Source Free Unsupervised Graph Domain Adaptation

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Abstract

Graph Neural Networks (GNNs) have achieved great success on a variety of tasks with graph-structural data, among which node classification is an essential one. Unsupervised Graph Domain Adaptation (UGDA) shows its practical value of reducing the labeling cost for node classification. It leverages knowledge from a labeled graph (i.e., source domain) to tackle the same task on another unlabeled graph (i.e., target domain). Most existing UGDA methods heavily rely on the labeled graph in the source domain. They utilize labels from the source domain as the supervision signal and are jointly trained on both the source graph and the target graph. However, in some real-world scenarios, the source graph is inaccessible because of either unavailability or privacy issues. Therefore, we propose a novel scenario named Source Free Unsupervised Graph Domain Adaptation (SFUGDA). In this scenario, the only information we can leverage from the source domain is the well-trained source model, without any exposure to the source graph and its labels. As a result, existing UGDA methods are not feasible anymore. To address the non-trivial adaptation challenges in this practical scenario, we propose a model-agnostic algorithm for domain adaptation to fully exploit the discriminative ability of the source model while preserving the consistency of structural proximity on the target graph. We prove the effectiveness of the proposed algorithm both theoretically and empirically. The experimental results on four cross-domain tasks show consistent improvements of the Macro-F1 score up to 0.17.

Introduction

Node classification is a crucial task on graph-structural data such as social networks (Kipf and Welling 2017), biology networks (Borgwardt et al. 2005) and so on. Recently, Graph Neural Networks have greatly advanced the performance on node classification. However, most existing studies only concentrate on how to classify well on one given graph of a specific domain, while ignoring its performance degradation when applying it to graphs from other domains due to the domain gap. For example, regarding two real-world citation networks with papers as nodes and edges represent their citations, papers published within 2010 - 2020 may have significant differences from the following two aspects: (1) Feature distribution shift as the advanced research topics and high-frequency keywords change over time. (2) Discrepancy between graph structures: due to the great success of Deep Learning, papers on machine learning and neuro-science have been more frequently cited in recent years. The above problems, i.e., feature distribution shift and graph structure discrepancy, lead to unsatisfactory performance when transferring the GNN model across graphs from different domains to handle the same task. The naive way to achieve good results on the target graph from different domain is to label the graph manually and retrain a new model from scratch, which is expensive and time-consuming. To solve this problem, unsupervised Domain Adaptation (UDA), a transfer learning technique leveraging knowledge learned from a sufficiently labeled source domain to enhance the performance on an unlabeled target domain, has raised increasing attention recently.

UDA has shown great success on image data (Tzeng et al. 2014; Ganin and Lempitsky 2015; Saito, Ushiku, and Harada 2017) and text data (Jiang and Zhai 2007; Dai et al. 2007). Recently, Unsupervised Graph Domain Adaptation (UGDA) is proposed as a new application of UDA on graph data. It utilizes different important properties of graphs, especially the structural information indicating the correlation between nodes. Generally speaking, most existing UGDA methods (Yang et al. 2020a; Shen et al. 2020; Zhang et al. 2019) utilize a joint learning framework: (1) A feature encoder is trained to align the feature distributions between the source domain and the target domain for mitigating the domain gap. (2) A classifier is trained on the encoded features with the cross entropy loss, supervised by source labels. Then the model can achieve satisfying results on the target graph with its strong discriminative ability on the aligned feature distribution.

However, a crucial requirement for these joint learning methods is the access permission to the source data, which might be problematic for both accessibility and privacy issues (Voigt and Von dem Bussche 2017). In the real-world scenario, access to the source domain is not always available (e.g., domain adaptation between two different platforms). The usage of sensitive attributes on graphs may lead to potential data leakage and other severe privacy issues. There-
fore, we propose a new scenario, **Source Free Unsupervised Graph Domain Adaptation** (SFUGDA), in which only the unlabeled target data and the GNN model trained from source data are available for adaptation.

The key challenges in this scenario are two-fold: (1) How can the model adapt well to the shifted target data distribution without accessing the source graph for aligning the feature distributions. (2) How to enhance the discriminative ability of the source model without accessing source labels for supervision. In this paper, we propose SOGA, a model agnostic SOurce free domain Graph Adaptation algorithm, which could enable the GNN model trained on the labeled source graph to perform on the unlabeled target graph. SOGA addresses these challenges by the following two components: (1) Structure Consistency (SC) optimization objective is proposed to adapt the source model to the shifted target data distribution by leveraging the structure information of the target graph. To be specific, the SC objective can guide the model to preserve the structural consistency, for which node pairs with high structural proximity should have similar predictions. (2) To enhance the discriminative ability of the source model, we propose Information Maximization (IM) optimization objective that maximizes the mutual information between the target graph and its corresponding output. We prove that IM can improve the confidence of prediction and raise the lower bound of the AUC metric.

Moreover, our algorithm is model agnostic so that it can be applied to arbitrary GNN models. This property is of great necessity because we cannot determine the source model architecture and its training procedure.

In summary, the main contributions of our work are as follows:

• We first articulate a new scenario called SFUGDA when we have no access to the source graph and its labels. To the best of our knowledge, this is the first work in SFUGDA.

• We propose a model agnostic unsupervised algorithm called SOGA to tackle the challenges in SFUGDA. It can both adapt the source model to the shifted target distribution and enhance its discriminative ability with a theoretical guarantee.

• Extensive experiments are conducted on real-world datasets. Our SOGA outperforms all the baselines on four cross-domain tasks, and the largest improvement on Macro-F1 score is 0.17. Moreover, the evaluation results verify the model agnostic property as SOGA can be applied with different representative GNN models successfully.

**Related Work**

Unsupervised Graph Domain Adaptation (UGDA) aims to transfer the knowledge learnt on a labeled graph from the source domain to an unlabeled graph from the target domain tackling the same task. Most existing UGDA methods aim to mitigate the domain gap by aligning the source feature distribution and the target one. According to different alignment approaches, they can be roughly divided into two categories.(1) Distance based methods like (Shen et al. 2020; Yang et al. 2020a) incorporate maximum mean discrepancy (MMD) (Borgwardt et al. 2006) as a domain distance loss to match the distribution statistical moments at different order. (2) Domain adversarial methods follow the guidance of adversarial training, which confuse generated features across the source domain and the target one to mitigate the domain discrepancy. DANE (Zhang et al. 2019) adds an adversarial regularizer inspired by LSGAN (Mao et al. 2017), while UDAGCN (Wu et al. 2020) uses Gradient Reversal Layer (Ganin and Lempitsky 2015) and domain adversarial loss to extract cross-domain node embedding.

However, all the above UGDA methods heavily rely on access to source data, which leads to failure in the SFUGDA scenario where source data is not available anymore.

In computer vision, Source Free Unsupervised Domain Adaptation is a new research task with practical value. Most of the existing studies focus on different strategies to generate pseudo labels on image data inspired by (Saito, Ushiku, and Harada 2017). SHOT (Liang, Hu, and Feng 2020) utilizes the Deep Cluster algorithm to assign cleaner pseudo labels iteratively with a global view on the target domain. PrDA (Kim et al. 2020) uses a set-to-set distance to filter confident pseudo labels. MA (Li et al. 2020) focuses on how to adapt the feature distribution on the target domain by generating similar feature samples from a GAN-based model.

However, the above methods designed for image data are not suitable for graph-structural data. Since graph node samples are naturally structured by dependencies (i.e., edges) between nodes, strategies focusing on i.i.d. data, such as images, cannot be well adopted. For example, even when the feature distribution stays the same, graph-based data may still suffer from domain gaps between various structure patterns. Thus, methods for SFUGDA should be able to handle structural dependencies well. It is worth noting that although the graph structure leads to new challenges, using it to help with adaptation is intuitive and promising. The various properties of the graph structure, such as structural proximity, could help the adaptation if modeled properly.

**Preliminary and Problem Definition**

**Definition 1 (Node Classification)** Node classification is a task to learn a conditional probability $Q(Y|G;\Theta)$ to distinguish the category of each unlabeled node on a single graph $G = (V, E, X, Y)$, where $\Theta$ is the model parameters. $V = \{v_1, \cdots, v_n\}$ is the node set with $n$ nodes and $E$ is the edge set. $X$ is the node feature set, $Y$ is the partial observed node label set which satisfies $\forall y_i \in Y, y_i \in \{1, k\}$, and $k$ is the number of categories.

Node classification differs from typical classification tasks since the latter usually assumes that different samples are i.i.d (independent identical distribution), whereas samples in the former case are correlated through edges. In deep learning, we use Graph Neural Networks (GNNs) (Hamilton, Ying, and Leskovec 2017) to model $Q(Y|G;\Theta)$ for capturing such relationships, where the predicted conditional distribution is usually decomposed for the performance reason, i.e., $Q(Y|G;\Theta) = \prod_{v_i \in V} q(y_i|x_i, N_i;\Theta)$ and $N_i$ is
the neighbor information of the node \( v_i \). Followed by the GNN model, Cross Entropy is usually adopted as the loss function:

\[
E_{v_i \sim p(v)} \left[ -\sum_{y=1}^{k} p(y|x_i,N_i) \log q(y|x_i,N_i; \Theta) \right], \quad (1)
\]

where \( p(v) \) is the prior distribution and \( p(y|x,N) \) is the oracle conditional distribution.

According to the Def. 1, a typical node classification task is defined on a single graph with partial supervision. To better leverage the knowledge from a labeled graph (namely source graph) to tackle the same node classification task on another unlabeled graph (namely target graph), Unsupervised Graph Domain Adaptation (UGDA) (Zhang et al., 2019) is proposed and defined as follows:

**Definition 2 (Unsupervised Graph Domain Adaptation)**

Unsupervised Graph Domain Adaptation aims to learn a node classification model \( \mathcal{Q}(Y|G; \Theta) \) based on a source graph \( G_s = (V_s, E_s, X_s, Y_s) \), and the model performs well on a target graph \( G_t = (V_t, E_t, X_t, Y_t) \) where the following conditions need to be satisfied: (1) \( Y_t \) is unknown, (2) edges of both graphs are homogeneous, (3) node features express the same meaning, (4) exactly the same set of node labels are shared, and (5) the prediction tasks are almost same, i.e., the oracle conditional distributions for source graph \( p_s(y|x,N) \) and for target graph \( p_t(y|x,N) \) are almost equal.

According to the Eq. (1), since \( p_s(y|x,N) \) and \( p_t(y|x,N) \) are almost equal, the main challenges for UGDA are the misalignment between prior distributions \( p_s(v) \) of the source graph and \( p_t(v) \) of the target graph. Thus, all of the existing works try to align these two distributions as a part of their techniques, which heavily relies on access to the source data. Considering privacy constraints, we formally define the following research problem.

**Problem Statement: Source Free Unsupervised Graph Domain Adaptation** aims to learn a well-performed node classification model \( \mathcal{Q}(Y|G; \Theta_t) \) on the target graph \( G_t \), while the accessible information only contains a well trained source model \( \mathcal{Q}(Y|G; \Theta_s) \) and \( G_s \) without any supervision. The source model architecture could be an arbitrary GNN as we could not determine.

**Methodology**

**Overall Framework**

As shown in Fig. 1 the whole framework is composed of two components, i.e., inaccessible training procedure on the source graph and model adaptation procedure on the target graph. Our work focuses on the latter procedure without any assumption on the first procedure such as the GNN model architecture, the prior distribution of the source data, the optimization method and so on.

To adapt the given source model, we design two optimization objectives. One is to leverage the information stored in the given model, namely Information Maximization (IM) optimization objective, the other is to utilize the target graph structure, namely the Structure Consistency (SC) optimization objective, to enhance the discriminative ability of the model on the target graph. The overall objective is defined as follows:

\[
\max \mathcal{L} = \mathcal{L}_{IM} + \mathcal{L}_{SC} \quad (2)
\]

More details about two objectives will be presented in the following sections.

**Information Maximization Optimization Objective**

We define the IM objective as the mutual information between the input and the output of the model for enhancing the discriminative ability:

\[
\mathcal{L}_{IM} = MI(V_t, \hat{Y}_t) = -H(\hat{Y}_t|V_t) + H(\hat{Y}_t), \quad (3)
\]

where \( \hat{Y}_t \) is the prediction on target domain and \( V_t \) is information of input nodes containing node feature \( X_t \) and information from node neighbor \( X_e \). \( MI(\cdot, \cdot) \) is the mutual information, and \( H(\cdot) \) and \( H(\cdot|\cdot) \) are entropy and conditional entropy, respectively. The objective can be divided into two parts, one is to minimize the conditional entropy and the other is to maximize the entropy of the marginal distribution of \( \hat{Y}_t \). We will introduce the implementation and the idea behind such a design for these two parts, respectively.
Conditional Entropy  The conditional entropy can be implemented by the following equation:

$$H(\hat{Y}_t | X_t) = \mathbb{E}_{x_t \sim p_t(x)} \left[ - \sum_{y=1}^{k} q(y|x_t, N_t; \Theta) \log q(y|x_t, N_t; \Theta) \right]$$  \hspace{1cm} (4)$$

which can be easily optimized by sampling nodes from the prior distribution $p_t(x)$ on the target graph.

This objective strengthens the confidence of the prediction on the target graph, just like using pseudo labels. Theoretically, we have the following Lemma:

**Lemma 1** When the source model is optimized by the objective Eq. (4) with a gradient descent optimizer and the capacity of the source model is sufficiently large, for each node $v_i$ on the target graph, the predicted conditional distribution $q(y|x_t, N_t; \Theta)$ will converge to a vector $q$, where the value of $q$ elements will be $\frac{1}{N}$, and the other elements will be 0. $q$ is determined by the number of categories with the maximum probability value predicted by the original source model $q(y|x_t, N_t; \Theta)$. Similarly, the non-zero positions of $q$ are the indices of categories with the maximum probability value.

In most cases, $q$ equals one, and hence the prediction $q$ will be a one-hot encoding vector. The proof will be listed in the Appendix. For further verifying the effectiveness of the objective, we theoretically analyze its effect to the Area Under Curve (AUC) metric on a binary classification problem:

**Lemma 2** When the original source model is trained for a binary classification problem with the discriminative ability of $r_p$ and $r_n$ accuracy for positive samples and negative samples on the target graph respectively, the lower bound of AUC can be raised from $r_p \times r_n$ to $\frac{1}{2}(r_p + r_n)$ by using the conditional entropy objective Eq. (4).

The proof will be listed in the Appendix. Raising the lower bound of AUC from $r_p \times r_n$ to $\frac{1}{2}(r_p + r_n)$ is significant, for instance, if $r_p = r_n = 0.7$, then the absolute improvement will be 0.21.

Entropy of Marginal Distribution  The entropy of marginal distribution $\mathbb{E}_t$ can be calculated as:

$$H(\hat{Y}_t) = - \sum_y q(y) \log q(y),$$  \hspace{1cm} (5)$$

where $q(y) = \mathbb{E}_{v_t \sim p_t(v)} [q(y|x_t, N_t; \Theta)]$.

This objective is designed for avoiding concentrating predictions on the same category. If we have additional knowledge about the prior distribution of labels $p_t(y)$ on the target graph, a KL-divergence objective can be a replacement for the Eq. (5):

$$KL(p_t(y) || q(y)) = \sum_y p_t(y) \log \frac{p_t(y)}{q(y)}. $$  \hspace{1cm} (6)$$

Structure Consistency Optimization Objective  Since we do not have any supervision on the target graph, leveraging the structural information of the target graph becomes the key solution. Thus, we design a Structure Consistency (SC) objective based on two hypotheses, i.e., (1) the probability of sharing the same label for local neighbors is relatively high; (2) the probability of sharing the same label for the nodes with the same structural role is relatively high. These two hypotheses are commonly used in lots of Graph Embedding works (Perozzi, Al-Rfou, and Skiena 2014 Grover and Leskovec 2016 Ribeiro, Saverese, and Figueiredo 2017) where several structure preserving losses based on the above hypotheses are designed for learning node representations.

To be specific, the SC objective is designed as follows:

$$\max - \sum_{v_i \in \mathbb{V}_t} \sum_{v_j \in \mathbb{V}_t} \lambda_1 H(p_t^{(i,j)}, q_t^{(i,j)}) + \lambda_2 H(p_s^{(i,j)}, q_c^{(i,j)}),$$  \hspace{1cm} (7)$$

where $H(\cdot, \cdot)$ is the cross entropy, $\lambda_1$ and $\lambda_2$ are hyperparameters to control the importance of two sub-objectives, and $p_t^{(i,j)}$, $p_s^{(i,j)}$, and $q_c^{(i,j)}$ are Bernoulli distributions for each node pair. $p_t^{(i,j)}$ and $p_s^{(i,j)}$ are the oracle distributions defined by the local neighbor similarity and structural role similarity. $q_c^{(i,j)}$ is the prediction vector for the $i$th node, and $\langle \cdot, \cdot \rangle$ is a similarity function within the range of $[0, 1]$.

Specifically, if $(v_i, v_j) \in \mathbb{E}_t$, then $p_t^{(i,j)} = 1$, otherwise $p_t^{(i,j)} = 0$. Similarly, if $(v_i, v_j) \in \mathbb{S}_t$ then $p_s^{(i,j)} = 1$, otherwise $p_s^{(i,j)} = 0$, where $\mathbb{S}_t$ is a set containing the top $\kappa$ structurally similar node pairs. We follow struc2vec (Ribeiro, Saverese, and Figueiredo 2017) to define the structural similarity that can be roughly understood as calculating the similarity of the sorted degree sequences around two given nodes. In order to reduce the number of hyperparameters, $\kappa$ is set as the size of the edge set $|\mathbb{E}_t|$ by default in all of our experiments while it can be adjusted as needed. $f(\hat{Y}_t, \hat{Y}_t)$ is defined as $\sigma(\langle \hat{Y}_t, \hat{Y}_t \rangle)$ without any additional parameter where $\sigma(x) = 1/(1+e^{-x})$ and $\langle \cdot, \cdot \rangle$ is the inner product.

Finally, we use the negative sampling technique to avoid calculating the objective function for each node pair for acceleration. The final SC objective is formulated as follows:

$$L_{SC} = \lambda_1 \sum_{(v_i, v_j) \in \mathbb{E}_t} \log J_{ij} - \epsilon \cdot \mathbb{E}_{v_n \sim p_n} \log J_{in}$$

$$+ \lambda_2 \sum_{(v_i, v_j) \in \mathbb{S}_t} \log J_{ij} - \epsilon \cdot \mathbb{E}_{v_n \sim p_n} \log J_{in} $$  \hspace{1cm} (8)$$

where $J_{ij} = \sigma(\langle \hat{Y}_t^{(i)}, \hat{Y}_t^{(j)} \rangle)$, $p_n$ and $p_n'$ are the distributions for negative samples, and $\epsilon$ is the number of negative samples. We use uniform distributions for $p_n$ and $p_n'$ while they can be adjusted if needed. $\epsilon$ is set as 5 in our experiments.

Combining the objectives Eq. (2), Eq. (4), Eq. (5), and Eq. (8), we obtain the overall differentiable objective of the model parameters $\Theta$. We adopt the adaptive moment estimation method (i.e., Adam) (Kingma and Ba 2015) to optimize the overall objective.
Table 1: Statistics of the experimental datasets

| Datasets | # Nodes | # Edges | # Features | # Labels |
|----------|---------|---------|------------|----------|
| DBLPv8   | 5578    | 7341    | 7537       | 6        |
| ACMv9    | 7410    | 11135   | 7537       | 6        |
| ACM-D    | 1500    | 4960    | 300        | 4        |
| ACM-S    | 1500    | 759     | 300        | 4        |

Experiments

We conduct experiments on real-world datasets to study our proposed algorithm SOGA. We design a series of experiments to answer the following research questions:

- **RQ1**: How does the GCN-SOGA compare with other state-of-the-art node classification methods? (GCN-SOGA indicates SOGA applying on the default source domain model: GCN)

- **RQ2**: Can SOGA still achieve satisfactory results when being applied to different source domain GNN models other than GCN?

- **RQ3**: How do different components in SOGA contribute to its effectiveness?

- **RQ4**: How do different choices of hyperparameters \( \lambda_1 \) and \( \lambda_2 \) affect the performance of SOGA?

**Experiment Settings**

**Datasets.** We use two groups of real-world graph datasets for our experiments. The detailed statistics of these datasets are illustrated on Tab. [1]. DBLPv8 and ACMv9 are the first group of citation networks collected by [Zhang et al., 2019] from arnetMiner ([Tang et al., 2008]). Their domain gap mainly comes from different origins (DBLP, ACM respectively) and different publication time periods, i.e. DBLPv8 (after 2010), ACMv9 (between years 2000 and 2010). ACM-D (Dense) and ACM-S (Sparse) are the second group of citation networks from the ACM dataset collected by [Yang et al., 2020b]. Their domain gap mainly comes from their structural difference as the number of edges per node of ACM-D is 6.5 times larger than ACM-S. More details about datasets are shown in the Appendix.

**Baselines.** We select some state-of-the-art node classification methods as baselines to verify the effectiveness of our SOGA.

They are (1) Graph embedding methods including DeepWalk, LINE, and Node2vec ([Perozzi, Al-Rfou, and Skiena, 2014] [Tang et al., 2015] [Grover and Leskovec, 2016]). (2) GNN methods including GCN, GraphSAGE, and GAT ([Kipf and Welling, 2017] [Hamilton, Ying, and Leskovec, 2017] [Velickovic et al., 2018]). (3) UGDA methods including DANE and UDAGCN ([Zhang et al., 2019] [Wu et al., 2020]). Notice that DANE and UDAGCN utilize GCN as encoder.

**Reproducibility Settings.** To ensure the validity of experiments, each source dataset is randomly split into training and validation sets with the ratio 4:1. All the experimental results are averaged over 5 runs with different random seeds [1, 3, 5, 7, 9]. Notice that, for a fair comparison, we set the hyperparameters \( \lambda_1 \) and \( \lambda_2 \) in SOGA to the default value: 1, without any additional hyperparameter search. We will provide further hyperparameter sensitivity analysis in the later section.

For baseline methods, we apply the large-scale hyperparameter grid search on GraphSAGE, GAT, DANE, and UDAGCN. Our reproducing settings are different from some baseline methods reported in their papers like five different random seeds and the validation partition. After checking with their authors, we consider that this may induce a different experimental result from the one in the original paper. The details of hyperparameter, hardware, and software settings can be found in the appendix.

**Evaluation Methods.** We conduct the stability evaluation to verify the stability of different methods. The main reason is that models trained with different epochs may have large performance differences. Generally speaking, there should be an additional validation set used to select the best training epoch. However, the validation set is not available on the unlabeled target domain. Therefore, it is of great importance to evaluate the stability of model performance on the target domain. With good stability, it is easy for models to achieve satisfying performance for stability prevents significant performance fluctuations after convergence. On the contrary, the performance of the unstable method will drop quickly after reaching the peak or fluctuate continuously. Concretely speaking, we (1) plot the line chart describing the Macro-F1 score on the target domain in each training epoch. (2) calculate the mean and standard deviation of the Macro-F1 scores on the target domain across the epochs. To avoid the initial fluctuation before convergence, we choose the epochs after the first \( n \) ones for calculation (set to 20 by default). A flat curve with little fluctuation indicates good stability, similar to the statistics results with the large expectation and small standard deviation.

**Results and Analysis**

**Overall Results (RQ1).** The experimental results of all baseline methods and GCN-SOGA (applying SOGA on GCN) on Macro-F1 score are illustrated on Tab. [2]. Results on the Micro-F1 score are shown in the Appendix. Notice that UGDA methods other than GCN-SOGA require additional information, i.e., the access permission to the source graph. Therefore, these methods are not feasible in the SFUGDA scenario. When reproducing these methods, we give them additional access to the source graph and its labels.

Experimental results on four cross-domain tasks show consistent improvements on Macro-F1 score, with a maximum gain of 0.17. From the perspective of different cross-domain tasks, we can find the performance on the DBLPv8 \( \rightarrow \) ACMv9 and ACM-D \( \rightarrow \) ACM-S is much lower than the other two tasks which indicates its difficulties. We will mainly focus on these two difficult tasks and conduct further experiments on them in the later section. From the perspective of different methods, we can see that the graph embedding methods perform poorly, probably for the lack of preserving cross-graph similarity. Though the relative position between nodes is preserved by structural proximity, similar nodes may have entirely different absolute positions in different graphs. GNN methods perform better for the message...
passing mechanism like graph convolution can preserve the similarity of nodes if their local sub-graphs are similar as proven by (Donnat et al. 2018).

Moreover, we conduct stability evaluation on UGDA methods to explicitly show the strength of GCN-SOGA in detail. From Fig. 2, we can see that GCN-SOGA in red illustrates stability with high Macro-F1 score, while DANE in blue reveals a slower convergence. The performance of UDAGCN in green illustrates a violent fluctuation. It will cause great difficulty to decide which epoch to stop the training procedure.

**Effectiveness of SOGA on different GNN models (RQ2).** To demonstrate the efficacy and the model agnostic property of our proposed SOGA, we evaluate SOGA with different representative GNN models. Specifically, we combine SOGA with GCN, GraphSAGE and GAT, named GCN-SOGA, GraphSAGE-SOGA, and GAT-SOGA, respectively. The experimental results are shown in Tab. 2.

| Methods   | Group1 | Group2 |
|-----------|--------|--------|
|           | DBLPv8→ACMv9 | ACMv9→DBLPv8 | ACM-D→ACM-S | ACM-S→ACM-D |
| DeepWalk  | 0.135 ± 0.012 | 0.112 ± 0.012 | 0.183 ± 0.012 | 0.237 ± 0.012 |
| LINE      | 0.135 ± 0.012 | 0.112 ± 0.012 | 0.183 ± 0.012 | 0.237 ± 0.013 |
| Node2vec  | 0.128 ± 0.023 | 0.080 ± 0.018 | 0.134 ± 0.012 | 0.219 ± 0.014 |
| GCN       | 0.583 ± 0.002 | 0.668 ± 0.015 | 0.685 ± 0.005 | 0.796 ± 0.030 |
| GraphSAGE | 0.418 ± 0.057 | 0.752 ± 0.010 | 0.407 ± 0.042 | 0.743 ± 0.015 |
| GAT       | 0.227 ± 0.004 | 0.745 ± 0.036 | 0.681 ± 0.006 | 0.804 ± 0.007 |
| DANE      | 0.614 ± 0.017 | 0.452 ± 0.020 | 0.722 ± 0.004 | 0.821 ± 0.004 |
| UDAGCN    | 0.626 ± 0.070 | 0.696 ± 0.009 | 0.665 ± 0.010 | 0.822 ± 0.018 |
| GCN-SOGA  | 0.636 ± 0.003 | 0.928 ± 0.018 | 0.733 ± 0.005 | 0.841 ± 0.009 |

Figure 2: The comparison of learning curves of different UGDA methods on the DBLPv8 → ACMv9 task. The x axis denotes the training epoch, whereas the y axis denotes the Macro-F1 score on the target graph.

Figure 3: The comparison of learning curves of GCN-SOGA and its variants on the DBLPv8 → ACMv9 task. The x axis denotes the training epoch, whereas the y axis denotes the Macro-F1 score in the target graph.

most the same with the best result: 0.736. It indicates that SOGA can help to achieve a comparable good performance regardless of the poor origin GNN model.

**Ablation Study (RQ3).** We conduct an ablation study to investigate the contribution of each component. First, we verify the effectiveness of the indispensable component: the well-trained source model. Experiments show that only applying two unsupervised objectives with a randomly initialized model leads to failure where the highest Macro-F1 score among all tasks is no more than 0.20, similar to random guess. Therefore, it is of great significance to utilize the primary discriminative ability of the well-trained source model.

Then we further explore the different roles of two unsupervised objectives by stability evaluation. We propose the variants of our proposed SOGA called SOGA-IM and SOGA-SC corresponding to the algorithm trained with only IM or SC objective, respectively. The curves on DBLPv8 → ACMv9 are shown in Fig. 3. We can find the following observations: (1) For our GCN-SOGA in red, it shows significant performance gain and strong stability with a flat curve after the first few epochs. (2) For GCN-SOGA-IM in blue, there has been an evident drop after reaching the peak around 10 epochs. This unstable phenomenon reveals the difficulty and uncertainty to achieve a good result. (3) For GCN-SOGA-SC in green, the curve is smooth after reaching the peak with only a little gain. Overall speaking, IM
Table 3: The performance comparison on the Macro-F1 score of different GNN models with or without applying SOGA.

| Methods  | Group1          | Group2          |
|----------|-----------------|-----------------|
|          | DBLPv8→ACMv9  | ACMv9→DBLPv8  | ACM-D→ACM-S | ACM-S→ACM-D |
| GCN      | 0.583 ± 0.002  | 0.668 ± 0.015  | 0.685 ± 0.005 | 0.796 ± 0.030 |
| GCN-SOGA | 0.636 ± 0.003  | 0.928 ± 0.018  | 0.736 ± 0.007 | 0.838 ± 0.008 |
| GraphSAGE| 0.418 ± 0.057  | 0.752 ± 0.010  | 0.407 ± 0.042 | 0.743 ± 0.015 |
| GraphSAGE-SOGA | 0.594 ± 0.086  | 0.947 ± 0.002  | 0.734 ± 0.006 | 0.820 ± 0.020 |
| GAT      | 0.227 ± 0.004  | 0.745 ± 0.036  | 0.681 ± 0.006 | 0.804 ± 0.007 |
| GAT-SOGA | 0.592 ± 0.086  | 0.946 ± 0.001  | 0.736 ± 0.006 | 0.824 ± 0.027 |

Table 4: Statistical results of stability evaluation on GCN-SOGA and its variants. The reported results are expectation and standard derivation of Macro-F1 scores on the training procedure after 20 epochs.

| Methods  | Group1          | Group2          |
|----------|-----------------|-----------------|
|          | DBLPv8→ACMv9  | ACMv9→DBLPv8  | ACM-D→ACM-S | ACM-S→ACM-D |
| GCN-SOGA | 0.6151 ± 0.0005 | 0.9382 ± 0.0002 | 0.7323 ± 0.0017 | 0.8244 ± 0.0056 |
| GCN-SOGA-IM | 0.5823 ± 0.0007 | 0.9406 ± 3.6397 | 0.7227 ± 0.0170 | 0.8263 ± 0.0060 |
| GAT-SOGA-SC | 0.5576 ± 0.0004 | 0.6491 ± 0.0653 | 0.7160 ± 0.0026 | 0.3182 ± 0.0013 |

Figure 4: Performances on the target domain with different choices of $\lambda_1$ and $\lambda_2$. The orange solid line and the corresponding shadow indicate the mean value and the standard deviation of the results, respectively, when $\lambda_2 > \lambda_1$, which means more attention on the neighborhood. The blue ones are similar except $\lambda_1 > \lambda_2$.

and SC objectives show a complementary effect. IM could enhance the discriminative ability to achieve better results while SC takes charge of maintaining stability to keep the good performance consistently in the training procedure.

The detailed statistical results of stability evaluation on all tasks are illustrated on Tab. 4. We can find that on the easy tasks like ACMv9 → DBLPv8, GCN-SOGA-IM can achieve similar results with GCN-SOGA. However, on more difficult tasks, which are DBLPv8 → ACMv9 and ACM-D → ACM-S, GCN-SOGA could achieve more significant and stable improvement than GCN-SOGA-IM. It further indicates the necessity of SC especially on more difficult tasks, which are DBLPv8, ACM-S, GCN-SOGA-IM can achieve more significant performance than GCN-SOGA. However, on more difficult tasks, which are DBLPv8 → ACMv9 and ACM-D → ACM-S, GCN-SOGA could achieve more significant and stable improvement than GCN-SOGA-IM. It further indicates the necessity of SC especially on more difficult task.

Hyperparameter sensitivity. (RQ4) Though we have achieved impressive results with the default hyperparameter setting as $\lambda_1 = \lambda_2 = 1$, it is still noteworthy to examine how the different choices of $\lambda_1$ and $\lambda_2$ affect the performance of SOGA. Specifically, we focus on the Macro-F1 score performance of GCN-SOGA as well as its stability in the training procedure with different hyperparameter settings. Revolving around this goal, we conduct neighborhood evaluation and structure role evaluation which spare larger weight to $\lambda_1$ and $\lambda_2$, respectively. For neighborhood evaluation, we run experiments 10 times with different choices where $\lambda_1 > \lambda_2$. The details of hyperparameter choices are shown in the Appendix. Then we plot the line chart describing the Macro-F1 score on the target domain after the first 10 training epochs, which skips initial fluctuations for brevity. Structure role evaluation is similar except $\lambda_2 > \lambda_1$. The experimental results on DBLPv8 → ACMv9 and ACM-D → ACM-S are illustrated in Fig. 4. The solid line is the average result of the 10 experiments while the shadow one represents the corresponding standard deviation. We can see that curves stay in a high level and the shadow area is narrow, which indicates good performance with stability in the training procedure. We can conclude that our performance is robust to different choices of $\lambda_1$ and $\lambda_2$.

Conclusion

In this work, we articulate a new scenario called Source Free Unsupervised Graph Domain Adaptation (SFUGDA) with no access to the source graph because of practical reasons like privacy policies. Most existing methods cannot work
well as it is impossible for feature alignment anymore. Facing the challenges in SFUGDA, we propose our algorithm SOGA, which could be applied to arbitrary GNN model by adapting to the shifted target domain distribution and enhancing the discriminative ability of the source model.
References

Borgwardt, K. M.; Gretton, A.; Rasch, M. J.; Kriegel, H.-P.; Schölkopf, B.; and Smola, A. J. 2006. Integrating structured biological data by kernel maximum mean discrepancy. Bioinformatics, 22(14): e49–e57.

Borgwardt, K. M.; Ong, C. S.; Schönauer, S.; Vishwanathan, S.; Smola, A. J.; and Kriegel, H.-P. 2005. Protein function prediction via graph kernels. Bioinformatics, 21(suppl_1): i47–i56.

Dai, W.; Xue, G.-R.; Yang, Q.; and Yu, Y. 2007. Co-clustering based classification for out-of-domain documents. In Association for Computing Machinery Special Interest Group on Knowledge Discovery and Data Mining, 210–219.

Donnat, C.; Zitnik, M.; Hallac, D.; and Leskovec, J. 2018. Learning structural node embeddings via diffusion wavelets. In Association for Computing Machinery Special Interest Group on Knowledge Discovery and Data Mining, 1320–1329.

Ganin, Y.; and Lempitsky, V. 2015. Unsupervised domain adaptation by backpropagation. In International Conference on Machine Learning, 1180–1189. PMLR.

Grover, A.; and Leskovec, J. 2016. node2vec: Scalable feature learning for networks. In Association for Computing Machinery Special Interest Group on Knowledge Discovery and Data Mining, 855–864.

Hamilton, W. L.; Ying, R.; and Leskovec, J. 2017. Inductive representation learning on large graphs. In International Conference on Neural Information Processing Systems, 1025–1035.

Jiang, J.; and Zhai, C. 2007. Instance weighting for domain adaptation in NLP. In Association of Computational Linguistics, 264–271.

Kim, Y.; Cho, D.; Panda, P.; and Hong, S. 2020. Progressive Domain Adaptation from a Source Pre-trained Model. arXiv preprint arXiv:2007.01524.

Kingma, D. P.; and Ba, J. 2015. Adam: A method for stochastic optimization. International Conference on Learning Representations.

Kipf, T. N.; and Welling, M. 2017. Semi-supervised classification with graph convolutional networks. International Conference on Learning Representations.

Li, R.; Jiao, Q.; Cao, W.; Wong, H.-S.; and Wu, S. 2020. Model adaptation: Unsupervised domain adaptation without source data. In IEEE/CVF Conference on Computer Vision and Pattern Recognition, 9641–9650.

Liang, J.; Hu, D.; and Feng, J. 2020. Do we really need to access the source data? source hypothesis transfer for unsupervised domain adaptation. In International Conference on Machine Learning, 6028–6039. PMLR.

Mao, X.; Li, Q.; Xie, H.; Lau, R. Y.; Wang, Z.; and Paul Smolley, S. 2017. Least squares generative adversarial networks. In IEEE International Conference on Computer Vision, 2794–2802.

Perozzi, B.; Al-Rfou, R.; and Skiena, S. 2014. Deepwalk: Online learning of social representations. In Association for Computing Machinery Special Interest Group on Knowledge Discovery and Data Mining, 701–710.

Ribeiro, L. F.; Saverese, P. H.; and Figueiredo, D. R. 2017. struc2vec: Learning node representations from structural identity. In Association for Computing Machinery Special Interest Group on Knowledge Discovery and Data Mining, 385–394.

Saito, K.; Ushiku, Y.; and Harada, T. 2017. Asymmetric tri-training for unsupervised domain adaptation. In International Conference on Machine Learning, 2988–2997. PMLR.

Shen, X.; Dai, Q.; Mao, S.; Chung, F.-I.; and Choi, K.-S. 2020. Network together: Node classification via cross-network deep network embedding. IEEE Transactions on Neural Networks and Learning Systems, 32(5): 1935–1948.

Tang, J.; Qu, M.; Wang, M.; Zhang, M.; Yan, J.; and Mei, Q. 2015. Line: Large-scale information network embedding. In International Conference on World Wide Web, 1067–1077.

Tang, J.; Zhang, J.; Yao, L.; Li, J.; Zhang, L.; and Su, Z. 2008. Arnetminer: extraction and mining of academic social networks. In Association for Computing Machinery Special Interest Group on Knowledge Discovery and Data Mining, 990–998.

Tzeng, E.; Hoffman, J.; Zhang, N.; Saenko, K.; and Darrell, T. 2014. Deep domain confusion: Maximizing for domain invariance. Computer Science.

Veličković, P.; Cucurull, G.; Casanova, A.; Romero, A.; Lio, P.; and Bengio, Y. 2018. Graph attention networks. ArXiv preprint arXiv:1710.10903.

Voigt, P.; and Von dem Bussche, A. 2017. The eu general data protection regulation (gdpr). A Practical Guide, 1st Ed., Cham: Springer International Publishing, 10: 3152676.

Wu, M.; Pan, S.; Zhou, C.; Chang, X.; and Zhu, X. 2020. Unsupervised domain adaptive graph convolutional networks. In The Web Conference 2020, 1457–1467.

Yang, S.; Song, G.; Jin, Y.; and Du, L. 2020a. Domain Adaptive Classification on Heterogeneous Information Networks. In International Joint Conference on Artificial Intelligence, 1410–1416.

Yang, S.; Wang, Y.; van de Weijer, J.; Herranz, L.; and Jui, S. 2020b. Unsupervised domain adaptation without source data by casting a bait. Computer Vision and Pattern Recognition.

Zhang, Y.; Song, G.; Du, L.; Yang, S.; and Jin, Y. 2019. Dane: Domain adaptive network embedding. International Joint Conference on Artificial Intelligence, 4362–4368.