g., $\ell(h_\theta(G_f(\mathbf{A})[i, :]\mathbf{X}), y_i)$ is the loss function for i-th node in the graph where $h_\theta : \mathcal{X} \mapsto \mathcal{Y}$ is the hypothesis of our parameterized model which belongs to $\mathcal{H}$ with $\theta \in \Theta$.

True and empirical risks: The empirical risk function for labeled node samples $\mathbf{X}_m$ is given by

$$R(\mathbf{Z}_m, h_\theta) := \frac{1}{m} \sum_{i=1}^m \ell(h_\theta(G_f(\mathbf{A})[i, :]\mathbf{X}_m), y_i). \tag{1}$$

We also define the true risk as the average of loss function over unlabeled nodes, $\mathbf{X}_u$, in transductive learning,

$$R(\mathbf{Z}_u, h_\theta) := \frac{1}{u} \sum_{i=m+1}^{m+u} \ell(h_\theta(G_f(\mathbf{A})[i, :]\mathbf{X}_u), y_i). \tag{2}$$

We would like to study the performance of the model trained with the labeled data set $\mathbf{Z}_m = \{(\mathbf{X}_i, Y_i)\}_{i=1}^m$ and evaluated against the unlabeled dataset $\mathbf{Z}_u = \{(X_i, Y_i)\}_{i=m+1}^{m+u}$ loss, using transductive Rademacher complexity analysis (El-Yaniv & Pechyony, 2009).

4 The Generalization Error of Imbalanced Transductive Node Classification

This section provides a generalization error upper bound under an imbalance scenario for transductive node classification via Rademacher complexity analysis. All proof details are deferred to Appendix C.

For theoretical analysis, we need the following assumptions.

Assumption 4.1 (Bounded node features). For every node, the features are contained in an ℓ_2-ball of radius B_f. In particular, $\|\mathbf{X}[i;]\|_2 \leq B_f$ for all nodes.

Assumption 4.2 (Bounded norm of parameters). There exists $U_F(i) \in \mathbb{R}$ such that $\|\theta_i\|_F \leq U_F(i)$ where θ_i is parameter matrix of i-th layer.

Assumption 4.3 (Activation functions). The activation function $\varphi : \mathbb{R} \mapsto \mathbb{R}$ is 1-Lipschitz [1], so that $|\varphi(x_1) - \varphi(x_2)| \leq |x_1 - x_2|$ for all $x_1, x_2 \in \mathbb{R}$, and zero-centered, i.e., $\varphi(0) = 0$.

In theoretical analysis, we consider binary classification, based on (Bartlett et al., 2017), where γ-margin loss function for binary classification is proposed. For a positive $\gamma \in \mathbb{R}^+$, we have, $\ell_\gamma(y_1, y_2) = 0$ and $\ell_\gamma(y_1, y_2) = \min(1, 1 - \frac{y_1 y_2}{\gamma})$ for $y_1 y_2 \geq \gamma$ and $y_1 y_2 < \gamma$, respectively.

For transductive learning analysis, inspired by El-Yaniv & Pechyony (2009), we define empirical transductive Rademacher complexity as for $p \in [0, 1/2]$ and let the set $\boldsymbol{\epsilon} := \{\epsilon_i\}_{i=1}^{m+u}$ be i.i.d. with probability $P(\epsilon_i = 1) = P(\epsilon_i = -1) = p$ and $P(\epsilon_i = 0) = 1 - 2p$ for all $i \in [m+u]$ and assuming $p = \frac{m+u}{(m+u)^2}$,

$$\mathfrak{R}_{m+u}(\mathcal{H}) := \left(\frac{1}{m} + \frac{1}{u}\right) \mathbb{E}_{\boldsymbol{\epsilon}} \left[\sum_{i=1}^{m+u} \epsilon_i h_\theta(x_i) \right].$$

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[1] For the Tanh and Relu activation function satisfy this assumption.

Similarly, we can define the empirical transductive Rademacher complexity for i-th class with $\mathfrak{R}_{m_i+u_i}(\mathcal{H})$. Furthermore, in transductive learning, we consider m_i and u_i as labeled nodes and unlabeled nodes belong to the i-th class. We first provide an upper bound on population risk for transductive learning under the imbalance scenario.

Proposition 4.4. *Let $Q_i = (\frac{1}{u_i} + \frac{1}{m_i})$, $S_i = \frac{m_i+u_i}{(m_i+u_i-1/2)(1-1/(2\max(m_i,u_i)))}$ for $i = 1, 2$. Then, with probability at least $(1-\delta)$ over the choice of the training set from nodes of graphs, for all $h_\theta \in \mathcal{H}$,*

$$R(\mathbf{Z}_u, h_\theta) \leq \sum_{i=1}^{2} R_\gamma(\mathbf{Z}_{m_i}, h_\theta) + \frac{u_i}{u}\Big(\frac{1}{\gamma}\mathfrak{R}_{m_i+u_i}(\mathcal{H}) + c_0 Q_i\sqrt{\min(m_i, u_i)} + \sqrt{\frac{S_i Q_i}{2}\log(1/\delta)}\Big),$$

where $\mathfrak{R}_{m_i+u_i}(\mathcal{H})$ is the transductive Rademacher complexity for i-th class, $R_\gamma(\mathbf{Z}_{m_i}, h_\theta)$ is the empirical risk based on γ-margin loss for i-th class and $c_0 = \sqrt{\frac{32\ln(4e)}{3}}$.

Next, we provide an upper bound on the transductive Rademacher complexity for general deep GNN.

Proposition 4.5. *Given Assumptions 4.1, 4.2 and 4.3, then the following upper bound holds on the transductive Rademacher complexity of node classification for GNN with depth d and graph filter $\mathrm{G}_f(\mathbf{A})$,*

$$\mathfrak{R}_{m_i+u_i}(\mathcal{H}) \leq \frac{C_1\|\mathrm{G}_f(\mathbf{A})[i]\|_\infty^{2(d-1)}\Pi_{j=1}^d U_F(j)}{\sqrt{m_i+u_i}},$$

where $C_1 = B_f(\sqrt{2\log(2)d}+1)$ and $\|\mathrm{G}_f(\mathbf{A})[i]\|_\infty$ is the infinite norm of graph filter among i-th class.

Combining Proposition 4.5 with Proposition 4.4, we can derive the following upper bound on population risk.

Theorem 4.6. *Under the same Assumptions in Proposition 4.4 and Proposition 4.5, the following upper bound holds on population risk for imbalanced transductive node classification under a GCN model,*

$$R(\mathbf{Z}_u, h_\theta) \leq \sum_{i=1}^{2} R_\gamma(\mathbf{Z}_{m_i}, h_\theta) + c_0 Q_i\sqrt{\min(m_i, u_i)} + \sqrt{\frac{S_i Q_i}{2}\log(1/\delta)}\Big)$$
$$+ \frac{u_i}{u}\Big(\frac{B_f(\sqrt{2\log(2)d}+1)\Pi_{j=1}^d U_F(j)}{\gamma\sqrt{(m_i+u_i)}} \times \Big(\frac{\deg_i^{\max}+1}{\deg^{\min}+1}\Big)^{d-1}\Big),$$

where $U_F(i)$ is the maximum of Frobenius norm of i-th layer parameter.

Convergence rate discussion: For large values of u_i and m_i ($i \in 1, 2$), the value of S_i approaches one. Moreover, we find $Q_i = O(1/\min(m_i, u_i))$ and $\mathfrak{R}_{m_i+u_i}(\mathcal{H}) = O(1/(\sqrt{m_i+u_i}))$. Consequently, assuming $u_i \ll m_i$ for both $i = 1, 2$, yields an overall convergence rate of $O(1/u)$. Conversely, when $m_i \ll u_i$, the convergence rate becomes $O(\max(\frac{1}{\sqrt{m_1}}, \frac{1}{\sqrt{m_2}}))$. It's noteworthy that in the balanced case, where $u_1 = u_2$ and $m_1 = m_2$, assuming $m_i \ll u_i$ for $i = 1, 2$ recover the convergence rate applicable to balanced node classification, dependent on the maximum degree per class and the minimum degree.

Maximum and Minimum Degrees: In balance transductive node classification, e.g., (Oono & Suzuki, 2019; Cong et al., 2021; Tang & Liu, 2023), the upper bound on population risk is dependent on the maximum and minimum degree of all nodes. Our bound in Theorem 4.6 reveals that for an imbalance scenario, the upper bound depends on the maximum degree of nodes per class and the minimum degree of all graph nodes. Note that, this result can also be applied to balance scenario by assuming $m_i = m$ for all classes.

Discussion: Theorem 4.6 reveals that the population risk upper bound is fundamentally dominated by the number of samples in the minority class. This theoretical insight suggests a straightforward yet powerful approach: increasing the representation of minority classes can improve classification performance. While this observation emerges directly from our theoretical analysis, its implications are significant as it applies broadly to any transductive imbalanced node classification task. In the following section, we propose an algorithm that leverages this insight by strategically assigning pseudo-labels to unlabeled nodes, thereby effectively augmenting the minority class representation and improving node-classification performance.

Figure 1: Pipeline of the UPL Algorithm

5 UPL Algorithm

In this section, we introduce the Uncertainty-aware Pseudo-labeling (UPL) Algorithm to mitigate the imbalance effect in transductive node classification.

In the UPL algorithm, we add pseudo-labels to unlabeled nodes of minority classes to mitigate the effect of imbalance node classification. Our UPL algorithm contains two blocks: uncertainty-aware pseudo-labeling, and balanced-softmax loss function. The pipeline of the UPL algorithm is shown in Figure 1. Our UPL algorithm involves an iterative training approach, leveraging the pseudo-labeling technique to enhance the model's performance on graph-based data.

5.1 Uncertainty-aware Pseudo-labeling

Pseudo-labeling is a semi-supervised learning technique that enhances model performance by generating synthetic labels for unlabeled data using a previously trained model. This method effectively expands the training dataset, allowing the model to learn from a broader range of examples and improve accuracy. Different strategies for Pseudo-labeling are proposed. In this work inspired by the technique in (Rizve et al., 2021), we propose an iterative uncertainty-aware pseudo-labeling method where the uncertainty is computed based on the graph's topology.

Pseudo-labeling: To refine the selection of pseudo-labels, we incorporate two thresholds: a lower threshold (η_l) and an upper threshold (η_u). As proposed by Rizve et al. (2021), the lower threshold selects high-confidence samples. To avoid overfitting to these high-confidence samples, we introduce an upper threshold, η_u, which selects samples with intermediate confidence levels. This can be seen as a band-pass filter on the nodes, including those within a specific probability range. This method balances the use of confident predictions with the exploration of less certain ones, preventing the model from becoming biased towards the nodes' most confident nodes. To mitigate, the noise of pseudo-lableling process, we also add pseudo-labels to minority classes and avoid the pseudo-labels for majority classes during training.

Uncertainty-Aware: Our proposed Selective Edge Removal (SER) method addresses the challenge of poor calibration in GNN pseudo-labeling by introducing a topology-aware uncertainty estimation approach. The method works by strategically removing edges based on node degrees, where highly-connected nodes have a higher probability of edge removal, then making multiple inferences on these perturbed graph versions. By measuring the entropy of predictions across different perturbed versions and computing the variance of these entropy values, we can effectively estimate prediction uncertainty for each unlabeled node. Nodes

showing consistent predictions (low entropy variance) across perturbations are considered more reliable and selected for pseudo-labeling, specifically retaining the lowest 90% based on uncertainty values. This approach naturally accounts for both aleatoric and epistemic uncertainty while preserving the graph's core structure, offering a computationally efficient way to improve pseudo-label quality in GNN applications.

Finally, combining the thresholds for the pseudo-labeling process and the uncertainty estimation, we can select the pseudo-label for an unlabeled node, i.e.,

$$\tilde{Y}_i = \mathbb{1}(P(\hat{Y}_i|X_i) \geq \eta_l)\mathbb{1}(P(\hat{Y}_i|X_i) \leq \eta_u)\mathbb{1}\big(\mathrm{U}(P(\hat{Y}_i|X_i)) \leq Q_\alpha\big), \tag{3}$$

where $P(\hat{Y}_i|X_i)$ is the prediction of our model for node sample X_i over classes and $\mathrm{U}(\cdot)$ is variance of entropy of each nodes predictions among different perturbations, $\mathrm{U}(P(\hat{Y}_i|X_i)) = \mathbb{VAR}_k(H_k(i))$ where $H_k(i)$ is the entropy of predictions for i-th node in the k-th perturbed graph. Also Q_α represent the quantile function for some $\alpha \in (0, 1)$ as follows:

$$Q_\alpha = \mathrm{quantile}\big(\mathrm{U}(P(\hat{Y}_j|X_j)) : j = 1, \ldots, n, \alpha\big). \tag{4}$$

5.2 Balanced Softmax loss function

The balanced softmax loss function (Ren et al., 2020) is a variant of the traditional softmax loss designed to address the issue of class imbalance in multi-class classification problems. The primary idea is to introduce a class-specific weighting factor, β_c, which adjusts the contribution of each class to the overall loss. This weighting factor is inversely proportional to the class frequency, assigning higher weights to underrepresented classes and lower weights to overrepresented classes. The formulation of the balanced softmax loss is given by

$$-\frac{1}{N}\sum_{i=1}^{N}\sum_{c=1}^{k}\beta_c y_{ic}\log(p_{ic}), \tag{5}$$

where N is the number of training samples, k is the number of classes, y_{ic} is the ground truth label (0 or 1) for sample i and class c, p_{ic} is the predicted probability for sample i and c-th class , and β_c is the weighting factor calculated as $\beta_c = \frac{(1-\alpha)}{(1-\alpha^{m_c})}\alpha^{(1-m_c)}$. Here, α is a hyperparameter controlling the degree of balancing, and m_c is the number of training samples belonging to c-th class. This adjustment ensures that the model pays more attention to the minority classes during training, improving performance on imbalanced datasets. Finally, the details and operational steps of the UPL algorithm are outlined in Appendix D.

Guided by our theoretical analysis, UPL introduces three novel mechanisms to specifically address the limitations of existing imbalanced learning methods:

1. **Topology-Aware Uncertainty (SER):** To ensure reliable pseudo-labels, we introduce Selective Edge Removal (SER). Rather than relying on simple softmax confidence, SER estimates uncertainty by observing prediction variance across topologically perturbed versions of the graph, capturing local structural stability.

2. **Band-Pass Pseudo-Label Filtering:** We employ a dual-threshold strategy (upper η_u and lower η_l) that acts as a *band-pass* filter. This selects informative, mid-confidence nodes rather than just the *easiest* high-confidence samples, preventing the reinforcement of existing model biases.

3. **Minority-Class Augmentation:** Consistent with our risk bound findings, UPL exclusively targets unlabeled nodes predicted to belong to minority classes for pseudo-labeling. This directly mitigates the representation gap that dominates the generalization error.

Furthermore, our approach eliminates the need for computationally expensive clustering or node-reordering steps used in prior works like UNREAL, resulting in significant efficiency gains.

6 Experiment

In this section, we provide the results of experiments for our UPL algorithm. All experiments setup details are provided in Appendix E and F. All experiments are conducted on GCN models. More GNN architectures, e.g., GAT, GraphSage and GIN are studied in Appendix G.

Baselines: In our experiments, we compare our proposed method against a blend of both foundational and state-of-the-art (SOTA) methods. In particular, we include foundational baselines: Vanilla, Re-weight (Japkowicz & Stephen, 2002), DR-GCN (Shi et al., 2020) and Balanced Softmax (Ren et al., 2020). Furthermore, we also consider recent SOTA methods, including, PC Softmax (Hong et al., 2021), GraphSMOTE (Zhao et al., 2021b), GraphENS (Park et al., 2022), TAM (Song et al., 2022), BAT1 (Liu et al., 2023), Graphsha (Li et al., 2023a), and Unreal (Yan et al., 2023).

Datasets: In our experiments, we utilize citation network datasets—CiteSeer, Cora, and Pubmed (Sen et al., 2008)—which we categorize as homophilic graphs, where nodes represent documents and edges represent citation links. For heterophilic graphs, we employ Chameleon and Squirrel (Rozemberczki et al., 2021), where nodes represent Wikipedia pages and edges denote links between them, as well as Wisconsin, a graph composed of web pages crawled from the Internet by Craven et al. (2000). Furthermore, we use the Amazon Computers and Amazon Photos datasets Shchur et al. (2019) in Appendix G.

Imbalance Learning: In a classification scenario with training dataset $z = \{z_1, \ldots, z_n\}$ where $z_i = (x_i, y_i)$, the imbalance occurs when the distribution $\mathbf{P}_k$ over k classes within the dataset has larger probability mass points over some classes. The imbalance severity is often quantified using an imbalance ratio ρ, which measures the ratio between the number of samples in the most populated class (majority class) and the least populated class (minority class) and can be defined as follows,

$$\rho = \frac{\max_{j \in [k]} |m_j|}{\min_{j \in [k]} |m_j|}. \tag{6}$$

More information regarding Imbalance ratio definition and minority class discrimination can be found in Appendix F.3.

Hyper-parameter Sensitivity: We conducted a sensitivity analysis on the two thresholds used in pseudo-labeling to evaluate the model's performance at various values of η_l and η_u. The results of this parameter sweep are presented in Figure 2.
The chart on the left shows the F1-score as η_l is varied within the range $(0.25, 1.0)$, while η_u is set to $\min(\eta_l + 0.3, 1.0)$. Based on this lower-threshold sweep, we observe that the optimal value of η_l for this case lies within the range $(0.25, 0.45)$. A similar trend is observed across other datasets.
The right plot in Figure 2 depicts the results of varying η_u within the range $(0.3, 1.0)$, with η_l fixed at 0.3. These results further support the importance of using an upper threshold. Specifically, setting η_u within the range $(0.35, 0.45)$ improves the overall F1-score on both the validation and test sets.

6.1 Experiment results

To further study the effect of UPL, we have conducted experiments on multiple datasets, a fraction of which has been shown in Table 1 and 2. We report averaged balanced accuracy (bAcc)[2] and F1-score with the standard errors for 10 repetitions on the GCN model. In our experiments, datasets are generated with an imbalance ratio of $\rho = 10$. We explore other imbalance ratios in Appendix G.

As shown in Tables 1 and 2, our UPL algorithm outperforms other baselines across both homophilic and heterophilic datasets in most cases. Notably, UPL demonstrates significantly lower performance variance than competing methods, indicating better reliability in its predictions. Table 2 also highlights a common challenge which is a marked decline in performance on heterophilic datasets. In contrast, our method consistently delivers better results in most cases, even in these challenging scenarios. Moreover, based on theoretical

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[2]Balanced accuracy is calculated as $\frac{1}{2}\left(\frac{\text{TP}}{\text{TP+FN}} + \frac{\text{TN}}{\text{TN+FP}}\right)$ where TP is true positive, FN is false negative and TN is true negative.

Figure 2: F1-score for different values of upper and lower thresholds for pseudo-labeling. The Figure on the left indicates the sweeping over η_l while $\eta_u = 0.3 + \eta_l$ for the CiteSeer dataset. The Figure on the right represents sweeping over η_u from 0.3 to 1.0 for Cora. In both Figures, the red line represents the validation results, and blue shows the result for the test set.

Table 1: Experimental results of our algorithm (UPL) compared to other baselines. All the experiments have been done using the GCN architecture. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for Cora, CiteSeer and PubMed datasets. All the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

Dataset	Cora		CiteSeer		PubMed	
Imbalance Ratio ($\rho = 10$)	bAcc.	F1	bAcc.	F1	bAcc.	F1
Vanilla	53.58 ±0.70	48.52 ±1.09	35.29 ±0.34	22.62 ±0.39	62.22 ±0.35	48.99 ±1.02
Re-Weight(Japkowicz & Stephen, 2002)	65.52 ±0.84	65.54 ±1.20	44.52 ±1.22	38.85 ±1.62	70.17 ±1.25	66.37 ±1.73
PC Softmax Hong et al. (2021)	67.79 ±0.92	67.39 ±1.08	49.81 ±1.12	45.55 ±1.26	70.20 ±0.60	68.83 ±0.73
DR-GCN Shi et al. (2020)	60.17 ±0.83	59.31 ±0.97	42.64 ±0.75	38.22 ±1.22	65.51 ±0.81	64.95 ±0.53
GraphSMOTE Zhao et al. (2021b)	62.66 ±0.83	61.76 ±0.96	34.26 ±0.89	28.31 ±1.48	68.94 ±0.89	64.17 ±1.43
BalancedSoftmax Ren et al. (2020)	67.75 ±1.09	66.47 ±1.27	52.09 ±1.61	48.55 ±2.01	71.78 ±0.82	71.18 ±0.94
GraphENS Park et al. (2022)+ TAM Song et al. (2022)	69.42 ±0.90	68.70 ±1.08	53.10 ±1.82	50.67 ±2.28	71.70 ±0.95	69.01 ±1.72
GraphSHA Li et al. (2023a)	39.82 ±0.85	34.88 ±0.92	33.20 ±1.10	24.74 ±1.25	66.55 ±0.70	66.74 ±0.68
BAT1 Liu et al. (2023)	72.32 ±0.52	71.10 ±0.55	59.23 ±0.90	58.48 ±0.87	73.37 ±0.45	72.60 ±0.48
Unreal Yan et al. (2023)	**78.33** ±1.04	**76.44** ±1.06	65.63 ±1.38	64.94 ±1.38	75.35 ±1.41	73.65 ±1.43
UPL	76.16 ±0.76	74.53 ±0.85	**68.18** ±0.27	**67.78** ±0.25	**77.50** ±0.44	**77.19** ±0.43

Table 2: Experimental results of our algorithm (UPL) compared to other baselines. All the experiments have been done using the GCN architecture. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for Cora, CiteSeer and PubMed datasets. All the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

Dataset	Chameleon		Squirrel		Wisconsin	
Imbalance Ratio ($\rho = 10$)	bAcc.	F1	bAcc.	F1	bAcc.	F1
Vanilla	57.01 ±0.53	55.61 ±0.67	38.07 ±0.57	34.81 ±0.69	34.51 ±2.31	31.45 ±2.66
Re-Weight Japkowicz & Stephen (2002)	36.07 ±0.87	35.61 ±0.81	26.92 ±0.53	25.04 ±0.59	44.13 ±3.08	40.74 ±3.27
PC Softmax Hong et al. (2021)	36.86 ±1.04	36.24 ±1.01	26.49 ±0.59	25.73 ±0.49	30.90 ±3.10	28.15 ±2.16
DR-GCN Shi et al. (2020)	33.34 ±0.81	29.60 ±0.79	23.34 ±0.43	18.20 ±0.49	29.44 ±1.36	27.08 ±1.37
GraphSMOTE Zhao et al. (2021b)	52.38 ±0.77	50.03 ±0.76	41.30 ±0.47	39.07 ±0.60	45.36 ±4.21	40.91 ±4.39
BalancedSoftmax Ren et al. (2020)	58.60 ±1.06	58.20 ±1.00	41.81 ±0.64	41.27 ±0.71	44.44 ±3.46	41.29 ±2.85
GraphENS Park et al. (2022)+ TAM Song et al. (2022)	40.98 ±0.85	38.93 ±0.84	27.98 ±0.90	24.04 ±0.70	41.38 ±2.78	34.56 ±2.22
Unreal	58.18 ±0.94	56.98 ±1.03	**45.65** ±1.08	**44.78** ±1.07	41.26 ±5.19	32.14 ±2.15
UPL	**61.19** ±0.66	**60.71** ±0.71	43.34 ±0.25	42.82 ±0.07	**48.70** ±2.88	**42.72** ±2.38

results and the fact that the maximum degree of nodes per class in heterophilic datasets is large, then we expect lower accuracy over these datasets. A detailed comparison with Unreal is provided in App. H.

6.2 Ablation study

We evaluate key components' individual and combined effects on our UPL algorithm to discover their contributions in transductive node classification tasks under imbalance scenario, for both homophilic and heterophilic datasets, in Table 3, respectively. For this purpose, we use BalancedSoftmax **(BS)**, which adjusts softmax to favor minority classes; Uncertainty-aware Pseudo-labeling **(UPL)**, which uses generated pseudo-labeled samples to generate more training data; aiming to align predicted class distributions with

Table 3: Experimental results of Ablation study of our proposed algorithm. All the experiments have been done using the GCN architecture. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for all datasets.

Dataset	Cora		CiteSeer		PubMed		Chameleon		Squirrel		Wisconsin	
Imbalance Ratio ($\rho = 10$)	bAcc.	F1	bAcc.	F1	bAcc.	F1	bAcc.	F1	bAcc.	F1	bAcc.	F1
Vanilla	53.28 ±0.65	48.12 ±1.03	35.53 ±0.33	22.67 ±0.41	61.96 ±0.33	48.97 ±0.89	57.24 ±0.63	55.82 ±0.75	37.70 ±0.58	34.45 ±0.71	34.51 ±2.31	31.45 ±2.66
+ BS	67.51 ±1.27	66.29 ±1.32	51.83 ±1.58	48.56 ±1.87	72.22 ±0.83	71.31 ±0.99	58.98 ±0.86	58.44 ±0.87	41.76 ±0.49	40.91 ±0.50	44.44 ±3.46	41.29 ±2.85
+ PL	68.86 ±1.51	66.45 ±1.86	48.81 ±2.62	41.75 ±3.74	73.19 ±1.42	71.98 ±2.08	60.24 ±0.90	59.63 ±0.95	39.34 ±0.56	37.15 ±0.58	38.62 ±2.28	36.51 ±2.54
+ Uncertainty	53.28 ±0.65	48.12 ±1.03	35.53 ±0.33	22.67 ±0.41	61.96 ±0.33	48.97 ±0.89	57.02 ±0.76	55.78 ±0.95	37.78 ±0.57	34.68 ±0.75	34.51 ±2.31	31.45 ±2.66
+ BS + PL	75.27 ±0.92	73.59 ±1.02	64.70 ±1.17	64.34 ±1.26	76.08 ±0.28	76.08 ±0.29	**61.26** ±0.73	**60.73** ±0.74	41.83 ±0.42	41.04 ±0.48	47.72 ±4.08	**44.03** ±3.44
+ Uncertainty + BS	67.51 ±1.27	66.29 ±1.32	51.83 ±1.58	48.56 ±1.87	72.22 ±0.83	71.31 ±0.99	59.04 ±0.85	58.44 ±0.88	41.70 ±0.48	40.88 ±0.54	44.44 ±3.46	41.29 ±2.85
+ Uncertainty + PL	67.51 ±2.16	65.28 ±2.59	40.01 ±2.01	28.25 ±2.31	74.85 ±0.75	73.80 ±0.89	59.21 ±0.74	58.14 ±0.77	38.39 ±0.67	35.86 ±0.87	36.92 ±2.62	34.74 ±2.76
UPL	**76.16** ±0.76	**74.53** ±0.85	**68.18** ±0.27	**67.78** ±0.25	**77.50** ±0.44	**77.19** ±0.43	61.19 ±0.66	60.71 ±0.71	**42.34** ±0.67	**41.76** ±0.68	**48.70** ±2.88	42.72 ±2.38

actual distributions. In Tables 3, The Vanilla model serves as our baseline which is log-loss function. We further study other uncertainty method in App. G.

The results demonstrate the effectiveness of various strategies for addressing class imbalance in node classification tasks. Across all datasets, the UPL method consistently excels, showcasing the robustness of integrating approaches. Notably, combinations like BS + UPL frequently lead to significant performance improvements, highlighting the synergy between direct imbalance mitigation and the strategic use of pseudo-labeled data.

7 Conclusion and Future Work

In this study, we make several key contributions to transductive node classification in imbalanced scenarios. First, we establish a theoretical upper bound on the population risk that depends on the maximum degree node within each class. Second, we develop an uncertainty-aware algorithm for identifying pseudo-labels for minority class nodes, introducing a novel selective edge removal method for uncertainty estimation. Our approach demonstrates superior performance compared to baseline methods across both homophilic and heterophilic datasets.

While our theoretical analysis currently focuses on γ-margin loss functions in binary classification, several promising directions emerge for future work. From a theoretical perspective, we aim to extend our results to multi-class scenarios and broader loss functions, as well as expand the analysis to inductive node classification settings where unlabeled nodes are not observed during training. Additionally, we plan to investigate theoretical bounds for heterophilic graphs to strengthen our framework's theoretical foundation.

As future work, we envision integrating our approach with H2GCN approach (Zhu et al., 2020) to enhance performance on heterophilic datasets. We also plan to incorporate advanced pseudo-labeling techniques such as Meta-Pseudo Label (Pham et al., 2021) or Flexmatch (Zhang et al., 2021a) to improve label quality. Finally, we intend to explore subgraph-based selective edge removal approaches for more sophisticated uncertainty estimation.

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A   Notations

Notations in this paper are summarized in Table 4.

Table 4: Summary of notations in the paper

Notation	Definition	Notation	Definition
$\mathcal{A}$	Adjacency matrices space	X_i	i-th node feature
$\deg_i^{\max}$	Maximum node degree i-th class	$\deg_i^{\min}$	Minimum node degree i-th class
Y_i	i-th node's label	Z_i	i-th node sample pair (X_i, Y_i)
$\mathbf{Z}_m$	The set of data training samples	$\mathbf{Z}_u$	The unlabeled samples
$P(.)$	Prediction of model	m_i	Number of nodes in i-th class
k	Number of classes	P_j	$\frac{|m_j|}{\sum_{i=1}^{k}|m_i|}$
$d_{\min}$	Minimum node degree of among all classes	$G_f(\mathbf{A})$	Graph filter with input matrix $\mathbf{A}$
$l(\hat{y}, y)$	Loss function	h_θ	Parameterized model
B_f	l_2-ball of radius	θ_i	Parameter matrix of i-th layer
φ	Activation function	$\mathfrak{R}_{m+u}(\mathcal{H})$	Empirical Rademacher complexity
$R(Z_u, h_\theta)$	True risk over unlabeled dataset	$R(Z_m, h_\theta)$	Empirical risk over labeled dataset
$U_F(i)$	Maximum of Frobenius norm i-th layer parameters	$U(.)$	Uncertainty Function
η_l	Lower thresholds of Pseudo-labeling process	η_u	Upper thresholds of Pseudo-labeling process
$\mathrm{KL}(P\|Q)$	$\int_{\mathbb{Z}} \log(\mathrm{d}P/\mathrm{d}Q)\mathrm{d}P$	$H(P,Q)$	$\int_{\mathbb{Z}} \log(\mathrm{d}P)\mathrm{d}Q$
B_f	Bound on node features	ρ	Imbalance Ratio
$\|\mathbf{Y}\|_F$	$\sqrt{\sum_{j=1}^{k}\sum_{i=1}^{q}\mathbf{Y}^2[j,i]}$	$\|\mathbf{Y}\|_\infty$	$\max_{1\leq j\leq k}\sum_{i=1}^{q}|\mathbf{Y}[j,i]|$
$\|\mathbf{Y}\|_2$	$\left(\sum_{j=1}^{q}|q|x_j^2\right)^{1/2}$	Q_α	Quantile of order α
t	Number of itterations	S_k	Number of edges removed in each itteration

B   Other Related Works

Pseudo-labeling in semi-supervised learning: Pseudo-labeling, introduced in (Lee et al., 2013), involves training a model using labeled data and assigning pseudo-labels to the unlabeled data based on the model's predictions. These pseudo-labels are then used to construct another model, which is trained in a supervised manner using both labeled and pseudo-labeled data. Under different scenarios, it is shown that the pseudo-labeling is effective, (Arazo et al., 2020) and (Rizve et al., 2021). (Kou et al., 2023) shows that semi-supervised learning with pseudo-labeling can achieve near-zero test loss under some conditions. The study by Pham et al. (2021) introduced meta pseudo-labeling. This method enhanced pseudo-labels' accuracy by incorporating feedback from the student model. (Rizve et al., 2021) proposed confidential-based pseudo-label generation for training a network with unlabeled data. (Arazo et al., 2020) suggests soft-labeling with the MixUp method to reduce over-fitting to model predictions and confirmation bias. In contrast, our work is focused on transductive node classification, and we employed the Pseudo-labels to mitigate the imbalance effect.

Imbalance Classification: Effective classification in the presence of imbalanced data is an important research field in supervised and semi-supervised learning, given that a significant class imbalance is commonly found in numerous real-world contexts (Herland et al., 2018; Rao et al., 2006; Cieslak et al., 2006) such as fraud detection in finance applications (Wei et al., 2013). This imbalance often presents challenges, as many classifiers tend to prefer the majority class, sometimes to the extent of completely overlooking the minority class. Traditional Class Imbalance Learning methods typically fall into two broad categories: data-level methods and algorithm-level methods. Data-level techniques aim to rebalance the training data itself to mitigate class imbalance. This includes strategies like over-sampling the minority class (Chawla et al., 2002; He et al., 2008; Mullick et al., 2019), under-sampling the majority class (Laurikkala, 2001; Mani & Zhang, 2003), and hybrid methods that combine both over-sampling and under-sampling (Ramentol et al., 2012; Sáez et al., 2015). On the other hand, algorithm-level methods focus on modifying the learning algorithms to better handle class imbalance. These methods encompass cost-sensitive learning (Tang et al., 2008; Zhou & Liu, 2005), ensemble learning (Seiffert et al., 2009; Guo & Viktor, 2004; Chawla et al., 2003), and engineering of specialized loss functions (Cao et al., 2019; Dong et al., 2018; Cui et al., 2019).

C   Proof and details of Section 4

Lemma C.1 (Bound on infinite norm of the symmetric normalized graph filter). *Consider a graph sample G with adjacency matrix A. For the symmetric normalized graph filter, we have $\left\|\tilde{D}^{-1/2}(A+I)\tilde{D}^{-1/2}\right\|_\infty[k] \leq \sqrt{\frac{\deg_k^{\max}+1}{\deg^{\min}+1}}$ where $\deg_k^{\max}$ is the maximum degree of graph G with adjacency matrix A among the nodes in k-th class.*

Proof. Recall that $\tilde{A} = A + I$. We have,

$$
\begin{aligned}
\left\|\tilde{L}\right\|_\infty[k] &= \left\|\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2}\right\|_\infty[k] \\
&= \max_{i\in[N_k]} \sum_{j=1}^{N} \frac{\tilde{A}_{ij}}{\sqrt{\deg_i+1}\sqrt{\deg_j+1}} \\
&\leq \frac{1}{\sqrt{\deg^{\min}+1}} \max_{i\in[N_k]} \sum_{j=1}^{N} \frac{\tilde{A}_{ij}}{\sqrt{\deg_i+1}} \\
&\leq \sqrt{\frac{\deg_k^{\max}+1}{\deg^{\min}+1}}.
\end{aligned}
\tag{7}
$$

where N_k is the number nodes in k-th class. $\qquad\square$

Proposition 4.4 (**Restated**). *Let $Q_i = (\frac{1}{u_i} + \frac{1}{m_i})$, $S_i = \frac{m_i+u_i}{(m_i+u_i-1/2)(1-1/(2\max(m_i,u_i)))}$ for $i = 1,2$. Then, with probability at least $(1-\delta)$ over the choice of the training set from nodes of graphs, for all $h_\theta \in \mathcal{H}$,*

$$
R(\mathbf{Z}_u, h_\theta) \leq \sum_{i=1}^{2} R_\gamma(\mathbf{Z}_{m_i}, h_\theta) + \frac{u_i}{u}\left(\frac{1}{\gamma}\mathfrak{R}_{m_i+u_i}(\mathcal{H}) + c_0 Q_i\sqrt{\min(m_i,u_i)} + \sqrt{\frac{S_i Q_i}{2}\log(1/\delta)}\right),
$$

where $\mathfrak{R}_{m_i+u_i}(\mathcal{H})$ is the transductive Rademacher complexity for i-th class, $R_\gamma(\mathbf{Z}_{m_i}, h_\theta)$ is the empirical risk based on γ-margin loss for i-th class and $c_0 = \sqrt{\frac{32\ln(4e)}{3}}$.

Proof. Let's decompose the true risk as follows,

$$
R(\mathbf{Z}_u, h_\theta) = \sum_{i=1}^{2} \frac{u_i}{u} R(\mathbf{Z}_{u_i}, h_\theta),
\tag{8}
$$

where $R(\mathbf{Z}_{u_i}, h_\theta)$ is true risk of i-th class. Inspired by (El-Yaniv & Pechyony, 2009, Corollary 1), we have,

$$
R(\mathbf{Z}_{u_i}, h_\theta) \leq R_\gamma(\mathbf{Z}_{m_i}, h_\theta) + \frac{1}{\gamma}\mathfrak{R}_{m_i+u_i}(\mathcal{H}) + c_0 Q_i\sqrt{\min(m_i,u_i)} + \sqrt{\frac{S_i Q_i}{2}\log(1/\delta)}.
\tag{9}
$$

Combining equation 9 with equation 8, we have,

$$
\begin{aligned}
R(\mathbf{Z}_u, h_\theta) &= \sum_{i=1}^{2} \frac{u_i}{u} R(\mathbf{Z}_{u_i}, h_\theta) \\
&\leq \sum_{i=1}^{2} \frac{u_i}{u}\left(R_\gamma(\mathbf{Z}_{m_i}, h_\theta) + \frac{1}{\gamma}\mathfrak{R}_{m_i+u_i}(\mathcal{H}) + c_0 Q_i\sqrt{\min(m_i,u_i)} + \sqrt{\frac{S_i Q_i}{2}\log(1/\delta)}\right).
\end{aligned}
\tag{10}
$$

It completes the proof by considering $\frac{u_i}{u} \leq 1$. $\qquad\square$

Proposition 4.5 (**Restated**). *Given Assumptions 4.1 , 4.2 and 4.3, then the following upper bound holds on the transductive Rademacher complexity of node classification,*

$$
\mathfrak{R}_{m_k+u_k}(\mathcal{H}) \leq \frac{B_f(\sqrt{2\log(2)d}+1)\Pi_{j=1}^{d} U_F(i)\|\mathrm{G}_f(\mathbf{A})[i]\|_\infty^{2(d-1)}}{\sqrt{m_k+u_k}}
$$

where $\|\mathrm{G}_f(\mathbf{A})[k]\|_\infty$ is the infinite norm of graph filter among k-th class.

Proof. Fix $\lambda > 0$, to be chosen later. Let us denote the output of q-th layer of GCN as,

$$N_{\theta_q}(\mathbf{X}_{u_k+m_k}) = \sigma(\theta_{q-1}\mathrm{G}_f(\mathbf{A})[i,:](\cdots\sigma(\theta_1\mathrm{G}_f(\mathbf{A})[i,:]\mathbf{X}_{u_k+m_k}))).$$

For the last layer, we do not consider aggregation. The Rademacher complexity can be upper bounded as

$$\left(\frac{m_k u_k}{m_k+u_k}\right)\mathfrak{R}_{m_k+u_k}(\mathcal{H}) = \mathbb{E}_{\boldsymbol{\epsilon}} \sup_{N_{\theta_{d-1}},\theta_d} \sum_{i=1}^{m_k+u_k} \epsilon_i \theta_d \sigma(\theta_{d-1}\mathrm{G}_f(\mathbf{A})[i,:]N_{\theta_{d-1}}(\mathbf{X}_{u_k+m_k}))$$

$$\leq \frac{1}{\lambda} \log \mathbb{E}_{\boldsymbol{\epsilon}} \sup \exp\left(\lambda \sum_{i=1}^{m_k+u_k} \epsilon_i \theta_d \sigma(\theta_{d-1}\mathrm{G}_f(\mathbf{A})[i,:]N_{\theta_{d-1}}(\mathbf{X}_{u_k+m_k}))\right)$$

$$\leq \frac{1}{\lambda} \log \mathbb{E}_{\boldsymbol{\epsilon}} \sup \exp\left(U_F(d) \cdot \left\|\lambda \sum_{i=1}^{m_k+u_k} \epsilon_i \sigma\left(\theta_{d-1}\mathrm{G}_f(\mathbf{A})[i,:]N_{\theta_{d-1}}(\mathbf{X}_{u_k+m_k})\right)\right\|\right).$$

We write this last expression as

$$\frac{1}{\lambda} \log \mathbb{E}_{\boldsymbol{\epsilon}} \sup_{f,\|\theta_{d-1}\|_F \leq U_F(d-1)} \exp\left(U_F(d) \cdot \lambda \left\|\sum_{i=1}^{m_k+u_k} \epsilon_i \sigma(\theta_{d-1}\mathrm{G}_f(\mathbf{A})[i,:]N_{\theta_{d-1}}(\mathbf{X}_{u_k+m_k}))\right\|\right)$$

$$\leq \frac{1}{\lambda} \log\left(2 \cdot \mathbb{E}_{\boldsymbol{\epsilon}} \sup_f \exp\left(U_F(d) \cdot U_F(d-1) \cdot \|\mathrm{G}_f(\mathbf{A})\|_\infty^2 \lambda \left\|\sum_{i=1}^{m_k+u_k} \epsilon_i N_{\theta_{d-1}}(\mathbf{X}_{u_k+m_k})\right\|\right)\right).$$

Repeating the process, we arrive at

$$\left(\frac{m_k u_k}{m_k+u_k}\right)\hat{\mathcal{R}}_{m_i+u_i}(\mathcal{H}) \leq \frac{1}{\lambda} \log\left(2^d \cdot \mathbb{E}_{\boldsymbol{\epsilon}} \exp\left(M\lambda \left\|\sum_{i=1}^{m_k+u_k} \epsilon_i \mathbf{X}_i\right\|\right)\right). \tag{11}$$

where $V = \|\mathrm{G}_f(\mathbf{A})\|_\infty^{2(d-1)} \prod_{j=1}^d U_F(j)$. Define a random variable

$$Z = V \cdot \left\|\sum_{i=1}^m \epsilon_i \mathbf{X}_i\right\|,$$

(random as a function of the random variables $\epsilon_1, \ldots, \epsilon_m$). Then

$$\frac{1}{\lambda} \log\left\{2^d \cdot \mathbb{E} \exp \lambda Z\right\} = \frac{d\log(2)}{\lambda} + \frac{1}{\lambda} \log\left\{\mathbb{E} \exp \lambda(Z - \mathbb{E}Z)\right\} + \mathbb{E}Z. \tag{12}$$

By Jensen's inequality, $\mathbb{E}[Z]$ can be upper bounded by using the Rademacher complexity random variables

$$V\sqrt{\mathbb{E}_{\boldsymbol{\epsilon}}\left[\left\|\sum_{i=1}^m \epsilon_i \mathbf{X}_i\right\|^2\right]} = V\sqrt{\mathbb{E}_{\boldsymbol{\epsilon}}\left[\sum_{i,i'=1}^m \epsilon_i \epsilon_{i'} \mathbf{X}_i^\top \mathbf{x}_{i'}\right]} = 2Vp\sqrt{\sum_{i=1}^m \|\mathbf{X}_i\|^2},$$

where $p = \frac{m_k u_k}{(m_k+u_k)^2}$. To handle the $\log\left\{\mathbb{E} \exp \lambda(Z - \mathbb{E}Z)\right\}$ term in equation 12, note that Z is a deterministic function of the i.i.d. random variables $\epsilon_1, \ldots, \epsilon_m$, and satisfies

$$Z(\epsilon_1, \ldots, \epsilon_i, \ldots, \epsilon_m) - Z(\epsilon_1, \ldots, -\epsilon_i, \ldots, \epsilon_m) \leq 2V\|\mathbf{X}_i\|.$$

This means that Z satisfies a bounded-difference condition, which by the proof of Theorem 6.2 in (Boucheron et al., 2003), implies that Z is sub-Gaussian, with variance factor

$$v = \frac{1}{4} \sum_{i=1}^{m_k+u_k} (2V\|\mathbf{X}_i\|)^2 = 4p^2V^2 \sum_{i=1}^{m_k+u_k} \|\mathbf{X}_i\|^2,$$

and satisfies

$$\frac{1}{\lambda} \log \{\mathbb{E} \exp \lambda(Z - \mathbb{E}Z)\} \leq \frac{1}{\lambda} \frac{\lambda^2 4 V^2 p^2 \sum_{i=1}^{m_k+u_k} \|\mathbf{X}_i\|^2}{2} = \frac{\lambda 4 V^2 p^2 \sum_{i=1}^{m_k+u_k} \|\mathbf{X}_i\|^2}{2}.$$

Choosing $\lambda = \dfrac{\sqrt{2\log(2)d}}{2pV\sqrt{\sum_{i=1}^{m_k+u_k}\|\mathbf{X}_i\|^2}}$ and using the above, we get that equation 11 can be upper bounded as follows:

$$\frac{1}{\lambda} \log \{2^d \cdot \mathbb{E} \exp \lambda Z\} \leq \mathbb{E}Z + \sqrt{2\log(2)d} \cdot 2pV \sqrt{\sum_{i=1}^{m_k+u_k} \|\mathbf{X}_i\|^2}$$

$$\leq 2pV \left(\sqrt{2\log(2)d} + 1\right) \sqrt{\sum_{i=1}^{m_k+u_k} \|\mathbf{X}_i\|^2}$$

$$\leq 2pV \left(\sqrt{2\log(2)d} + 1\right) B_f \sqrt{m_k + u_k}$$

$$= 2pV \left(\sqrt{2\log(2)d} + 1\right) B_f \sqrt{m_k + u_k},$$

from which the result follows. $\qquad \square$

Theorem 4.6 (Restated). *Under the same Assumptions in Proposition 4.4 and Proposition 4.5, the following upper bound holds on population risk for imbalanced transductive node classification under a GCN model,*

$$R(\mathbf{Z}_u, h_\theta) \leq \sum_{i=1}^{2} R_\gamma(\mathbf{Z}_{m_i}, h_\theta) + \frac{u_i}{u} \Big(\frac{B_f(\sqrt{2\log(2)d}+1)\Pi_{j=1}^d U_F(j)}{\gamma\sqrt{(m_i+u_i)}} \times \left(\frac{\deg_i^{\max} + 1}{\deg^{\min} + 1} \right)^{d-1}$$

$$+ c_0 Q_i \sqrt{\min(m_i, u_i)} + \sqrt{\frac{S_i Q_i}{2} \log(1/\delta)} \Big),$$

where $U_F(i)$ is the maximum of Frobenius norm of i-th layer parameter.

Proof. The proof follows directly from combining Proposition 4.4 with Proposition 4.5 and substituting $\|\mathrm{G}_f(\mathbf{A})\|_\infty$ for the GCN model using Lemma C.1. $\qquad \square$

D UPL Algorithm Details

Algorithm 1 Uncertainty-aware Pseudo-labeling (UPL) Algorithm

---

1: **Input:** Graph $G(X, V, E, Y)$, set of known train labels $\mathcal{Y}_t$, Number of classes C, set of edges $\mathcal{E}$, Number of Iterations k
2: **Output:** Model parameters
3: Initialize empty pseudo labels set $\mathcal{Y}_p$
4: **for** 1 to k **do**
5:     Initialize new model
6:     Train *model* on $\mathcal{Y}_t \cup \mathcal{Y}_p$ utilizing BS
7:     Initialize results set R with known labels
8:     **for** $i \leftarrow 1$ to t **do**
9:         $G_{\text{Aug}} \leftarrow$ Selective Edge Removal on G for S_k times
10:         $R_i \leftarrow \{$Inference Model on $G_{\text{Aug}}\}$ ▷ Add output to R
11:     **end for**
12:     $P \leftarrow \{$Inference Model on $G\}$ ▷ class-wise probabilities
13:     Initialize the set $\mathcal{Y}^{\text{new}}$ for new pseudo labels
14:     **for** each v in $G(V)$ **do**
15:         **if** $v \notin \mathcal{Y}_t$ **then**
16:             **if** $\eta_l < \max(P_k^v) < \eta_u$ **then**
17:                 **if** $U(v) < Q_\alpha$ **then**
18:                     Add v and $\arg\max(P_k^v)$ to $\mathcal{Y}^{\text{new}}$ as node and pseudo label
19:                 **end if**
20:             **end if**
21:         **end if**
22:     **end for**
23:     $\mathcal{Y}^p \leftarrow \mathcal{Y}^{\text{new}}$
24: **end for**
25: **return** *best_model* parameters

E Experiment Details

Datasets: We summarized the dataset statistics in Table 5. Note that in the Amazon Computers and Amazon Photos datasets Shchur et al. (2019), nodes represent products and edges denote co-purchasing relationships between them. We have included the Flickr dataset Zeng et al. (2019) to demonstrate our model's performance among the large datasets.

Table 5: Dataset statistics.

Dataset	Nodes	Edges	Classes	Features
CiteSeer	3,327	4,732	6	3,703
Cora	2,708	5,429	7	1,433
Pubmed	19,717	44,338	3	500
Chameleon	2,277	36,101	5	2,325
Squirrel	5,201	217,073	5	2,089
Wisconsin	251	515	5	1,703
Computers	13,381	245,778	10	767
Photo	7,650	119,081	8	745
Flickr	89,250	899,756	7	500

Hyperparameters: To attain the best results we have fine-tuned three hyperparameters for our model. These hyperparameters and their tune range along with hyperparameters from some of the previous have been displayed in Table 6.

Table 6: Tuned hyperparameters used in our work compared with those from previous methods

Methods	Hyperparameters Range
GraphENS	$\lambda \in \beta(2,2)$
	$k \in \{1,5,10\}$
	$\tau \in \{1,2\}$
	warm up $\in \{1,5\}$
TAM	$\alpha \in \{0.25, 0.5, 1.5, 2.5\}$
	$\beta \in \{0.125, 0.25, 0.5\}$
	$\phi \in \{0.8, 1.2\}$
Unreal	$K \in \{100, 300, 500, 700, 900\}$
	$T \in \{40, 50, 60, 70, 80, 100\}$
	$\alpha \in \{4, 6, 8, 10\}$
	$p \in \{0.5, 0.75, 0.98\}$
	DGIN threshold $\in \{0.25, 0.5, 0.75, 1.00\}$
UPL	$\eta_l \in \{0.25 + 0.05n \mid n \leq 9, n \in \mathbb{N} \cup \{0\}\}$
	$\eta_u \in \{min(\eta_l + 0.25n, 1.00) \mid n \leq 3, n \in \mathbb{N}\}$
	$Q_\alpha \in \{Q_{0.8}, Q_{0.9}\}$

F   Experiments Setup

UPL contains two tunable hyperparameters used for the pseudo labels threshold and three fixed ones which have approximated using a few experiments. Other extra hyperparameters have been adjusted according to (Song et al., 2022). We will discuss the setting for these parameters in the following sections.

F.1   UPL

We employ two thresholds for pseudo-labeling. As mentioned in Table 6, η_l and η_u are chosen respectively from $\{0.25 + 0.05n \mid 0 \leq n \leq 8, n \in \mathbb{N}\}$ and $\eta_u \in \{min(\eta_l + 0.25n, 1) \mid n \leq 3, n \in \mathbb{N}\}$. Both S_k and t are fixed to 100, and the quantile for uncertainty-based node selection is chosen from $\{Q_{0.8}, Q_{0.9}\}$.

F.2   BalancedSoftmax

Another part of UPL is BalancedSoftmax (BS) presented in (Ren et al., 2020). We have used the same values found in (Song et al., 2022) to prevent increasing the number of hyperparameters in the UPL algorithm.

F.3   Imbalance Ratio and Class Discrimination

In our experiments, the distinction between minority and majority classes is determined from the labeled training set. The **imbalance ratio (ρ)** is formally defined as the ratio of the size of the largest class to that of the smallest class. This is calculated as:

$$\rho = \frac{\max_{j \in [k]} |m_j|}{\min_{j \in [k]} |m_j|} \tag{13}$$

where $|m_j|$ is the number of training samples in class j.

Following this, we define a "minority class" as any class whose size is approximately $\frac{|m_{\max}|}{\rho}$, where $|m_{\max}|$ is the size of the largest class. In our UPL framework, we exclusively add pseudo-labels for nodes that the model predicts to belong to one of these identified minority classes.

We also note that for certain datasets like **Wisconsin**, which are naturally imbalanced and where training set size may vary significantly across different experimental runs, we take an additional step for robustness. To establish a stable imbalance ratio, we first calculate the average size of each class across all experimental

runs and then apply the formula above to these averaged sizes. This ensures a consistent and representative definition of minority and majority classes throughout our experiments.

Imbalance Ratio: The distribution of training sets for each dataset can be seen in Table 7. All datasets follow a 10:1 imbalance ratio, except for Wisconsin, which has an imbalance ratio (ρ) of 11.63. By analyzing Table 7, it is evident from the results in Tables 9 and 10 that our model generally performs significantly better when the node with the maximum degree is present in one of the majority classes.

F.4 Other Details

More minor details concerning the experiments have been explained in the following sections.

Table 7: Number of training nodes per class

Dataset ($\rho = 10$)	C_0	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9
Cora	20	20	20	20	2	2	2	-	-	-
CiteSeer	20	20	20	2	2	2	-	-	-	-
PubMed	20	20	2	-	-	-	-	-	-	-
Chameleon	225	220	218	22	22	-	-	-	-	-
Squirrel	487	494	501	50	50	-	-	-	-	-
Wisconsin ($\rho = 11.63$)	4	38	50	5	5	-	-	-	-	-
Computers	20	20	20	20	20	2	2	2	2	2
Photo	20	20	20	20	2	2	2	2	-	-
Flickr	2628	4321	3164	2431	432	432	432	-	-	-

Table 8: Size of maximum degree node per class

Dataset	C_0	C_1	C_2	C_3	C_4	C_5	C_6
Cora	36	78	168	74	40	23	31
CiteSeer	15	21	99	18	51	17	-
PubMed	80	171	154	-	-	-	-
Chameleon	207	269	322	531	732	-	-
Squirrel	1041	1054	1081	1060	1904	-	-
Wisconsin	5	122	10	13	11	-	-

Hardware and setup: All of our Experiments were conducted on a single server containing an Nvidia RTX 3090 GPU, AMD Ryzen 5 3600x CPU @ 3.80GHz, and 48GB of RAM.

Training: To choose the training mask, we use the training masks provided by Pytorch Geometric. We train each model for 1000 epochs with an early stopping patience of 100. For each dataset η_l is chosen from $(0.25, 0.90)$ and the value of η_u is chosen from $(\eta_u, 1.00)$. We also perform each experiment with 10 iterations of pseudo-labeling.

Optimizer: we use PyTorch Adaptive Moment Estimation (ADAM) as the optimizer. Also, ℓ_2 regularization with weight decay of $5e^{-4}$ for the first layer and dropout in some layers are used to prevent over-fitting. We use a learning rate of 0.01.

G More Experiments

G.1 Other Imbalance Ratios

In this section, we present the performance outcomes for four prominent GNN architectures: Graph Convolutional Network (GCN), Graph Attention Network (GAT), Graph SAGE (SAGE), and Graph Isomorphism Network (GIN). These models were evaluated across six diverse datasets with four different imbalance ratios

to assess their effectiveness in various scenarios. The results for the imbalance ratio of 10 are detailed in Table 9 and Table 10.

Tables 11 and 12 present the performance evaluation of UPL with an imbalance ratio of 5, while Tables 13 and 14 show the corresponding results for a lower imbalance ratio of $\rho = 2$.

We have also assessed our performance under an imbalance ratio of 20. These results are presented in Tables 15 and 16 for the Homophilic and Heterophilic datasets, respectively.

Table 9: Experimental results of our regularization methods and other baselines on three class-imbalanced node classification benchmark datasets: Cora, CiteSeer and PubMed. We report averaged balanced accuracy (bAcc.) and F1-score with the standard errors for 10 repetitions on three representative GNN architectures, i.e., GCN, GAT, Sage and GIN.

	Dataset	Cora		CiteSeer		PubMed	
	Imbalance Ratio ($\rho = 10$)	bAcc.	F1	bAcc.	F1	bAcc.	F1
GCN	Vanilla	53.58 ±0.70	48.52 ±1.09	35.29 ±0.34	22.62 ±0.39	62.22 ±0.35	48.99 ±1.02
	Re-Weight	65.52 ±0.84	65.54 ±1.20	44.52 ±1.22	38.85 ±1.62	70.17 ±1.25	66.37 ±1.73
	PC Softmax	67.79 ±0.92	67.39 ±1.08	49.81 ±1.12	45.55 ±1.26	70.20 ±0.60	68.83 ±0.73
	DR-GCN	60.17 ±0.83	59.31 ±0.97	42.64 ±0.75	38.22 ±1.22	65.51 ±0.81	64.95 ±0.53
	GraphSMOTE	62.66 ±0.83	61.76 ±0.96	34.26 ±0.89	28.31 ±1.48	68.94 ±0.89	64.17 ±1.43
	BalancedSoftmax	67.75 ±1.09	66.47 ±1.27	52.09 ±1.61	48.55 ±2.01	71.78 ±0.82	71.18 ±0.94
	GraphENS + TAM	69.42 ±0.90	68.70 ±1.08	53.10 ±1.82	50.67 ±2.28	71.70 ±0.95	69.01 ±1.72
	GraphSHA	39.82 ±0.85	34.88 ±0.92	33.20 ±1.10	24.74 ±1.25	66.55 ±0.70	66.74 ±0.68
	BAT1	72.32 ±0.52	71.10 ±0.55	59.23 ±0.90	58.48 ±0.87	73.37 ±0.45	72.60 ±0.48
	Unreal	**78.33** ±1.04	**76.44** ±1.06	65.63 ±1.38	64.94 ±1.38	75.35 ±1.41	73.65 ±1.43
	UPL	76.16 ±0.76	74.53 ±0.85	**68.18** ±0.27	**67.78** ±0.25	**77.50** ±0.44	**77.19** ±0.43
GAT	Vanilla	49.47 ±0.74	45.14 ±1.04	33.67 ±0.27	21.70 ±0.25	59.98 ±0.33	47.05 ±0.81
	Re-Weight	66.72 ±0.80	66.52 ±1.06	45.59 ±1.73	39.43 ±2.03	69.13 ±1.25	64.81 ±1.70
	PC Softmax	67.02 ±0.65	66.57 ±0.89	50.70 ±1.73	47.14 ±1.85	72.20 ±0.49	70.95 ±0.82
	DR-GCN	59.30 ±0.76	57.79 ±1.03	44.04 ±1.26	39.44 ±1.76	69.56 ±1.01	68.49 ±0.71
	GraphSMOTE	56.50 ±0.71	54.27 ±1.09	44.94 ±1.36	41.63 ±1.78	62.86 ±0.53	53.00 ±1.17
	BalancedSoftmax	66.63 ±0.91	65.66 ±0.98	52.51 ±1.28	49.71 ±1.80	71.09 ±0.74	68.95 ±0.97
	GraphENS + TAM	69.35 ±0.85	68.20 ±0.94	53.50 ±1.21	51.15 ±1.58	71.27 ±0.85	68.43 ±1.65
	GraphSHA	39.39 ±0.75	34.97 ±0.80	27.13 ±1.15	19.61 ±1.20	66.11 ±0.65	65.91 ±0.68
	BAT1	71.4 ±0.50	70.2 ±0.53	60.6 ±0.75	59.9 ±0.79	74.6 ±0.35	73.9 ±0.38
	Unreal	**78.91** ±0.59	**75.99** ±0.47	64.10 ±1.49	63.44 ±1.47	74.68 ±1.43	72.78 ±0.89
	UPL	76.28 ±0.75	75.55 ±0.79	**66.44** ±0.59	**65.98** ±0.57	**75.27** ±0.42	**74.43** ±0.61
Sage	Vanilla	50.82 ±0.47	43.77 ±0.75	34.95 ±0.19	22.54 ±0.24	61.63 ±0.63	49.58 ±1.24
	Re-Weight	63.76 ±0.98	63.46 ±1.22	46.64 ±1.92	41.38 ±2.76	69.03 ±1.17	64.01 ±2.18
	PC Softmax	64.03 ±0.81	63.73 ±0.99	50.14 ±1.89	47.38 ±2.13	71.39 ±0.84	70.25 ±1.02
	DR-GCN	61.05 ±1.17	60.17 ±1.23	46.00 ±0.93	47.73 ±1.12	69.23 ±0.68	67.35 ±0.90
	GraphSMOTE	65.37 ±0.55	65.13 ±0.68	38.94 ±1.05	33.60 ±1.68	64.15 ±0.55	54.00 ±1.14
	BalancedSoftmax	63.91 ±0.88	63.01 ±1.00	49.45 ±1.65	46.08 ±2.08	70.20 ±0.72	69.60 ±0.86
	GraphENS + TAM	65.36 ±0.96	64.63 ±1.16	50.37 ±1.62	47.41 ±1.99	70.48 ±0.87	68.65 ±1.61
	GraphSHA	38.11 ±0.78	34.76 ±0.82	34.10 ±1.10	25.85 ±1.25	65.81 ±0.60	66.61 ±0.63
	BAT1	71.4 ±0.51	70.1 ±0.54	60.0 ±0.78	59.3 ±0.81	**76.3** ±0.33	**75.8** ±0.36
	Unreal	**75.99** ±0.98	73.63 ±1.23	66.45 ±0.39	65.83 ±0.30	74.78 ±1.30	72.80 ±0.54
	UPL	75.06 ±0.84	**73.93** ±0.86	**67.41** ±0.51	**67.06** ±0.51	74.84 ±0.42	74.26 ±0.54
GIN	Vanilla	58.7 ±1.03	55.77 ±1.46	36.3 ±0.86	26.71 ±1.45	66.16 ±0.78	58.10 ±1.60
	BalancedSoftmax	66.78 ±0.79	65.67 ±1.02	46.02 ±2.19	41.76 ±2.77	70.22 ±0.80	66.95 ±0.92
	UPL	**72.72** ±0.60	**71.81** ±0.76	**58.6** ±1.39	**58.36** ±1.39	**72.89** ±1.00	**72.59** ±0.92

Table 10: Experimental results of our UPL algorithm and other baselines on three class-imbalanced node classification benchmark datasets: Chameleon, Squirrel and Wisconsin. We report averaged balanced accuracy (bAcc.) and F1-score with the standard errors for 10 repetitions on three representative GNN architectures, i.e., GCN, GAT, Sage and GIN

	Dataset	Chameleon		Squirrel		Wisconsin ($\rho = 11.63$)	
	Imbalance Ratio ($\rho = 10$)	bAcc.	F1	bAcc.	F1	bAcc.	F1
GCN	Vanilla	57.01 ±0.53	55.61 ±0.67	38.07 ±0.57	34.81 ±0.69	34.51 ±2.31	31.45 ±2.66
	Re-Weight	36.07 ±0.87	35.61 ±0.81	26.92 ±0.53	25.04 ±0.59	44.13 ±3.08	40.74 ±3.27
	PC Softmax	36.86 ±1.04	36.24 ±1.01	26.49 ±0.59	25.73 ±0.49	30.90 ±3.10	28.15 ±2.16
	DR-GCN	33.34 ±0.81	29.60 ±0.79	23.34 ±0.43	18.20 ±0.49	29.44 ±1.36	27.08 ±1.37
	GraphSMOTE	52.38 ±0.77	50.03 ±0.76	41.30 ±0.47	39.07 ±0.60	45.36 ±4.21	40.91 ±4.39
	BalancedSoftmax	58.60 ±1.06	58.20 ±1.00	41.81 ±0.64	41.27 ±0.71	44.44 ±3.46	41.29 ±2.85
	GraphENS + TAM	40.98 ±0.85	38.93 ±0.84	27.98 ±0.90	24.04 ±0.70	41.38 ±2.78	34.56 ±2.22
	Unreal	58.18 ±0.94	56.98 ±1.03	**45.65** ±1.08	**44.78** ±1.07	41.26 ±5.19	32.14 ±2.15
	UPL	**61.19** ±0.66	**60.71** ±0.71	43.34 ±0.25	42.82 ±0.07	**48.70** ±2.88	**42.72** ±2.38
GAT	Vanilla	48.17 ±0.91	44.01 ±1.48	29.12 ±0.68	22.05 ±0.58	33.25 ±1.83	31.50 ±2.29
	Re-Weight	35.72 ±0.65	34.19 ±0.74	25.79 ±0.52	24.32 ±0.62	42.15 ±2.33	37.66 ±2.27
	PC Softmax	38.32 ±0.88	37.46 ±0.84	26.52 ±0.31	25.71 ±0.44	41.89 ±3.95	38.03 ±3.35
	DR-GCN	34.84 ±0.72	31.53 ±0.86	24.69 ±0.46	21.81 ±0.42	33.93 ±2.34	31.75 ±2.50
	GraphSMOTE	40.72 ±0.83	33.44 ±1.28	27.10 ±0.49	26.63 ±0.63	40.77 ±2.24	38.96 ±2.48
	BalancedSoftmax	54.37 ±0.87	53.91 ±0.89	33.73 ±1.11	32.82 ±1.12	41.05 ±2.87	38.65 ±2.48
	GraphENS + TAM	49.13 ±0.73	48.61 ±0.71	29.01 ±0.41	26.99 ±0.67	39.34 ±3.36	35.11 ±2.64
	Unreal	58.79 ±0.54	57.91 ±0.44	43.02 ±1.18	41.57 ±1.15	38.33 ±5.25	31.61 ±2.92
	UPL	**58.87** ±0.48	**58.72** ±0.44	**43.62** ±0.47	**43.07** ±0.48	**48.35** ±3.16	**43.34** ±2.49
Sage	Vanilla	45.61 ±0.41	40.52 ±0.71	27.55 ±0.41	21.43 ±0.29	50.08 ±3.41	49.39 ±4.14
	Re-Weight	36.49 ±1.21	34.84 ±1.30	29.83 ±0.59	25.88 ±0.42	68.13 ±3.19	63.45 ±2.27
	PC Softmax	40.71 ±0.82	39.95 ±0.98	29.23 ±0.50	28.19 ±0.54	**70.57** ±3.34	**67.13** ±2.91
	DR-GCN	39.58 ±0.58	38.37 ±0.72	28.78 ±0.50	25.01 ±0.70	69.30 ±1.99	64.60 ±2.00
	GraphSMOTE	33.31 ±0.63	30.83 ±0.67	25.51 ±0.43	19.79 ±0.49	65.14 ±3.84	62.53 ±3.40
	BalancedSoftmax	54.01 ±0.54	53.72 ±0.52	32.70 ±0.50	32.37 ±0.51	63.51 ±3.67	62.50 ±2.97
	GraphENS + TAM	48.01 ±0.97	47.19 ±1.05	30.75 ±0.51	30.54 ±0.53	59.69 ±3.04	53.28 ±2.61
	Unreal	50.21 ±1.63	49.35 ±1.84	**33.43** ±0.53	32.30 ±0.49	62.20 ±6.83	51.52 ±4.14
	UPL	**54.68** ±0.63	**54.22** ±0.67	33.19 ±0.75	**32.74** ±0.75	70.19 ±4.50	67.09 ±3.78
GIN	Vanilla	53.21 ±0.66	50.65 ±0.87	25.07 ±1.57	17.65 ±1.64	33.42 ±2.27	30.10 ±1.79
	BalancedSoftmax	57.43 ±1.04	56.81 ±1.02	24.24 ±1.40	17.10 ±1.56	**41.12** ±2.28	**36.54** ±1.77
	UPL	**59.16** ±0.95	**58.73** ±0.96	**39.17** ±0.84	**38.18** ±0.78	39.25 ±2.44	35.68 ±1.63

Table 11: Experimental results of our algorithm (UPL) compared to baselines for $\rho = 5$. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for Cora, CiteSeer and PubMed datasets. All the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

	Datasets	Cora		CiteSeer		PubMed	
	Imbalance Ratio ($\rho = 5$)	bAcc.	F1	bAcc.	F1	bAcc.	F1
GCN	Vanilla	63.07 ±0.76	62.12 ±0.98	39.11 ±1.21	30.01 ±1.89	67.37 ±0.96	59.63 ±1.76
	BalancedSoftmax	73.31 ±0.76	72.77 ±0.68	58.82 ±1.27	57.09 ±1.64	74.29 ±0.97	73.60 ±0.91
	GraphENS + TAM	75.25 ±0.82	75.00 ±0.61	60.68 ±1.05	59.86 ±1.17	74.18 ±0.63	73.21 ±0.68
	UPL	**78.66** ±0.52	**77.62** ±0.55	**68.29** ±0.13	**67.92** ±0.15	**77.81** ±0.38	**77.49** ±0.4
GAT	Vanilla	57.19 ±0.65	56.18 ±0.83	36.17 ±0.59	26.86 ±1.12	65.18 ±1.12	56.75 ±2.43
	BalancedSoftmax	72.48 ±0.71	72.05 ±0.57	57.74 ±0.90	56.17 ±1.11	73.77 ±0.43	72.85 ±0.80
	GraphENS + TAM	74.27 ±0.59	73.19 ±0.55	58.98 ±1.11	58.05 ±1.41	73.67 ±0.60	72.08 ±0.88
	UPL	**78.94** ±0.81	**77.8** ±0.73	**66.92** ±0.26	**66.44** ±0.28	**75.83** ±0.45	**75.63** ±0.48
Sage	Vanilla	59.30 ±0.92	57.30 ±1.41	37.21 ±0.92	26.80 ±1.56	65.88 ±0.85	57.60 ±1.52
	BalancedSoftmax	70.41 ±0.60	69.84 ±0.52	56.53 ±1.19	54.88 ±1.48	72.89 ±0.39	71.69 ±0.62
	GraphENS + TAM	72.93 ±0.35	72.43 ±0.41	59.08 ±1.19	58.39 ±1.27	74.05 ±0.79	73.01 ±0.97
	UPL	**77.54** ±0.56	**76.37** ±0.56	**67.23** ±0.45	**66.81** ±0.41	**75.96** ±0.58	**75.42** ±0.54

Table 12: Experimental results of our algorithm (UPL) compared to baselines for $\rho = 5$. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for Chameleon, Squirrel and Wisconsin datasets. All the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

	Datasets	Chameleon		Squirrel		Wisconsin	
	Imbalance Ratio ($\rho = 5$)	bAcc.	F1	bAcc.	F1	bAcc.	F1
GCN	Vanilla	62.03 ±0.62	61.62 ±0.65	41.48 ±0.85	40.38 ±0.85	41.03 ±2.00	38.97 ±1.91
	BalancedSoftmax	63.23 ±0.64	62.94 ±0.64	45.36 ±0.71	45.04 ±0.74	43.20 ±2.90	38.81 ±2.19
	GraphENS + TAM	43.42 ±1.05	41.57 ±0.95	27.78 ±0.46	23.29 ±0.74	40.85 ±2.93	36.32 ±1.78
	UPL	63.7 ±0.74	63.48 ±0.71	45.49 ±0.48	45.16 ±0.48	46.51 ±2.63	41.54 ±2.27
GAT	Vanilla	56.11 ±0.91	55.45 ±0.87	29.93 ±0.49	22.58 ±0.42	37.69 ±2.71	34.61 ±2.26
	BalancedSoftmax	57.55 ±0.96	57.50 ±0.85	39.08 ±1.38	38.58 ±1.43	39.82 ±2.30	37.01 ±3.14
	GraphENS + TAM	50.02 ±0.50	49.68 ±0.57	29.27 ±0.40	26.43 ±0.88	45.10 ±2.30	37.04 ±1.47
	UPL	61.78 ±0.8	61.48 ±0.8	46.35 ±0.58	46.07 ±0.57	44.92 ±3.18	41.95 ±2.84
Sage	Vanilla	49.86 ±0.40	48.12 ±0.61	29.41 ±0.51	25.90 ±0.58	61.13 ±2.03	62.47 ±2.21
	BalancedSoftmax	56.57 ±0.49	56.10 ±0.53	34.27 ±0.58	34.04 ±0.57	68.17 ±3.38	66.74 ±3.50
	GraphENS + TAM	49.14 ±0.69	48.42 ±0.74	31.90 ±0.80	31.39 ±0.83	56.33 ±4.20	50.60 ±3.27
	UPL	57.42 ±0.60	56.94 ±0.60	34.49 ±0.49	34.33 ±0.51	73.61 ±2.99	71.3 ±2.89

Table 13: Experimental results of our algorithm (UPL) compared to baselines for $\rho = 2$. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for Cora, CiteSeer and PubMed datasets. All the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

	Datasets	Cora		CiteSeer		PubMed	
	Imbalance Ratio ($\rho = 2$)	bAcc.	F1	bAcc.	F1	bAcc.	F1
GCN	Vanilla	77.09 ±0.43	77.18 ±0.39	63.29 ±0.93	62.74 ±0.98	76.93 ±0.33	75.70 ±0.40
	BalancedSoftmax	79.46 ±0.28	78.58 ±0.30	67.26 ±0.49	66.84 ±0.53	78.25 ±0.28	77.78 ±0.29
	GraphENS + TAM	79.88 ±0.32	79.15 ±0.35	67.27 ±0.34	66.87 ±0.36	76.42 ±0.48	76.15 ±0.51
	UPL	81.24 ±0.31	80.27 ±0.30	68.58 ±0.29	68.16 ±0.31	78.37 ±0.21	77.88 ±0.21
GAT	Vanilla	73.61 ±0.49	74.45 ±0.49	60.76 ±1.19	59.84 ±1.49	74.43 ±0.55	72.14 ±0.81
	BalancedSoftmax	78.68 ±0.28	77.64 ±0.35	65.71 ±0.39	65.14 ±0.40	76.54 ±0.37	75.49 ±0.49
	GraphENS + TAM	79.25 ±0.27	78.13 ±0.28	66.62 ±0.40	66.24 ±0.40	76.28 ±0.47	75.87 ±0.46
	UPL	80.53 ±0.32	79.76 ±0.19	67.69 ±0.23	67.31 ±0.21	77.83 ±0.22	77.04 ±0.29
Sage	Vanilla	74.44 ±0.25	74.63 ±0.24	62.32 ±0.70	61.63 ±0.80	75.65 ±0.68	74.41 ±0.76
	BalancedSoftmax	77.56 ±0.27	76.61 ±0.25	65.74 ±0.48	65.24 ±0.49	75.68 ±0.40	74.97 ±0.38
	GraphENS + TAM	78.79 ±0.41	77.07 ±0.42	66.83 ±0.27	66.32 ±0.30	76.28 ±0.46	75.71 ±0.47
	UPL	80.12 ±0.26	78.67 ±0.31	68.98 ±0.20	68.62 ±0.19	76.90 ±0.30	76.45 ±0.26

Table 14: Experimental results of our algorithm (UPL) compared to baselines for $\rho = 2$. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for Chameleon, Squirrel and Wisconsin datasets. Same as other experiments, all the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

	Datasets	Chameleon		Squirrel		Wisconsin	
	Imbalance Ratio ($\rho = 2$)	bAcc.	F1	bAcc.	F1	bAcc.	F1
GCN	Vanilla	66.95 ±0.73	66.67 ±0.69	49.53 ±0.38	49.59 ±0.38	39.63 ±2.14	38.28 ±2.26
	BalancedSoftmax	67.10 ±0.79	66.78 ±0.73	50.00 ±0.47	49.74 ±0.48	44.81 ±3.18	41.32 ±2.32
	Graphens + TAM	43.76 ±1.08	41.49 ±1.38	26.98 ±0.79	23.69 ±0.67	43.86 ±2.89	37.68 ±2.15
	UPL	67.58 ±0.56	67.37 ±0.54	51.26 ±0.62	51.01 ±0.56	44.32 ±3.27	40.30 ±2.41
GAT	Vanilla	63.44 ±0.50	63.06 ±0.45	39.20 ±1.24	38.06 ±1.55	34.40 ±2.06	32.28 ±1.72
	BalancedSoftmax	62.81 ±0.93	62.39 ±0.89	43.99 ±1.95	43.55 ±1.98	42.17 ±2.41	37.66 ±2.74
	Graphens + TAM	53.21 ±0.84	52.86 ±0.93	33.21 ±0.58	32.81 ±0.65	44.02 ±2.16	36.57 ±1.60
	UPL	65.68 ±0.57	65.39 ±0.55	50.13 ±0.39	49.68 ±0.35	44.40 ±2.51	41.34 ±2.44
Sage	Vanilla	59.18 ±0.42	58.85 ±0.41	36.10 ±0.63	35.98 ±0.63	65.57 ±2.81	66.42 ±2.48
	BalancedSoftmax	59.17 ±0.52	58.55 ±0.50	37.22 ±0.53	37.00 ±0.52	74.10 ±2.77	70.37 ±3.04
	Graphens + TAM	51.25 ±0.90	50.87 ±0.93	32.86 ±0.49	32.52 ±0.51	63.35 ±3.53	53.89 ±3.07
	UPL	60.01 ±0.56	59.59 ±0.57	37.30 ±0.58	36.94 ±0.58	75.21 ±3.21	73.20 ±2.86

Table 15: Experimental results of our algorithm (UPL) compared to baselines for $\rho = 20$. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for Cora, CiteSeer and PubMed datasets. All the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

	Datasets	Cora		CiteSeer		PubMed	
	Imbalance Ratio ($\rho = 20$)	bAcc.	F1	bAcc.	F1	bAcc.	F1
GCN	Vanilla	50.01 ±0.18	42.37 ±0.28	34.95 ±0.23	21.83 ±0.11	61.11 ±0.19	46.91 ±0.43
	BalancedSoftmax	63.75 ±1.11	62.67 ±1.18	47.83 ±1.67	42.52 ±1.88	69.52 ±1.03	68.00 ±0.89
	Graphens + Tam	64.29 ±1.42	62.85 ±1.55	48.66 ±1.78	45.03 ±2.19	66.65 ±1.26	60.53 ±2.42
	UPL	**73.92** ±0.90	**73.48** ±0.98	**64.97** ±1.18	**64.18** ±1.29	**76.67** ±0.20	**76.61** ±0.20
GAT	Vanilla	48.27 ±0.26	41.45 ±0.21	34.28 ±0.22	21.80 ±0.18	59.43 ±0.27	45.36 ±0.32
	BalancedSoftmax	61.22 ±1.07	60.64 ±1.08	47.21 ±0.95	43.03 ±1.16	68.55 ±0.69	65.84 ±0.91
	Graphens + Tam	64.28 ±1.47	62.80 ±1.70	48.71 ±1.48	44.67 ±1.76	67.15 ±1.66	60.29 ±2.95
	UPL	**72.15** ±0.74	**71.48** ±0.73	**60.75** ±1.46	**60.25** ±1.47	**75.39** ±0.42	**75.13** ±0.38
Sage	Vanilla	49.50 ±0.17	41.93 ±0.32	34.65 ±0.09	22.05 ±0.08	60.15 ±0.36	46.89 ±0.75
	BalancedSoftmax	60.55 ±1.14	59.39 ±1.40	44.23 ±1.21	38.60 ±1.37	67.10 ±0.44	66.58 ±0.55
	Graphens + Tam	59.39 ±1.01	57.18 ±1.25	42.26 ±1.54	35.89 ±1.91	66.03 ±1.01	59.67 ±2.06
	UPL	**72.45** ±1.02	**71.80** ±1.13	**65.39** ±0.75	**64.89** ±0.90	**73.09** ±0.55	**73.19** ±0.49
GIN	Vanilla	51.24 ±0.95	45.53 ±1.39	34.16 ±0.23	22.49 ±0.36	61.8 ±0.63	49.47 ±1.44
	BalancedSoftmax	61.23 ±0.79	59.58 ±1.08	42.12 ±1.39	36.85 ±1.75	65.24 ±1.37	60.24 ±1.51
	UPL	**68.92** ±0.65	**67.94** ±0.70	**54.06** ±1.35	**53.65** ±1.41	**75.92** ±0.37	**75.23** ±0.36

Table 16: Experimental results of our algorithm (UPL) compared to baselines for $\rho = 20$. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for Chameleon, Squirrel and Wisconsin datasets. All the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

	Datasets	Chameleon		Squirrel		Wisconsin	
	Imbalance Ratio ($\rho = 20$)	bAcc.	F1	bAcc.	F1	bAcc.	F1
GCN	Vanilla	52.14 ±0.62	48.43 ±0.97	36.25 ±0.48	31.02 ±0.63	32.28 ±1.24	28.84 ±1.54
	BalancedSoftmax	54.63 ±0.79	53.10 ±0.70	**39.66** ±0.53	**38.51** ±0.55	40.18 ±3.31	36.53 ±2.35
	Graphens + Tam	53.27 ±0.74	52.34 ±0.80	38.87 ±0.41	38.01 ±0.46	**44.43** ±4.13	37.20 ±2.01
	UPL	**55.98** ±0.80	**54.99** ±0.83	39.01 ±0.60	38.10 ±0.60	42.61 ±3.35	**38.16** ±2.78
GAT	Vanilla	43.82 ±0.54	36.15 ±0.91	29.84 ±0.76	22.42 ±0.63	30.98 ±0.99	27.92 ±1.15
	BalancedSoftmax	51.26 ±0.55	50.94 ±0.65	31.72 ±1.08	30.80 ±1.08	38.63 ±3.28	35.45 ±2.19
	Graphens + Tam	47.19 ±0.82	46.19 ±0.92	28.80 ±0.60	26.86 ±0.99	43.27 ±4.25	34.73 ±2.05
	UPL	**54.62** ±0.67	**54.07** ±0.71	**40.83** ±0.51	**39.68** ±0.50	**43.60** ±3.14	**41.69** ±2.68
Sage	Vanilla	43.98 ±0.58	36.68 ±1.12	27.33 ±0.46	20.69 ±0.37	42.45 ±2.71	39.62 ±2.99
	BalancedSoftmax	49.21 ±0.97	48.94 ±0.83	32.17 ±0.55	31.63 ±0.58	54.16 ±4.31	52.16 ±4.16
	Graphens + Tam	44.62 ±0.98	43.60 ±0.86	30.04 ±0.45	29.31 ±0.39	48.54 ±4.17	44.28 ±2.58
	UPL	**50.63** ±0.63	**50.58** ±0.53	**32.50** ±0.52	**32.08** ±0.54	**55.47** ±2.89	**52.76** ±2.32
GIN	Vanilla	49.15 ±0.64	44.38 ±0.83	25.23 ±1.52	18.03 ±1.38	32.47 ±0.66	30.35 ±0.78
	BalancedSoftmax	52.39 ±1.05	51.17 ±1.13	23.7 ±1.24	18.32 ±1.81	**41.17** ±2.27	**37.95** ±1.60
	UPL	**54.41** ±1.05	**53.52** ±1.05	**31.69** ±1.02	**30.08** ±1.08	39.27 ±2.25	35.85 ±1.31

G.2 Additional Datasets

To further test UPL, we have included additional experiments with Amazon datasets (Shchur et al., 2019), comparing them to other previous works in Table 17, Table 18, and ablation studies in Table 19.

Table 17: Experimental results of our algorithm (UPL) compared to baselines for $\rho = 10$. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for Computers and Photo datasets. All the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

	Datasets	Computers		Photo	
	Imbalance Ratio ($\rho = 10$)	bAcc.	F1	bAcc.	F1
GCN	Vanilla	47.11 ± 2.28	36.53 ± 3.27	53.80 ± 3.09	44.83 ± 4.50
	BalancedSoftmax	74.35 ± 1.30	73.73 ± 1.35	74.86 ± 1.20	74.33 ± 1.39
	GraphENS + TAM	73.82 ± 2.76	72.68 ± 3.02	**82.34** ± 1.76	**81.39** ± 2.26
	UPL	**75.53** ± 0.94	**75.84** ± 0.97	79.27 ± 0.93	78.67 ± 0.93
GAT	Vanilla	41.24 ± 1.24	32.45 ± 1.92	46.52 ± 0.67	37.62 ± 1.55
	BalancedSoftmax	64.11 ± 2.09	63.01 ± 2.70	71.36 ± 1.90	69.78 ± 2.07
	GraphENS + TAM	64.55 ± 0.95	62.59 ± 1.34	68.86 ± 1.34	65.52 ± 1.60
	UPL	**74.62** ± 1.08	**74.20** ± 1.10	**81.93** ± 0.87	**81.60** ± 0.91
Sage	Vanilla	48.16 ± 1.84	38.56 ± 2.70	60.43 ± 2.83	52.07 ± 3.69
	BalancedSoftmax	73.18 ± 1.51	72.19 ± 1.71	78.55 ± 1.41	77.46 ± 1.59
	GraphENS + TAM	75.20 ± 1.47	73.96 ± 1.72	81.36 ± 1.54	80.67 ± 1.64
	UPL	**81.56** ± 0.94	**81.49** ± 1.01	**89.00** ± 0.44	**88.90** ± 0.46
GIN	Vanilla	51.76 ± 6.22	47.36 ± 6.82	74.3 ± 1.20	74.25 ± 1.37
	BalancedSoftmax	47.27 ± 7.61	43.37 ± 8.70	79.66 ± 1.02	79.43 ± 1.08
	UPL	**75.84** ± 1.19	**75.61** ± 1.34	**82.7** ± 0.71	**82.66** ± 0.71

Table 18: Experimental results of our algorithm (UPL) compared to baselines for $\rho = 20$. We report the averaged balanced accuracy, averaged F1-score and the standard error of each experiment for Computers and Photo datasets. All the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

	Datasets	Computers		Photo	
	Imbalance Ratio ($\rho = 20$)	bAcc.	F1	bAcc.	F1
GCN	Vanilla	42.85 ± 0.37	30.79 ± 0.33	45.82 ± 0.23	33.49 ± 0.21
	BalancedSoftmax	64.33 ± 1.63	63.93 ± 1.78	66.27 ± 2.54	64.84 ± 2.68
	Graphens + Tam	**73.38** ± 1.72	**71.33** ± 2.06	**78.50** ± 1.48	**77.24** ± 1.78
	UPL	66.29 ± 1.65	65.65 ± 1.93	71.86 ± 1.87	70.60 ± 1.97
GAT	Vanilla	40.95 ± 0.78	31.45 ± 0.48	44.82 ± 0.62	34.36 ± 0.47
	BalancedSoftmax	59.27 ± 1.71	57.27 ± 2.29	60.73 ± 1.62	58.45 ± 1.83
	Graphens + Tam	58.76 ± 1.54	57.52 ± 1.71	67.59 ± 1.84	65.23 ± 2.04
	UPL	**66.67** ± 1.31	**65.78** ± 1.36	**76.41** ± 0.99	**75.10** ± 1.25
Sage	Vanilla	45.36 ± 0.28	33.79 ± 0.20	46.75 ± 0.18	34.34 ± 0.23
	BalancedSoftmax	67.15 ± 1.30	65.60 ± 1.40	72.39 ± 1.62	71.49 ± 1.75
	Graphens + Tam	67.16 ± 2.19	64.69 ± 2.41	72.05 ± 2.73	69.94 ± 3.14
	UPL	**75.95** ± 1.33	**74.94** ± 1.57	**85.80** ± 1.22	**85.15** ± 1.45
GIN	Vanilla	37.98 ± 4.74	31.59 ± 4.83	64.91 ± 0.88	62.29 ± 1.14
	BalancedSoftmax	45.71 ± 6.12	43.55 ± 6.74	72.82 ± 1.60	71.62 ± 2.01
	UPL	**71.71** ± 2.34	**71.04** ± 2.58	**77.52** ± 1.47	**77.10** ± 1.53

We have also included some experiments to compare our performance with Unreal under massive graph datasets flickr. These result are displayed in Table 20.

G.3 Impact of Pseudo-Labeling Scope

A fundamental design choice in the UPL framework is the restriction of pseudo-labeling exclusively to minority classes. Our core hypothesis is that in imbalanced semi-supervised scenarios, the classifier is inherently biased

Table 19: We conducted an ablation study on our UPL algorithm, comparing it to baselines by systematically removing key components. We report the averaged balanced accuracy, averaged F1-score, and the standard error for each experiment on the Computers and Photo datasets. The results were calculated over 10 repetitions and 10 pseudo-labeling iterations.

	Datasets	Computers		Photo	
	Imbalance Ratio ($\rho = 10$)	bAcc.	F1	bAcc.	F1
GCN	Vanilla	46.15 ±1.61	35.25 ±2.37	48.30 ±2.46	36.86 ±3.46
	+ BS	74.24 ±0.92	74.57 ±0.92	76.86 ±0.87	75.97 ±0.92
	+ PL	61.95 ±1.55	57.85 ±1.92	63.95 ±2.97	58.74 ±4.17
	+ Uncertainty	47.96 ±2.25	37.78 ±3.19	48.25 ±2.42	36.79 ±3.40
	+ BS + PL	73.56 ±1.17	73.74 ±1.14	76.86 ±0.99	75.92 ±1.08
	+ Uncertainty + BS	74.44 ±1.02	74.54 ±1.07	76.61 ±0.92	75.91 ±0.96
	+ Uncertainty + PL	62.20 ±3.10	55.43 ±3.83	72.14 ±2.93	68.49 ±3.95
	UPL	**75.53** ±0.94	**75.84** ±0.97	**79.27** ±0.93	**78.67** ±0.93

Table 20: Experimental results of our algorithm (UPL) compared to Unreal for the large dataset of Flickr. We report the averaged balanced accuracy, averaged F1-score and the standard error. All the results have been calculated over 10 repetitions and 10 pseudo-labeling iterations.

Backbone	GCN		GAT		SAGE	
	bAcc.	F1	bAcc.	F1	bAcc.	F1
Unreal	22.82 ±0.27	21.31 ±0.47	23.82 ±1.62	18.64 ±1.18	24.57 ±0.41	22.88 ±0.50
UPL	**28.57** ±0.34	**24.07** ±0.44	**27.32** ±0.17	**23.46** ±0.28	**30.60** ±0.08	**25.97** ±0.23

toward majority classes. Consequently, indiscriminate pseudo-labeling (applying labels to all classes) risks amplifying this bias, as the model is likely to confidently misclassify ambiguous nodes as majority class samples.

To empirically validate this hypothesis, we evaluated a variant of our method termed **UPL-AC (UPL-All Classes)**, where the minority-only constraint is removed, allowing pseudo-labels to be assigned to any node satisfying the uncertainty thresholds. We tested this variant both with and without the Balanced Softmax (BS) loss function.

The results, detailed in Table 21, provide strong evidence supporting the minority-only strategy. We observe the following key trends:

1. **Degradation via Indiscriminate Labeling:** Across all backbones (GCN, GAT, SAGE, GIN), applying pseudo-labels to all classes consistently degrades performance compared to the proposed UPL. For instance, on the Cora dataset using GCN, UPL-AC results in a 4.47% drop in balanced accuracy compared to UPL.

2. **Confirmation Bias without Re-weighting:** The effect is most severe when the Balanced Softmax loss is removed (`UPL-AC w/o BS`). In this setting, the model's performance collapses (e.g., F1 score drops to 47.82 on Cora). This confirms that without the minority-only constraint, the self-training loop simply reinforces the majority class dominance, effectively ignoring the minority samples.

3. **Synergy of UPL components:** Even when Balanced Softmax is used to mitigate loss-level imbalance (`UPL-AC + BS`), the performance remains inferior to the proposed UPL. This indicates that loss re-weighting alone is insufficient to counteract the noise introduced by majority-class pseudo-labels.

These findings demonstrate that "more data" is not intrinsically better in imbalanced graph learning; rather, the distributional alignment of the pseudo-labeled set is the governing factor for success.

Table 21: This table compares the outcome of applying pseudo labeling to all classes with BS (UPL-AC + BS) and without BS (UPL-AC w/o BS) to proposed method (UPL).

$\rho = 10$		UPL		UPL-AC + BS (Δ from UPL)		UPL-AC w/o BS (Δ from UPL-AC+BS)	
		bAcc.	F1	bAcc.	F1	bAcc.	F1
GCN	Cora	**76.16**	**74.53**	71.69 (-4.47)	71.26 (-3.27)	53.12 (-18.57)	47.82 (-23.44)
	CiteSeer	**68.18**	**67.78**	65.38 (-2.80)	64.02 (-3.76)	35.37 (-30.01)	22.76 (-41.26)
	PubMed	**77.50**	**77.19**	76.07 (-1.43)	73.58 (-3.61)	62.08 (-13.99)	49.04 (-24.54)
GAT	Cora	**76.28**	**75.55**	71.24 (-5.04)	70.14 (-5.41)	49.65 (-21.59)	45.05 (-25.09)
	CiteSeer	**66.44**	**65.98**	63.03 (-3.41)	62.16 (-3.82)	34.15 (-28.88)	22.88 (-39.28)
	PubMed	**75.27**	**74.43**	72.71 (-2.56)	70.77 (-3.66)	62.03 (-10.68)	53.03 (-17.74)
SAGE	Cora	**75.06**	**73.93**	69.90 (-5.16)	69.35 (-4.58)	49.95 (-19.95)	43.70 (-25.65)
	CiteSeer	**67.41**	**67.06**	63.79 (-3.62)	63.11 (-3.95)	33.85 (-29.94)	21.93 (-41.18)
	PubMed	**74.84**	**74.26**	73.69 (-1.15)	71.11 (-3.15)	61.65 (-12.04)	49.90 (-21.21)

G.4 Uncertainty methods

We evaluate our approach's uncertainty estimation on the Cora dataset, comparing against two uncertainty estimation methods for GNN as baselines: CaGCN Wang et al. (2021) and ALG Zhang et al. (2021b) in Table 22. Our results show that imbalanced data significantly impacts uncertainty estimation performance in existing graph-based models.

Table 22: Comparison of our model with CaGCN and Alg as uncertainty estimation in GNN utilizing uncertainty in graphs has been tested under the imbalance scenario with ratio $\rho = 10$.

Methods	Cora	CiteSeer
CaGCN	46.23 $_{\pm 0.49}$	23.42 $_{\pm 0.74}$
Alg	67.48 $_{\pm 0.76}$	27.50 $_{\pm 0.85}$
UPL	74.51 $_{\pm 0.65}$	67.78 $_{\pm 0.25}$

G.5 Discussion

Both Table 9 and Table 10 demonstrate a clear superiority of our method across various architectures and datasets. A particularly notable aspect of our experiments is the significant margin by which our results surpass the second-best outcomes. This pronounced difference underscores the effectiveness of our approach, setting a new benchmark for performance in this field.

Our experimental analysis investigated the impact of varying the number of edge removal iterations (t) and the number of edges removed in each iteration (S_k) on model performance. The results, provided in Figure 3, demonstrate that choosing both $t = 100$ and $S_k = 100$ yields the best results in both studied datasets. Notably, the computation of uncertainty values does not require any training steps, which significantly reduces the computational overhead. Given that typical model training procedures require over 1000 epochs, the time needed to calculate uncertainty values is negligible in comparison to the overall training process.

For a summary of the performance of UPL, we have provided Table 23, comparing our model with previous methods in term of F1 score ranking based on topological nature of the dataset and the employed backbone. Performance ranking is measured in terms of Best|Second. It is worth noting that this ranking is adequate as UPL hasn't performed lower than second compared to previous methods in any of the experiments.

Figure 3: Selection Edge Removal: F1 score versus number of iterations and number of edges for removal. Each plot is normalized to it's lowest value.

Table 23: UPL performance summary: Comparison of UPL in terms of the number of Best|Second rank performance.

Datasets Types	GCN	GAT	SAGE
Homophilic	12|4	15|1	15|1
Heterophilic	9|3	12|0	9|3
Total	21|7	27|1	24|4

H Detailed Comparison with UNREAL

Comparison with UNREAL: Our algorithm, UPL, demonstrates notable computational advantages over the UNREAL algorithm (Yan et al., 2023). UPL's efficiency stems from two key factors: first, it employs a more selective pseudo-labeling process that focuses on minority classes, resulting in fewer pseudo-labeled nodes overall. Second, UPL eliminates the need for two computationally intensive components present in UNREAL—node reordering and clustering—which contribute significantly to that algorithm's complexity. Instead, UPL introduces a novel framework that incorporates uncertainty estimation and an upper threshold for pseudo-labeling. In contrast, the UNREAL algorithm operates through a series of three main steps,

- Dual Pseudo-tag Alignment Mechanism (DPAM): This step involves clustering all nodes, which inherently have a complexity of $O(N^2)$ for N nodes, and then inferring the GCN model.

- Node-Reordering: Utilizes the Rank-Biased Overlap (RBO) algorithm (Webber et al., 2010) to merge two sorted lists generated by clustering and GCN inference. This merging process also presents a complexity of $O(N^2)$ for N nodes.

- Discarding Geometrically Imbalanced Nodes (DGIN): This step computes the second nearest cluster center for each node, leading to a complexity of $O(Nk)$, where k is the predefined number of clusters,

where each is iterated T times, potentially leading to increased computational overhead. By reducing both the number of operations each step, UPL achieves improved efficiency without sacrificing performance. In particular, our UPL algorithm simplifies the computational process significantly:

- Uncertainty estimation: UPL involves sampling the edges to be removed based on their distribution to estimate the uncertainty. This process is iterated S_k times.

- Subsequently, similar to UNREAL, we infer the GCN model.

Notably our complexity is less than the UNREAL, as we avoid DGIN and RBO processes in UNREAL.

Furthermore, to assess practical efficiency, we conducted time measurements for both UNREAL and UPL under identical experimental conditions. Our findings demonstrate that UPL's streamlined approach, which

employs fewer and less complex iterative processes, substantially reduces both time and computational resource requirements, resulting in superior empirical efficiency. This advantage is clearly illustrated in our experiments with the PubMed dataset: UPL completed 10 runs in an average runtime of 0.66 minutes, while UNREAL required an average runtime of 14.1 minutes for the same number of runs. These timing tests were performed on a server equipped with an Nvidia RTX 3090 GPU and AMD Ryzen 5 3600x CPU @ 3.80GHz, ensuring consistent and comparable results. While UPL uses less time to run, it also delivers better performance, as shown in Tables 1, 2, 9, and 10. Our extensive evaluation across 24 different experimental setups reveals that UPL consistently outperforms UNREAL. In 17 out of these 24 setups, UPL achieved better results in both balanced accuracy and F1 score, while in the remaining cases, it secured second place, highlighting its robustness and consistent performance across a variety of conditions.