Gradient-Based Clean Label Backdoor Attack to Graph Neural Networks

Ryo Meguro[1], Hiroya Kato[2], Shintaro Narisada[2], Seira Hidano[2], Kazuhide Fukushima[2], Takuo Suganuma[1] and Masahiro Hiji[1]
[1]*Tohoku University, Miyagi, Japan*
[2]*KDDI Research, Inc., Saitama, Japan*

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Abstract: Graph neural networks (GNNs) can obtain useful information from graph structured data. Although its great capability is promising, GNNs are vulnerable to backdoor attacks, which plant a marker called trigger in victims' models to cause them to misclassify poisoned data with triggers into a target class. In particular, a clean label backdoor attack (CLBA) on the GNNs remains largely unexplored. Revealing characteristics of the CLBA is vital from the perspective of defense. In this paper, we propose the first gradient based CLBA on GNNs for graph classification tasks. Our attack consists of two important phases, the graph embedding based pairing and the gradient based trigger injection. Our pairing makes pairs from graphs of the target class and the others to successfully plant the backdoor in the target class area in the graph embedding space. Our trigger injection embeds triggers in graphs with gradient-based scores, yielding effective poisoned graphs. We conduct experiments on multiple datasets and GNN models. Our results demonstrate that our attack outperforms the existing CLBA using fixed triggers. Our attack surpasses attack success rates of the existing CLBA by up to 50%. Furthermore, we show that our attack is difficult to detect with an existing defense.

1 INTRODUCTION

Graph structured data appear in various fields, such as molecular structures, social networks, and web analysis. In recent years, GNNs have been researched and utilized in fields such as security and commerce, indicating their broad potential applications to graph structured data. For example, research has been conducted on the detection of fake news (Zhang et al., 2020) and malware detection based on call graphs (Feng et al., 2020). There are also many studies on the application of GNNs in recommendation systems (RSs), demonstrating the advantages of GNN-based RSs over traditional methods (Qiu et al., 2020; Yang et al., 2021; Guo et al., 2021).

However, as with other machine learning systems, GNNs have been recognized to be vulnerable to adversarial examples and poisoning attacks (Chen et al., 2020; Zügner et al., 2018; Kwon et al., 2019; Jiang et al., 2022). Furthermore, studies on backdoor attacks on GNNs (Zhang et al., 2021; Xi et al., 2021; Yang et al., 2022; Xu and Picek, 2022) have been presented recently. The backdoor attacks plant a marker called trigger in victims' models to cause them to misclassify poisoned data with triggers into a target class. In the context of graph domains, the trigger denotes modified information such as edges or node features in the graph. Backdoored models behaves normally when clean data is given. This is why the backdoor attack is highly favorable for attackers in terms of stealthiness. Consequently, attackers may conduct the backdoor attack on GNNs with the motive for disrupting security or gaining financial benefits. However, effective defensive methods against backdoor attacks have not been established in the GNN domain. From the perspective of defense, revealing characteristics of backdoor attacks is vital. Therefore, it is essential to work on a study on backdoor attacks so as to ensure robustness and security of GNNs.

There are two types of backdoor attacks, namely a label flipping attack and a clean label backdoor attack (CLBA). In the label flipping attack, labels of poisoned data injected into victim's dataset are changed to a target label. The CLBA does not alter labels of poisoned data. In the GNN domain, the majority of studies on backdoor attacks are based on label flipping attacks (Zhang et al., 2021; Xi et al., 2021; Yang et al., 2022). The potential risks of CLBAs remain

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largely unexplored. To our knowledge, there is only one study (Xu and Picek, 2022) regarding CLBAs on GNNs for graph classification tasks that utilizes fixed subgraphs as triggers. There are two problems with that existing CLBA (Xu and Picek, 2022). The first problem is that the CLBA ignores the topological attributes in each graph. Since ER model (Erdos, 1959) is used to generate a trigger with a random structure, the performance of the attack is solely dependent on the trigger density. Thus, there are cases where the attack does not succeed for certain datasets. The second problem is that a fixed subgraph is utilized as the trigger. The fixed trigger may be easily detected because the same structure always appears in all poisoned graphs. Therefore, assigning more adaptive triggers to each graph is favorable for the effective backdoor attack.

In this paper, we propose the first gradient based CLBA on GNNs for graph classification tasks. Our attack consists of two important phases, namely (1) *graph embedding based pairing*, and (2) *gradient based trigger injection*. In the graph embedding based pairing, the attacker makes pairs from graphs of the target class and the others on the basis of their distance in the graph embedding space. This pairing is helpful in clarifying the direction of movement in the graph embedding space during the trigger injection phase, enabling a more successful attack. In the gradient based trigger injection, the attacker injects tailored trigger edges on paired graphs chosen in the pairing phase to create effective poisoned graphs. In this part, gradient based edge scoring is introduced in order to create triggers that enables the pairs to appropriately approach each other in the graph embedding space. This trigger injection is performed on a graph-by-graph basis to enhance the attack effectiveness. These phases realize topology-aware and graph-adaptive triggers, which can address problems posed by the existing CLBA.

Our Contributions. The main contributions of this work are summarized as follows:

- We propose the first gradient-based CLBA on GNNs for graph classification tasks. We introduce the graph embedding based pairing and the gradient based trigger injection to our CLBA for creating effective poisoned graphs.
- We uniquely redefine the threat model of the CLBA to correct the overestimation of the existing attack on GNNs.
- We conduct experiments on multiple datasets and multiple experimental conditions, demonstrating the effectiveness of our attack. Our attack improves the attack success rate by up to over 50% compared with the existing CLBA.
- We show that our attack is difficult to detect by an existing defense method.

2 RELATED WORK

2.1 Backdoor Attacks

Backdoor attacks aim to change the model prediction only for poisoned data that include triggers from a true label to a desired label. These true and desired labels are referred to as source and target labels, respectively. In a backdoor attack, an attacker is involved in both the training and inference phases of a victim model. In the training phase, poisoned data are generated by applying triggers to clean data. After that, in order to poison victim's model, the poisoned data are injected into training datasets of victims in some way. In the inference phase, the attacker injects similar triggers to clean data with source labels which leads to misclassification of those data.

BadNets (Gu et al., 2019) is a backdoor attack on the image domain. In this attack, road signs are misclassified into the labels intended by the attacker using small image instances as triggers. Another backdoor attack on CNNs for image classification tasks exists (Liao et al., 2018). In that backdoor attack, the attacker generates adaptive trigger pixels, making it more difficult for humans to visually identify the poisoned data. A more advanced backdoor attack that utilizes encoders is proposed in (Li et al., 2021). That attack is inspired by DNN-based image steganography and designed to avoid trigger detection. As mentioned above, in the field of image processing, various techniques for backdoor attacks have been studied, revealing the presence of certain threats.

2.2 Backdoor Attacks on GNNs

Recently, backdoor attacks intended for GNNs have been studied. In the graph domain, a subgraph is utilized as a trigger for backdoor attacks. The poisoned graphs are injected into the training dataset to make a victim model associate the trigger edges or nodes with the target labels during the model training. In the inference phase, poisoned graphs for which attackers desire to change the prediction are created by assigning trigger edges or nodes to clean graphs with source labels. As a result, trained models yield incorrect prediction for input data with triggers while making correct predictions for clean data. For the sake of simplicity, we refer to clean graphs with source labels as "sources" and clean graphs with target labels as "targets". In addition, we call sources with

triggers "poisoned sources" and targets with triggers "poisoned targets".

There are multiple scenarios of backdoor attacks. In particular, existing backdoor attacks in the graph domain are mainly divided into two directions, namely a label flipping backdoor attack, and a CLBA depending on whether attackers change labels of poisoned graphs. This label manipulation has a significant impact on the difficulty of the attacks.

2.2.1 Label Flipping Backdoor Attacks

In label flipping backdoor attacks, an attacker changes the labels of the poisoned graphs. In particular, the attacker first generates poisoned data by embedding trigger edges into sources. Then, their labels are changed to target labels, and the poisoned data become poisoned targets. As with general backdoor attacks, such poisoned targets are injected into training datasets to plant a hidden backdoor in victim models. In the inference phase, poisoned sources that have similar triggers are input into victim models with backdoors. A subgraph based backdoor attack (Zhang et al., 2021) uses a fixed subgraph that is pregenerated by connecting existing nodes randomly as the trigger. In the above paper, experiments are conducted on various trigger sizes, trigger densities, and other parameters to show the effectiveness of the backdoor attack using fixed triggers. GTA (Xi et al., 2021) is a backdoor attack against pretrained GNN models that optimizes both attack effectiveness and evasivenss by bi-level optimization. That attack shows the high attack performance in multiple datasets. Furthermore, their results reveal that existing defense mechanisms in other domains are ineffective in preventing that attack. In a TRAP attack (Yang et al., 2022), graph edges are perturbed on the basis of specific scores. These scores are calculated using gradients of an attacker's model. The utilization of gradient information to select modified edges is effective.

Since the original labels of poisoned targets are the source labels in label flipping backdoor attacks, it is relatively easy for the attacker to change decision boundary of the victim model and to induce the model to misclassify the poisoned sources. However, since the labels and characteristics of data themselves are inconsistent compared to those from legitimate targets, it is possible that poisoned targets are detected as outliers, which is a limitation of label flipping attacks.

2.2.2 Clean Label Backdoor Attack (CLBA)

To realize a more sophisticated attack, a CLBA is proposed in the graph domain. In CLBAs, attackers create poisoned targets by injecting triggers into targets. In other words, their labels are consistent throughout the entire attack process from beginning to end. This is why their features tend to be almost consistent with those of clean targets, meaning that poisoned targets are more difficult to detect as outliers. These poisoned targets are injected into training dataset. Then, as with label flipping backdoor attacks, triggers are attached to sources so as to create poisoned sources which are input during the inference phase. Although there are some CLBAs targeting node classification tasks (Dai et al., 2023; Yang et al., 2023), there is currently only one CLBA (Xu and Picek, 2022) targeting graph classification tasks. In that CLBA, a small, fixed random graph is generated by utilizing the Erdős-Rényi (ER) model in advance (Erdos, 1959). This subgraph is used as a common trigger among all poisoned graphs for CLBAs.

2.3 Defense Against Backdoor Attacks

A defense method has been proposed in (Liu et al., 2018). In this approach, a defender checks the distribution of erroneously predicted results. However, this approach has been shown to be ineffective in subsequent research. Neural Cleanse (Wang et al., 2019) is a defense mechanism that has been shown to be effective in preventing backdoor attacks against DNNs. In that method, a defender mitigates backdoor attacks by utilizing reverse-engineered triggers.

Currently, there are a few defense mechanisms against backdoor attacks in GNNs. For example, there is randomized subsampling (Zhang et al., 2021) that changes edge information of a graph to mitigate the impact of trigger edges. However, such a defense is not effective because the accuracy of the clean model often decreases greatly or it cannot prevent attacks in almost all cases (Yang et al., 2022). There is another existing defense mechanism (Jiang and Li, 2022) against label flipping backdoor attacks. That defense utilizes the explanation score and achieves high detection rates of poisoned data in their experiment. However, we find that that defense cannot work well for our attack as shown in Section 5. Thus, more effective defense methods against backdoor attacks are still needed. To devise such effective methods, we argue that the study of the backdoor attack is quite important because it can reveal characteristics of poisoned data. Such revealed characteristics regarding the topological structures allow us to utilize them for defensive strategies.

3 PRELIMINARIES

3.1 Graph Neural Networks (GNNs)

In this work, we consider graph classification as the task. This type of task can be widely utilized for various purposes such as the prediction of the existence of enzymes in a protein molecule and cell lung cancer in chemicals. Let $\mathcal{D}_{\text{train}} = \{(G_1, y_1), (G_2, y_2), ..., (G_n, y_n)\}$ denote a training dataset. $\mathcal{D}_{\text{train}}$ contains graphs $G_i = (\boldsymbol{A}_i, \boldsymbol{X}_i)$ and their labels y_i. $\boldsymbol{A}_i \in \{0,1\}^{N \times N}$ is the adjacency matrix of the graph data that has N nodes, where the existence of each edge is represented as 1. $\boldsymbol{X}_i$ is the feature matrix of nodes in G_i. The goal of the graph classification is to learn a model F that outputs a predicted label y_{c_i} for a class out of classes in $\mathcal{C} = \{c_1, c_2, ..., c_K\}$. K is the number of classes. In fact, F consists of two components, namely the graph representation module f_{GNN} and the classifier module f_{fc}, which means $F = (f_{\text{fc}} \circ f_{\text{GNN}})$. f_{GNN} is utilized so as to learn useful information from graph structured data. In general, f_{GNN} generates node embeddings, which are numerical vectors regarding node features. On the other hand, f_{fc} is equivalent to a fully connected neural network or a traditional classifier such as support vector machine.

As representative graph representation modules, there are two GNN models for graph classification tasks. The first one is Graph Convolutional Network (GCN) (Kipf and Welling, 2016). In GCN architecture, the one step of node embeddings generation is formulated as follows:

$$h^{(l+1)} = \sigma(\hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2}h^{(l)}W^{(l)}). \quad (1)$$

Here, σ is a nonlinear activation function like ReLU, $\hat{A}$ is the addition of an adjacency matrix A and the identity matrix I. D is the the diagonal node degree matrix of $\hat{A}$, and $W^{(l)}$ is a weight matrix for the l-th GNN layer. The other one is Graph Isomorphism Network (GIN) (Xu et al., 2018). In GIN architecture, the one step of node embeddings generation is formulated as follows:

$$h_i{}^{(l+1)} = \text{MLP}\left((1+\varepsilon^{(l)}) \cdot h_i{}^{(l)} + \sum_{j \in N(i)} h_j{}^{(l)}\right). \quad (2)$$

Here, MLP is multi-layer perceptrons, $h_i{}^l$ is the l-th node embedding of node i and $N(i)$ is the set of nodes adjacent to node i.

In the graph classification, f_{GNN} outputs a entire graph representation h_{G_i} obtained by aggregating features of nodes in each graph. To this end, a readout function is applied to h_i^l. A simple summation or a more sophisticated graph-level pooling function can be utilized as a readout function. The resulting h_{G_i} is input to f_{fc} for predicting a label of G_i.

3.2 Threat Model

Attacker's Goal. The attacker has two goals. The first goal is to improve the attack effectiveness. This goal is intended to ensure that the poisoned sources input by the attacker during the inference phase are misclassified to the target label y_t. The second goal is to improve the attack evasiveness. With this goal, the attack is accomplished without the victim being aware of it. To achieve these goals, the attacker plants triggers in the victim's model by poisoning their training dataset with poisoned targets disseminated to public.

Attacker's Capability. The attacker has his own GNN model. We assume two attack scenarios for this model, namely white- and gray-box scenarios. The white- and gray-box scenarios are defined as follows:

White-Box. Attackers can access the whole information about parameters of victim models and what graph data are used for training dataset in this scenario. This scenario is the worst-case scenario for victims in the real world.

Gray-Box. Attackers cannot access any information about victim models, as they know only about what graph data are used for training. In other words, attackers need to prepare surrogate models with different architectures and parameters to conduct attacks. For example, if the victim model is a GCN model, then the attacker's model is a GIN model, and vice versa.

Unlike existing work (Xu and Picek, 2022), we uniquely assume that the attacker has the following constraint on both the existing and proposed CLBAs.

Maintenance of the Clean Label Scenario. In the CLBA, poisoned targets are injected into the training dataset of the victim model. Thus, an attacker should select only from the targets that are correctly classified as the target labels by the attacker's model. Choosing targets classified as source labels leads to the association of source-like graphs with triggers, despite the target labels being assigned to them. If such targets mutate into poisoned targets to plant triggers in the victim models, then the genuine CLBA is not realized. In such a case, the success of the attack is purely dependent on misclassification and label flipping ability. In other words, the attack performance of the existing attack is overestimated. This is why we set up the above two scenarios both in the existing attack and our attack to properly evaluate the CLBA in our experiments while the attacker does not necessarily need to utilize the information of models in the existing attack.

3.3 Problem Formulation

We formulate CLBAs that achieves the goal described in Section 3.2 as follows:

$$F_{\theta'}(G^g_{y_s}) = y_t$$
$$\text{s.t. } \theta' = \underset{\theta}{\operatorname{argmin}}\, \mathcal{L}_{\text{train}}(F_\theta, \mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{poison}}), \tag{3}$$

$$F_{\theta'}(G_{y_s}) = F_{\theta_c}(G_{y_s}), \tag{4}$$

where $F_{\theta'}$ and F_{θ_c} denote a backdoored model with model parameters θ' and a clean one with model parameters θ_c, respectively. Furthermore, y_s is the source label. Let $\mathcal{D}_{\text{poison}}$ denote the poisoned dataset containing poisoned targets with y_t. A poisoned target $G^g_{y_t}$ is created by injecting a trigger g into a clean target G_{y_t}. Similarly, a poisoned source $G^g_{y_s}$ is created by injecting g into a clean source G_{y_s}. $\mathcal{L}_{\text{train}}$ is the loss for training F_θ on $\mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{poison}}$. Eq.(3) represents the situation where the poisoned sources are misclassified as the target labels by the backdoored model. This equation is related to the attack effectiveness of backdoor attacks. Moreover, Eq.(4) represents the situation where the backdoored model correctly outputs the prediction for clean sources. This equation guarantees attack evasiveness.

4 PROPOSED ATTACK

4.1 Attack Overview

We propose the first gradient based CLBA on GNNs for graph classification tasks. Our attack consists of two important phases, namely, (1) *graph embedding based pairing* and (2) *gradient based trigger injection*. In the first phase, the attacker forms pairs of sources and targets on the basis of their distance in the graph embedding space. This phase is divided into two parts. First, the attacker selects the same number of sources as the number of targets that have been correctly predicted by the attacker's model. Second, a source is paired with a target in a one-to-one correspondence considering their positions in graph embedding space. This pairing is helpful in clarifying the direction of movement in the graph embedding space during the trigger injection phase, enabling a more successful attack. In the second phase, the attacker attaches trigger edges on the graphs chosen in the pairing phase to create poisoned sources and poisoned targets. In this part, gradient-based triggers are assigned to the selected graphs, and the pairs are appropriately guided to approach each other in the graph embedding space. This optimization is performed on a graph-by-graph basis to enhance attack effectiveness. We provide an overview diagram of our attack in Fig.1.

4.2 Graph Embedding Based Pairing

As shown in Subsection 4.1, this phase has two parts. First, attackers select p sources which have smallest prediction probability with respect to the source label by the attacker's model. The process of choosing a source is described as follows:

$$\underset{G_{y_s} \in S}{\operatorname{argmin}}\, F'(G_{y_s})_{y_s}, \tag{5}$$

where $F'(G)_l$ represents the prediction probability of the attacker's model F' for graph G regarding a label l, and S is the set of sources. This data selection approach is repeated p times. We refer to these selected p sources as $\mathcal{S}$ (different from S).

Attackers also choose the same number of p targets which are farthest from decision boundary. The process of choosing such a target is described as follows:

$$\underset{G_{y_t} \in T}{\operatorname{argmax}}\, F'(G_{y_t})_{y_t}, \tag{6}$$

where T is the set of targets. We refer to these p targets as $\mathcal{T}$ (different from T). The reason for selecting data on the basis of distance from the decision boundary is that moving sources in the direction of paired targets is expected to cause the sources to invade the target region when trigger edges are injected into them.

Second, attackers pair sources and targets in a one-to-one correspondence based on a greedy algorithm. The greedy algorithm assigns $G_{y_t} \in \mathcal{T}$ that is the closest to $G_{y_s} \in \mathcal{S}$ in the graph embedding space one by one. Let $h_{G_{y_t}}$ and $h_{G_{y_s}}$ denote the graph embeddings of targets and sources, respectively. $h_{G_{y_t}}$ and $h_{G_{y_s}}$ are obtained through F'_θ that is attacker's model trained on $\mathcal{D}_{\text{train}}$. In other words, $h_{G_{y_t}} = f'_{\text{GNN}}(G_{y_t})$ and $h_{G_{y_s}} = f'_{\text{GNN}}(G_{y_s})$ where f'_{GNN} is a graph representation module of the attacker's model.

In this approach, G_{y_t} is paired with G_{y_s} as follows:

$$\underset{G_{y_t}}{\operatorname{argmin}}\, \ell(h_{G_{y_s}}, h_{G_{y_t}}), \tag{7}$$

where $\ell(\cdot,\cdot)$ is the loss function based on the cosine similarity and is defined as

$$\ell(h_{G_{y_s}}, h_{G_{y_t}}) = 1 - \gamma(h_{G_{y_s}}, h_{G_{y_t}}). \tag{8}$$

Note that $\gamma(\cdot,\cdot)$ is the cosine similarity.

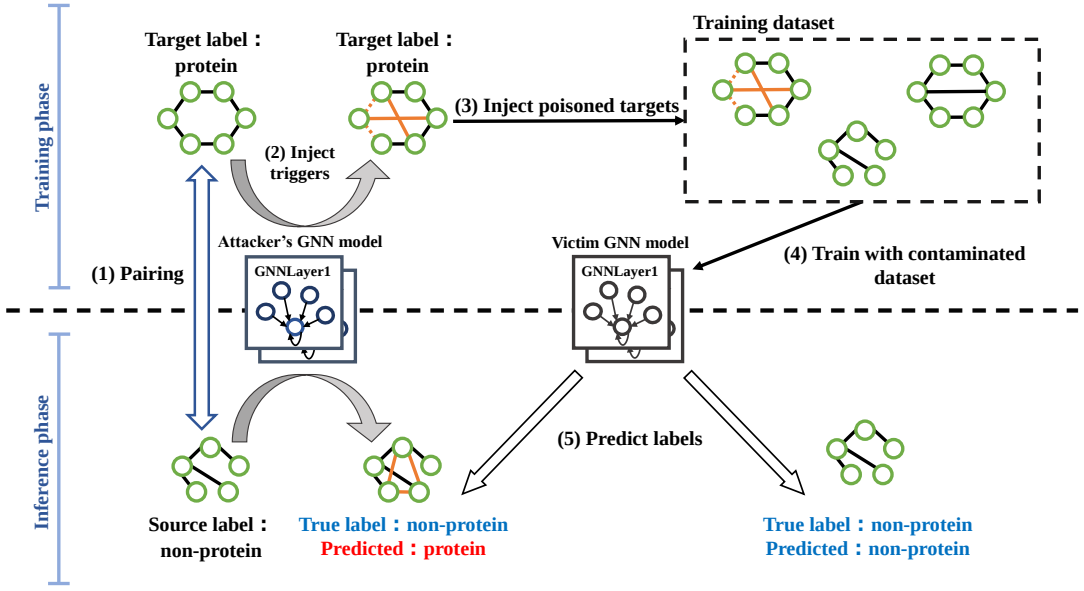


Figure 1: The proposed gradient-based CLBA.

4.3 Gradient Based Trigger Injection

Our trigger injection has two important points, namely a gradient based edge scoring and the order of trigger injection. In what follows, we elaborate on them.

The gradient based edge scoring is useful in selecting appropriate edges that constitute a trigger. Let Score_i denote the scores for edges in a graph G_i. Score_i is calculated as follows:

$$\text{Score}_i = (2 \cdot \boldsymbol{A}_i - 1) \cdot \nabla_{\boldsymbol{A}_i}, \tag{9}$$

where $\nabla_{\boldsymbol{A}_i}$ means the gradient of Eq.(8) with respect to $\boldsymbol{A}_i$ corresponding to edges in G_i. The meaning of this score is explained from here. First, consider the existent edges. If the edge connecting nodes a and b has a positive gradient value, deleting this edge reduces the loss in Eq.(8), which brings the graph data closer to the paired data in the graph embedding space. If the gradient is negative, then we do not delete the edge because doing so only increases the loss. Next, we consider nonexistent edges. If the gradient of the nonexistent edge between nodes a and b is positive, then we do not connect them because doing so only increases the loss. On the other hand, if the gradient value is negative, then adding the edge brings the graph data closer to the paired data in the graph embedding space. In short, by inverting the information of "existent edges with positive gradients" and "nonexistent edges with negative gradients", the pairs can be approached efficiently in the graph embedding space. The larger the absolute values of the gradients are, the closer to the paired data are when these edges are changed. Therefore, to assign higher scores to these edges, the sign is adjusted in the first term in Eq.(9). The above score is calculated for each value in $\boldsymbol{A}_i$ to generate the score list. On the basis of that score list, edge information with top m scores is changed to attach triggers to graphs.

As for the order of trigger injection, the trigger edges are first assigned to $\mathcal{S}$ to create poisoned sources $\hat{\mathcal{S}}$. This is because the above order allows the sources to move to the paired targets significantly, which results in invading the target area in graph embedding space. After that, poisoned targets $\hat{\mathcal{T}}$ are created by making $\mathcal{T}$ close to paired poisoned sources in $\hat{\mathcal{S}}$. This process allows for the creation of effective poisoned targets. As a result, when the poisoned targets are used for training the victim model, target label area can be further expanded, causing misclassification of the poisoned sources.

4.4 Algorithm

The complete attack process is presented in Algorithm 1. After the initialization procedure (Line 1) and obtaining F'_θ trained on $\mathcal{D}_{\text{train}}$ (Line 2), poisoned graphs are generated. In our attack, $\hat{\mathcal{S}}$ is generated prior to $\hat{\mathcal{T}}$. Let $\mathcal{G}^{\text{mod}}$ and $\mathcal{G}^{\text{anch}}$ denote the set of p modified graphs and that of p anchor graphs, respectively. Triggers are embedded in $G_i^{\text{mod}} \in \mathcal{G}^{\text{mod}}$ so that G_i^{mod} are close to $G_i^{\text{anch}} \in \mathcal{G}^{\text{anch}}$. $\mathcal{G}^{\text{mod}}$ and $\mathcal{G}^{\text{anch}}$ are changed depending on the type of graph that triggers are embedded in. When $\hat{\mathcal{S}}$ is generated, $\mathcal{G}^{\text{mod}}$ and $\mathcal{G}^{\text{anch}}$ are $\mathcal{S}$ and $\mathcal{T}$, respectively (Line 5). On the other

Algorithm 1: Proposed gradient-based CLBA.

Input : $\mathcal{S}$, $\mathcal{T}$, F'_θ, and $\mathcal{D}_{\text{train}}$
Output: Poisoned sources and targets $(\hat{\mathcal{S}}, \hat{\mathcal{T}})$

1 $(\hat{\mathcal{S}}, \hat{\mathcal{T}}) \leftarrow (\emptyset, \emptyset)$
2 Obtain F'_θ trained on $\mathcal{D}_{\text{train}}$
3 **while** $\hat{\mathcal{S}} = \emptyset$ or $\hat{\mathcal{T}} = \emptyset$ **do**
4 **if** $\hat{\mathcal{S}} = \emptyset$ **then**
5 $\mathcal{G}^{\text{mod}} \leftarrow \mathcal{S}$ and $\mathcal{G}^{\text{anch}} \leftarrow \mathcal{T}$
6 **else**
7 $\mathcal{G}^{\text{mod}} \leftarrow \mathcal{T}$ and $\mathcal{G}^{\text{anch}} \leftarrow \hat{\mathcal{S}}$
8 $\mathcal{P}, \mathcal{G}^{\text{tmp}} \leftarrow \emptyset, \emptyset$
9 **for** $i = 1$ *to* p **do**
10 Select $G_i^{\text{mod}} \in \mathcal{G}^{\text{mod}}$ paired with $G_i^{\text{anch}} \in \mathcal{G}^{\text{anch}}$ based on Eq.(7)
11 $\mathcal{P} \leftarrow \mathcal{P} \cup (G_i^{\text{mod}}, G_i^{\text{anch}})$
12 **for** each pair $(G_i^{\text{mod}}, G_i^{\text{anch}}) \in \mathcal{P}$ **do**
13 $\nabla_{A_i^{\text{mod}}} \leftarrow \nabla_{A_i^{\text{mod}}} \ell(h_{G_i^{\text{mod}}}, h_{G_i^{\text{anch}}})$
14 $\text{Score}_i \leftarrow (2 \cdot A_i^{\text{mod}} - 1) \cdot \nabla_{A_i^{\text{mod}}}$
15 Create $\hat{G}_i^{\text{mod}}$ by reversing elements with top m values of Score_i in A_i^{mod}
16 $\mathcal{G}^{\text{tmp}} \leftarrow \mathcal{G}^{\text{tmp}} \cup \{\hat{G}_i^{\text{mod}}\}$
17 **if** $\hat{\mathcal{S}} = \emptyset$ **then**
18 $\hat{\mathcal{S}} \leftarrow \mathcal{G}^{\text{tmp}}$
19 **else**
20 $\hat{\mathcal{T}} \leftarrow \mathcal{G}^{\text{tmp}}$
21 **return** $(\hat{\mathcal{S}}, \hat{\mathcal{T}})$

hand, when $\hat{\mathcal{T}}$ is generated, $\mathcal{G}^{\text{mod}}$ is $\mathcal{T}$, and $\mathcal{G}^{\text{anch}}$ is $\hat{\mathcal{S}}$ (Line 7). A set of paired graphs $\mathcal{P}$ is created by pairing G_i^{mod} with G_i^{anch} on the basis of the greedy algorithm (Lines 9-11). For each pair $(G_i^{\text{mod}}, G_i^{\text{anch}}) \in \mathcal{P}$, the gradient $\nabla_{A_i^{\text{mod}}}$ of the loss function ℓ with respect to the adjacency matrix A_i^{mod} of G_i^{mod} is calculated (Lines 13). Then, Score_i is calculated on the basis of $\nabla_{A_i^{\text{mod}}}$ to determine the edges to reverse (Line 14). After that, a poison graph $\hat{G}_i^{\text{mod}}$ is created on the basis of Score_i (Line 15). $\hat{G}_i^{\text{mod}}$ is stored in a temporary set $\mathcal{G}^{\text{tmp}}$ (Line 16). The above procedures are repeatedly conducted for creating each of $\hat{\mathcal{S}}$ and $\hat{\mathcal{T}}$. Finally, $\hat{\mathcal{S}}$ and $\hat{\mathcal{T}}$ are returned.

5 ATTACK EVALUATION

In this section, we evaluate our attack effectiveness and evasiveness. Specifically, in this experiment, we aim to address the following questions.

1. How much does our attack effectiveness and evasiveness improve compared to those in the existing method?
2. To what extent does the threat model impact attack performance?
3. Do existing defense methods effectively work against our attack?

5.1 Experimental Settings

5.1.1 Datasets

We utilized four real-world datasets to evaluate our attack effectiveness and evasiveness. The datasets are MUTAG (Debnath et al., 1991), DHFR (Wale et al., 2008), NCI1 (Dobson and Doig, 2003) and PROTEINS-full (Morris et al., 2020). We now refer to PROTEINS-full as PROTEINS. Table 1 presents the summary of the datasets. The label of graph with fewer instances is selected as the target label.

We use 80% of graphs for the training dataset and the remaining 20% for the test dataset. When we divide the dataset, we ensure that the ratio of labels is maintained during the split. Both the attacker and the victim train their models according to the above data split scenario. The datasets are binary classification datasets with labels 0 and 1. The labels refer to the classification results of the molecular data in each graph dataset.

5.1.2 Metrics

We use two metrics to evaluate our attack effectiveness and evasiveness.

The first metric is the Attack Success Rate (ASR), which is the proportion of misclassified samples in the poisoned sources by the victim model and is described as follows:

$$ASR = \frac{\sum_{i=1}^{|\hat{\mathcal{S}}|} [F_{\theta'}(\hat{\mathcal{S}}_i) = y_t]}{|\hat{\mathcal{S}}|}.$$

$\hat{\mathcal{S}}$ is the set of poisoned sources, and $F_{\theta'}$ is the contaminated victim model. [A] represents 1 if proposition A is true and 0 otherwise. Note here that the attacks are considered successful only when a clean model correctly classifies clean data before the trigger edges are inserted as the source label; however, the backdoored model misclassifies poisoned data as the target label. Although this scenario is challenging for attackers, it is appropriate because it helps avoid overestimation of the ASR due to coincidental misclassifications.

The second metric is the Clean Accuracy Drop (CAD), which is the drop from clean accuracy to

Table 1: Datasets summary.

Dataset	Graphs in class	Avg. nodes	Avg. edges	Node features	Target label
NCI1	2053(0), 2057(1)	29.86	64.60	37	0
PROTEINS	663(0), 450(1)	39.05	145.63	32	1
DHFR	295(0), 461(1)	42.42	89.08	3	0
MUTAG	63(0), 125(1)	17.93	39.58	7	0

Table 2: GNN model.

GNN	Parameter	Settings
GCN, GIN	Architecture	2 Layers(16, 8)
	Classifier	Linear
	Aggregator	Max Pooling
	Optimizer	Adam
	Scheduler	StepLR

Table 3: Clean Accuracy (%).

Dataset	GCN	GIN
NCI1	65.43	70.91
PROTEINS	74.43	74.61
DHFR	70.72	72.43
MUTAG	74.73	79.47

backdoored accuracy. Here, clean accuracy is the accuracy of the model trained without poisoned targets, while backdoored accuracy is that of the model trained with poisoned targets.

We evaluate the experimental values of the ASR and CAD by taking the average of 10 repetitions for each experimental condition. The existing attack is executed in the condition that edge density for fixed triggers is 0.8.

5.1.3 Model Settings

The composition of the GNN model is shown in the Table 2. We use the Adam Optimizer and StepLR scheduler in the training process. The model parameters are selected on the basis of the results of the grid search, with those that yield the maximum accuracies being chosen. Table 3 shows the clean accuracy by the models with the selected parameters.

5.2 Experimental Results

How Much Does our Attack Effectiveness and Evasiveness Improve Compared to Those in the Existing Method? Table 4 and Table 5 summarize the experimental values for the 10% poisoning rate (or the maximum poisoning rate) as numerical data. Our attack outperforms the existing attack under almost all conditions in terms of the ASR. We achieve an increase of over 50% compared to the existing attack in the gray-box scenario where the dataset is MUTAG. This improvement is achieved due to the following reason. In our attack, it is possible to induce misclassification effectively because our attack assigns appropriate trigger edges tailored to each graph. In contrast, the existing attack ignores the characteristics of each graph and assigns a fixed trigger, which is why its attack performance is considered unstable.

Fig.2–5 show the comparison of the ASR and the CAD in our gray-box and white-box attacks when the poisoning rate is varied at 1%, 3%, 5%, 7%, 9%, and 10%. Due to the limited number of graphs for creating poisoned data, there are cases where the maximum poisoning rate is less than 10%, and in such cases, we stop the evaluation of metrics at the maximum data size. Regarding the increase in the ASR with respect to poisoning rate, our attack method shows a strong upward trend as shown in Fig.2 and Fig.4. On the other hand, the existing attack appears to remain relatively stable. This suggests that our attack is capable of generating effective poisoned data, which the existing attack is unable to produce. For example, when the poisoning rate increased from 1% to 10%, the increase of the ASR in the existing attack reaches at most about 20%. In contrast, with our attack, the increase can be over 40% at its maximum. Regarding CAD as shown in Fig.3 and Fig.5, for the MUTAG dataset, our attack shows an upward trend, indicating suboptimal evasion performance. However, for other datasets, even when compared to the existing attack, CAD remains at similarly low levels of less than 5% in most datasets. Therefore, it becomes possible to execute our attack without being detected by the victim.

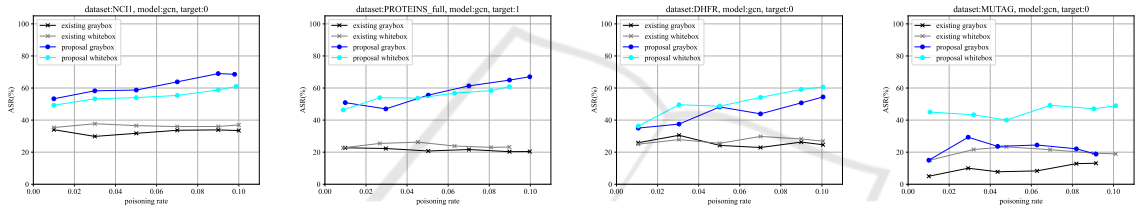
To What Extent Does the Threat Model Impact Attack Performance? As shown in Fig.2, there is a case where the ASR of our gray-box attack dropped by more than 20% compared to that of our white-box attack when the dataset is MUTAG. However, in other datasets, our attack maintains a high attack success rate even in the gray-box scenario, demonstrating that our attack is feasible for attackers who do not possess detailed information about the model. Furthermore, there are cases where the gray-box scenario shows better attack performance, but this finding can be attributed to $\mathcal{S}$ whose labels are originally misclas-

Table 4: ASR comparison of the existing attack, our whitebox and graybox attacks (poisoning rate=10%). Highest ASR cells are grayed out.

Dataset	Existing (graybox)		Existing (whitebox)		Proposal (graybox)		Proposal (whitebox)	
	GCN	GIN	GCN	GIN	GCN	GIN	GCN	GIN
NCI1	33.48	37.45	36.97	48.29	68.56	73.44	61.01	68.51
PROTEINS	20.39	30.49	23.24	28.10	67.03	66.82	60.80	71.25
DHFR	24.63	35.62	26.84	50.65	54.43	72.99	60.65	68.94
MUTAG	13.11	21.05	18.94	33.68	18.77	73.24	48.94	58.42

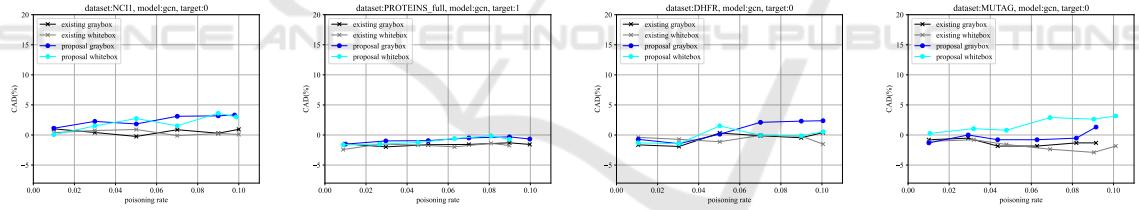
Table 5: CAD comparison of the existing attack, our whitebox and graybox attacks(poisoning rate=10%). Lowest CAD are grayed out.

Dataset	Existing (graybox)		Existing (whitebox)		Proposal (graybox)		Proposal (whitebox)	
	GCN	GIN	GCN	GIN	GCN	GIN	GCN	GIN
NCI1	0.93	0.75	0.09	2.00	3.31	2.83	3.00	2.91
PROTEINS	-1.56	1.79	-1.74	0.98	-0.67	2.55	-0.71	3.45
DHFR	0.39	1.38	-1.51	1.57	2.36	-0.59	0.52	2.30
MUTAG	-1.31	0.00	-1.84	1.57	1.31	7.89	3.15	2.89



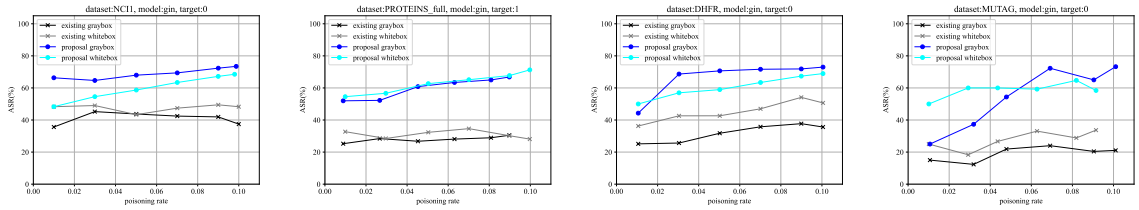
(a) NCI1 (b) PROTEINS (c) DHFR (d) MUTAG

Figure 2: Comparison of the ASR in our attack and the existing attack (GCN).



(a) NCI1 (b) PEOTEINS (c) DHFR (d) MUTAG

Figure 3: Comparison of the CAD in our attack and the existing attack (GCN).

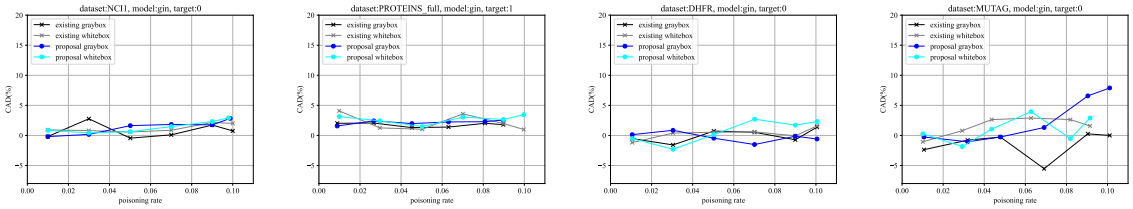


(a) NCI1 (b) PROTEINS (c) DHFR (d) MUTAG

Figure 4: Comparison of the ASR in our attack and the existing attack (GIN).

sified by the victim model, leading to the inability to maintain the clean-label scenario. Therefore, it is not always straightforward that the gray-box scenario is superior to the white-box scenario.

Next, we explain the difference between the results reported in the existing attack's paper (Xu and Picek, 2022) and the results of our verification experiments. In that paper (Xu and Picek, 2022), the ASR is over 80% when datasets are NCI1 and MUTAG in the condition that poisoning rate is 10%. However,



(a) NCI1 (b) PEOTEINS (c) DHFR (d) MUTAG

Figure 5: Comparison of the CAD in our attack and the existing attack (GIN).

according to our experimental results, the ASR is less than 50% in all cases. This is because change of the threat model enables proper evaluation of the ASR, which corrects the overestimation. As a result, it is revealed that the existing attack is not so successful in practice.

Do Existing Defense Methods Effectively Work Against our Attack? To evaluate our attack evasiveness, we apply an existing defense mechanism (Jiang and Li, 2022) against label flipping backdoor attacks. That defense utilizes explanation scores and shows a high detection rate of poisoned data. In this defense approach, the defender first adopts edges that serve as explanations for the model's predictions. The explanations mean important edges that dictate the prediction. Subsequently, based on explanation-based scores, the defender detects the presence of trigger edges in poisoned sources and removes those edges. To be more specific, the defender calculates an explanability score (ES) for each graph, identifying graphs with high ESs as poisoned sources. The threshold is set as the maximum value of benign data in the test dataset, and any data with ESs exceeding this threshold are considered malicious. The detection rate is the number of detected poisoned sources divided by the number of all poisoned sources. Then, the defender proceeds to guide predictions in the correct direction by removing the edges on the basis of explanations. In this experiment, the number of removed edges is equal to the trigger size of our attack. We utilize the same dataset to evaluate our attack and take this defensive approach under the condition that the poisoning rate is the maximum value.

The results of defense by explanation are shown in Fig.6 and Fig.7. The detection rate of the attack is below 20% in most cases, indicating a high level of attack evasiveness. There are conditions where the partial detection rate is higher (Dataset: MUTAG, Model: GCN, our whitebox attack). There are two possible reasons for this. First, the average graph size of MUTAG dataset is smaller than that of other datasets. As a result, the trigger size decreases, and the detection rate increases because the importance of edges concentrated on specific edges. However, it is important to note that in this case, the number of edges adopted for explanation is equal to the trigger size, and this defense is carried out under conditions favorable to the defender. Therefore, in practice, detection may be more challenging.

6 CONCLUSION

In this paper, we propose the first gradient based CLBA on GNNs for graph classification tasks. Our attack introduces the graph embedding based pairing and the gradient based trigger injection. We also reconsider the threat model of backdoor attacks, define a more practical threat model, and eliminate the overestimation of attack performance in the existing attack. Under this threat model, our results demonstrate that our attack outperforms the existing CLBA in terms of the ASR metric and the existing CLBA is not so successful in practice. We validate our attack performance on multiple datasets and experimental conditions, demonstrating the generalizability of our attack approach. Furthermore, we confirm that the existing defense cannot sufficiently detect our attack. Therefore, the results clarify that devising more effective defense mechanisms against CLBAs are needed, which stimulates further research in this area.

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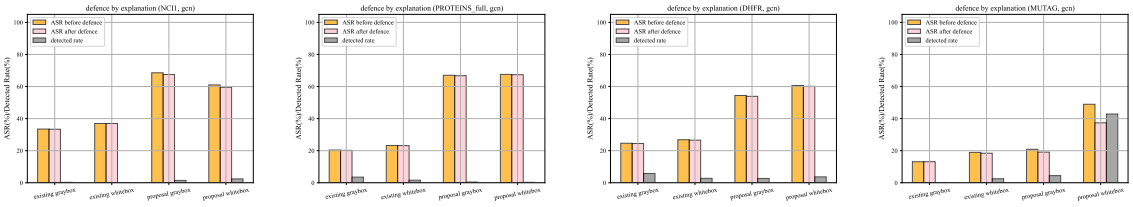
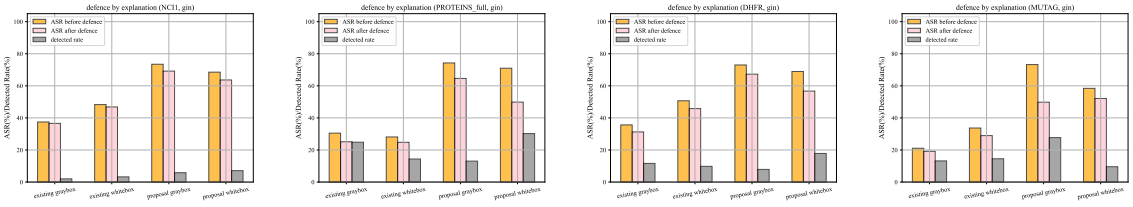


(a) NCI1 (b) PROTEINS (c) DHFR (d) MUTAG

Figure 6: Comparison of Defense results (GCN).



(a) NCI1 (b) PROTEINS (c) DHFR (d) MUTAG

Figure 7: Comparison of Defense results (GIN).

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