

Compressing Deep Graph Neural Networks via Adversarial Knowledge Distillation

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ABSTRACT

Deep graph neural networks (GNNs) have been shown to be expressive for modeling graph-structured data. Nevertheless, the over-stacked architecture of deep graph models makes it difficult to deploy and rapidly test on mobile or embedded systems. To compress over-stacked GNNs, knowledge distillation via a teacher-student architecture turns out to be an effective technique, where the key step is to measure the discrepancy between teacher and student networks with predefined distance functions. However, using the same distance for graphs of various structures may be unfit, and the optimal distance formulation is hard to determine. To tackle these problems, we propose a novel Adversarial Knowledge Distillation framework for graph models named GraphAKD, which adversarially trains a discriminator and a generator to adaptively detect and decrease the discrepancy. Specifically, noticing that the well-captured inter-node and inter-class correlations favor the success of deep GNNs, we propose to criticize the inherited knowledge from node-level and class-level views with a trainable discriminator. The discriminator distinguishes between teacher knowledge and what the student inherits, while the student GNN works as a generator and aims to fool the discriminator. To our best knowledge, GraphAKD is the first to introduce adversarial training to knowledge distillation in graph domains. Experiments on node-level and graph-level classification benchmarks demonstrate that GraphAKD improves the student performance by a large margin. The results imply that GraphAKD can precisely transfer knowledge from a complicated teacher GNN to a compact student GNN.

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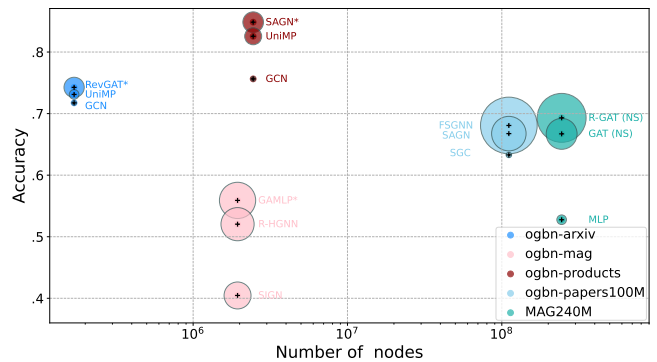


Figure 1: Node classification accuracy v.s. graph size. Each bubble’s area is proportional to the number of parameters of a model. Model name with * means the variant. The statistics are collected from OGB leaderboards.

CCS CONCEPTS

• Computing methodologies → Machine learning; • Networks → Network algorithms.

KEYWORDS

Graph Neural Networks, Knowledge Distillation, Adversarial Training, Network Compression

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1 INTRODUCTION

In recent years, graph neural networks (GNNs) have become the standard toolkit for graph-related applications including recommender systems [20, 57], social network [19, 29], and biochemistry [10, 13]. However, GNNs that show great expressive power on large-scale graphs tend to be over-parameterized [22]. As large-scale

graph benchmarks including Microsoft Academic Graph (MAG) [45] and Open Graph Benchmark (OGB) [23] spring up, complicated and over-stacked GNNs [5, 30] have been developed to achieve state-of-the-art performance. Figure 1 illustrates model performance versus graph size (i.e., the number of nodes in a graph). We note that deep and complicated GNNs significantly outperform shallow models on large-scale graphs, implying the great expressive power of over-parameterized GNNs. However, the over-stacked architecture frequently and inevitably degrades both parameter-efficiency and time-efficiency of GNNs [30], which makes them inapplicable to computationally limited platforms such as mobile or embedded systems. To compress deep GNNs and preserve their expressive power, we explore the knowledge distillation technique in graph domains, which has attracted growing attention in recent years.

Knowledge distillation has been shown to be powerful for compressing huge neural networks in both visual learning and language modeling tasks [2, 25], especially with a teacher-student architecture. The main idea is that the student network mimics the behavior of the teacher network to obtain a competitive or even a superior performance [14, 37], while the teacher network transfers soft targets, hidden feature maps, or relations between pair of layers as distilled knowledge to the shallow student network. However, existing algorithms that adapt knowledge distillation to graph domains [53, 55, 59] mainly propose specially designed and fixed distance functions to measure the discrepancy between teacher and student graph models, which results in following two inherent limitations.

- They force the student network to mimic the teacher network with hand-crafted distance functions, of which the optimal formulation is hard to determine [48]. Even worse, Wang et al. [46, 47] have pointed out that the performance of the student trained this way is always suboptimal because it is difficult to learn the exact distribution from the teacher.
- The predefined and fixed distance is unfit to measure the distribution discrepancy of teacher and student representations in different feature spaces. For example, citation networks and image networks have distinct feature spaces due to the intrinsic difference between textual data and visual data. Experiments in Section 4.2 also confirm this claim.

In this paper, we propose a novel adversarial knowledge distillation framework named GraphAKD to tackle the aforementioned problems. Specifically, instead of forcing the student network to exactly mimic the teacher network with hand-designed distance functions, we develop a trainable discriminator to distinguish between student and teacher from the views of node representations and logits. The discriminator modifies the teacher-student architecture into generative adversarial networks (GANs) [17], where the student model works as a generator. Two identifiers constitute the discriminator, namely the representation identifier and the logit identifier. The representation identifier tells student and teacher node representations apart via criticizing the local affinity of connected nodes and the global affinity of patch-summary pairs, while the logit identifier distinguishes between teacher and student logits with a residual multi-layer perceptron (MLP). We think the proposed discriminator is topology-aware as it considers graph structures. The generator, i.e., the student network, is trained to produce node representations and logits similar to the teacher’s distributions so that

Table 1: Glossary of notations.

Notation	Description
$\mathcal{G} = (\mathcal{V}, \mathcal{E})$	a graph composed of node set \mathcal{V} and edge set \mathcal{E}
$y_v; Y_{\mathcal{G}}$	labels of node v and graph \mathcal{G} , respectively
$m_{\mathcal{N}(v)}$	message aggregated from v 's neighborhood $\mathcal{N}(v)$
$\mathbf{X}; \mathbf{H}^{(k)}$	node embeddings of initial and k -th layers, respectively
$\mathbf{h}_v; \mathbf{z}_v$	representation vector and logit of node v , respectively
$\mathbf{s}_{\mathcal{G}}; \mathbf{z}_{\mathcal{G}}$	summary vector and logit of graph \mathcal{G} , respectively
$G^T; G^S$	GNN models of teacher and student, respectively
$\mathbf{H}^T; \mathbf{H}^S$	node embeddings of teacher and student, respectively
$\mathbf{Z}^T; \mathbf{Z}^S$	logits of teacher and student, respectively
$D_e; D_{\ell}$	identifiers of node embeddings and logits, respectively

the discriminator cannot distinguish. By alternately optimizing the discriminator and the generator, GraphAKD is able to transfer both inter-node and inter-class correlations from a complicated teacher GNN to a compact student GNN. We further note that the discriminator is more tolerant than predefined distance formulations such as Kullback-Leibler (KL) divergence and Euclidean distance. We can view the trainable discriminator as a teaching assistant that helps bridge the capacity gap between teacher and student models. Moreover, the proposed topology-aware discriminator can lower the risk of over-fitting.

To evaluate the effectiveness of our proposed GraphAKD, we conduct extensive experiments on eight node classification benchmarks and two graph classification benchmarks. Experiments demonstrate that GraphAKD enables compact student GNNs to achieve satisfying results on par with or sometimes even superior to those of the deep teacher models, while requiring only 10 ~ 40% parameters of their corresponding teachers.

2 BACKGROUND

In this part, we review the basic concepts of GNNs. Main notations are summarized in Table 1. GNNs are designed as an extension of convolutions to non-Euclidean data [4]. In this paper, we mainly select message passing based GNNs [16] as both teacher and student models, where messages are exchanged between nodes and updated with neural networks [16]. Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ denote a graph with feature vector \mathbf{X}_v for node $v \in \mathcal{V}$. We are interested in two tasks, namely (1) *Node classification*, where each node $v \in \mathcal{V}$ has an associated label y_v and the goal is to learn a representation vector \mathbf{h}_v of v that aids in predicting v 's label as $\hat{y}_v = f(\mathbf{h}_v)$; and (2) *Graph classification*, where we are given a set of graphs $\{\mathcal{G}_1, \dots, \mathcal{G}_N\}$ with corresponding labels $\{y_{\mathcal{G}_1}, \dots, y_{\mathcal{G}_N}\}$ and the goal is to learn a summary vector $\mathbf{s}_{\mathcal{G}}$ such that the label of an entire graph can be predicted as $\hat{y}_{\mathcal{G}} = f(\mathbf{s}_{\mathcal{G}})$. Therefore, we decompose a general GNN into an encoder and a classifier. The encoder follows a message-passing scheme, where the hidden embedding $\mathbf{h}_v^{(k+1)}$ of node $v \in \mathcal{V}$ is updated according to information aggregated from v 's graph neighborhood $\mathcal{N}(v)$ at k -th iteration. This message-passing update [18] can be expressed as

$$\mathbf{h}_v^{(k+1)} = \text{UPDATE}^{(k)} \left(\mathbf{h}_v^{(k)}, m_{\mathcal{N}(v)}^{(k)} \right),$$

$$\text{where } m_{\mathcal{N}(v)}^{(k)} = \text{AGGREGATE}^{(k)} \left(\{\mathbf{h}_u^{(k)} \mid \forall u \in \mathcal{N}(v)\} \right).$$

Note that the initial embeddings are set to the input features for all the nodes if $k = 0$, i.e., $\mathbf{h}_v^{(0)} = \mathbf{X}_v, \forall v \in \mathcal{V}$. After running K iterations of the GNN message passing, we derive the final representation $\mathbf{h}_v = \mathbf{h}_v^{(K)}$ for each node $v \in \mathcal{V}$. For graph-level classification, the READOUT function aggregates final node embeddings to obtain the summary vector $\mathbf{s}_{\mathcal{G}}$ of the entire graph, i.e.,

$$\mathbf{s}_{\mathcal{G}} = \text{READOUT}(\{\mathbf{h}_v \mid \forall v \in \mathcal{V}\}),$$

where the READOUT function can be a simple permutation invariant function such as max-pooling and mean-pooling [19, 50]. The classifier then reads into the final representation of a node or a graph for node-level or graph-level classification, i.e.,

$$\begin{aligned} \mathbf{z} &= g(\mathbf{h}), \\ \hat{\mathbf{y}} &= \text{softmax}(\mathbf{z}), \end{aligned}$$

where we usually interpret \mathbf{z}_v (or $\mathbf{z}_{\mathcal{G}}$) and $\hat{\mathbf{y}}_v$ (or $\hat{\mathbf{y}}_{\mathcal{G}}$) as logit and prediction of a node (or a graph), respectively.

3 METHODOLOGY

In this part, we first introduce our adversarial knowledge distillation framework in Section 3.1. Next, we detail the proposed representation identifier in Section 3.2 and logit identifier in Section 3.3.

3.1 An Adversarial Knowledge Distillation Framework for Graph Neural Networks

We note that a powerful knowledge distillation method in graph domains should be able to 1) adaptively detect the difference between teacher and student on graphs of various fields; 2) inherit the teacher knowledge as much as possible; and 3) transfer teacher knowledge in a topology-aware manner.

Previous work [8, 46, 52] has demonstrated that distance functions such as ℓ_p distance and KL-divergence are too vigorous for student models with a small capacity. Even worse, Wang et al. [48] declared that it is hard to determine which distance formulation is optimal. Therefore, we develop the first adversarial distillation framework in graph domains to meet the first requirement. Furthermore, inspired by the fact that intermediate representations can provide hints for knowledge transfer [37], we take advantage of node representations and logits derived from deep teacher models to improve the training of compact student networks. Finally, to meet the third requirement, we develop a topology-aware discriminator, which stimulates student networks to mimic teachers and produce similar local affinity of connected nodes and global affinity of patch-summary pairs.

Figure 2 illustrates the overall architecture of GraphAKD, which adversarially trains the student model against a topology-aware discriminator in a two-player minimax game. The student GNN serves as a generator and produces node embeddings and logits that are similar to teacher output, while the discriminator aims to distinguish between teacher output and what the generator produces. The minimax game ensures the student network to perfectly model the probability distribution of teacher knowledge at the equilibrium via adversarial losses [46, 47].

In addition to teacher and student GNNs, GraphAKD includes a novel discriminator as well, which can be decomposed into a representation identifier and a logit identifier. As the node classification

Algorithm 1 GraphAKD for node-level classification.

Require: Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, adjacent matrix \mathbf{A} , node features \mathbf{X} and the pretrained teacher model G^T .

Ensure: The learnt student model G^S .

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1:  $\mathbf{H}^T, \mathbf{Z}^T = G^T(\mathbf{X}, \mathbf{A}); \mathbf{s}^T = \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \mathbf{h}_v^T$ 
2: while not converge do
3:    $\mathbf{H}^S, \mathbf{Z}^S = G^S(\mathbf{X}, \mathbf{A}); \mathbf{s}^S = \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \mathbf{h}_v^S$ 
4:   for all node  $v \in \mathcal{V}$  do
5:     Update  $D_e$  to distinguish  $(\mathbf{h}_v^T, \mathbf{s}^T)$  and  $(\mathbf{h}_v^S, \mathbf{s}^T)$ 
6:     Update  $D_e$  to distinguish  $(\mathbf{h}_v^S, \mathbf{s}^S)$  and  $(\mathbf{h}_v^T, \mathbf{s}^S)$ 
7:     for node  $u \in \mathcal{N}(v)$  do
8:       Update  $D_e$  to distinguish  $(\mathbf{h}_v^T, \mathbf{h}_u^T)$  and  $(\mathbf{h}_v^S, \mathbf{h}_u^S)$ 
9:       Update the parameters of  $G^S$  to fool  $D_e$  via Eq. 1
10:      Update  $D_\ell$  to distinguish  $\mathbf{z}_v^T$  and  $\mathbf{z}_v^S$ 
11:      Update the parameters of  $G^S$  to fool  $D_\ell$  via Eq. 4
12: return  $G^S$ 

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task is popular in existing distillation literature [53, 55, 59], we take node classification for an example and represent the training procedure of GraphAKD for node-level classification in Algorithm 1. As for the graph-level algorithm, please refer to Appendix A. Let D_e and D_ℓ be the two identifiers that operate on node embeddings and logits, respectively. Suppose we have a pretrained teacher GNN G^T and accompanying knowledge, i.e., node representations \mathbf{H}^T and logits \mathbf{Z}^T . The objective is to train a student GNN G^S with much less parameters while preserving the expressive power of the teacher G^T . That is, we expect that the student G^S can generate high-quality node representations \mathbf{H}^S and logits \mathbf{Z}^S to achieve competitive performance against the teacher. As the trainable discriminator is more flexible and tolerant than most specific distance including KL-divergence and ℓ_p distance [8, 52], GraphAKD enables student GNNs to capture inter-node and inter-class correlations instead of mimicking the exact distribution of teacher knowledge.

3.2 The Representation Identifier

In this section, we introduce our topology-aware representation identifier. Note that we decompose a GNN into an encoder and a classifier in Section 2. The representation identifier focuses on the output of the GNN encoder, i.e., the final node embeddings. Instead of directly matching the feature maps of teacher and student [55], we adversarially distill node representations of teacher models from both local and global views.

Given the node representations of teacher and student GNNs, namely $\mathbf{H}^T \in \mathbb{R}^{|\mathcal{V}| \times d^T}$ and $\mathbf{H}^S \in \mathbb{R}^{|\mathcal{V}| \times d^S}$, we perform mean-pooling to obtain the corresponding summary vectors for a graph as $\mathbf{s}^T \in \mathbb{R}^{d^T}$ and $\mathbf{s}^S \in \mathbb{R}^{d^S}$. In practice we set the dimension of student's node representations equal to that of teacher's, i.e., $d^S = d^T = d$. For each node v , the representation learned by the student GNN G^S is criticized by the identifier D_e through both local and global views. Specifically, reading in connected node pair $\{\mathbf{h}_v, \mathbf{h}_u\}$ or patch-summary pair $\{\mathbf{h}_v, \mathbf{s}\}$, the identifier D_e is expected to predict a binary value "Real/Fake" that indicates whether the pair is real or fake. Fake node pair implies that the representations of the two adjacent nodes are produced by the student GNN G^S ; while

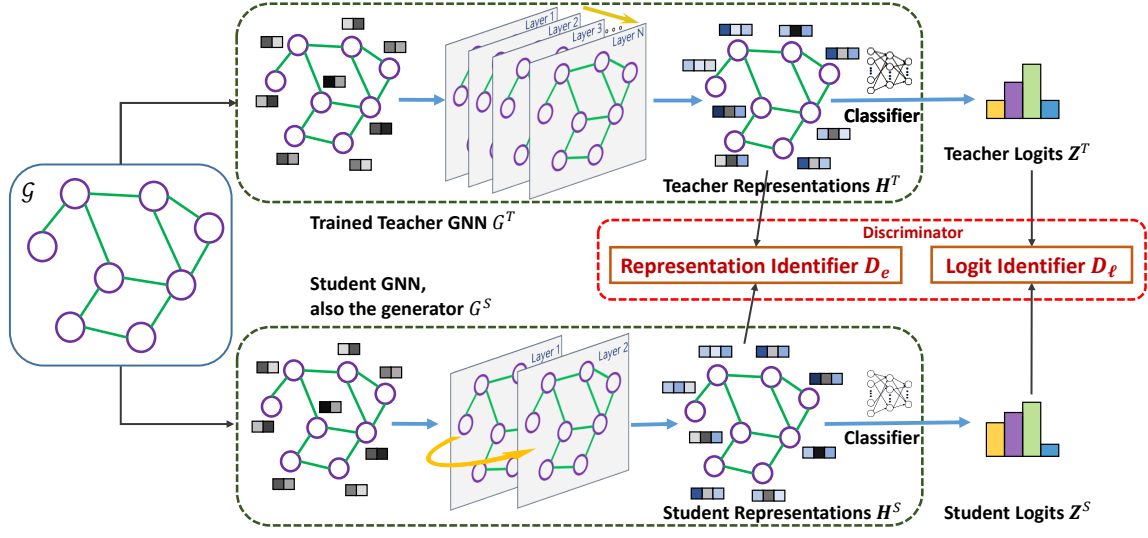


Figure 2: Illustration of the proposed adversarial knowledge distillation framework GraphAKD.

fake patch-summary pair implies that the patch representation and summary representation are produced by GNNs of different roles.

Formally, the topology-aware identifier D_e consists of D_e^{local} and D_e^{global} . If nodes v and u form an edge on the graph \mathcal{G} , then D_e^{local} maps representations of the two connected nodes to the real value that we interpret as affinity between connected nodes. On the other hand, for each node v on the graph, D_e^{global} maps the patch-summary pair to the real value that we interpret as affinity between node and graph. That is,

$$\begin{aligned} D_e^{local}(\mathbf{h}_v^T, \mathbf{h}_u^T) &= \langle \mathbf{h}_v^T, \mathbf{W}^{local} \mathbf{h}_u^T \rangle \in [0, 1], \\ D_e^{local}(\mathbf{h}_v^S, \mathbf{h}_u^S) &= \langle \mathbf{h}_v^S, \mathbf{W}^{local} \mathbf{h}_u^S \rangle \in [0, 1], \quad \forall (v, u) \in \mathcal{E}, \\ D_e^{global}(\mathbf{h}_v^{T/S}, \mathbf{s}_{\mathcal{G}}^T) &= \langle \mathbf{h}_v^{T/S}, \mathbf{W}^{global} \mathbf{s}_{\mathcal{G}}^T \rangle \in [0, 1], \\ D_e^{global}(\mathbf{h}_v^{T/S}, \mathbf{s}_{\mathcal{G}}^S) &= \langle \mathbf{h}_v^{T/S}, \mathbf{W}^{global} \mathbf{s}_{\mathcal{G}}^S \rangle \in [0, 1], \quad \forall v \in \mathcal{V} \subset \mathcal{G}, \end{aligned}$$

where \mathbf{W}^{local} and \mathbf{W}^{global} are learnable diagonal matrices. By this means, D_e^{local} encourages the student to inherit the local affinity hidden in teacher's node embeddings, while D_e^{global} encourages the student to inherit the global affinity.

As the student GNN aims to fool the representation identifier D_e , we view G^S as a generator. Under the guidance of the identifier D_e , the generator strives to yield indistinguishable node representations. The adversarial training process can be formulated as a two-player minimax game, i.e.,

$$\min_{G^S} \max_{D_e} \mathcal{J}^{local} + \mathcal{J}^{global}, \quad (1)$$

where \mathcal{J}^{local} is written as

$$\frac{1}{|\mathcal{E}|} \sum_{(v,u) \in \mathcal{E}} \left(\log P(\text{Real} | D_e^l(\mathbf{h}_v^T, \mathbf{h}_u^T)) + \log P(\text{Fake} | D_e^l(\mathbf{h}_v^S, \mathbf{h}_u^S)) \right),$$

and \mathcal{J}^{global} is written as

$$\begin{aligned} \frac{1}{2|\mathcal{V}|} \sum_{v \in \mathcal{V}} \left(\log P(\text{Real} | D_e^g(\mathbf{h}_v^T, \mathbf{s}_{\mathcal{G}}^T)) + \log P(\text{Fake} | D_e^g(\mathbf{h}_v^S, \mathbf{s}_{\mathcal{G}}^T)) \right) \\ + \log P(\text{Real} | D_e^g(\mathbf{h}_v^S, \mathbf{s}_{\mathcal{G}}^S)) + \log P(\text{Fake} | D_e^g(\mathbf{h}_v^T, \mathbf{s}_{\mathcal{G}}^S)), \end{aligned}$$

where D_e^l and D_e^g denote D_e^{local} and D_e^{global} , respectively. By alternately maximizing and minimizing the objective function, we finally obtain an expressive student GNN when it converges.

It is worth noting that we can understand the representation identifier D_e from different perspectives. In fact, D_e^{local} can degenerate into a bilinear distance function. If we modify the trainable diagonal matrix to the identity matrix and normalize the input vectors, then the local affinity calculated by D_e^{local} is equivalent to cosine similarity between node embeddings. That is, if $\mathbf{W}^{local} = \mathbf{I}$ and $\hat{\mathbf{h}}_v = \mathbf{h}_v / \|\mathbf{h}_v\|_2$, then

$$\langle \hat{\mathbf{h}}_v, \mathbf{W}^{local} \hat{\mathbf{h}}_u \rangle = \text{cosine_sim}(\mathbf{h}_v, \mathbf{h}_u), \quad \forall (v, u) \in \mathcal{E}.$$

Apart from that, we can perceive the training process of D_e^{global} as the maximization of the mutual information between the graph-level representation (i.e., the summary vector $\mathbf{s}_{\mathcal{G}}$) and the node-level representation (i.e., the patch vector \mathbf{h}_v). Likewise, Velickovic et al. [43] propose a discriminator to maximize the mutual information between graph representations of different levels. However, our proposed D_e^{global} differs from DGI [43] in two aspects. First, the performance of DGI [43] heavily relies on how to draw negative samples, while D_e^{global} exempts the need of negative sampling. Second, DGI [43] judges the representations produced by the same encoder for unsupervised graph learning, while D_e^{global} discriminates the representations produced by teacher and student for adversarial knowledge distillation.

Compared with existing distance-based embedding distillation in graph domains [55], we replace predefined distance formulations with a more flexible and tolerant identifier. Instead of mimicking the exact distribution of teacher node embeddings, our representation

identifier enables student GNN to capture the inter-node correlation, which is proved to be of crucial importance in graph domains [26].

3.3 The Logit Identifier

In this section, we introduce the second identifier of the proposed framework, which operates on the output logits. For notation convenience, we introduce the logit identifier in the context of node-level classification. Output of the GNN-based classifier is a probability distribution over categories. The probability is derived by applying a softmax function over the output of the last fully connected layer, which is also known as logits. By leveraging adversarial training, we aim to transfer inter-class correlation [54] from complicated teacher GNNs to compact student GNNs.

Instead of forcing the student to exactly mimic the teacher by minimizing KL-divergence [21] or other predefined distance, we transfer the inter-class correlation hidden in teacher logits through a logit identifier. Inspired by adversarial training in visual representation learning [48, 52], our logit identifier is trained to distinguish student logits from teacher logits, while the generator (i.e., the student GNN) is adversarially trained to fool the identifier. That is, we expect the compact student GNN to output logits similar to the teacher logits so that the identifier cannot distinguish.

As residual learning can mitigate the gap between teacher and student [15], we use an MLP with residual connections as our logit identifier D_ℓ . The number of hidden units in each layer is the same as the dimension of logit, which is equal to the number of categories C . A plain identifier reads into the logit of each node and predicts a binary value “Real/Fake” that indicates whether the logit is derived by teacher or student. Denote the logit of node v derived by teacher and student as z_v^T and z_v^S , respectively. A plain identifier D aims to maximize the log-likelihood as

$$\max_D \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \left(\log P(\text{Real} \mid D(z_v^T)) + \log P(\text{Fake} \mid D(z_v^S)) \right). \quad (2)$$

As Xu et al. [52] pointed out that the plain version is slow and unstable, we follow [36, 52] and modify the objective to also predict the specific node labels. Therefore, the output of D_ℓ is a $C + 1$ dimensional vector with the first C for label prediction and the last for Real/Fake (namely teacher/student) indicator. We thus maximize following objective for the training of D_ℓ :

$$\begin{aligned} \max_{D_\ell} \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} & \left(\log P(\text{Real} \mid D_\ell(z_v^T)) + \log P(\text{Fake} \mid D_\ell(z_v^S)) \right. \\ & \left. + \log P(y_v \mid D_\ell(z_v^T)) + \log P(y_v \mid D_\ell(z_v^S)) \right). \end{aligned} \quad (3)$$

As for the training of generator, i.e., the student GNN G^S , we follow [24, 52] and introduce instance-level alignment between teacher and student logits besides the category-level alignment. We thus minimize the loss function for the training of G^S as

$$\begin{aligned} \min_{G^S} \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} & \left(\log P(\text{Real} \mid D_\ell(z_v^T)) + \log P(\text{Fake} \mid D_\ell(z_v^S)) \right. \\ & \left. - \left[\log P(y_v \mid D_\ell(z_v^T)) + \log P(y_v \mid D_\ell(z_v^S)) \right] \right. \\ & \left. + \|z_v^S - z_v^T\|_1 \right). \end{aligned} \quad (4)$$

Table 2: Statistics of the eight node classification benchmarks.

Datasets	#Nodes	#Edges	#Feat.	Data Split
Cora [3, 34]	2,708	5,429	1,433	140/500/1K
CiteSeer [40]	3,327	4,732	3,703	120/500/1K
PubMed [35]	19,717	44,338	500	60/500/1K
Flickr [33, 58]	89,250	899,756	500	44K/22K/22K
Arxiv [23]	169,343	1,166,243	128	90K/29K/48K
Reddit [19, 58]	232,965	23,213,838	602	153K/23K/55K
Yelp [58]	716,847	13,954,819	300	537K/107K/71K
Products [23]	2,449,029	61,859,140	100	196K/39K/2M

Compared to existing knowledge distillation models for GNNs [53, 59], the logit identifier relaxes the rigid coupling between student and teacher. Besides, the adversarial training approach relieves the pain for hand-engineering the loss.

4 EXPERIMENTS

In this part, we conduct extensive experiments to evaluate the capability of our proposed GraphAKD. Our experiments are intended to answer the following five research questions.

- RQ1:** How does GraphAKD perform on node-level classification?
- RQ2:** How does GraphAKD perform on graph-level classification?
- RQ3:** How efficient are the student GNNs trained by GraphAKD?
- RQ4:** How do different components (i.e., D_e or D_ℓ) affect the performance of GraphAKD?
- RQ5:** Do student GNNs learn better node representations when equipped with GraphAKD?

4.1 Experimental Setup

4.1.1 Datasets. For a comprehensive comparison, in Section 4.2 we perform node classification on eight widely-used datasets, covering graphs of various sizes. The statistics are summarized in Table 2. To evaluate the effectiveness of GraphAKD on graph-level classification, we benchmark GraphAKD against traditional knowledge distillation methods on two molecular property prediction datasets [23] in Section 4.3. For detailed information on the ten datasets, please refer to Appendix B. In a nutshell, all datasets are collected from real-world networks in different domains, including social networks, citation networks, molecular graphs, and trading networks. We conduct experiments under both transductive and inductive settings, involving both textual and visual features.

4.1.2 Model Selection for Student and Teacher. In fact, GraphAKD is applicable to all message passing based GNNs. For node-level classification, we select two simple and famous GNNs as the student models. Specifically, we choose GCN [28] for Cora [3, 34], CiteSeer [40], PubMed [35], Flickr [33, 58], Arxiv [23] and Reddit [19, 58], while Cluster-GCN [7] is selected for large-scale datasets including Yelp [58] and Products [23]. On the other hand, we employ two deep teacher GNNs on different graphs, namely GMLP [60] for Products and GCNII [5] for other seven datasets. As for graph-level classification, we test both GCN [28] and GIN [50] as students on

Table 3: Performance on Node Classification (metric: F1-micro (%)). “O. Perf.” and “R. Perf.” refer to performance reported in original papers and reproduced by our own, respectively. Higher of these two columns are underlined. “Perf. Impv.” and “#Params Decr.” refer to the absolute improvement of student performance (w.r.t. the underlined results) and the relative decrease of teacher parameters, respectively. Results of previous work are mainly taken from [58], [12], and OGB Leaderboards. We report the average performance and std. across 10 random seeds.

Datasets	Teacher			Vanilla Student			Student trained with GraphAKD			
	Model	Perf.	#Params	Model	O. Perf.	R. Perf.	Perf.	#Params	Perf. Impv. (%)	#Params Decr.
Cora	GCNII	85.5	616,519	GCN	<u>81.5</u>	78.3 ±0.9	83.6 ±0.8	96,633	2.1	84.3%
CiteSeer	GCNII	73.4	5,144,070	GCN	<u>71.1</u>	68.6 ±1.1	72.9 ±0.4	1,016,156	1.8	80.2%
PubMed	GCNII	80.3	1,177,603	GCN	<u>79.0</u>	78.1 ±1.0	81.3 ±0.4	195,357	2.3	83.4%
Flickr	GCNII	56.20	1,182,727	GCN	49.20	<u>49.63</u> ±1.19	52.95 ±0.24	196,473	3.32	83.4%
Arxiv	GCNII	72.74	2,148,648	GCN	<u>71.74</u>	71.43 ±0.13	73.05 ±0.22	242,426	1.31	88.7%
Reddit	GCNII	96.77	691,241	GCN	<u>93.30</u>	<u>94.12</u> ±0.04	95.15 ±0.02	234,655	1.03	66.1%
Yelp	GCNII	65.14	2,306,660	Cluster-GCN	59.15	<u>59.63</u> ±0.51	60.63 ±0.42	431,950	1.00	81.3%
Products	GAMLN	84.59	3,335,831	Cluster-GCN	<u>76.21</u>	74.99 ±0.76	81.45 ±0.47	682,449	5.24	79.5%

Molhiv [23] and Molpcba [23]. Simultaneously, we choose HIG¹ as the sole teacher model for the graph-level task. Note that we execute the teacher models during pre-computation, which prepares node representations and logits for student training. For more implementation details and the information on the mentioned teacher and student graph models, please refer to Appendix C.

4.2 Performance on Node Classification (RQ1)

To evaluate the capability of our proposed adversarial knowledge distillation framework, we conduct node classification across graphs of various sizes. Empirical results on eight datasets are presented in Table 3. Note that we follow the standard data split of previous work [7, 12, 28, 58]. As a node in the graph may belong to multiple classes (e.g., Yelp [58]), we use F1-micro score to measure the performance.

In general, deep and complex GNNs have great expressive power and perform well on node classification task, especially for large graphs. For example, GCNII [5] outperforms the vanilla GCN [28] by a large margin. However, deep and wide GNNs usually suffer from prohibitive time and space complexity [30]. By contrast, shallow and thin GNNs have small model capacity while they can easily scale to large datasets. Tabel 3 shows that the proposed GraphAKD enables shallow student GNNs to achieve comparable or even superior performance to their teachers while maintaining the computational efficiency. Concretely, the GCN student outperforms the over-stacked teacher (i.e., GCNII) on PubMed and Arxiv with the knowledge transferred by GraphAKD. As for large-scale graphs such as Flickr and Products, GraphAKD consistently and significantly improves the performance of student GNNs. We notice that to achieve superior accuracy on PubMed and Arxiv, the student GCN only requires less than 20% parameters of its teacher. However, the reason why GraphAKD can achieve superior performance to the teacher GNNs is intriguing. Cheng et al. [6] have pointed out that knowledge distillation makes students learn various concepts simultaneously, rather than learn concepts from raw data sequentially. Therefore, GraphAKD enables students learn both node-level and class-level views simultaneously, alleviating the problem that

Table 4: Comparison with other distillation algorithms.

Datasets	Student	KD [21]	FitNet [37]	LSP [55]	GraphAKD
Cora	81.5	83.2	82.4	81.7	83.6
CiteSeer	71.1	71.4	71.6	68.8	72.9
PubMed	79.0	80.3	81.3	80.8	81.3
Flickr	49.20	50.58	50.69	50.02	52.95
Arxiv	71.74	73.03	71.83	OOM	73.05
Reddit	93.30	94.01	94.99	OOM	95.15
Yelp	59.15	59.14	59.92	49.24	60.63
Products	76.21	79.19	76.57	70.86	81.45

deep teacher GNNs tend to gradually discard views through layers according to the information-bottleneck theory [41, 49].

To further demonstrate the effectiveness of GraphAKD, we compare the proposed framework with several distillation methods including the traditional logit-based knowledge distillation (KD) [21], the feature mimicking algorithm FitNet [37] and the recent local structure preserving (LSP) method [55]. We reproduce them and present comparisons in Table 4. Highest performance of each row is highlighted with boldface. As graphs in different fields own distinct feature spaces, the three distance-based approaches fail to yield consistent improvement across all fields, which support the claim that a predefined and fixed distance is unfit to measure the discrepancy between teacher and student in different feature spaces. Specifically, KD [21] performs even inferior than the vanilla student on Yelp; LSP [55] achieves poor performance on two trading networks (namely Yelp and Products); and FitNet [37] barely yields gains on two citation networks (namely CiteSeer and Arxiv). On the other hand, GraphAKD outperforms three baselines by a large margin on most of the eight datasets. Moreover, we note that LSP incurs the out-of-memory (OOM) issue on Arxiv and Reddit, while the GCN students equipped with GraphAKD survive.

To understand why the proposed framework outperforms other baselines, we delve deeper into the four competitors. We note that KD [21], FitNet [37] and LSP [55] take advantage of teacher knowledge from different aspects. Specifically, KD [21] only uses

¹<https://github.com/TencentYoutuResearch/HIG-GraphClassification>.

teacher logits as soft targets, while FitNet [37] and LSP [55] are proposed to leverage intermediate node embeddings. Contrary to them, GraphAKD leverages both aspects of teacher knowledge to distill inter-class and inter-node correlations. Another important reason comes from the different ways they transfer teacher knowledge to student. Concretely, KD [21], FitNet [37] and LSP [55] force the student to mimic the exact distribution of teacher output (logits or intermediate embeddings) with fixed distance formulations, namely KL-divergence, Euclidean distance, and kernel functions. GraphAKD differs from KD [21], FitNet [37] and LSP [55] as it transfers teacher knowledge via adversarial training, which is more tolerant and is less sensitive to parameters than the metric selection or temperature setting in traditional distance-based distillation.

Table 5: Graph classification on Molhiv [23] (metric: ROC-AUC (%)) and Molpcba [23] (metric: AP (%)). Results of teacher and student are taken from OGB Leaderboards. We report the average performance and std. across 10 random seeds.

Dataset	Molhiv		Molpcba	
	HIG with DeeperGCN	HIG with Graphormer	HIG with DeeperGCN	HIG with Graphormer
Teacher	GCN	GIN	GCN	GIN
Teacher	84.03 ±0.21	84.03 ±0.21	31.67 ±0.34	31.67 ±0.34
Student	76.06 ±0.97	75.58 ±1.40	20.20 ±0.24	22.66 ±0.28
KD [21]	74.98 ±1.09	75.08 ±1.76	21.35 ±0.42	23.56 ±0.16
FitNet [37]	79.05 ±0.96	77.93 ±0.61	21.25 ±0.91	23.74 ±0.19
GraphAKD	79.46 ±0.97	79.16 ±1.50	22.56 ±0.23	25.85 ±0.17

4.3 Performance on Graph Classification (RQ2)

To evaluate the capability of GraphAKD on graph-level tasks, we conduct molecular property prediction across two benchmarks, namely Molhiv [23] and Molpcba [23]. Table 5 summarizes the empirical results. Note that the teacher model HIG on Molhiv [23] is based on DeeperGCN [31], while the teacher model on Molpcba [23] is built upon Graphormer [56]. Our student architectures are GCN and GIN, which do not use virtual nodes and are considered to be less expressive but more efficient than HIG.

In Table 5, we compare the proposed GraphAKD with knowledge distillation approaches including the traditional logit-based KD [21] and the representation-based FitNet [37]. We observe that GraphAKD consistently improves student performance and outperforms the two distillation baselines. Notably, as Graphormer [56] is different from typical GNNs, both KD and FitNet yield minor performance boosts on Molpcba [23]. However, GraphAKD yields significant improvement against the vanilla student models across the two graph-level benchmarks, which implies that GraphAKD is promising to bridge graph models of different architectures.

4.4 Analysis of Model Efficiency (RQ3)

For practical applications, apart from effectiveness, the usability of a neural network also depends on model efficiency. We investigate the efficiency of GraphAKD with three criteria: 1) parameter-efficiency, 2) computation-efficiency, and 3) time-efficiency. Specifically, we

Table 6: Comparison of efficiency between student GNNs and the corresponding teachers.

Datasets	#Params		GPU Memory		Inference time	
	Teacher	Student	Teacher	Student	Teacher	Student
Cora	0.6M	0.1M	0.22G	0.03G	40.3ms	4.1ms
PubMed	1.2M	0.2M	1.23G	0.33G	57.3ms	5.7ms
Flickr	1.2M	0.2M	2.79G	1.49G	309.7ms	11.9ms
Yelp	2.3M	0.4M	6.28G	4.73G	3.0s	1.5s
Products	3.3M	0.7M	6.25G	6.20G	16.1s	7.0s

compare the student GNNs trained by GraphAKD against their teachers in terms of the aforementioned three criteria. We select five graph benchmarks (namely Cora, PubMed, Flickr, Yelp, and Products) and summarize the efficiency comparison in Table 6. Note that we conduct full-batch testing for both teacher and student on Cora, PubMed and Flickr. As for Yelp and Products, we align the batch size of teacher and student for a fair comparison. We provide detailed analyses as follows.

4.4.1 Parameter efficiency. For resource limited device, the amount of memory occupied by the model becomes critical to deployment. Here we use the number of parameters to measure the memory consumption for both teacher and student models. We observe that the number of node features, network layers, and hidden dimensions contribute to the number of parameters. By drastically lessening hidden dimensions and network layers, GraphAKD reduces the model size of teacher GNNs to less than 20% on average.

4.4.2 Computation efficiency. In addition to storage consumption, the dynamic memory usage is important as well. The reported GPU memory is the peak GPU memory usage during the first training epoch, which is also used in [30]. Restricted to the size and weight of mobile or embedded systems, neural networks that consume huge memory may be inapplicable to many practical situations. We note that the GPU memory is highly related to the hidden dimensions and the number of network layers. As mentioned in Section 4.4.1, GraphAKD significantly reduces hidden dimensions and network layers of over-stacked teacher GNNs, which brings about portable and flexible student graph models.

4.4.3 Time efficiency. As low latency is sometimes demanded in real-world applications, we also evaluate the inference time of both teacher and student GNNs, which refers to the time consumption of inference on testing dataset. Table 6 shows that GraphAKD significantly reduces the inference time for deep GNNs. On Flickr, in particular, GraphAKD even cuts down more than 90% inference time of the GCNII teacher, which shows that GraphAKD trades off a reasonable amount of accuracy to reduce latency. The acceleration may originate from the sharp decrease in the number of network layers. In a nutshell, Table 6 shows that GraphAKD is able to compress over-parameterized teacher GNNs into compact and computationally efficient student GNNs with relatively low latency.

4.5 Ablation Studies (RQ4)

To thoroughly evaluate our framework, in this section we provide ablation studies to show the influence of the two identifiers. Specifically, we separately test the capability of the two identifiers (D_e and

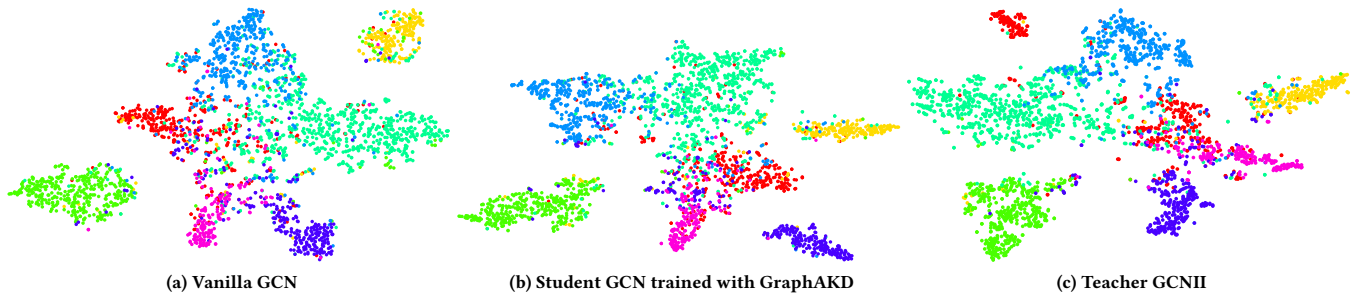


Figure 3: t-SNE embeddings of the nodes in the Cora dataset from the vanilla GCN embeddings (left), embeddings from the student GCN that trained by GraphAKD (middle), and GCNII (right). The Silhouette scores [38] of the embeddings learned by three models are 0.2196, 0.2638, and 0.3033, respectively.

Table 7: Ablation studies on the impacts of each identifier.

Datasets	Cora	PubMed	Flickr	Yelp	Products	Molhiv
Teacher	85.5	80.3	56.20	65.14	84.59	84.03
Student	81.5	79.0	49.20	59.15	76.21	75.58
Only D_e	82.9	80.6	52.20	59.63	81.13	78.28
Only D_ℓ	82.3	81.0	52.52	60.03	79.76	78.09
GraphAKD	83.6	81.3	52.95	60.63	81.45	79.16

D_ℓ) to clarify the essential improvement of each component. We conduct our analysis on the same five node-level benchmarks used in Section 4.4 as well as a graph-level dataset. Highest performance of each column is highlighted in Table 7.

We can conclude that the improvements benefit from both the representation identifier and the logit identifier. Another valuable observation in Table 7 is that both D_e and D_ℓ enable a vanilla GCN to achieve results superior to the GCNII teacher on PubMed. The fact that GraphAKD outperforms each of the identifiers demonstrates the importance of both node representations and logits. Either of the two identifiers captures orthogonal yet valuable knowledge via adversarial training. Specifically, the representation identifier excels at capturing inter-node correlation, while the logit identifier specializes in capturing inter-class correlation.

4.6 Visualization (RQ5)

We further perform qualitative analysis on the embeddings learnt by the GCN student in order to better understand the properties of our GraphAKD. We follow [43] and focus our analysis exclusively on Cora [3, 34] because it has the smallest number of nodes among the node-level benchmarks, which notably aids clarity.

Figure 3 gives a standard set of “evolving” t-SNE plots of the embeddings learnt by three models, namely the vanilla GCN, the student GCN trained with our GraphAKD, and the teacher GCNII, respectively. For all the three subfigures, we can observe that the learnt embeddings’ 2D projections exhibit discernible clustering in the projected space, which corresponds to the seven topic classes of Cora. We further notice that the 7-category scientific papers can be differentiated more effectively by student GCN equipped with GraphAKD than by a vanilla GCN.

Figure 3 qualitatively shows that GraphAKD not only increases the accuracy of classification, but also enables the student GCN to

learn high-quality node representations. To obtain a more accurate and convincing conclusion, we calculate Silhouette scores [38] for the three projections. Specifically, the Silhouette score [38] of the embeddings learned by student GCN is 0.2638, which compares favorably with the score of 0.2196 for the vanilla GCN.

5 RELATED WORK

In this part, we first introduce existing work that adapts knowledge distillation to graph domains in Section 5.1. Next, we review applications of adversarial training in graph domains in Section 5.2.

5.1 Knowledge Distillation for Graph Models

Knowledge distillation has achieved great success for network compression in visual learning and language modeling tasks [2, 25, 37, 39]. However, directly applying the established approaches in visual learning and language modeling to graph domains is not applicable as graphs contain both features and topological structures.

Recent success in GNNs impels the advent of knowledge distillation for GNNs. Among existing work, [53, 55, 59] are the most relevant to this paper as they all use the teacher-student architecture and focus on node classification. However, the adaptive distillation strategy makes our work distinct from existing research [53, 55, 59]. Specifically, LSP [55] aligns node representations of teacher and student with kernel function based distance; Zhang et al. [59] and Yang et al. [53] use Euclidean distance to match the probability distributions of teacher and student. Contrary to them, our proposed GraphAKD adversarially trains a discriminator and a generator to adaptively detect and decrease the discrepancy between teacher and student. Moreover, [53, 55, 59] merely conduct node-level classification and focus on graphs with less than 100K nodes, while the proposed GraphAKD is widely applicable to both node-level and graph-level classification tasks and performs well on graphs with number of nodes varying from 2K to 2M.

5.2 Adversarial Training for Graph Models

The idea of adversarial training originates from generative adversarial networks (GANs) [17], where the generator and discriminator compete with each other to improve their performance.

In recent years, adversarial training has demonstrated superior performance in graph domains for different aims. Specifically, Wang et al. [44] and Feng et al. [11] leverage the adversarial architecture

to learn universal and robust graph representations, while Dai et al. [9] explore adversarial attack on graph structured data. Alam et al. [1] perform adversarial domain adaptation with graph models, while Suresh et al. [42] develop adversarial graph augmentation to improve the performance of self-supervised learning. Different from them, this work aims to conduct adversarial knowledge distillation for graph models, which leads to the contribution.

6 CONCLUSION

Over-stacked GNNs are usually expressive and powerful on large-scale graph data. To compress deep GNNs, we present a novel adversarial knowledge distillation framework in graph domains, namely GraphAKD, which introduces adversarial training to topology-aware knowledge transfer for the first time. By adversarially training a discriminator and a generator, GraphAKD is able to transfer both inter-node and inter-class correlations from a complicated teacher GNN to a compact student GNN (i.e., the generator). Experiments demonstrate that GraphAKD yields consistent and significant improvements across node-level and graph-level tasks on ten benchmark datasets. The student GNNs trained this way achieve competitive or even superior results to their teacher graph models, while requiring only a small proportion of parameters. In the future work, we plan to explore the potential application of GraphAKD on graph tasks beyond classification.

REFERENCES

- [1] Firoz Alam, Shafiq Joty, and Muhammad Imran. 2018. Domain Adaptation with Adversarial Training and Graph Embeddings. In *Proc. of ACL*.
- [2] Paul Bergmann, Michael Fauser, David Sattler, and Carsten Steger. 2020. Uninformed Students: Student-Teacher Anomaly Detection With Discriminative Latent Embeddings. In *Proc. of CVPR*.
- [3] Aleksandar Bojchevski and Stephan Günnemann. 2018. Deep Gaussian Embedding of Graphs: Unsupervised Inductive Learning via Ranking. In *Proc. of ICLR*.
- [4] Joan Bruna, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. 2014. Spectral Networks and Locally Connected Networks on Graphs. In *Proc. of ICLR*.
- [5] Ming Chen, Zhewei Wei, Zengfeng Huang, Bolin Ding, and Yaliang Li. 2020. Simple and Deep Graph Convolutional Networks. In *Proc. of ICML*.
- [6] Xu Cheng, Zhefan Rao, Yilan Chen, and Quanshi Zhang. 2020. Explaining knowledge distillation by quantifying the knowledge. In *Proc. of CVPR*.
- [7] Wei-Lin Chiang, Xuanqing Liu, Si Si, Yang Li, Samy Bengio, and Cho-Jui Hsieh. 2019. Cluster-GCN: An Efficient Algorithm for Training Deep and Large Graph Convolutional Networks. In *Proc. of KDD*.
- [8] Inseop Chung, Seonguk Park, Jangho Kim, and Nojun Kwak. 2020. Feature-map-level Online Adversarial Knowledge Distillation. In *Proc. of ICML*.
- [9] Hanjun Dai, Hui Li, Tian Tian, Xin Huang, Lin Wang, Jun Zhu, and Le Song. 2018. Adversarial attack on graph structured data. In *International conference on machine learning*.
- [10] David Duvenaud, Dougal Maclaurin, Jorge Aguilera-Iparraguirre, Rafael Gómez-Bombarelli, Timothy Hirzel, Alán Aspuru-Guzik, and Ryan P. Adams. 2015. Convolutional Networks on Graphs for Learning Molecular Fingerprints. In *Proc. of NeurIPS*.
- [11] Fuli Feng, Xiangnan He, Jie Tang, and Tat-Seng Chua. 2019. Graph Adversarial Training: Dynamically Regularizing Based on Graph Structure. *IEEE Transactions on Knowledge & Data Engineering* (2019).
- [12] Matthias Fey, Jan Eric Lenssen, Frank Weichert, and Jure Leskovec. 2021. GN-NAutoScale: Scalable and Expressive Graph Neural Networks via Historical Embeddings. In *Proc. of ICML*.
- [13] Alex Fout, Jonathon Byrd, Basir Shariat, and Asa Ben-Hur. 2017. Protein Interface Prediction using Graph Convolutional Networks. In *Proc. of NeurIPS*.
- [14] Tommaso Furlanello, Zachary Chase Lipton, Michael Tschannen, Laurent Itti, and Anima Anandkumar. 2018. Born-Again Neural Networks. In *Proc. of ICML*.
- [15] Mengya Gao, Yujun Wang, and Liang Wan. 2021. Residual error based knowledge distillation. *Neurocomputing* (2021).
- [16] Justin Gilmer, Samuel S. Schoenholz, Patrick F. Riley, Oriol Vinyals, and George E. Dahl. 2017. Neural Message Passing for Quantum Chemistry. In *Proc. of ICML*.
- [17] Ian J. Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron C. Courville, and Yoshua Bengio. 2014. Generative Adversarial Nets. In *Proc. of NeurIPS*.
- [18] William L. Hamilton. 2020. *Graph Representation Learning*. Morgan & Claypool Publishers.
- [19] William L. Hamilton, Zitao Ying, and Jure Leskovec. 2017. Inductive Representation Learning on Large Graphs. In *Proc. of NeurIPS*.
- [20] Xiangnan He, Kuan Deng, Xiang Wang, Yan Li, Yong-Dong Zhang, and Meng Wang. 2020. LightGCN: Simplifying and Powering Graph Convolution Network for Recommendation. In *Proc. of SIGIR*.
- [21] Geoffrey E. Hinton, Oriol Vinyals, and Jeffrey Dean. 2015. Distilling the Knowledge in a Neural Network. *CoRR* (2015).
- [22] Weihua Hu, Matthias Fey, Hongyu Ren, Maho Nakata, Yuxiao Dong, and Jure Leskovec. 2021. OGB-LSC: A Large-Scale Challenge for Machine Learning on Graphs. *CoRR* (2021).
- [23] Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. 2020. Open Graph Benchmark: Datasets for Machine Learning on Graphs. In *Proc. of NeurIPS*.
- [24] Phillip Isola, Jun-Yan Zhu, Tinghui Zhou, and Alexei A. Efros. 2017. Image-to-Image Translation with Conditional Adversarial Networks. In *Proc. of CVPR*.
- [25] Xiaojie Jiao, Yichun Yin, Lifeng Shang, Xin Jiang, Xiao Chen, Linlin Li, Fang Wang, and Qun Liu. 2020. TinyBERT: Distilling BERT for Natural Language Understanding. In *Proc. of ACL*.
- [26] Wei Jin, Tyler Derr, Yiqi Wang, Yao Ma, Zitao Liu, and Jiliang Tang. 2021. Node Similarity Preserving Graph Convolutional Networks. In *Proc. of WSDM*.
- [27] Diederick P Kingma and Jimmy Ba. 2015. Adam: A method for stochastic optimization. In *Proc. of ICLR*.
- [28] Thomas N. Kipf and Max Welling. 2017. Semi-Supervised Classification with Graph Convolutional Networks. In *Proc. of ICLR*.
- [29] Chang Li and Dan Goldwasser. 2019. Encoding Social Information with Graph Convolutional Networks for Political Perspective Detection in News Media. In *Proc. of ACL*.
- [30] Guohao Li, Matthias Müller, Bernard Ghanem, and Vladlen Koltun. 2021. Training Graph Neural Networks with 1000 Layers. In *Proc. of ICML*.
- [31] Guohao Li, Chenxin Xiong, Ali Thabet, and Bernard Ghanem. 2020. Deepergcn: All you need to train deeper gens. *arXiv preprint arXiv:2006.07739* (2020).
- [32] Qimai Li, Zhichao Han, and Xiao-Ming Wu. 2018. Deeper Insights Into Graph Convolutional Networks for Semi-Supervised Learning. In *Proc. of AAAI*.
- [33] Julian J. McAuley and Jure Leskovec. 2012. Image Labeling on a Network: Using Social-Network Metadata for Image Classification. In *Proc. of ECCV*.
- [34] Andrew McCallum, Kamal Nigam, Jason Rennie, and Kristie Seymore. 2000. Automating the Construction of Internet Portals with Machine Learning. *Inf. Retr.* (2000).
- [35] Galileo Namata, Ben London, Lise Getoor, Bert Huang, and UMD EDU. 2012. Query-driven active surveying for collective classification. In *10th International Workshop on Mining and Learning with Graphs*.
- [36] Augustus Odena, Christopher Olah, and Jonathon Shlens. 2017. Conditional Image Synthesis with Auxiliary Classifier GANs. In *Proc. of ICML*.
- [37] Adriana Romero, Nicolas Ballas, Samira Ebrahimi Kahou, Antoine Chassang, Carlo Gatta, and Yoshua Bengio. 2015. FitNets: Hints for Thin Deep Nets. In *Proc. of ICLR*.
- [38] Peter J Rousseeuw. 1987. Silhouettes: a graphical aid to the interpretation and validation of cluster analysis. *Journal of computational and applied mathematics* (1987).
- [39] Victor Sanh, Lysandre Debut, Julien Chaumond, and Thomas Wolf. 2019. DistilBERT, a distilled version of BERT: smaller, faster, cheaper and lighter. *CoRR* (2019).
- [40] Prithviraj Sen, Galileo Namata, Mustafa Bilgic, Lise Getoor, Brian Gallagher, and Tina Eliassi-Rad. 2008. Collective Classification in Network Data. *AI Mag.* (2008).
- [41] Ravid Shwartz-Ziv and Naftali Tishby. 2017. Opening the black box of deep neural networks via information. *arXiv preprint arXiv:1703.00810* (2017).
- [42] Susheel Suresh, Pan Li, Cong Hao, and Jennifer Neville. 2021. Adversarial graph augmentation to improve graph contrastive learning. *Advances in Neural Information Processing Systems* (2021).
- [43] Petar Velickovic, William Fedus, William L. Hamilton, Pietro Liò, Yoshua Bengio, and R. Devon Hjelm. 2019. Deep Graph Infomax. In *Proc. of ICLR*.
- [44] Hongwei Wang, Jia Wang, Jialin Wang, Miao Zhao, Weinan Zhang, Fuzheng Zhang, Xing Xie, and Minyi Guo. 2018. Graphgan: Graph representation learning with generative adversarial nets. In *Proc. of AAAI*.
- [45] Kuansan Wang, Zhihong Shen, Chiyuan Huang, Chieh-Han Wu, Yuxiao Dong, and Anshul Kanakia. 2020. Microsoft academic graph: When experts are not enough. *Quantitative Science Studies* (2020).
- [46] Xiaojie Wang, Rui Zhang, Yu Sun, and Jianzhong Qi. 2018. KDGAN: Knowledge Distillation with Generative Adversarial Networks. In *Proc. of NeurIPS*.
- [47] Xiaojie Wang, Rui Zhang, Yu Sun, and Jianzhong Qi. 2021. Adversarial Distillation for Learning with Privileged Provisions. *IEEE Trans. Pattern Anal. Mach. Intell.* (2021).
- [48] Yunhe Wang, Chang Xu, Chao Xu, and Dacheng Tao. 2018. Adversarial Learning of Portable Student Networks. In *Proc. of AAAI*.

- [49] Natalie Wolchover and Lucy Reading. 2017. New theory cracks open the black box of deep learning. *Quanta Magazine* (2017).
- [50] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. 2019. How Powerful are Graph Neural Networks?. In *Proc. of ICLR*.
- [51] Keyulu Xu, Chengtao Li, Yonglong Tian, Tomohiro Sonobe, Ken-ichi Kawarabayashi, and Stefanie Jegelka. 2018. Representation Learning on Graphs with Jumping Knowledge Networks?. In *Proc. of ICML*.
- [52] Zheng Xu, Yen-Chang Hsu, and Jiawei Huang. 2018. Training Shallow and Thin Networks for Acceleration via Knowledge Distillation with Conditional Adversarial Networks. In *Proc. of ICLR Workshop*.
- [53] Cheng Yang, Jiawei Liu, and Chuan Shi. 2021. Extract the Knowledge of Graph Neural Networks and Go Beyond it: An Effective Knowledge Distillation Framework. In *Proc. of WWW*.
- [54] Chenglin Yang, Lingxi Xie, Siyuan Qiao, and Alan L. Yuille. 2019. Training Deep Neural Networks in Generations: A More Tolerant Teacher Educates Better Students. In *Proc. of AAAI*.
- [55] Yiding Yang, Jiayan Qiu, Mingli Song, Dacheng Tao, and Xinchao Wang. 2020. Distilling Knowledge From Graph Convolutional Networks. In *Proc. of CVPR*.
- [56] Chengxuan Ying, Tianle Cai, Shengjie Luo, Shuxin Zheng, Guolin Ke, Di He, Yanming Shen, and Tie-Yan Liu. 2021. Do Transformers Really Perform Bad for Graph Representation? *arXiv preprint arXiv:2106.05234* (2021).
- [57] Rex Ying, Ruining He, Kaifeng Chen, Pong Eksombatchai, William L. Hamilton, and Jure Leskovec. 2018. Graph Convolutional Neural Networks for Web-Scale Recommender Systems. In *Proc. of KDD*.
- [58] Hanqing Zeng, Hongkuan Zhou, Ajitesh Srivastava, Rajgopal Kannan, and Viktor K. Prasanna. 2020. GraphSAINT: Graph Sampling Based Inductive Learning Method. In *Proc. of ICLR*.
- [59] Wentao Zhang, Xupeng Miao, Yingxia Shao, Jiawei Jiang, Lei Chen, Olivier Ruas, and Bin Cui. 2020. Reliable Data Distillation on Graph Convolutional Network. In *Proc. of SIGMOD*.
- [60] Wentao Zhang, Ziqi Yin, Zeang Sheng, Wen Ouyang, Xiaosen Li, Yangyu Tao, Zhi Yang, and Bin Cui. 2021. Graph Attention Multi-Layer Perceptron. *CoRR* (2021).

A CODE FOR GRAPH CLASSIFICATION

Algorithm 2 GraphAKD for graph-level classification.

Require: Graphs $\{\mathcal{G}_1, \dots, \mathcal{G}_N\}$, and the pretrained teacher G^T .

Ensure: The learnt student model G^S .

```

1: while not converge do
2:   for all graph  $\mathcal{G} \in \{\mathcal{G}_1, \dots, \mathcal{G}_N\}$  do
3:      $\mathbf{H}^T, \mathbf{z}_{\mathcal{G}}^T = G^T(\mathbf{X}_{\mathcal{G}}, \mathbf{A}_{\mathcal{G}}); \mathbf{s}_{\mathcal{G}}^T = \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \mathbf{h}_v^T$ 
4:      $\mathbf{H}^S, \mathbf{z}_{\mathcal{G}}^S = G^S(\mathbf{X}_{\mathcal{G}}, \mathbf{A}_{\mathcal{G}}); \mathbf{s}_{\mathcal{G}}^S = \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \mathbf{h}_v^S$ 
5:     for all node  $v \in \mathcal{V} \subset \mathcal{G}$  do
6:       Update  $D_e$  to distinguish  $(\mathbf{h}_v^T, \mathbf{s}_{\mathcal{G}}^T)$  and  $(\mathbf{h}_v^S, \mathbf{s}_{\mathcal{G}}^T)$ 
7:       Update  $D_e$  to distinguish  $(\mathbf{h}_v^T, \mathbf{s}_{\mathcal{G}}^S)$  and  $(\mathbf{h}_v^S, \mathbf{s}_{\mathcal{G}}^S)$ 
8:       for node  $u \in \mathcal{N}(v)$  do
9:         Update  $D_e$  to distinguish  $(\mathbf{h}_v^T, \mathbf{h}_u^T)$  and  $(\mathbf{h}_v^S, \mathbf{h}_u^S)$ 
10:      Update the parameters of  $G^S$  to fool  $D_e$  via Eq. 1
11:     Update  $D_\ell$  to distinguish  $\mathbf{z}_{\mathcal{G}}^T$  and  $\mathbf{z}_{\mathcal{G}}^S$ 
12:     Update the parameters of  $G^S$  to fool  $D_\ell$  via Eq. 4
13: return  $G^S$ 

```

B DATASETS

We detail all datasets as follows.

- **Cora** [3, 34] and **CiteSeer** [40] are networks of computer science publications. Each node in the two networks represents a publication and each directed edge means a citation. Each node is annotated with a vector of binary word indicators and a label indicating the paper topic.

- **PubMed** [35] is a set of articles related to diabetes from the PubMed database. Node features are TF/IDF-weighted word frequencies and the labels specify the type of diabetes.
- **Flickr** [33, 58] is an undirected graph of images. Nodes are *images*, and edges indicate the connected two images share some common properties (e.g., geographic location, gallery, and users commented, etc.). Node features are the 500-dimensional bag-of-words representation of the images. We adopt the labels and dataset split in [58].
- **Arxiv** [23] is a directed graph that represents the citation network between all computer science arXiv papers indexed by MAG [45]. Node features are the averaged skip-gram word embeddings of the paper title and abstract.
- **Reddit** [19, 58] is an undirected graph constructed from an online discussion forum. Nodes are posts belonging to different communities and each edge indicates the connected posts are commented by the same user. We use the sparse version of Reddit dataset, which contains about 23M edges instead of more than 114M edges [12, 58]. Besides, we follow the same inductive setting in [12, 19, 58], i.e., we do not require all nodes in the graph are present during training.
- **Yelp** [58] is constructed with the data of business, users and reviews provided in the open challenge website. Each node is a customer and each edge implies the connected users are friends. Node features are Word2Vec embeddings of the user’s reviews. We follow [12, 58] to use the categories of the businesses reviewed by a user as the multi-class label of the corresponding node.
- **Products** [23] is an undirected graph that represents an Amazon product co-purchasing network. Nodes are products sold on Amazon, and edges indicate that the connected products are purchased together. Node features are bag-of-words vectors of the product descriptions, and node labels are categories of the products.
- **Molhiv** [23] and **Molpcba** [23] are two molecular property prediction datasets of different sizes. Each graph represents a molecule, where nodes are atoms, and edge are chemical bonds. Edge features indicate bond type, bond stereochemistry, and whether the bond is conjugated. Both node features and edge features are considered to predict the target molecular properties as accurately as possible.

C EXPERIMENTAL DETAILS

C.1 Implementation Details.

We implement GraphAKD in PyTorch and run it on a single NVIDIA GeForce RTX 2080Ti graphics card. Our implementation generally follows the open source codebases of deep graph library. We instantiate GraphAKD with a generator-discriminator architecture. For the generator part, we employ almost the same experimental settings including initialization, optimization and hyper-parameters as the corresponding vanilla student GNN. For convenience, we set the generator’s node embedding dimension to be the same as the teacher model’s embedding dimension. For the discriminator part, D_ℓ and D_e are uniformly initialized and all-one initialized, respectively. We sum the adversarial losses produced by D_ℓ and D_e without any tuned weight. We train the discriminator using Adam optimizer [27] with a learning rate varying from 0.05 to 0.001.

GraphAKD updates the parameters of generator and discriminator with a ratio of $k : 1$, which implies that the discriminator is update once after the generator is updated k times. We perform grid search to find a suitable k among $\{1, 5, 10, 20, 30\}$ for each dataset.

C.2 Model selection

We detail the teacher graph models as follows.

- **GCNII** [5] is an extension of the vanilla GCN [28]. Chen et al. [5] propose two effective techniques—namely initial residual and identity mapping—to deepen the graph convolution layers. GCNII increases the number of graph convolution layers from 2 to 64, while the performance on node classification is not affected by the over-smoothing issue [32, 51].
- **GAMLP** [60] is a powerful and over-parameterized graph learning model based on the reception field attention. Specifically, GAMLP [60] incorporates three principled attention mechanisms—namely smoothing attention, recursive attention, and jumping knowledge (JK) attention—into the representation learning process.
- **HIG**² is proposed as a node augmentation method to solve the graph classification task. HIG randomly selects nodes and

applies heterogeneous interpolation, then adds KL divergence constraint loss to make the distributions of augmented features be similar. For Molhiv [23], HIG built upon DeeperGCN [31] achieves state-of-the-art performance. For Molpcba [23], HIG that selects Graphormer [56] as the backbone achieves state-of-the-art performance.

We detail the student graph models as follows.

- **GCN** [28] simplifies graph convolutions by stacking layers of first-order Chebyshev polynomial filters. It has been proved to be one of the most popular baseline GNN architectures.
- **Cluster-GCN** [7] relieves the out-of-memory issue for GCN when scaling to large-scale graphs. Specifically, Cluster-GCN designs node batches based on efficient graph clustering algorithms, which leads to great computational benefits.
- **GIN** [50] generalizes the WL test and provably achieves great discriminative power among GNNs. Based on the theory of “deep multisets”, GIN learns to embed the subtrees in WL test to the low-dimensional space. By this means, GIN is able to discriminate different structures, and capture dependencies between graph structures as well.

²<https://github.com/TencentYoutuResearch/HIG-GraphClassification>.