
Relational Curriculum Learning for Graph Neural Network

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Abstract

1 Graph neural networks (GNNs) have achieved great success in representing data
2 with dependencies by recursively propagating and aggregating messages along
3 the edges. However, edges in real-world graphs often have varying degrees of
4 difficulty, and some edges may even be noisy to the downstream tasks. Therefore,
5 existing GNNs may lead to suboptimal learned representations because they usually
6 treat every edge in the graph equally. On the other hand, curriculum learning
7 (CL), which mimics the human learning principle of learning data samples in a
8 meaningful order, has been shown to be effective in improving the generalization
9 ability and robustness of representation learners by gradually proceeding from easy
10 to more difficult samples during training. Unfortunately, existing CL strategies
11 are designed for independent data samples and cannot be trivially generalized to
12 handle data dependencies. To address these issues, we propose a novel CL method
13 to gradually incorporate more edges into training according to their difficulty from
14 easy to hard, where the degree of difficulty is measured by how well the edges
15 are expected given the model training status. We demonstrate the strength of our
16 proposed method in improving the generalization ability and robustness of learned
17 representations through extensive experiments on nine synthetic datasets and nine
18 real-world datasets.

19 1 Introduction

20 Inspired by cognitive science studies [7, 28] that humans can benefit from the sequence of learning
21 basic (easy) concepts first and advanced (hard) concepts later, curriculum learning (CL) [2] suggests
22 training a machine learning model with easy data samples first and then gradually introducing more
23 hard samples into the model according to a designed pace, where the difficulty of samples can usually
24 be measured by their training loss [22]. Many previous studies have shown that this easy-to-hard
25 learning strategy can effectively improve the generalization ability of the model [2, 17, 13, 10, 30, 37],
26 and some studies [17, 13, 10] have shown that CL strategies can also increase the robustness of the
27 learned model against noisy training samples. An intuitive explanation is that in CL settings noisy
28 data samples correspond to harder samples and CL learner spends less time with the harder (noisy)
29 samples to achieve better generalization performance and robustness.

30 Although CL strategies have achieved great success in many fields such as computer vision and
31 natural language processing, existing methods are designed for independent data (such as images)
32 while designing effective CL methods for data with dependencies has been largely underexplored.
33 For example, in a citation network, two researchers with highly related research topics (e.g. machine
34 learning and data mining) are more likely to collaborate with each other, while the reason behind
35 a collaboration of two researchers with less related research topics (e.g. computer architecture and
36 social science) might be more difficult to understand. Prediction on one sample impacts that of
37 another, forming a graph structure that encompasses all samples connected by their dependencies.

38 There are many machine learning techniques for such graph-structured data, ranging from traditional
 39 models like conditional random field [31], graph kernels [32], to modern deep models like GNNs [40].
 40 However, traditional CL strategies are insufficient for them, which require not only considering the
 41 difficulty in individual samples but also the difficulty of their dependencies to determine how to
 42 gradually composite correlated samples for learning.

43 As previous CL strategies indicated that an easy-to-hard learning sequence on data samples can
 44 improve the generalization and robustness performance, an intuitive question is whether a similar
 45 strategy on data dependencies that iteratively involves easy-to-hard edges in learning can also benefit.
 46 Unfortunately, there exists no trivial way to directly generalize existing CL strategies on independent
 47 data to handle data dependencies due to several unique challenges: (1) **Difficulty in quantifying**
 48 **edge selection criteria**. Existing CL studies on independent data often use supervised computable
 49 metrics (e.g. training loss) to quantify sample difficulty, but how to quantify the difficulties of
 50 understanding the dependencies between data samples which has no supervision is challenging.
 51 (2) **Difficulty in designing an appropriate curriculum to gradually involve edges**. Existing CL
 52 methods usually design a fixed pacing function to include a certain ratio of samples during training.
 53 Similar to the human learning process, the model should ideally retain a certain degree of freedom to
 54 adjust the pacing of including edges according to its own learning status. (3) **Difficulty in ensuring**
 55 **convergence and a numerical steady process for CL in graphs**. Discrete changes in the number of
 56 edges can cause drift in the optimal model parameters between training iterations. How to guarantee
 57 a numerically stable learning process for CL on edges is challenging.

58 In order to address the aforementioned challenges, in this paper, we propose a novel CL algorithm
 59 named **Relational Curriculum Learning (RCL)** to improve the generalization ability and robustness
 60 of representation learners on data with dependencies. To address the first challenge, we propose an
 61 approach to select the edges by quantifying their corresponding difficulties in a self-supervised learn-
 62 ing manner. Specifically, for each training iteration, we choose K easiest edges whose corresponding
 63 relations are most well-expected by the current model. Second, to design an appropriate learning
 64 pace for gradually involving more edges in training, we present the learning process as a concise
 65 optimization model, which automatically lets the model gradually increase the number K to involve
 66 more edges in training according to its own status. Third, to ensure convergence of optimizing the
 67 model, we propose a proximal optimization algorithm with a theoretical convergence guarantee and
 68 an edge reweighting scheme to smooth the graph structure transition. Finally, we demonstrate the
 69 superior performance of RCL compared to state-of-the-art comparison methods through extensive
 70 experiments on both synthetic and real-world datasets.

71 2 Related work

72 **Curriculum learning (CL)**. [2] first proposed the idea of CL in the context of machine learning,
 73 aiming to improve model performance by gradually including easy to hard samples in training the
 74 model. Self-paced learning [22] measures the difficulty of samples by their training loss, which
 75 addressed the issue in previous works that difficulties of samples are generated by prior heuristic
 76 rules. Therefore, the model can adjust the curriculum of samples according to its own training
 77 status. Following works [16, 15, 44] further proposed many supervised measurement metrics for
 78 determining curriculums, for example, the diversity of samples [15] or the consistency of model
 79 predictions [44]. Meanwhile, many empirical and theoretical studies were proposed to explain why
 80 CL could lead to generalization improvement from different perspectives. For example, studies such
 81 as MentorNet [17] and Co-teaching [13] empirically found that utilizing CL strategy can achieve
 82 better generalization performance when the given training data are noisy. [10] provided theoretical
 83 explanations on the denoising mechanism that CL learners waste less time with the noisy samples as
 84 they are considered harder samples. Some studies [2, 30, 37, 11, 21] also realized that CL can help
 85 accelerate the optimization process of non-convex objectives and improve the speed of convergence
 86 in the early stages of training.

87 Despite great success, most of the existing designed CL strategies are for independent data such as
 88 images, and there is little work on generalizing CL strategies to handle samples with dependencies.
 89 Few existing attempts on graph-structured data [23], such as [35, 5, 36, 25], simply treat nodes as
 90 independent samples and then apply CL strategies on independent data, which ignore the fundamental
 91 and unique dependency information that carried by the structure in data, thus can not well handle the
 92 correlation between data samples. Furthermore, these models are mostly based on heuristic-based
 93 sample selection strategies [5, 36, 25], which largely limit the generalizability of these methods.

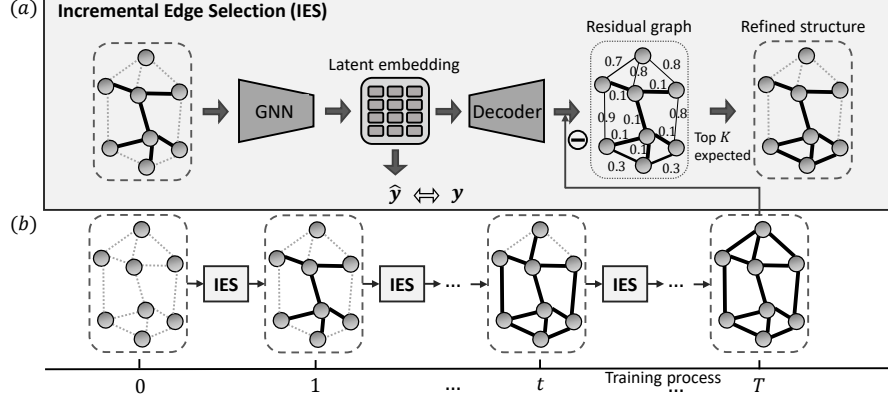


Figure 1: The overall framework of RCL. (a) The *Incremental Edge Selection* module first extracts the latent node embedding by the GNN model given the current training structure, then jointly learn the node prediction label y and reconstructs the input structure by a decoder. A small residual error on an edge indicates the corresponding dependency is well expected and thus can be added to the refined structure for the next iteration. (b) The iterative learning process of RCL. The model starts with an empty structure and gradually includes more edges until the training structure converges to the input structure.

Graph structure learning. Another stream of existing studies that are related to our work is *graph structure learning*. Recent studies have shown that GNN models are vulnerable to adversarial attacks on graph structure [6, 39]. In order to address this issue, studies in *graph structure learning* usually aim to jointly learn an optimized graph structure and corresponding graph representations. Existing works [8, 4, 18, 43, 26] typically consider the hypothesis that the intrinsic graph structure should be sparse or low rank from the original input graph by pruning “irrelevant” edges. Thus, they typically use pre-deterministic methods [6, 45, 8] to preprocess graph structure such as singular value decomposition (SVD), or dynamically remove “redundant” edges according to the downstream task performance on the current sparsified structure [4, 18, 26]. However, modifying the graph topology will inevitably lose potential useful information lying in the removed edges. More importantly, the modified graph structure is usually optimized for maximizing the performance on the training set, which can easily lead to overfitting issues.

3 Preliminaries

Graph Neural Networks Graph neural networks (GNNs) are a class of methods that have shown promising progress in representing structured data in which data samples are correlated with each other. Typically, the data samples are treated as nodes while their dependencies are treated as edges in the constructed graph. Formally, we denote a graph as $G = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V} = \{v_1, v_2, \dots, v_N\}$ is a set of nodes that $N = |\mathcal{V}|$ denotes the number of nodes in the graph and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ is the set of edges. We also let $\mathbf{X} \in \mathbb{R}^{N \times b}$ denote the node attribute matrix and $\mathbf{A} \in \mathbb{R}^{N \times N}$ represents the adjacency matrix. Specifically, $A_{ij} = 1$ denotes there is an edge connecting nodes v_i and $v_j \in \mathcal{V}$, otherwise $A_{ij} = 0$. A GNN model f maps node feature matrix \mathbf{X} associated with the adjacency matrix \mathbf{A} to the model predictions $\hat{\mathbf{y}} = f(\mathbf{X}, \mathbf{A})$, and get the loss $L_{\text{GNN}} = L(\hat{\mathbf{y}}, \mathbf{y})$, where L is the objective function and \mathbf{y} is the ground-truth label of nodes. The loss on one node v_i is denoted as $l_i = L(\hat{y}_i, y_i)$.

Curriculum Learning In order to leverage the information carried by the various difficulties of data samples into the training process, Curriculum Learning (CL) [2, 22], which is inspired by the cognitive process of human learning principles that learning concepts in a meaningful order [7], is a popular training strategy that can improve the generalization ability and robustness of representation learners. Specifically, instead of randomly presenting all training samples to the model as in traditional machine learning algorithms, CL learners start with easy samples and gradually include harder ones during the training process, where the difficulty of samples can be measured by a predetermined policy or a supervised computable metric (e.g. training loss).

4 Methodology

As previous CL methods have shown that an easy-to-hard learning sequence of independent data samples can improve the generalization ability and robustness of the representation learner, the goal

of this paper is to develop an effective CL method on data with dependencies, which is extremely difficult due to several unique challenges: (1) Difficulty in designing a feasible principle to select edges by properly quantifying their difficulties. (2) Difficulty in designing an appropriate pace of curriculum to gradually involve more edges in training based on model status. (3) Difficulty in ensuring convergence and a numerical steady process for optimizing the CL model.

In order to address the above challenges, we propose a novel CL method named **Relational Curriculum Learning (RCL)**. The sequence, which gradually includes edges from easy to hard, is called *curriculum* and learned in different grown-up stages of training. In order to address the first challenge, we propose a self-supervised module *Incremental Edge Selection (IES)*, which is shown in Figure 1(a), to select the K easiest edges at each training iteration that are mostly expected by the current model. The details are elaborated in Section 4.1. To address the second challenge, we present a joint optimization framework to automatically increase the number of selected edges K given its own training status. The framework is elaborated in Figure 1(b) and details can be found in Section 4.2. Finally, to ensure convergence of optimization and steady the numerical process, we propose a proximal optimization algorithm with theoretical convergence guarantee in Section 4.2 Algorithm 1 and an edge reweighting scheme to smooth the discrete edge incrementing process in Section 4.3.

4.1 Incremental edge selection by quantifying difficulties of sample dependencies

Here we propose a novel way to select edges by first quantifying their difficulty levels. Existing works on independent data typically use supervised metrics such as training loss of samples to quantify their difficulty level, but there exists no supervised metrics on edges. To address this issue, we propose a self-supervised module *Incremental Edge Selection (IES)*. We first quantify the difficulty of edges by measuring how well the edges are expected from the currently learned embeddings of their connected nodes. Then the most well-expected edges are selected as the easiest edges for the next iteration of training. As shown in Figure 1(a), given the currently selected edges at iteration t , we first feed them to the GNN model to extract the latent node embeddings. Then we restore the latent node embeddings to the original graph structure through a decoder, which is called the reconstruction of the original graph structure. The residual graph \mathbf{R} , which is defined as the degree of mismatch between the original adjacency matrix \mathbf{A} and the reconstructed adjacency matrix $\tilde{\mathbf{A}}^{(t)}$, can be considered a strong indicator for describing how well the edges are expected by the current model. Specifically, a smaller residual error indicates a higher probability of being a well-expected edge.

With the developed self-supervised method to measure the difficulties of edges, here we formulate the key learning paradigm of selecting the top K easiest edges. To obtain the training adjacency matrix $\mathbf{A}^{(t)}$ that will be fed into the GNN model $f^{(t)}$, we introduce a learnable binary mask matrix \mathbf{S} with each element $\mathbf{S}_{ij} \in \{0, 1\}$. Thus, the training adjacency matrix at iteration t can be represented as $\mathbf{A}^{(t)} = \mathbf{S}^{(t)} \odot \mathbf{A}$. To filter out the edges with K smallest residual error, we penalize the summarized residual errors over the selected edges, which can be represented as $\sum_{i,j} \mathbf{S}_{ij} \mathbf{R}_{ij}$. Therefore, the learning objective can be presented as follows:

$$\begin{aligned} \min_{\mathbf{w}} L_{\text{GNN}} + \beta \sum_{i,j} \mathbf{S}_{ij} \mathbf{R}_{ij}, \\ \text{s.t. } \|\mathbf{S}\|_1 \geq K, \end{aligned} \quad (1)$$

where the first term $L_{\text{GNN}} = L(f(\mathbf{X}, \mathbf{A}^{(t)}; \mathbf{w}), \mathbf{y})$ is the node-level predictive loss, e.g. cross-entropy loss for node classification task. The second term $\sum_{i,j} \mathbf{S}_{ij} \mathbf{R}_{ij}$ aims at penalizing the residual errors over the edges selected by the mask matrix \mathbf{S} . β is a hyperparameter to tune the balance between terms. The constraint is to guarantee only the most K well-expected edges are selected.

More concretely, the value of a residual edge $\tilde{\mathbf{A}}_{ij}^{(t)} \in [0, 1]$ can be computed by a non-parametric kernel function $\kappa(\mathbf{z}_i^{(t)}, \mathbf{z}_j^{(t)})$, e.g. the inner product kernel. Then the residual error \mathbf{R}_{ij} between the input structure and the reconstructed structure can be defined as $\|\tilde{\mathbf{A}}_{ij}^{(t)} - \mathbf{A}_{ij}\|$, where $\|\cdot\|$ is commonly chosen to be the squared ℓ_2 -norm.

4.2 Automatically control the pace of increasing edges

In order to dynamically include more edges into training, an intuitive way is to iteratively increase the value of K in Equation 1 to allow more edges to be selected. However, it is difficult to determine an appropriate value of K respect to the training status of the model. Besides, directly solving

Algorithm 1 Proximal Alternating Minimization Algorithm for Optimizing Equation 2

Input: Node features \mathbf{X} , adjacency matrix \mathbf{A} , a stepsize μ and hyperparameter γ

Output: The learnable parameter \mathbf{w} of GNN model f

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1: Initialize  $\mathbf{w}^{(0)}, \mathbf{S}^{(0)}, \lambda$ 
2: while Not converged do
3:    $\mathbf{w}^{(t)} = \arg \min_{\mathbf{w}} L(f(\mathbf{X}, \mathbf{A}^{(t-1)}; \mathbf{w}), \mathbf{y}) + \beta \sum_{i,j} \mathbf{S}_{ij} \left\| \tilde{\mathbf{A}}_{ij}^{(t-1)} - \mathbf{A}_{ij} \right\| + \frac{\gamma}{2} \left\| \mathbf{w} - \mathbf{w}^{(t-1)} \right\|$ 
4:   Given  $\mathbf{w}^{(t)}$ , extract latent nodes embedding  $\mathbf{Z}^{(t)}$  from GNN model  $f$ 
5:   Calculate reconstructed structure  $\tilde{\mathbf{A}}_{ij}^{(t)} = \kappa(\mathbf{z}_i^{(t)}, \mathbf{z}_j^{(t)})$  for all pairs of  $i, j$ 
6:    $\mathbf{S}^{(t)} = \arg \min_{\mathbf{S}} \beta \sum_{i,j} \mathbf{S}_{ij} \left\| \mathbf{A}_{ij} - \tilde{\mathbf{A}}_{ij}^{(t)} \right\| + g(\mathbf{S}; \lambda) + \frac{\gamma}{2} \left\| \mathbf{S} - \mathbf{S}^{(t-1)} \right\|$ 
7:   Compute  $\mathbf{A}^{(t)} = \mathbf{S}^{(t)} \odot \mathbf{A}$ 
8:   if  $\mathbf{A}^{(t)} \neq \mathbf{A}$  then
9:     Increase  $\lambda$  by stepsize  $\mu$ 
10:  end if
11: end while
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Equation 1 is difficult since \mathbf{S} is a binary matrix where each element $\mathbf{S}_{ij} \in \{0, 1\}$, optimizing \mathbf{S} would require solving a discrete constraint program at each iteration. To address this issue, we first relax the problem into continuous optimization so that each \mathbf{S}_{ij} can be allowed to take any value in the interval $[0, 1]$. Then we treat the constraint as a Lagrange multiplier and solve an equivalent problem by substituting the constraint to a regularization term $g(\mathbf{S}; \lambda)$, thus, our overall loss function can be rewritten as:

$$\min_{\mathbf{w}, \mathbf{S}} L_{\text{GNN}} + \beta \sum_{i,j} \mathbf{S}_{ij} \mathbf{R}_{ij} + g(\mathbf{S}; \lambda), \quad (2)$$

where $g(\mathbf{S}; \lambda) = \lambda \|\mathbf{S} - \mathbf{A}\|$ and $\|\cdot\|$ is commonly chosen to be the squared ℓ_2 -norm. Since the training adjacency matrix $\mathbf{A}^{(t)} = \mathbf{S}^{(t)} \odot \mathbf{A}$, as $\lambda \rightarrow \infty$, more edges in the input structure are included until the training adjacency matrix $\mathbf{A}^{(t)}$ converges to the input adjacency matrix \mathbf{A} . Specifically, the regularization term $g(\mathbf{S}; \lambda)$ controls the learning scheme by the *age parameter* λ , where $\lambda = \lambda(t)$ grows with the number of iterations. By monotonously increasing the value of λ , the regularization term $g(\mathbf{S}; \lambda)$ will push the mask matrix gradually converge to the input adjacency matrix \mathbf{A} , resulting in more edges automatically involved in the training structure.

Optimization of learning objective. It is worth noting that optimizing our objective function in Equation 2 requires jointly optimizing parameter \mathbf{w} of GNN model f and the mask matrix \mathbf{S} . In order to address this problem, we propose a proximal alternating optimization schema to iteratively update \mathbf{w} and \mathbf{S} in sequence. The full algorithm is presented in Algorithm 1. As we can see, our algorithm takes the input of node feature matrix \mathbf{X} and original adjacency matrix \mathbf{A} , a stepsize μ to control the increasing pace of age parameter λ , and a hyperparameter γ to tune the proximal terms. After initializing the parameters \mathbf{w} and \mathbf{S} , it alternates between two updating steps until it finally converges: (1) Step 3 first learns the optimal parameter of GNN model f with the current training adjacency matrix; (2) Step 4 & 5 extracts the latent node embedding by fixing the GNN model parameter and build the reconstructed adjacency matrix by the kernel function; (3) Step 6 learns the optimal mask matrix \mathbf{S} with the reconstructed adjacency matrix and regularization term; (4) Step 7 refines the training adjacency matrix with respect to the updated mask matrix; (5) The age parameter λ is increased when the training adjacency matrix $\mathbf{A}^{(t)}$ is still different from the input adjacency matrix \mathbf{A} , thus more edges will be included in the next iteration of the training.

Theorem 4.1. *We have the following convergence guarantees for Algorithm 1:*

- **Avoidance of Saddle Points.** *If the second derivatives of $L(f(\mathbf{X}, \mathbf{A}^{(t)}; \mathbf{w}), \mathbf{y})$ and $g(\mathbf{S}; \lambda)$ are continuous, then for sufficiently large γ , any bounded sequence $(\mathbf{w}^{(t)}, \mathbf{S}^{(t)})$ generated by Algorithm 1 with random initializations will not converge to a strict saddle point of F almost surely.*
- **Second Order Convergence.** *If the second derivatives of $L(f(\mathbf{X}, \mathbf{A}^{(t)}; \mathbf{w}), \mathbf{y})$ and $g(\mathbf{S}; \lambda)$ are continuous, and $L(f(\mathbf{X}, \mathbf{A}^{(t)}; \mathbf{w}), \mathbf{y})$ and $g(\mathbf{S}; \lambda)$ satisfy the Kurdyka-Łojasiewicz (KL) property [33], then for sufficiently large γ , any bounded sequence $(\mathbf{w}^{(t)}, \mathbf{S}^{(t)})$ generated by Algorithm 1 with random initialization will almost surely converge to a second-order stationary point of F .*

The detailed proof can be found in Appendix B.

4.3 Smooth structure transition by edge reweighting

Note that in the Algorithm 1, the optimization process requires iteratively updating the parameters \mathbf{w} of the GNN model f and training adjacency matrix $\mathbf{A}^{(t)}$, where $\mathbf{A}^{(t)}$ varies discretely between iterations. However, GNN models mostly work in a message-passing fashion, which computes node representations by recursively aggregating information along edges from neighboring nodes. Discretely modifying the number of edges will result in a great drift of the optimal model parameters between iterations. Therefore, it can increase the difficulty of finding optimal parameters and even hurt the generalization ability of the model in some cases. Besides the numerical problem caused by discretely increasing the number of edges, another issue raised by the CL strategy in Section 4.1 is the trustworthiness of the estimated edge difficulty, which is inferred by the residual error on the edges. Although the residual error can reflect how well edges are expected in the ideal case, the quality of the learned latent node embeddings may affect the validity of this metric and compromise the quality of the designed curriculum by the CL strategy.

To address both issues, we propose a novel edge reweighting scheme to (1) smooth the transition of the training structure between iterations, and (2) reduce the weight of edges that connect nodes with low-confidence latent embeddings. Formally, we use a smoothed version of structure $\bar{\mathbf{A}}^{(t)}$ to substitute $\mathbf{A}^{(t)}$ for training the GNN model f in step 3 of Algorithm 1, where the mapping from $\mathbf{A}^{(t)}$ to $\bar{\mathbf{A}}^{(t)}$ can be represented as:

$$\bar{\mathbf{A}}_{ij}^{(t)} = \pi_{ij}^{(t)} \mathbf{A}_{ij}^{(t)}, \quad (3)$$

where $\pi_{ij}^{(t)}$ is the weight imposed to edge e_{ij} at iteration t . $\pi_{ij}^{(t)}$ is calculated by considering the counted occurrences of edge e_{ij} until the iteration t and the confidence of the latent embedding for the connected pair of nodes v_i and v_j :

$$\pi_{ij}^{(t)} = \psi(e_{ij})\rho(v_i)\rho(v_j), \quad (4)$$

where ψ is a function that reflects the number of edge occurrences and ρ is a function to reflect the degree of confidence for the learned latent node embedding. The details of these two functions are described as follow.

Smooth the transition of the training structure between iterations. In order to obtain a smooth transition of the training structure between iterations, we take the learned curriculum of selected edges into consideration. Formally, we model ψ by a smooth function of the edge selected occurrences compared to the model iteration occurrences before the current iteration:

$$\psi(e_{ij}) = t(e_{ij})/t, \quad (5)$$

where t is the number of current iterations and $t(e_{ij})$ represents the counting number of selecting edge e_{ij} . Therefore, we transform the original discretely changing training structure into a smoothly changing one by taking the historical edge selection curriculum into consideration.

Reduce the influence of nodes with low confidence latent embeddings. As introduced in our Algorithm 1 line 6, the estimated structure $\hat{\mathbf{A}}$ is inferred from the latent embedding \mathbf{Z} , which is extracted from the trained GNN model f . Such estimated latent embedding may possibly shift from the true underlying embedding, which results in the inaccurately reconstructed structure around the node. In order to alleviate this issue, we model the function ρ by the training loss on nodes, which indicates the confidence of their learned latent embeddings. This idea is similar to previous CL strategies on inferring the difficulty of data samples by their supervised training loss. Specifically, a larger training loss indicates a low confident latent node embedding. Mathematically, the weights $\rho(v_i)$ on node v_i can be represented as a distribution of their training loss:

$$\rho(v_i) \sim e^{-l_i} \quad (6)$$

where l_i is the training loss on node v_i . Therefore, a node with a larger training loss will result in a smaller value of $\rho(v_i)$, which reduces the weight of its connecting edges.

5 Experiments

In this section, the experimental settings are introduced first in Section 5.1, then the performance of the proposed method on both synthetic and real-world datasets are presented in Section 5.2. We further present the robustness test on our CL method against topological structure adversarial attack in Section 5.3. Intuitive visualizations of the edge selection curriculum are shown in Section 5.4. In addition, we verify the effectiveness of framework components through ablation studies in Appendix A.2 and measure the parameter sensitivity in Appendix A.2 due to the space limit.

Homo ratio	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
GCN	50.84±1.03	56.50±0.50	65.17±0.48	77.94±0.54	87.15±0.44	93.27±0.24	97.48±0.25	99.10±0.17	99.93±0.03
GNNSVD	<u>54.96±0.76</u>	<u>58.45±0.56</u>	63.06±0.63	70.23±0.61	80.51±0.41	85.02±0.46	90.31±0.27	94.23±0.22	96.74±0.23
ProGNN	47.87±0.87	<u>54.59±0.55</u>	65.39±0.44	76.96±0.49	87.76±0.51	93.16±0.34	97.60±0.31	99.04±0.19	99.94±0.03
NeuralSparse	51.42±1.35	57.99±0.69	65.10±0.43	75.37±0.34	87.40±0.29	93.54±0.28	97.16±0.15	99.01±0.22	99.83±0.07
PTDNet	48.21±1.98	55.52±2.82	65.82±0.94	79.37±0.45	89.17±0.39	94.19±0.18	98.61±0.12	99.51±0.09	99.81±0.05
CLNodes	50.37±0.73	56.64±0.56	65.04±0.66	77.52±0.48	86.85±0.44	93.10±0.47	97.34±0.25	99.02±0.18	99.88±0.04
RCL	57.57±0.43	62.06±0.28	73.98±0.55	84.54±0.75	92.69±0.09	97.42±0.17	99.62±0.05	99.89±0.02	99.93±0.06
GIN	48.33±1.89	53.62±1.39	64.08±0.99	77.55±1.10	85.31±0.75	90.57±0.36	97.82±0.18	99.59±0.11	<u>99.91±0.02</u>
GNNSVD	43.21±1.60	45.68±1.66	54.90±1.16	68.29±0.79	79.76±0.52	85.63±0.44	93.65±0.39	97.22±0.17	98.94±0.17
ProGNN	45.76±1.40	52.96±1.01	64.12±1.07	76.95±0.87	85.13±0.71	89.96±0.55	96.54±0.48	99.51±0.12	99.78±0.05
NeuralSparse	50.23±2.05	54.12±1.52	62.81±0.75	76.98±1.17	85.14±0.94	92.57±0.44	98.02±0.20	99.61±0.12	99.91±0.05
PTDNet	<u>53.23±2.76</u>	<u>56.12±2.03</u>	<u>65.81±1.38</u>	<u>77.81±1.02</u>	86.14±0.65	93.21±0.74	97.08±0.41	99.51±0.18	99.91±0.03
CLNodes	45.36±1.42	<u>51.10±1.15</u>	62.53±0.88	<u>75.83±1.07</u>	87.76±0.90	94.25±0.44	98.30±0.26	99.60±0.09	99.92±0.03
RCL	57.63±0.66	62.08±1.17	71.02±0.61	80.61±0.69	88.62±0.43	94.88±0.36	98.19±0.19	99.32±0.08	99.89±0.04
GraphSage	62.57±0.55	67.33±0.64	71.06±0.74	80.88±0.54	85.88±0.51	91.42±0.37	95.26±0.33	97.78±0.16	99.52±0.13
GNNSVD	64.42±0.80	65.71±0.39	67.12±0.58	68.47±0.50	77.70±0.65	82.86±0.50	87.81±0.71	91.61±0.55	95.01±0.50
ProGNN	58.57±2.09	66.75±0.91	72.14±0.64	81.27±0.44	<u>86.89±0.47</u>	<u>92.10±0.39</u>	95.21±0.30	97.51±0.23	99.50±0.11
NeuralSparse	61.70±0.77	66.65±0.66	70.60±0.79	79.65±0.45	84.19±0.91	91.31±0.54	94.86±0.53	97.16±0.23	99.55±0.19
PTDNet	65.72±1.08	69.25±0.92	72.60±0.77	79.65±0.45	86.54±0.56	91.79±0.53	96.10±0.58	97.98±0.13	99.78±0.08
CLNodes	69.41±0.66	70.83±0.58	75.51±0.36	82.65±0.43	87.08±0.56	91.58±0.41	95.91±0.38	98.33±0.26	99.57±0.14
RCL	68.03±0.37	71.39±0.51	76.99±0.99	83.76±0.55	88.24±0.30	93.34±0.56	97.66±0.52	98.86±0.28	99.64±0.08

Table 1: Node classification accuracy on synthetic datasets (%). The best-performing method on each backbone GNN model is highlighted in bold, while the second-best method is underlined. In situations where RCL’s performance is not strictly the best among all methods, we can see that almost all methods can achieve a near-perfect performance and RCL is still close to the best methods.

5.1 Experimental settings

Synthetic datasets. To evaluate the effectiveness of our proposed method on datasets with ground-truth difficulty labels on edges, we follow previous studies [19, 1] to generate a set of synthetic datasets, where the formation probability of an edge is designed to reflect its likelihood to positively contribute to the node classification job, which indicates its ground-truth difficulty level. Specifically, the nodes in a generated graph are divided into 10 equally sized node classes 1, 2, ..., 10, and the node features are sampled from overlapping multi-Gaussian distributions. Each generated graph is associated with a *homophily coefficient (homo)* which indicates the probability of a node forming an edge to another node with the same label. For the rest edges that are formed between nodes with different labels, the probability of forming an edge is inversely proportional to the distances between their labels. Nodes with close classes are more likely to be connected since the formation probability decreases with the distance of the node label, and connections from nodes with close classes can increase the likelihood of accurately classifying a node due to the homophily property of the designed node classification task. Therefore, an edge with a high formation probability indicates a higher chance to positively contribute to the node classification task because it connects a node with a close class, and thus can be considered an easy edge. We vary the value of *homo* to generate nine graphs in total. More details and visualization about the synthetic dataset can be found in Appendix A.1.

Real-world datasets. To further evaluate the performance of our proposed method in real-world scenarios, nine benchmark real-world attributed network datasets, including four citation network datasets Cora, Citeseer, Pubmed [42] and ogbn-arxiv [14], two coauthor network datasets CS and Physics [29], two Amazon co-purchase network datasets Photo and Computers [29], and one protein interaction network ogbn-proteins [14]. We follow the data splits from [3] on citation networks and use a 5-fold cross-validation setting on coauthor and Amazon co-purchase networks. All datasets are publicly available from Pytorch-geometric library [9] and Open Graph Benchmark (OGB) [14], where basic statistics are reported in Table 2.

Comparison methods. We incorporate three commonly used GNN models, including GCN [20], GraphSAGE [12], and GIN [41], as the baseline model and also the backbone model for RCL. In addition to evaluating our proposed method against the baseline GNNs, we further leverage two categories of state-of-the-art comparison methods in the experiments: (1) We incorporate four graph structure learning methods GNNSVD [8], ProGNN [18], NeuralSparse [43], and PTDNet [26]; (2) We further compare with a curriculum learning method named CLNode [36] which gradually select nodes in the order of the difficulties defined by a heuristic-based strategy. More details about the comparison methods can be found in Appendix A.1.

Initializing graph structure by a pre-trained model. It is worth noting that the model needs an initial training graph structure $A^{(0)}$ in the initial stage of training. An intuitive way is that we can initialize the model to work in a purely data-driven scenario that starts only with isolated nodes where no edges exist. However, an instructive initial structure can greatly reduce the search cost and computational burden. Inspired by many previous CL works [37, 11, 17, 44] that incorporate prior knowledge of a pre-trained model into designing curriculum for the current model, we initialize the

	Cora	Citeseer	Pubmed	CS	Physics	Photo	Computers	ogbn-arxiv	ogbn-proteins
# nodes	2,708	3,327	19,717	18,333	34,493	7,650	13,752	169,343	132,534
# edges	10,556	9,104	88,648	163,788	495,924	238,162	491,722	1,166,243	39,561,252
# features	1,433	3,703	500	6,805	8,415	745	767	100	8
GCN	85.74±0.42	78.93±0.32	87.91±0.09	93.03±0.32	96.55±0.15	93.25±0.70	88.09±0.40	71.74±0.29	72.51±0.35
GNNSVD	83.24±1.03	74.80±0.87	88.81±0.38	93.79±0.11	96.11±0.13	89.63±0.73	86.49±0.77	67.44±0.51	66.92±0.64
ProGNN	85.66±0.61	74.78±0.55	87.22±0.33	94.04±0.19	96.75±0.26	92.07±0.67	88.72±0.59	-	-
NeuralSparse	85.95±0.98	76.24±0.48	86.83±0.40	92.31±0.47	95.56±0.30	90.57±0.90	88.62±0.83	-	-
PTDNet	83.84±0.95	77.54±0.42	87.89±0.08	93.60±0.43	96.56±0.09	88.92±0.87	87.52±0.70	-	-
CLNode	85.67±0.33	78.99±0.57	89.50±0.28	93.83±0.24	95.76±0.16	93.39±0.83	89.28±0.38	70.95±0.18	71.40±0.32
RCL	87.15±0.44	79.79±0.55	89.79±0.12	94.66±0.32	97.02±0.23	94.41±0.76	90.23±0.23	74.08±0.33	75.19±0.26
GIN	84.43±0.65	74.87±0.20	85.72±0.40	91.48±0.36	95.62±0.30	93.02±0.91	86.94±1.58	69.26±0.34	74.51±0.32
GNNSVD	82.23±0.65	72.11±0.70	88.31±0.15	91.40±0.87	95.30±0.29	89.49±1.11	82.66±2.26	67.79±0.41	70.65±0.53
ProGNN	85.02±0.41	78.12±0.93	87.82±0.51	-	-	92.23±0.67	83.54±1.48	-	-
NeuralSparse	84.92±0.58	75.44±0.87	86.11±0.49	89.66±0.82	95.05±0.57	93.28±0.83	87.22±0.54	-	-
PTDNet	83.02±1.01	75.00±0.74	88.04±0.29	91.01±0.21	95.57±0.40	90.70±0.76	87.08±0.65	-	-
CLNode	83.52±0.77	75.82±0.58	86.92±0.61	91.71±0.41	95.75±0.46	92.78±0.90	85.93±1.53	70.58±0.17	73.97±0.31
RCL	86.64±0.39	77.60±0.18	89.17±0.29	93.92±0.27	96.75±0.17	93.88±0.51	89.76±0.19	72.55±0.15	78.76±0.22
GraphSage	86.22±0.27	77.27±0.23	88.50±0.16	94.22±0.18	96.26±0.34	93.82±0.51	88.62±0.21	71.49±0.27	77.68±0.20
GNNSVD	83.11±0.82	73.19±0.49	88.42±0.38	93.86±0.36	95.96±0.12	89.31±0.53	81.46±1.15	69.82±0.34	71.82±0.39
ProGNN	86.23±0.42	74.45±0.83	88.52±0.45	-	-	90.89±0.69	89.34±0.54	-	-
NeuralSparse	84.60±0.52	76.32±0.55	89.02±0.39	93.89±0.58	96.67±0.20	90.78±1.06	88.37±0.37	-	-
PTDNet	86.03±0.60	76.07±0.58	86.78±0.45	93.78±0.43	95.32±0.31	92.96±0.87	84.89±1.47	-	-
CLNode	86.60±0.64	77.23±0.54	88.76±0.57	94.13±0.34	96.87±0.45	93.90±0.42	89.57±0.62	71.54±0.20	78.40±0.41
RCL	86.90±0.39	78.95±0.18	90.14±0.43	95.05±0.23	96.88±0.19	95.06±0.52	90.47±0.38	73.13±0.14	79.89±0.35

Table 2: Node classification results on real-world datasets (%). The best-performing method on each backbone is highlighted in bold and second-best is underlined. (-) denotes an out-of-memory issue.

training structure $\mathbf{A}^{(0)}$ by a pre-trained vanilla GNN model f^* . Specifically, we follow the same steps from line 4 to line 7 in the algorithm 1 to obtain the initial training structure $\mathbf{A}^{(0)}$ but the latent node embedding is extracted from the pre-trained model f^* .

Implementation Details We use the baseline model (GCN, GIN, GraphSage) as the backbone model for both our RCL method and all comparison methods. For a fair comparison, we require all models follow the same GNN architecture with two convolution layers. For each split, we run each model 10 times to reduce the variance in particular data splits. Test results are according to the best validation results. General training hyperparameters (such as learning rate or the number of training epochs) are equal for all models.

5.2 Effectiveness results

Table 1 presents the node classification results of the synthetic datasets. We report the average accuracy and standard deviation for each model against the *homo* of generated graphs. From the table, we observe that our proposed method RCL consistently achieves the best or most competitive performance to all the comparison methods over three backbone GNN architectures. Specifically, RCL outperforms the second best method on average by 4.17%, 2.60%, and 1.06% on GCN, GIN, and GraphSage backbones, respectively. More importantly, the proposed RCL method performs significantly better than the second best model when the *homo* of generated graphs is low (≤ 0.5), on average by 6.55% on GCN, 4.17% on GIN, and 2.93% on GraphSage backbones. These demonstrate that our proposed RCL method significantly improves the model’s capability of learning an effective representation to downstream tasks especially when the edge difficulties vary largely in the data.

We report the experimental results of the real-world datasets in Table 2. The results demonstrate the strength of our proposed method by consistently achieving the best results in all 9 datasets by GCN backbone architecture, all 9 datasets by GraphSage backbone architecture, and 8 out of 9 datasets by GIN backbone architecture. Specifically, our proposed method improved the performance of baseline models on average by 1.86%, 2.83%, and 1.62% over GCN, GIN, and GraphSage, and outperformed the second best models model on average by 1.37%, 2.49%, and 1.22% over the three backbone models, respectively. The results demonstrate that the proposed RCL method consistently improves the performance of GNN models in real-world scenarios.

Our experimental results are statically sound. In 43 out of 48 tasks our method outperforms the second-best performing model with strong statistical significance. Specifically, we have in 30 out of 43 cases with a significance $p < 0.001$, in 8 out of 43 cases with a significance $p < 0.01$, and in 5 out of 43 cases with a significance $p < 0.05$. Such statistical significance results can demonstrate that our proposed method can consistently perform better than the baseline models in both scenarios.

5.3 Robustness analysis against adversarial topological structure attack

To further examine the robustness of the RCL method on extracting powerful representation from correlated data samples, we follow previous works [18, 26] to randomly inject fake edges into real-world graphs. This adversarial attack can be viewed as adding random noise to the topological structure of graphs. Specifically, we randomly connect M pairs of previously unlinked nodes in the

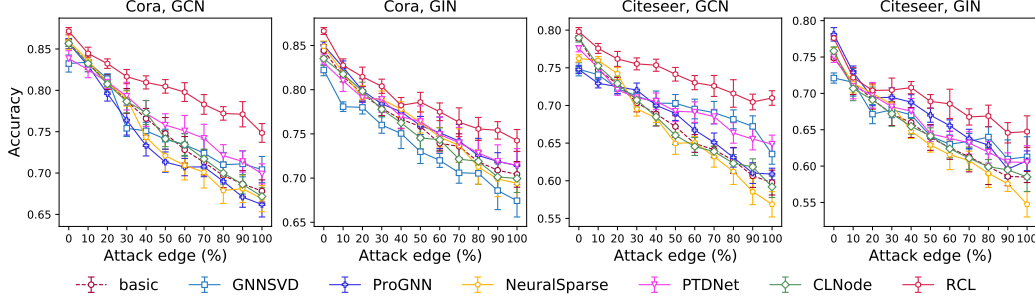


Figure 2: Node classification accuracy (%) on Cora and Citeseer under random structure attack. The attack edge ratio is computed versus the original number of edges, where 100% means that the number of inserted edges is equal to the number of original edges.

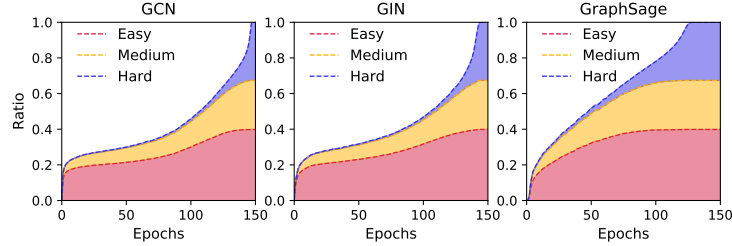


Figure 3: Visualization of edge selection process during training.

341 real-world datasets, where the value of M varies from 10% to 100% of the original edges. We then
342 train RCL and all the comparison methods on the attacked graph and evaluate the node classification
343 performance. The results are shown in Figure 2, we can observe that RCL shows strong robustness to
344 adversarial structural attacks by consistently outperforming all compared methods on all datasets.
345 Especially, when the proportion of added noisy edges is large ($> 50\%$), the improvement becomes
346 more significant. For instance, under the extremely noisy ratio at 100%, RCL outperforms the second
347 best model by 4.43% and 2.83% on Cora dataset, and by 6.13%, 3.47% on Citeseer dataset, with
348 GCN and GIN backbone models, respectively.

349 5.4 Visualization of learned edge selection curriculum

350 Besides the effectiveness and robustness of the RCL method on downstream classification results,
351 it is also interesting to verify whether the learned edge selection curriculum satisfies the rule from
352 easy to hard. Since real-world datasets do not have ground-truth labels of difficulty on edges, we
353 conduct visualization experiments on synthetic datasets, where the difficulty of each edge can be
354 indicated by its formation probability. Specifically, we classify edges into three balanced categories
355 according to their difficulty: easy, medium, and hard. Here, we define all homogenous edges that
356 connect nodes with the same class as easy, edges connecting nodes with adjacent classes as medium,
357 and the remaining edges connecting nodes with far away classes as hard. We report the proportion of
358 edges selected for each category during training in Figure 3. We can observe that RCL can effectively
359 select most of the easy edges at the early stage of training, then more easy edges and most medium
360 edges are gradually included during training, and most hard edges are left unselected until the end
361 stage of training. Such edge selection behavior is highly consistent with the core idea of designing
362 a curriculum for edge selection, which verifies that our proposed method can effectively design
363 curriculums to select edges according to their difficulty from easy to hard.

364 6 Conclusion

365 This paper focuses on developing a novel CL method to improve the generalization ability and
366 robustness of GNN models on learning representations of data samples with dependencies. The
367 proposed method **Relational Curriculum Learning (RCL)** effectively addresses the unique challenges
368 in designing CL strategy for handling dependencies. First, a self-supervised learning module is
369 developed to select appropriate edges that are expected by the model. Then an optimization model is
370 presented to iteratively increment the edges according to the model training status and a theoretical
371 guarantee of the convergence on the optimization algorithm is given. Finally, an edge reweighting
372 scheme is proposed to steady the numerical process by smoothing the training structure transition.
373 Extensive experiments on synthetic and real-world datasets demonstrate the strength of RCL in
374 improving the generalization ability and robustness.

References

- [1] Sami Abu-El-Haija, Bryan Perozzi, Amol Kapoor, Nazanin Alipourfard, Kristina Lerman, Hrayr Harutyunyan, Greg Ver Steeg, and Aram Galstyan. Mixhop: Higher-order graph convolutional architectures via sparsified neighborhood mixing. In *international conference on machine learning*, pages 21–29. PMLR, 2019.
- [2] Yoshua Bengio, Jérôme Louradour, Ronan Collobert, and Jason Weston. Curriculum learning. In *Proceedings of the 26th annual international conference on machine learning*, pages 41–48, 2009.
- [3] Jie Chen, Tengfei Ma, and Cao Xiao. Fastgcn: Fast learning with graph convolutional networks via importance sampling. In *International Conference on Learning Representations*, 2018.
- [4] Yu Chen, Lingfei Wu, and Mohammed Zaki. Iterative deep graph learning for graph neural networks: Better and robust node embeddings. *Advances in neural information processing systems*, 33:19314–19326, 2020.
- [5] Guanyi Chu, Xiao Wang, Chuan Shi, and Xunqiang Jiang. Cuco: Graph representation with curriculum contrastive learning. In *IJCAI*, pages 2300–2306, 2021.
- [6] Hanjun Dai, Hui Li, Tian Tian, Xin Huang, Lin Wang, Jun Zhu, and Le Song. Adversarial attack on graph structured data. In *International conference on machine learning*, pages 1115–1124. PMLR, 2018.
- [7] Jeffrey L Elman. Learning and development in neural networks: The importance of starting small. *Cognition*, 48(1):71–99, 1993.
- [8] Negin Entezari, Saba A Al-Sayouri, Amirali Darvishzadeh, and Evangelos E Papalexakis. All you need is low (rank) defending against adversarial attacks on graphs. In *Proceedings of the 13th International Conference on Web Search and Data Mining*, pages 169–177, 2020.
- [9] Matthias Fey and Jan Eric Lenssen. Fast graph representation learning with pytorch geometric. *arXiv preprint arXiv:1903.02428*, 2019.
- [10] Tieliang Gong, Qian Zhao, Deyu Meng, and Zongben Xu. Why curriculum learning & self-paced learning work in big/noisy data: A theoretical perspective. *Big Data & Information Analytics*, 1(1):111, 2016.
- [11] Guy Hacoheh and Daphna Weinshall. On the power of curriculum learning in training deep networks. In *International Conference on Machine Learning*, pages 2535–2544. PMLR, 2019.
- [12] Will Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs. *Advances in neural information processing systems*, 30, 2017.
- [13] Bo Han, Quanming Yao, Xingrui Yu, Gang Niu, Miao Xu, Weihua Hu, Ivor Tsang, and Masashi Sugiyama. Co-teaching: Robust training of deep neural networks with extremely noisy labels. *Advances in neural information processing systems*, 31, 2018.
- [14] Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. Open graph benchmark: Datasets for machine learning on graphs. *arXiv preprint arXiv:2005.00687*, 2020.
- [15] Lu Jiang, Deyu Meng, Shou-I Yu, Zhenzhong Lan, Shiguang Shan, and Alexander Hauptmann. Self-paced learning with diversity. *Advances in neural information processing systems*, 27, 2014.
- [16] Lu Jiang, Deyu Meng, Qian Zhao, Shiguang Shan, and Alexander G Hauptmann. Self-paced curriculum learning. In *Twenty-ninth AAAI conference on artificial intelligence*, 2015.
- [17] Lu Jiang, Zhengyuan Zhou, Thomas Leung, Li-Jia Li, and Li Fei-Fei. Mentornet: Learning data-driven curriculum for very deep neural networks on corrupted labels. In *International conference on machine learning*, pages 2304–2313. PMLR, 2018.

- [18] Wei Jin, Yao Ma, Xiaorui Liu, Xianfeng Tang, Suhang Wang, and Jiliang Tang. Graph structure learning for robust graph neural networks. In *Proceedings of the 26th ACM SIGKDD international conference on knowledge discovery & data mining*, pages 66–74, 2020.
- [19] Fariba Karimi, Mathieu Génois, Claudia Wagner, Philipp Singer, and Markus Strohmaier. Homophily influences ranking of minorities in social networks. *Scientific reports*, 8(1):1–12, 2018.
- [20] Thomas N. Kipf and Max Welling. Semi-Supervised Classification with Graph Convolutional Networks. In *Proceedings of the 5th International Conference on Learning Representations*, 2017.
- [21] Yajing Kong, Liu Liu, Jun Wang, and Dacheng Tao. Adaptive curriculum learning. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 5067–5076, 2021.
- [22] M Kumar, Benjamin Packer, and Daphne Koller. Self-paced learning for latent variable models. *Advances in neural information processing systems*, 23, 2010.
- [23] Haoyang Li, Xin Wang, and Wenwu Zhu. Curriculum graph machine learning: A survey. *arXiv preprint arXiv:2302.02926*, 2023.
- [24] Qiuwei Li, Zhihui Zhu, and Gongguo Tang. Alternating minimizations converge to second-order optimal solutions. In *International Conference on Machine Learning*, pages 3935–3943. PMLR, 2019.
- [25] Xiaohe Li, Lijie Wen, Yawen Deng, Fuli Feng, Xuming Hu, Lei Wang, and Zide Fan. Graph neural network with curriculum learning for imbalanced node classification. *arXiv preprint arXiv:2202.02529*, 2022.
- [26] Dongsheng Luo, Wei Cheng, Wenchao Yu, Bo Zong, Jingchao Ni, Haifeng Chen, and Xiang Zhang. Learning to drop: Robust graph neural network via topological denoising. In *Proceedings of the 14th ACM international conference on web search and data mining*, pages 779–787, 2021.
- [27] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, et al. Pytorch: An imperative style, high-performance deep learning library. *Advances in neural information processing systems*, 32, 2019.
- [28] Douglas LT Rohde and David C Plaut. Language acquisition in the absence of explicit negative evidence: How important is starting small? *Cognition*, 72(1):67–109, 1999.
- [29] Oleksandr Shchur, Maximilian Mumme, Aleksandar Bojchevski, and Stephan Günnemann. Pitfalls of graph neural network evaluation. *arXiv preprint arXiv:1811.05868*, 2018.
- [30] Abhinav Shrivastava, Abhinav Gupta, and Ross Girshick. Training region-based object detectors with online hard example mining. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 761–769, 2016.
- [31] Charles Sutton, Andrew McCallum, et al. An introduction to conditional random fields. *Foundations and Trends® in Machine Learning*, 4(4):267–373, 2012.
- [32] S Vichy N Vishwanathan, Nicol N Schraudolph, Risi Kondor, and Karsten M Borgwardt. Graph kernels. *Journal of Machine Learning Research*, 11:1201–1242, 2010.
- [33] Junxiang Wang, Hongyi Li, and Liang Zhao. Accelerated gradient-free neural network training by multi-convex alternating optimization. *Neurocomputing*, 487:130–143, 2022.
- [34] Xin Wang, Yudong Chen, and Wenwu Zhu. A survey on curriculum learning. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 44(9):4555–4576, 2021.
- [35] Yiwei Wang, Wei Wang, Yuxuan Liang, Yujun Cai, and Bryan Hooi. Curgraph: Curriculum learning for graph classification. In *Proceedings of the Web Conference 2021*, pages 1238–1248, 2021.

- 469 [36] Xiaowen Wei, Weiwei Liu, Yibing Zhan, Du Bo, and Wenbin Hu. Clnode: Curriculum learning
470 for node classification. *arXiv preprint arXiv:2206.07258*, 2022.
- 471 [37] Daphna Weinshall, Gad Cohen, and Dan Amir. Curriculum learning by transfer learning: Theory
472 and experiments with deep networks. In *International Conference on Machine Learning*, pages
473 5238–5246. PMLR, 2018.
- 474 [38] Richard Lee Wheeden and Antoni Zygmund. *Measure and integral*, volume 26. Dekker New
475 York, 1977.
- 476 [39] Huijun Wu, Chen Wang, Yuriy Tyshetskiy, Andrew Docherty, Kai Lu, and Liming Zhu. Ad-
477 versarial examples for graph data: deep insights into attack and defense. In *Proceedings of the*
478 *28th International Joint Conference on Artificial Intelligence*, pages 4816–4823, 2019.
- 479 [40] Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and S Yu Philip. A
480 comprehensive survey on graph neural networks. *IEEE transactions on neural networks and*
481 *learning systems*, 32(1):4–24, 2020.
- 482 [41] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural
483 networks? In *International Conference on Learning Representations*, 2018.
- 484 [42] Zhilin Yang, William Cohen, and Ruslan Salakhudinov. Revisiting semi-supervised learning
485 with graph embeddings. In *International conference on machine learning*, pages 40–48. PMLR,
486 2016.
- 487 [43] Cheng Zheng, Bo Zong, Wei Cheng, Dongjin Song, Jingchao Ni, Wenchao Yu, Haifeng Chen,
488 and Wei Wang. Robust graph representation learning via neural sparsification. In *International*
489 *Conference on Machine Learning*, pages 11458–11468. PMLR, 2020.
- 490 [44] Tianyi Zhou, Shengjie Wang, and Jeff Bilmes. Robust curriculum learning: from clean label de-
491 tection to noisy label self-correction. In *International Conference on Learning Representations*,
492 2020.
- 493 [45] Daniel Zügner, Amir Akbarnejad, and Stephan Günnemann. Adversarial attacks on neural
494 networks for graph data. In *Proceedings of the 24th ACM SIGKDD international conference on*
495 *knowledge discovery & data mining*, pages 2847–2856, 2018.

A Additional experimental settings and results

A.1 Additional experimental settings

Synthetic datasets To evaluate the effectiveness of our proposed method on datasets with ground-truth difficulty labels on structure, we first follow previous studies [19, 1] to generate a set of synthetic datasets, where the difficulty of edges in generated graphs are indicated by their formation probability. Specifically, as shown in Figure 4, each generated graph is with 5,000 nodes, which are divided into 10 equally sized node classes 1, 2, \dots , 10. The node features are sampled from overlapping multi-Gaussian distributions. Each generated graph is associated with a *homophily coefficient* (*homo*) which indicates the likelihood of a node forming a connection to another node with the same label (same color in Figure 4). For example, a generated graph with *homo* = 0.5 will have on average half of the edges formed between nodes with the same label. For the rest edges that are formed between nodes with different labels (different colors in Figure 4), the probability of forming an edge is inversely proportional to the distances between their labels. Mathematically, the probability of forming an edge between node u and node v follows $p_{u \rightarrow v} \propto e^{-|c_u - c_v|}$, where the distances between labels $|c_u - c_v|$ means shortest distance of two classes on a circle. Therefore, the probability of forming an edge in the synthetic graph can reflect how well this edge is expected. Specifically, edges with a higher formation probability, e.g. connecting nodes with the same label or close labels, meaning that there is a higher chance that this connection will positively contribute to the prediction (less chance to be a noisy edge). Conversely, edges with a lower formation probability, e.g., connecting nodes with faraway labels, mean that there is a higher chance that this connection will negatively contribute to the prediction (higher chance to be a noisy edge). We vary the value of *homo* from 0.1, 0.2, \dots , 0.9 to generate nine graphs in total. Similar to previous works [19, 1], we randomly partition each synthetic graph into equal-sized train, validation, and test node splits.

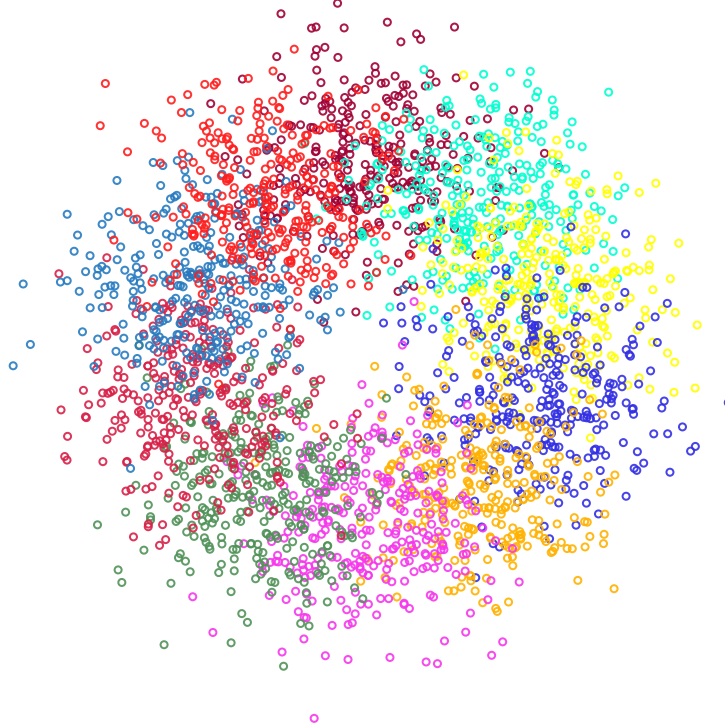


Figure 4: Visualization of synthetic datasets. Each color represents a class of nodes. Node attributes are sampled from overlapping multi-Gaussian distributions, where the attributes of nodes with close labels are likely to have short distances. Homogeneous edges represent edges that connect nodes of the same class (with the same color). The probability of connecting two nodes of different classes decreases with the distance between the center points of their class distribution. Therefore, the formation probability of a node denotes the edge difficulty, since edges between nodes with close classes are more likely to positively contribute to the prediction under the homogeneous assumption.

519 **Initializing graph structure by a pre-trained model.** It is worth noting that the model needs
 520 an initial training graph structure $\mathbf{A}^{(0)}$ in the initial stage of training. An intuitive way is that we
 521 can initialize the model to work in a purely data-driven scenario that starts only with isolated nodes
 522 where no edges exist. However, an instructive initial structure can greatly reduce the search cost and
 523 computational burden. Inspired by many previous CL works [37, 11, 17, 44] that incorporate prior
 524 knowledge of a pre-trained model into designing curriculum for the current model, we initialize the
 525 training structure $\mathbf{A}^{(0)}$ by a pre-trained vanilla GNN model f^* . Specifically, we follow the same
 526 steps from line 4 to line 7 in the algorithm 1 to obtain the initial training structure $\mathbf{A}^{(0)}$ but the latent
 527 node embedding is extracted from the pre-trained model f^* .

528 **Implementation Details** We use the baseline model (GCN, GIN, GraphSage) as the backbone
 529 model for both our RCL method and all comparison methods. For a fair comparison, we require all
 530 models follow the same GNN architecture with two convolution layers. For each split, we run each
 531 model 10 times to reduce the variance in particular data splits. Test results are according to the best
 532 validation results. General training hyperparameters (such as learning rate or the number of training
 533 epochs) are equal for all models. For the pre-trained model to initialize the training structure, we
 534 utilize the same model as the backbone model utilized by our method. For example, if we use GCN
 535 as the backbone model for RCL, the pre-trained model to initialize is also GCN. All experiments are
 536 conducted on a 64-bit machine with four NVIDIA Quadro RTX 8000 GPUs. The proposed method is
 537 implemented with Pytorch deep learning framework [27].

538 The following describes the details of our comparison models.

539 **Graph Neural Networks (GNNs).** We first introduce three baseline GNN models as follows.

540 (i) **GCN.** Graph Convolutional Networks (GCN) [20] is a commonly used GNN, which introduces a
 541 first-order approximation architecture of the Chebyshev spectral convolution operator;

542 (ii) **GIN.** Graph Isomorphism Networks (GIN) [41] is a variant of GNN, which has provably powerful
 543 discriminating power among the class of 1-order GNNs;

544 (iii) **GraphSage.** GraphSage [12] is a GNN method that computes the hidden representation of the
 545 root node by aggregating the hidden node representations hierarchically from bottom to top.

546 **Graph structure learning.** We then introduce four state-of-the-art methods for jointly learning the
 547 optimal graph structure and downstream tasks.

548 (i) **GNNSVD.** GNNSVD [8] first apply singular value decomposition (SVD) on the graph adjacency
 549 matrix to obtain a low-rank graph structure and apply GNN on the obtained low-rank structure;

550 (ii) **ProGNN.** ProGNN [18] is a method to defend against graph adversarial attacks by obtaining a
 551 sparse and low-rank graph structure from the input structure;

552 (iii) **NeuralSparse.** NeuralSparse [43] is a method to learn robust graph representations by iteratively
 553 sampling k -neighbor subgraphs for each node and sparsifying the graph according to the performance
 554 on the node classification;

555 (iv) **PTDNet.** PTDNet [26] learns a sparsified graph by pruning task-irrelevant edges, where sparsity
 556 is controlled by regulating the number of edges.

557 **Curriculum learning on graph data.** We introduce a recent curriculum learning work on node
 558 classification as follows.

559 (i) **CLNode.** CLNode [36] regards nodes as data samples and gradually incorporates more nodes into
 560 training according to their difficulty. They apply a heuristic-based strategy to measure the difficulty of
 561 nodes, where the nodes that connect neighboring nodes with different classes are considered difficult.

562 **Searching space for hyperparameters.**

563 Number of epochs trained: $\{150, 500\}$;

564 Learning rate for model: $\{1e-2, 5e-3, 1e-3\}$;

565 Number of GNN layers: $\{2\}$;

566 Dimension of hidden state: $\{64\}$;

567 Age parameter $\lambda : \{1, 2, 3, 4, 5\}$ (A larger value indicates faster pacing for adding edges, where 1
 568 denotes the training structure will converge to the input structure at the final iteration).

	Synthetic	Citeseer	Computers	ogbn-arxiv	ogbn-proteins
Vanilla	7.32s	3.90s	16.88s	55.22s	1438.23s
GNNsVD	11.49s	3.82s	35.96s	135.72s	2632.42s
CLNode	6.29s	3.96s	17.02s	58.53s	1545.53s
ProGNN	220.25s	72.42s	1953.23s	(-)	(-)
NeuralSparse	310.02s	88.91s	6553.34s	(-)	(-)
PTDNet	153.43s	48.42s	2942.02s	(-)	(-)
Ours	4.07s	2.42s	14.62s	71.49s	2239.05s

Table 3: Running time of our method and comparison methods. Here (-) denotes an out-of-memory error and Vanilla denotes the standard GNN model.

	Synthetic1	Synthetic2	Citeseer	CS	Computers
Full	73.98±0.55	97.42±0.17	79.79±0.55	94.66±0.22	90.23±0.23
Curriculum-linear	70.93±0.54	95.19±0.19	79.04±0.38	94.14±0.26	89.28±0.21
Curriculum-root	70.13±0.72	95.50±0.18	78.27±0.54	94.47±0.34	89.27±0.15
Random-linear	58.76±0.46	89.78±0.11	77.43±0.49	92.76±0.14	88.76±0.18
Random-root	61.04±0.20	91.04±0.09	76.81±0.35	92.92±0.15	88.81±0.28
w/o edge appearance	70.70±0.43	95.77±0.16	77.77±0.65	94.39±0.21	89.56±0.30
w/o node confidence	72.38±0.41	96.86±0.17	78.72±0.72	94.34±0.13	90.03±0.62
w/o pre-trained model	72.56±0.69	93.89±0.14	78.28±0.77	94.50±0.14	89.80±0.55

Table 4: Ablation study. Here “Full” represents the original method without removing any component. The best-performing method on each dataset is highlighted in bold.

A.2 Additional experiments

Time complexity analysis Here we consider GCN as the backbone. First, the time complexity of an L -layer GCN is $O(L|\mathcal{E}|b + L|\mathcal{V}|b^2)$, where b is the number of node attributes. Second, the time complexity of measuring the difficulty levels of edges by reconstruction is $O(|\mathcal{E}|d)$ where d is the number of latent embedding dimensions. Third, the time complexity of selecting the edges to add is $O(|\mathcal{E}|)$. Therefore, the total time complexity of our algorithm is $O(|\mathcal{E}|(Lb + d) + L|\mathcal{V}|b^2)$.

In addition, we compare the total running time of our method and all comparison methods in the Table 3. We can observe that the running time of our proposed method is comparable to that of standard GNN models in all datasets. Notably, our method is even faster than standard GNN models in some datasets. One possible reason is that at the beginning of training, the graphs in our model have much fewer edges than those in standard GNN models. Therefore, the computational cost of the GNN model is also reduced.

Ablation study To investigate the effectiveness of our proposed model with some simpler heuristics, we deploy a series of synthetic analysis. We first train the model with node classification task purely and select the top K expected edges as suggested by the reviewer. Specifically, we follow previous works [34, 36] using two classical selection pacing functions as follows:

$$\begin{aligned} \text{Linear: } K_{\text{linear}}(t) &= \frac{t}{T}|\mathcal{E}|; \\ \text{Root: } K_{\text{root}}(t) &= \sqrt{\frac{t}{T}}|\mathcal{E}|, \end{aligned}$$

where t is the number of current iterations and T is the number of total iterations, and $|\mathcal{E}|$ is the number of total edges. We name these two variants Curriculum-linear and Curriculum-root, respectively. In addition, we also remove the edge difficulty measurement module and use random selection instead. Specifically, we gradually incorporate more edges into training in random order to verify the effectiveness of the learned curriculum. We name two variants as Random-linear and Random-root with the above two mentioned pacing functions, respectively.

In order to further investigate the impact of the proposed components of RCL. We also first consider variants of removing the edge smoothing components mentioned in Section 4.3. Specifically, we consider two variants *w/o EC* and *w/o NC*, which remove the smoothing function of the edge occurrence ratio and the component to reflect the degree of confidence for the latent node embedding in RCL, respectively. In addition to examining the effectiveness of edge smoothing components, we further consider a variant *w/o pre-trained model* that avoids using a pre-trained model to initialize

model, which is mentioned in Appendix A.1, to initialize the training structure by a pre-trained model and instead starts with inferred structure from isolated nodes with no connections.

We present the results of two synthetic datasets (*homophily coefficient*= 0.3, 0.6) and three real-world datasets in Table 4. We summarize our findings from the above table as below: (i) Our full model consistently outperforms the two variants Curriculum-linear and Curriculum-root by an average of 1.59% on all datasets, suggesting that our pacing module can benefit model training. It is worth noting that these two variants also outperform the baseline vanilla GNN model Vanilla by an average of 1.92%, which supports the assumption that even a simple curriculum learning strategy can still improve model performance. (ii) We observe that the performance of the two variants Random-linear and Random-root on all datasets drops by 3.86% on average compared to the variants Curriculum-linear and Curriculum-root. Such behavior demonstrates the effectiveness of our proposed edge difficulty quantification module by showing that randomly involving edges into training cannot benefit model performance. (iii) We can observe a significant performance drop consistently for all variants that remove the structural smoothing techniques and initialization components. The results validate that all structural smoothing and initialization components can benefit the performance of RCL on the downstream tasks.

Parameter sensitivity analysis Recall that RCL learns a curriculum to gradually add edges in a given input graph structure to the training process until all edges are included. An interesting question is how the speed of adding edges will affect the performance of the model. Here we conduct experiments to explore the impact of age parameter λ which controls the speed of adding edges to the model performance. Here a larger value of λ means that the training structure will converge to the input structure earlier. For example, $\lambda = 1$ means that the training structure will probably not converge to the input structure until the last iteration, and $\lambda = 5$ means that the training structure will converge to the input structure around half of the iterations are complete, and then the model will be trained with the full input structure for the remaining iterations. We present the results on two synthetic datasets (*homophily coefficient*= 0.3, 0.6) and two real-world datasets in Figure 5. As can be seen from the figure, the classification results are steady that the average standard deviation is only 0.41%. It is also worth noting that the peak values for all datasets consistently appear around $\lambda = 3$, which indicates that the best performance is when the training structure converges to the full input structure around two-thirds of the iterations are completed.

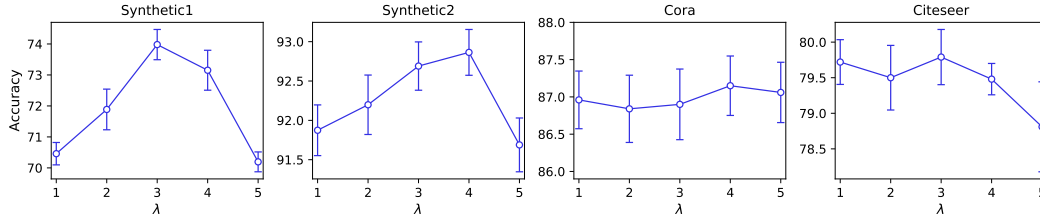


Figure 5: Parameter sensitivity analysis on four datasets. Here a larger value of λ means the training structure will converge to the original structure at an earlier training stage.

627

628 B Mathematical proof

629 **Theorem 1.** We have the following convergence guarantees for Algorithm 1:

- 630 • **Avoidance of Saddle Points** If the second derivatives of $L(f(\mathbf{X}, \mathbf{A}^{(t)}; \mathbf{w}), \mathbf{y})$ and $g(\mathbf{S}; \lambda)$ are continuous, then for sufficiently large γ , any bounded sequence $(\mathbf{w}^{(t)}, \mathbf{S}^{(t)})$ generated by Algorithm 1 with random initializations will not converge to a strict saddle point of F almost surely.
- 633 • **Second Order Convergence** If the second derivatives of $L(f(\mathbf{X}, \mathbf{A}^{(t)}; \mathbf{w}), \mathbf{y})$ and $g(\mathbf{S}; \lambda)$ are continuous, and $L(f(\mathbf{X}, \mathbf{A}^{(t)}; \mathbf{w}), \mathbf{y})$ and $g(\mathbf{S}; \lambda)$ satisfy the Kurdyka-Łojasiewicz (KL) property [33], then for sufficiently large γ , any bounded sequence $(\mathbf{w}^{(t)}, \mathbf{S}^{(t)})$ generated by Algorithm 1 with random initialization will almost surely converges to a second-order stationary point of F .

637 *Proof.* We prove this theorem by Theorem 10 and Corollary 3 from [24].

638 **[Avoidance of Saddle Points]** Because the sequence $(\mathbf{w}^{(t)}, \mathbf{S}^{(t)})$ is bounded, and the second derivatives of L and g are continuous, then they are bounded. In other words, we have

639

640 $\max\{\|\nabla_{\mathbf{w}}^2 L(f(\mathbf{X}, \mathbf{A}^{(t)}; \mathbf{w}^{(t)}), \mathbf{y})\|, \|\nabla_{\mathbf{S}}^2 g(S^{(t)}; \lambda)\|\} \leq p$, where $p > 0$ is a constant. Simi-
 641 larly, it is easy to check that the second derivative of the term $\sum_{i,j} \mathbf{S}_{ij} \|\tilde{\mathbf{A}}_{ij}^{(t)} - \mathbf{A}_{ij}\|_2^2$ is bounded,
 642 i.e., $\max\{\|\nabla_{\mathbf{w}}^2 \sum_{i,j} \mathbf{S}_{ij} \|\tilde{\mathbf{A}}_{ij}^{(t)} - \mathbf{A}_{ij}\|_2^2\|, \|\nabla_{\mathbf{S}}^2 \sum_{i,j} \mathbf{S}_{ij} \|\tilde{\mathbf{A}}_{ij}^{(t)} - \mathbf{A}_{ij}\|_2^2\| \} \leq q$, where $q > 0$ is
 643 constant and $\tilde{\mathbf{A}}$ is a function of \mathbf{w} . Therefore, it means that the objective F is bi-smooth, i.e.
 644 $\max\{\|\nabla_{\mathbf{w}}^2 F\|, \|\nabla_{\mathbf{S}}^2 F\|\} \leq p + q$. In other words, F satisfies Assumption 4 from [24]. Moreover,
 645 the second derivative of F is continuous. For any $\gamma > p + q$, any bounded sequence $(\mathbf{w}^{(t)}, \mathbf{S}^{(t)})$
 646 generated by Algorithm 1 will not converge to a strict saddle of F almost surely by Theorem 10 from
 647 [24].
 648 **[Second Order Convergence]** From the above proof of avoidance of saddle points, we know that F
 649 satisfies Assumption 4 from [24]. Moreover, because L and g satisfy the KL property, and the term
 650 $\sum_{i,j} \mathbf{S}_{ij} \|\tilde{\mathbf{A}}_{ij}^{(t)} - \mathbf{A}_{ij}\|_2^2$ satisfies the KL property, we conclude that F satisfy the KL property as
 651 well. From the proof above, we also know that the second derivative of F is continuous. Because
 652 continuous differentiability implies Lipschitz continuity [38], it infers that the first derivative of
 653 F is Lipschitz continuous. As a result, F satisfies Assumption 1 from [24]. Because F satisfies
 654 Assumptions 1 and 4, then for any $\gamma > p + q$, any bounded sequence $(\mathbf{w}^{(t)}, \mathbf{S}^{(t)})$ generated by
 655 Algorithm 1 will almost surely converges to a second-order stationary point of F by Corollary 3 from
 656 [24]. \square

657 While the convergence of Algorithm 1 entails the second-order optimality conditions of f and g ,
 658 some commonly used f such as the GNN with sigmoid or tanh activations and some commonly used
 659 g such as the squared ℓ_2 norm satisfy the KL property, and Algorithm 1 is guaranteed to avoid a strict
 660 saddle point and converges to a second-order stationary point.
 661