Graph Sanitation with Application to Node Classification

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ABSTRACT
The past decades have witnessed the prosperity of graph mining, with a multitude of sophisticated models and algorithms designed for various mining tasks, such as ranking, classification, clustering and anomaly detection. Generally speaking, the vast majority of the existing works aim to answer the following question, that is, given a graph, what is the best way to mine it?

In this paper, we introduce the graph sanitation problem, to answer an orthogonal question. That is, given a mining task and an initial graph, what is the best way to improve the initially provided graph? By learning a better graph as part of the input of the mining model, it is expected to benefit graph mining in a variety of settings, ranging from denoising, imputation to defense. We formulate the graph sanitation problem as a bilevel optimization problem, and further instantiate it by semi-supervised node classification, together with an effective solver named GaSoLiNe. Extensive experimental results demonstrate that the proposed method is (1) broadly applicable with respect to various graph neural network models and flexible graph modification strategies, (2) effective in improving the node classification accuracy on both the original and contaminated graphs in various perturbation scenarios. In particular, it brings up to 25% performance improvement over the existing robust graph neural network methods.

1 INTRODUCTION
Graph mining has become the cornerstone in a wealth of real-world applications, such as social media mining [44], brain connectivity analysis [1], computational epidemiology [19] and financial fraud detection [37]. For the vast majority of existing works, they essentially aim to answer the following question, that is, given a graph, what is the best model and/or algorithm to mine it? To name a few, PageRank [27] and its variants [13, 14, 16, 31] measure the node importance and node proximity based on multiple weighted paths; spectral clustering [30] minimizes inter-cluster connectivity and maximizes the intra-cluster connectivity to partition nodes into different groups; graph neural networks (GNNs) [20, 21, 34, 40] learn representation of nodes by aggregating information from the neighborhood. In all these works and many more, they require a given graph, including its topology and/or the associated attribute information, as part of the input of the corresponding mining model.

Despite tremendous success, some fundamental questions largely remain open, e.g., where does the input graph come from at the first place? To what extent does the quality of the given graph impact the effectiveness of the corresponding graph mining model? In response, we introduce the graph sanitation problem, which aims to improve the initially provided graph for a given graph mining model, so as to maximally boost its performance. The rationality is as follows. In many existing graph mining works, the initially provided graph is typically constructed manually based on some heuristics. The graph construction is often treated as a pre-processing step, without the consideration of the specific mining task. What is more, the initially constructed graph could be subject to various forms of contamination, such as missing information, noise and even adversarial attacks. This suggests that there might be under-explored space for improving the mining performance by learning a ‘better’ graph as the input of the corresponding task.

There are a few lines of existing works for modifying graphs. For example, network imputation [15, 25] and knowledge graph completion [4, 39] problems focus on restoring missing links in a partially observed graph; graph connectivity optimization [5] and computational immunization [6] problems aim to manipulate the graph connectivity in a desired way by changing the underlying topology; robust GNNs [9, 17, 41] utilize empirical properties of a benign graph to remove or assign lower weights to the poisoned graph elements (e.g., contaminated edges).

The graph sanitation problem introduced in this paper is related to but bears subtle difference from these existing work in the following sense. Most, if not all, of these existing works for modifying graphs assume the initially provided graph is impaired or perturbed in a specific way, e.g., due to missing links, or noise, or adversarial attacks. Some existing works further impose certain assumptions on the specific graph modification algorithms, such as the low-rank assumption behind many network imputation methods, the types of attacks and/or the empirical properties of the benign graph (e.g., topology sparsity, feature smoothness) behind some robust GNNs. In contrast, the proposed graph sanitation problem does not make any such assumptions, but instead pursues a different design principle. That is, we aim to let the performance of the downstream data mining task, measured on a validation set, dictate how we should optimally modify the initially provided graph. This is crucial, as it not only ensures that the modified graph will directly and maximally improve the mining performance, but also lends itself to be applicable to a variety of graph mining tasks.

Formally, we formulate the graph sanitation problem as a generic bilevel optimization problem, where the lower-level optimization problem corresponds to the specific mining task and the upper-level optimization problem encodes the supervision to modify the provided graph and maximally improve the mining performance. Based on that, we instantiate such a bilevel optimization problem by semi-supervised node classification with GNNs, where the lower-level objective function represents the cross-entropy classification loss over the training data and the upper-level objective function represents the loss over validation data, using the mining model trained from the lower-level optimization problem. We propose an effective solver (GaSoLiNe) which adopts an efficient approximation of hyper-gradient to guide the modification over the given graph. We carefully design the hyper-gradient aggregation mechanism...
Table 1: Node classification performance (Mean±Std Accuracy) boosting of existing defense methods on heavily poisoned graphs (25% edges perturbed by metattack [47]) by the proposed GaSoliNe.

| Data     | With GaSoliNe? | GAT | SVD | RGCN |
|----------|----------------|-----|-----|------|
| Cora     | N              | 48.8±0.2 | 60.1±0.6 | 50.6±0.8 |
|          | Y              | 63.7±0.6 | 79.7±0.6 | 62.6±0.6 |
| Citeseer | N              | 62.4±0.7 | 50.6±0.6 | 55.3±1.4 |
|          | Y              | 69.7±0.2 | 76.5±0.6 | 66.1±0.8 |
| Polblogs | N              | 48.2±0.6 | 77.3±3.3 | 50.8±0.9 |
|          | Y              | 70.8±0.6 | 89.2±0.7 | 67.7±0.3 |

respectively. Take the classification task as an example, $y_{ij} = 1$ if node $i$ belongs to class $j$ and $y_{ij} = 0$ otherwise; $\hat{y}_{ij}$ is the predicted probability that node $i$ belongs to class $j$. Furthermore, we use $Y_{\text{train}}$ and $Y_{\text{validd}}$ to denote the supervision information of all the nodes in the training set $T$ and the validation set $V$, respectively.

### B - Optimization-Based Graph Mining Models

For many graph mining models, they can be formulated from the optimization perspective [18] with a general goal to find an optimal solution $\theta^*$ so that a task-specific loss $L(G, \theta, T, Y_{\text{train}})$ is minimized. Here, $T$ and $Y_{\text{train}}$ are the training set and the associated ground truth (e.g., class labels for the classification task), which would be absent for the unsupervised graph mining tasks (e.g., clustering, ranking).

We give three concrete examples next.

**Example #1: personalized PageRank** [16] is a fundamental ranking model. When the adjacency matrix of the underlying graph is symmetrically normalized, the ranking vector $r$ can be obtained as:

$$r^* = \arg \min \ r^T (I - \hat{A} r + (1-q) [r - e])^2,$$

where $\hat{A}$ is the symmetrically normalized adjacency matrix; $q \in (0, 1]$ is the damping factor; $e$ is the preference vector; the ranking vector $r^*$ is the solution of the ranking model (i.e., $\theta^* = r^*$).

**Example #2: spectral clustering** [30] is a classic graph clustering model aiming to minimize the normalized cut between clusters:

$$u^* = \arg \min_u u^T L u \text{ s.t. } u^T D u = 1, D = D_u - I_u,$$

where $L$ is the Laplacian matrix of adjacency matrix $D$ is the diagonal degree matrix (i.e., $D[i, i] = \sum_j A[i, j]$); $D_u$ is one-all vector with the same size as $u$; the model solution $\theta^*$ is the cluster indicator vector $u^*$.

**Example #3: node classification** aims to construct a classification model based on the graph topology $A$ and feature $X$. A typical loss for node classification is cross-entropy (CE) over the training set:

$$\theta^* = \arg \min_{\theta} - \sum_{i \in T} \sum_{j=1}^K y_{ij} \ln \hat{y}_{ij},$$

where $c$ is the number of classes, $y_{ij}$ is the ground truth indicating if node $i$ belongs to class $j$, $T$ is the training set, $\hat{y}_{ij} = f(G, \theta)[i, j]$ is the predicted probability that node $i$ belongs to class $j$ by a classifier $f(G, \theta)$ parameterized by $\theta$. For example, classifier $f(G, \theta)$ can be a GNN whose trained model parameters form the solution $\theta^*$.

**Remarks.** Both the standard personalized PageRank and spectral clustering are unsupervised and therefore the training set $T$ and its supervision $Y_{\text{train}}$ are absent in the corresponding loss functions (i.e., Eq. (1) and (2)), respectively. Nonetheless, both personalized PageRank and spectral clustering have been generalized to further incorporate some forms of supervision, as we will show next.

### C - Graph Sanitation: Formulation and Instantiations

Given an initial graph $G$ and an optimization-based graph mining model $L(G, \theta, T, Y_{\text{train}})$, we aim to learn a modified graph $\hat{G}$ to boost the performance of the corresponding mining model and we name it as graph sanitation problem. The basic idea is to let the mining performance on a validation set $V$ guide the modification process. Formally, the graph sanitation problem is defined as follows.

**Problem 1: Graph Sanitation Problem**

**Given:** (1) a graph represented as $G = (A, X)$, (2) a graph mining task represented as $L(G, \theta, T, Y_{\text{train}})$, (3) a validation set $V$ and its supervision $Y_{\text{validd}}$, and (4) the sanitation budget $B$;
We formulate Problem 1 as a bilevel optimization problem:

\[
\begin{array}{l}
\text{min} \quad L_{\text{upper}}(G, 0^\ast, \mathcal{V}, Y_{\text{valid}}) \\
\text{s.t.} \quad 0^\ast = \text{arg min} \quad L_{\text{lower}}(G, 0, \mathcal{T}, Y_{\text{train}}), \quad D(\hat{G}, G) \leq B
\end{array}
\]

where the lower-level optimization is to train the model \(0^\ast\) based on the training set \(\mathcal{T}\); the upper-level optimization aims to optimize the performance of the trained model \(0^\ast\) on the validation set \(\mathcal{V}\), and there is no overlap between \(\mathcal{T}\) and \(\mathcal{V}\); the distance function \(D\) measures the distance between two graphs. For example, we can instantiate \(D(\hat{G}, G)\) as \(||A - A||_1\) or \(||X - X||_1\) based on scenarios. Notice that the loss function \(L_{\text{upper}}\) is the distance function \(D\) between the two graphs.

The proposed bilevel optimization problem in Eq. (4) is quite general. In principle, it is applicable to any graph model with differentiable \(L_{\text{upper}}\) and \(L_{\text{lower}}\). We give its instantiations with the three aforementioned mining tasks and summarize them in Table 2.

**Table 2: Instantiations of graph sanitation problem over various mining tasks**

| Mining Tasks | Personalized PageRank [2, 16, 24] | Spectral clustering [30, 38] | Semi-supervised node classification |
|--------------|-----------------------------------|-----------------------------|-----------------------------------|
| \(L_{\text{lower}}\) | \(\min_q \log(1 - A_r + (1 - q) ||r - e||^2)\) | \(\min_u \ Lu \) s.t. \(\text{tr} \ Du = 1, \ Du \perp 1\) | \(\min_c \sum_{i \in c} \sum_{j \in i} y_{ij} \ln y_{ij}\) |
| \(L_{\text{upper}}\) | \(\min_{A} \sum_{x \in P, y \in N} (1 + \exp \{r^\ast [x] - r^\ast [y]/w\})^{-1}\) | \(\min_{A} -u^\ast Qu^\ast\) | \(\min_{c} \sum_{i \in c} \sum_{j \in i} y_{ij} \ln y_{ij}\) |
| \(\mathcal{T}\) | none | none | training set \(\mathcal{T}\) |
| \(\mathcal{V}\) | positive node set \(P\) | 'must-link' set \(M\) | labels of training set \(Y_{\text{train}}\) |
| \(\mathcal{N}\) | negative node set \(N\) | 'cannot-link' set \(C\) | validation set \(\mathcal{V}\) |
| \(Y_{\text{valid}}\) | none | none | labels of validation set \(Y_{\text{valid}}\) |

Find: A modified graph \(\hat{G} = (\tilde{A}, \tilde{X})\) to boost the performance of input graph mining model.

We formulate Problem 1 as a bilevel optimization problem:

\[
\hat{G} = \arg \min_G L_{\text{upper}}(G, 0^\ast, \mathcal{V}, Y_{\text{valid}}), \quad D(\hat{G}, G) \leq B
\]

where the lower-level optimization is to train the model \(0^\ast\) based on the training set \(\mathcal{T}\); the upper-level optimization aims to optimize the performance of the trained model \(0^\ast\) on the validation set \(\mathcal{V}\), and there is no overlap between \(\mathcal{T}\) and \(\mathcal{V}\); the distance function \(D\) measures the distance between two graphs. For example, we can instantiate \(D(\hat{G}, G)\) as \(||A - A||_1\) or \(||X - X||_1\) based on scenarios. Notice that the loss function \(L_{\text{upper}}\) is the distance function \(D\) between the two graphs.

The proposed bilevel optimization problem in Eq. (4) is quite general. In principle, it is applicable to any graph model with differentiable \(L_{\text{upper}}\) and \(L_{\text{lower}}\). We give its instantiations with the three aforementioned mining tasks and summarize them in Table 2.

**Instantiation #1: supervised PageRank.** The original personalized PageRank [16] has been generalized to encode pair-wise ranking preference [2, 24]. For graph sanitation with supervised PageRank, the training set and its supervision is absent, and the lower-level loss \(L_{\text{lower}}\) is given in Eq. (1). The validation set \(\mathcal{V}\) is consisted of a positive node set \(P\) and a negative node set \(N\). The supervision of the upper-level problem is that ranking scores of nodes from \(P\) should be higher than that from \(N\), i.e., \(r[x] > r[y], \forall x \in P, \forall y \in N\). Several choices for the upper-level loss \(L_{\text{upper}}\) exist. For example, we can use Wilcoxon-Mann-Whitney loss [43]:

\[
\min_A \sum_{x \in P, y \in N} (1 + \exp \{r^\ast [x] - r^\ast [y]/w\})^{-1}
\]

where \(w\) is the width parameter. It is worth-mentioning that Eq. (5) only modifies graph topology \(A\). Although Eq. (5) does not contain variable \(A\), \(r^\ast\) is determined by \(A\) through the lower-level problem.

**Instantiation #2: supervised spectral clustering.** A typical way to encode supervision in spectral clustering is via 'must-link' and 'cannot-link' [35, 38]. For graph sanitation with supervised spectral clustering, the training set together with its supervision is absent, and the lower-level loss \(L_{\text{lower}}\) is given in Eq. (2). The validation set \(\mathcal{V}\) contains a 'must-link' set \(M\) and a 'cannot-link' set \(C\). For the upper-level loss, the idea is to encourage nodes from must-link set \(M\) to be grouped in the same cluster and in the meanwhile push nodes from cannot-link set \(C\) to be in different clusters. To be specific, \(L_{\text{upper}}\) can be instantiated as follows.

\[
\min_A -u^\ast Qu^\ast
\]

where \(Q\) encodes the 'must-link' and 'cannot-link', that is, \(Q[i, j] = 1\) if \((i, j) \in M\), \(Q[i, j] = -1\) if \((i, j) \in C\), and \(Q[i, j] = 0\) otherwise. This instantiation only modifies the graph topology \(A\).

**Instantiation #3: semi-supervised node classification.** For graph sanitation with semi-supervised node classification, its lower-level optimization problem is given in Eq. (3). We have cross-entropy loss over validation set \(\mathcal{V}\) as the upper-level problem:

\[
\min_G L_{\text{CE}}(G, 0^\ast, \mathcal{V}, Y_{\text{valid}}) = \sum_{i \in \mathcal{V}} \sum_{j \in i} y_{ij} \ln \hat{y}_{ij}
\]

As mentioned before, there should be no overlap between the training set \(\mathcal{T}\) and the validation set \(\mathcal{V}\). If both the topology \(A\) and node feature \(X\) are used for classification, then both components can be modified in this instantiation.

**Remarks.** If the initially given graph \(G\) is poisoned by adversarial attackers [46, 47], the graph sanitation problem with semi-supervised node classification can also be used as a defense strategy. However, it bears important difference from the existing robust GNNs [9, 17, 41] as it does not assume the given graph is poisoned or any specific way by which it is poisoned. Therefore, graph sanitation problem in this scenario can boost the performance under a wide range of attacking scenarios (e.g., non-poisoned graphs, lightly-poisoned graphs, and heavily-poisoned graphs) and has the potential to work hand-in-hand with existing robust GNNs model.

In the next section, we propose an effective algorithm to solve the graph sanitation problem with semi-supervised node classification.

### 3 PROPOSED ALGORITHMS: GASOLINE

In this section, we focus on graph sanitation problem in the context of semi-supervised node classification and propose an effective solver named GASOLiNe. The general workflow of GASOLiNe is as follows. First, we solve the lower-level problem (Eq. (3)) and obtain a solution \(0^\ast\) together with its corresponding updating trajectory. Then we compute the hyper-gradient of the upper-level loss function (Eq. (7)) w.r.t. the graph \(G\) and use a set of hyper-gradient-guided modification to solve the upper-level optimization problem. Recall that we need a classifier \(f\) to provide the predicted labels (in both the lower-level and upper-level problems) which is parameterized by \(\theta\) and we refer to this classifier as the backbone
classifier. Finally we test the performance of another classifier over the modified graph on the test set \( \mathcal{W} \) and this classifier is named as the downstream classifier. In the following subsections, we will introduce our proposed solution \textsc{GaSoliNe} in three parts, including (A) hyper-gradient computation, (B) hyper-gradient aggregation, (C) hyper-gradient-guided modification, and (D) low-rank speedup.

**A - Hyper-Gradient Computation.** Eq. (4) and its corresponding instantiations Eqs. (3)(7) fall into the family of bilevel optimization problem where the lower-level problem is to optimize \( \theta \) via minimizing the loss over the training set \( \{T, Y_{\text{train}}\} \) given \( G \) and the upper-level problem is to optimize \( G \) via minimizing the loss over \( \{V, Y_{\text{valid}}\} \). We compute gradient w.r.t. the upper-level problem and view the lower-level problem as a dynamic system:

\[
\theta^{t+1} = \Theta^{t+1}(G, \theta^t, T, Y_{\text{train}}), \quad \theta^1 = \Theta^1(G, T, Y_{\text{train}}),
\]

where \( \Theta^t \) is the initialization of \( \theta \) and \( \Theta^{t+1} (t \neq 0) \) is the updating formula which can be instantiated as an optimizer over the lower-level objective function on training set (Eq. (3)). Hence, in order to get the hyper-gradient of the upper-level problem \( \nabla_G \), we assume that the dynamic system converges in \( T \) iterations (i.e., \( \theta^T = \Theta^T \)). Then we can unroll the iterative solution of the lower-level problem and obtain the hyper-gradient \( \nabla_G \) via the chain rule as follows [3]. For brevity, we abbreviate cross-entropy loss over the validation set \( \mathcal{L}_{\text{CE}}(G, \theta^T, V, Y_{\text{valid}}) \) as \( \mathcal{L}_{\text{valid}}(\theta^T) \).

\[
\nabla_G \mathcal{L} = \nabla_G \mathcal{L}_{\text{valid}}(\theta^T) + \sum_{t=0}^{T-2} B_t A_{t+1} \cdots A_{T-1} \nabla_{\theta^T} \mathcal{L}_{\text{valid}}(\theta^T) \tag{9}
\]

where \( A_t = \nabla_{\theta^t} \theta^{t+1}, B_t = \nabla_G \theta^{t+1} \).

Our final goal is to improve the performance of converged downstream classifiers. Hence, \( T \) is set as a relatively large value (e.g., 200 in our experiments) to ensure the hyper-gradient from the upper-level problem is computed over a converged classifier. To balance the effectiveness and the efficiency, we adopt the truncated hyper-gradient [29] w.r.t. \( G \) and rewrite the second part of Eq. (9) as

\[
\sum_{t=0}^{T-2} B_t A_{t+1} \cdots A_{T-1} \nabla_{\theta^T} \mathcal{L}_{\text{valid}}(\theta^T) \equiv \nabla_{\theta^T} \mathcal{L}_{\text{valid}}(\hat{f}_G), \quad \hat{f}_G \text{ is an estimation of } f_G
\]

For brevity, we abbreviate \( \nabla_{\theta^T} \mathcal{L}_{\text{valid}}(\hat{f}_G) \) as \( \nabla_{\theta^T} \mathcal{L}_{\text{valid}}(\hat{f}_G) \). In order to achieve a faster estimation of the hyper-gradient, we further adopt a first-order approximation [26, 47] and the hyper-gradient \( \nabla_G \mathcal{L} \) can be computed as:

\[
\nabla_G \mathcal{L} = \sum_{t=0}^{T} \nabla_G \mathcal{L}_{\text{valid}}(\theta^t). \tag{10}
\]

where the updating trajectory of \( \theta^t \) is the same as Eq. (8). If the initially-provided graph \( G \) is undirected, it indicates that \( A = A' \). Hence, when we compute the hyper-gradient w.r.t. the undirected graph topology \( A \), we need to calibrate the partial derivative into the derivative [18] and update the hyper-gradient as follows:

\[
\nabla_A \mathcal{L} \leftarrow \nabla_A \mathcal{L} + (\nabla_A \mathcal{L})' - \text{diag}(\nabla_A \mathcal{L}). \tag{11}
\]

For the hyper-gradient w.r.t. feature \( X \) and directed graph topology \( A (A \neq A') \), the above calibration process is not needed.

**B - Hyper-Gradient Aggregation.** To ensure the quality of graph sanitization without introducing bias from a specific dataset split, we adopt \( K \)-fold training/validation split with similar settings as cross-validation [7]. The specific procedure is that during the training period, we split all the labeled nodes \( Z \) into \( K \) folds and alternately select one of them as \( V \) (with labels \( Y_{\text{valid}} \)) and the others as \( T \) (with labels \( Y_{\text{train}} \)). In total, there are \( K \) sets of training/validation splits. With the \( k \)-th dataset split, by Eq. (10), we obtain the hyper-gradient \( \nabla_G^k \mathcal{L} \). For the hyper-gradient \( \{\nabla_G^1 \mathcal{L}, \ldots, \nabla_G^K \mathcal{L}\} \) from the \( K \) sets of training/validation split, we sum them up as the aggregated hyper-gradient:

\[
\nabla_G = \sum_k \nabla_G^k \mathcal{L}. \tag{12}
\]

**C - Hyper-Gradient-Guided Modification.** With regard to modifying the graph based on the aggregated hyper-gradient \( \nabla_G \), we provide two variants, discretized modification and continuous modification. The discretized modification can work with binary inputs such as adjacency matrices of unweighted graphs and binary feature matrices. The continuous modification is suitable for both continuous and binary inputs. For the clarity of explanation, we replace the \( G \) with the adjacency matrix \( A \) as an example for the topology modification. It is straightforward to generalize that to the feature modification with feature matrix \( X \).

The discretized modification is guided by a hyper-gradient-based score matrix:

\[
S = (-\nabla_A) \circ (1 - 2A), \tag{13}
\]

where \( \circ \) denotes Hadamard product, 1 is an all-one matrix. This score matrix is composed by ‘preference’ (i.e., \(-\nabla_A\)) and ‘modifiability’ (i.e., \((1 - 2A)\)). Only entries with both high ‘preference’ and ‘modifiability’ can be assigned with high scores. For example, large positive \((1 - \nabla_A)[i, j] \) indicates strong preference of adding an edge between the \( i \)-th and the \( j \)-th nodes based on the hyper-gradient and if there was no edge between the \( i \)-th and the \( j \)-th nodes (i.e., \( A[i, j] = 0 \)), the signs of \((1 - \nabla_A)[i, j] \) and \((1 - 2A)[i, j] \) are the same which result in a large \( S[i, j] \). Then, corresponding \( B \) entries in \( A \) are modified by flipping the sign of them based on the indices of the top-\( B \) entries in \( S \).

The continuous modification is hyper-gradient descent with budget-adaptive learning rate:

\[
A \leftarrow A - \frac{B}{\sum_{i,j} |\nabla_A[i, j]|} \cdot \nabla_A. \tag{14}
\]

We compute the learning rate based on the ratio of the modification budget \( B \) to the sum of absolute values of the hyper-gradient matrix. In implementation, for both modification methods, we set the budget in every iteration as \( b \) and update the graph in multiple steps until we run out of the total budget \( B \) so as to balance the effectiveness and the efficiency. Algorithm 1 summarizes the detailed modification procedure. In addition, in our experiments, the \( B \) for topology \( (B_{\text{topo}}) \) and the \( B \) for feature \( (B_{\text{feat}}) \) are set separately since the modification cost on different elements of a graph may not be comparable.

**Remarks.** We notice that LDS [12] formulates the graph learning problem for GNN under the bilevel optimization context. Here, we claim the differences and advantages: (1) LDS focuses on learning graph topology, but \textsc{GaSoliNe} can handle any graph components (e.g., topology and feature); (2) LDS formulates the topology as a set of Bernoulli random variables, whose updating requires multiple samplings which are time-consuming, but \textsc{GaSoliNe} works in a deterministic and efficient way and also provides the discrete solutions; (3) in the following section we will introduce a speed-up variant of \textsc{GaSoliNe} which shows great efficacy.

**D - Speedup and Scale-up.** The core operation of our proposed \textsc{GaSoliNe} is to compute hyper-gradient w.r.t. the graph components (i.e., \( A \) and \( X \)) which leads into a gradient matrix (e.g., \( \nabla_A \)). In many real-world scenarios (e.g., malfunctions of certain nodes,
targeted adversarial attacks), perturbations are often around a small set of nodes, which leads to low-rank perturbation matrices. Hence, for topology modification, we propose to further decompose the incremental matrix (i.e., ∆A) into its low-rank representation (i.e., ∆A = UVr), and compute the hyper-gradient with respect to the low-rank matrices instead, which can significantly speedup and scale up the computation. Recall that the low-rank assumption is only held for the incremental matrix, but for the modified graph (i.e., A), it is not limited to be low-rank. Mathematically, the low-rank modification can be represented as:

$$\tilde{A} = A + ∆A = A + UV^r,$$

(14)

where U, V ∈ Rnxr, and r is the rank of ∆A. Hence, by substituting A with A + UV^r in Eq. (7) (i.e., G = (A + UV^r, X)) and changing the optimization variable from A into U and V, we can obtain hyper-gradient with respect to U and V (i.e., ∇U L and ∇V L) in the same manner as Eq.(10). By aggregating the hyper-gradients from different training/validation splits as we introduced in Sec. 3-B, we obtain aggregated hyper-gradients ∇U and ∇V. Any gradient descent-based method can then be used to update U and V.

In this way, we can significantly reduce the time and space complexity, which is summarized in the following lemma. Notice that n, m, d are number of nodes, number of edges and feature dimension, respectively and we have d ≪ n and m ≪ n^2. As a comparison, the time complexity of computing ∇A L is O(n^2d) and the space complexity of computing ∇A L is O(n^2). Hence, this low-rank method is much more efficient in both time and space.

**Lemma 1.** For computing ∇U L and ∇V L, the time complexity is O(n^2d^2 + md) and the space complexity is O(m + nd).

**Proof.** See Appendix. □

### 4 EXPERIMENTS

In this section, we perform empirical evaluations. All the experiments are designed to answer the following research questions:

- **RQ1** How applicable is the proposed GaSoliNe with respect to different backbone/downstream classifiers, as well as different modification strategies?
- **RQ2** How effective is the proposed GaSoliNe for initial graphs under various forms of perturbation? To what extent does the proposed GaSoliNe strengthen the existing robust GNNs?
- **RQ3** How efficient and effective is the low-rank GaSoliNe?

#### 4.1 Experiment Setups

We evaluate the proposed GaSoliNe on Cora, Citeseer, and Polblogs datasets [20, 46, 47]. Since the Polblogs dataset does not contain node features, we use an identity matrix as the node feature matrix. All the datasets are undirected unweighted graphs and we experiment on the largest connected component of every dataset.

In order to set fair modification budgets across different datasets, the modification budget on adjacency matrix Btopo is defined as Btopo = m × modification rate_topo and the budget on feature matrix Bfea is defined as Bfea = n × d × modification rate_fea, where m is the number of existing edges, n is the number of nodes, d is the node feature dimension. We set modification rate_topo = 0.1 and modification rate_fea = 0.001 throughout all the experiments. Detailed hyper-parameter settings are attached in Appendix.

We use the accuracy as the evaluation metric and repeat every set of experiment 10 times to report the mean ± std value.

#### 4.2 Applicability of GaSoliNe

In this subsection, we conduct an in-depth study about the property of modified graphs by GaSoliNe. The proposed GaSoliNe trains a backbone classifier in the lower-level problem and uses the trained backbone classifier to modify the initially-provided graph and improve the performance of the downstream classifier on the test nodes. In addition, GaSoliNe is capable of modifying both the graph topology (i.e., A) and feature (i.e., X) in both the discretized and continuous fashion. To verify that, we select three classic GNNs-based node classifiers, including GCN [20], SGC [40], and APPNP [21] to serve as the backbone classifiers and the downstream classifiers. The detailed experiment procedure is as follows.

First, we modify the given graph using proposed GaSoliNe algorithm with 4 modification strategies (i.e., modifying topology or node feature with discretized or continuous modification). Each variant is implemented with 3 backbone classifiers so that in total there are 12 sets of GaSoliNe settings. Second, with the 12 modified graphs, we test the performance of 3 downstream classifiers and report the result (mean±std Acc) under each setting. For the results in this subsection, the initially provided graph is Citeseer [20].
Table 3: Effectiveness of GaSoliNe under multiple variants (Mean±Std Accuracy). The first and second columns denote the modification strategies and backbone classifiers adopted by GaSoliNe respectively. The remaining columns show the performance of various downstream classifiers. • indicates significant improvement compared with results on the original graph (values in the second row) with a p-value<0.01 and ◦ indicates no statistically significant improvement.

| Variant | Backbone | GCN  | SGC  | APPNP |
|---------|----------|------|------|-------|
| None    | None     | 72.2±0.5 | 72.8±0.2 | 71.8±0.4 |
| DT      | GCN      | 74.7±0.3e | 74.8±0.1e | 75.4±0.2e |
|         | SGC      | 74.7±0.4e | 75.2±0.2e | 75.6±0.3e |
|         | APPNP    | 74.6±0.3e | 74.6±0.1e | 75.4±0.4e |
| DF      | GCN      | 72.4±0.3o | 72.7±0.2o | 72.8±0.3e |
|         | SGC      | 75.3±0.5e | 73.4±0.2e | 73.6±0.4e |
|         | APPNP    | 72.6±0.3o | 72.9±0.1o | 73.6±0.4e |
| CT      | GCN      | 73.1±0.4e | 73.6±0.1e | 74.8±0.2e |
|         | SGC      | 73.0±0.3e | 73.5±0.2e | 74.4±0.3e |
|         | APPNP    | 72.8±0.5o | 73.4±0.1e | 74.4±0.9e |
| CF      | GCN      | 72.7±0.4o | 73.6±0.1e | 73.8±0.3e |
|         | SGC      | 72.9±0.4e | 73.6±0.1e | 73.8±0.4e |
|         | APPNP    | 73.0±0.3e | 73.6±0.2e | 73.9±0.3e |

Figure 1: Visualization of node embeddings from original Citeseer graph (a) and modified Citeseer graph by GaSoliNe (b). Best viewed in color.

Experimental results are reported in Table 3 where ‘DT’ denotes ‘discretized topology modification’, ‘CT’ denotes ‘continuous topology modification’, ‘DF’ denotes ‘discretized feature modification’, and ‘CF’ denotes ‘continuous feature modification’. The second row of Table 3 shows the results on the initially-provided graph and the other rows denote the results on modified graphs with different settings. We use • to indicate that the improvement of the result is statistically significant compared with results on the initially-provided graph with a p-value<0.01, and we use ◦ to indicate no statistically significant improvement. We have the following observations. First, in the vast majority cases, the proposed GaSoliNe is able to statistically significantly improve the accuracy of the downstream classifier over the initially-provide graph, for every combination of the modification strategy (discretized vs. continuous) and the modification target (topology vs. feature). Second, the graphs modified by GaSoliNe with different backbone classifier can benefit different downstream classifiers, which demonstrates great transferability and broad applicability.

We further provide visualization of node embeddings before and after modification. We present the visualizations of initial Citeseer graph and the modified Citeseer graph from GaSoliNe discretized topology modification variant with backbone classifier as SGC [40]. The detailed visualization procedure is that we utilize the training set $\mathcal{F}$ (and corresponding labels $\mathcal{Y}_{\text{train}}$) of given initial/modified graphs to train a GCN [20] and use hidden representation of the trained GCN to encode every node into a high-dimensional vector. Then, we adopt t-SNE [33] method to map the high-dimensional node embeddings into two-dimensional ones for visualization. Figure 1 shows the visualization results of node embeddings of the original Citeseer graph and the modified Citeseer graph. Clearly, the node embeddings from modified graph are more discriminative than the embeddings from the original graph. In specific, the clusters are more cohesive and there is less overlap between clusters in the modified graphs (i.e., Figures 1b) compared with those on the original graph (i.e., Figure 1a). It further demonstrates that even we have no knowledge about the downstream classifiers (in this case the backbone classifier and downstream classifier are different), the proposed GaSoliNe can still improve the graph quality to benefit downstream classifiers.

4.3 Effectiveness of GaSoliNe

As we point out in Sec. 1, the defects of the initially-provided graph could be due to various reasons. In this subsection, we evaluate the effectiveness of the proposed GaSoliNe by (A) the comparison with baseline methods on various poisoned/noisy graphs and (B) integrating with existing robust GNNs methods. The attack methods we use to poison benign graphs are as follows: (1) Random Attack randomly flips entries of benign adjacency matrices with different perturbation rate; (2) NETTACK [46] attacks a set of target nodes with different perturbations/node; (3) metattack [47] poisons the performance of node classifiers by perturbing the overall benign graph topology with different perturbation rate.

A - Comparison with baseline methods. We compare GaSoliNe with the following baseline methods: APPNP [21], GAT [34], Jaccard [41], SVD [9], RGCN [45], DE [28], and LDS [12]. Recall that we feed all the graph modification-based methods (Jaccard, SVD, DE, LDS, GaSoliNe) with the exactly same downstream classifier (APPNP) for a fair comparison.

We set 3 variants of GaSoliNe to compare with the above baselines. To be specific, we refer to (1) GaSoliNe with discretized modification on topology as GaSoliNe-DT, (2) GaSoliNe with continuous modification on feature as GaSoliNe-CF, and (3) GaSoliNe with discretized modification on topology and continuous modification on feature as GaSoliNe-DTCF. All these GaSoliNe variants use APPNP [21] as both the backbone classifier and the downstream classifier. We test various perturbation rates (i.e., perturbation rate of metattack from 5% to 25% with a step of 5%, perturbation rate of random attack from 20% to 100% with a step of 20%, and perturbations/node of NETTACK from 1 to 5) to attack the Cora [20] dataset and report the accuracy (mean±std) in Figure 2. From experiment results we observe that: (1) with the increase of adversarial perturbation, the performance of all methods drops, which is consistent with our intuition; (2) variants of GaSoliNe consistently outperform the baselines under various adversarial/noisy scenarios; and (3) the proposed GaSoliNe even improves over the original, benign graphs (i.e., 0 perturbation rate and 0 perturbations/node).
Graph Sanitation with Application to Node Classification

Conference '17, July 2017, Washington, DC, USA

Figure 2: Performance of models under (a) metattack, (b) Nettack, and (c) random attack. Best viewed in color.

| Attack     | Data   | APPNP   | GAT    | Jaccard | SVD     | RGCN    | DE     | LDS    | G-DT   | G-CF   | G-DTCF |
|------------|--------|---------|--------|---------|---------|---------|--------|--------|--------|--------|--------|
| metattack  | Cora   | 47.0±0.7| 48.8±0.2| 65.4±0.9| 60.3±0.8| 50.6±0.8| 48.7±0.9| 58.7±1.3| 67.3±0.7| 57.0±0.9| 68.8±0.9|
|            | Citeseer| 49.4±2.2| 62.4±0.7| 57.1±1.0| 49.5±0.8| 55.5±1.4| 50.1±2.3| 58.2±2.3| 63.5±1.5| 58.4±1.5| 62.2±1.0|
|            | Polblogs| 58.4±3.6| 48.2±6.6| N/A     | 79.1±2.4| 50.8±0.9| 56.4±6.3| 63.7±5.7| 65.0±0.7| 55.0±4.1| 64.7±1.4|
| Nettack    | Cora   | 60.7±1.2| 54.2±2.3| 63.7±1.4| 52.9±2.8| 56.5±1.1| 60.8±1.0| 64.5±2.4| 64.5±2.2| 63.9±2.4| 66.1±1.9|
|            | Citeseer| 68.3±6.8| 61.9±4.4| 72.5±3.3| 50.2±6.6| 56.4±1.5| 63.3±4.7| 71.0±3.3| 71.6±3.9| 69.4±4.8| 74.3±1.6|
|            | Polblogs| 90.5±1.0| 91.1±0.7| N/A     | 93.6±1.2| 93.1±0.2| 89.1±2.4| 91.1±1.8| 92.3±1.6| 90.3±0.7| 92.4±1.7|
| random     | Cora   | 74.3±0.4| 58.1±1.0| 75.1±0.5| 72.6±0.3| 68.9±0.4| 73.9±0.6| 76.6±0.4| 77.1±0.3| 78.3±0.5| 77.8±0.2|
| attack     | Citeseer| 69.8±0.6| 60.8±1.6| 69.7±0.5| 66.7±0.4| 65.7±0.2| 69.4±0.5| 72.3±0.4| 73.8±0.2| 72.3±0.4| 73.4±0.5|
|            | Polblogs| 74.7±2.8| 84.5±1.0| N/A     | 83.3±2.8| 81.7±0.9| 75.9±1.4| 73.2±2.8| 73.4±4.1| 77.1±1.6| 77.6±2.9|

Table 4: Comparison with baselines on heavily poisoned datasets (Mean±Std Accuracy). Some results are not applicable since Jaccard requires node features which are absent on Polblogs graph. G denotes GASOLiNE for short.

An interesting question is, if the initially-provided graph is heavily poisoned/noisy, to what extent is the proposed GASOLiNE still effective? To answer this question, we study the performance of GASOLiNE and other baseline methods on heavily-poisoned graphs (100% perturbation rate of random attack, 25% perturbation rate of metattack, and 5 perturbations/node of Nettack). The detailed experiment results are presented in Table 4. In most cases, GASOLiNE can obtain competitive or even better performance against baseline methods. On the Polblogs graph, GASOLiNE does not perform as well as in the other two datasets. This is because, (1) the Polblogs graph does not have node feature which weakens the effectiveness of modification from GASOLiNE and (2) the Polblogs graph has strong low-rank structure, which can be further verified in Sec. 4.4. As flexible solutions, in the next subsection, we study that if GASOLiNE can work together with other graph defense methods.

B - Incorporating with graph defense strategies. GASOLiNE does not make any assumption about the property of the defects of the initially-provided graph. We further evaluate if GASOLiNE can help boost the performance of both model-based and data-based defense strategies under the heavily-poisoned settings. We use a data-based defense baseline SVD [9], a model-based defense baseline RGCN [45], and another strong baseline GAT [34] to integrate with GASOLiNE since they have shown competitive performance from Table 4 and Figure 2. The detailed procedure is that for model-based methods (i.e., GAT and RGCN), GASOLiNE modifies the graph at first, and then the baselines are implemented on the modified graphs to report the final results. For the data-based method (i.e.,
SVD), we first implement the baseline to preprocess graphs, and then we modify graphs again by GaSoliNe, and finally run the downstream classifiers (APPNP) on the twice-modified graphs. In this task, specifically, we use GaSoliNe-DTCF to integrate various defense methods. In order to heavily poison the graphs, we use metattack [47] with perturbation rate as 25% to attack the benign graphs. We report the results in Table 1 and observe that after integrating with GaSoliNe, performance of all the defense methods further improves significantly with a $p$-value<0.01.

**Remark.** A detailed case study about the behaviour of GaSoliNe and a set of sensitivity studies for the hyper-parameters are provided in Appendix.

### 4.4 Efficacy of Low-Rank GaSoliNe

In order to answer RQ3, we first compare the performance of APPNP [21] on two modified graphs from the low-rank GaSoliNe (denoted as GaSoliNe-LR) and the original GaSoliNe, respectively. Specifically, for the original GaSoliNe, we adopt its variant with continuous modification towards the network topology. Due to the space limitation, we only show the results given graphs perturbed by metattack [47] in Table 5. We observe that in most settings on both the Cora and Citeseer datasets, the GaSoliNe-LR can obtain promising performance against the original GaSoliNe. Surprisingly, on the Polblogs dataset, the GaSoliNe-LR shows great advantages over the original GaSoliNe. One possible explanation is that Polblogs dataset is inherently low-rank (which can be corroborated by Table 4 where SVD [9] obtains strong performance) and GaSoliNe-LR learns a low-rank incremental matrix which amplifies the advantage further.

To verify the efficiency of proposed GaSoliNe-LR, we generate a set of synthetic graphs with different number of nodes $n$. The wall-clock time for computing hyper-gradient is presented in Figure 3. Clearly, the GaSoliNe-LR is much more efficient compared with the original GaSoliNe especially when the network size is large.

### 5 RELATED WORK

#### A - Graph Modification

The vast majority of the existing works on graph modification assume the initially provided graph is impaired or perturbed in a specific way. Network imputation problems focus on restoring missing links in a partially observed graph. For example, Liben-Nowell and Kleinberg [25] study the property of a set of node topology proximity measures; Huisman [15] handles missing data in exponential random graphs. Besides, knowledge graph completion is to predict missing links between entities. The representative works include TransE [4], TransH [39], ComplEx [32] and many more. In another line of research, network enhancement and denoising problems delete irrelevant links for the

| Data | Polblogs | Rate (%) | APPNP | GaSoliNe | GaSoliNe-LR |
|------|----------|----------|-------|----------|-------------|
| 0 0  | 94.1±0.6 | 95.3±0.6 | 95.7±0.3 |
| 5 0  | 70.1±0.6 | 73.8±0.9 | 93.4±0.3 |
| 10 0 | 69.8±0.8 | 72.8±0.4 | 90.8±0.2 |
| 15 0 | 66.5±0.5 | 70.1±1.2 | 88.7±0.3 |
| 20 0 | 64.4±0.9 | 68.5±1.0 | 88.0±0.3 |
| 25 0 | 57.9±0.6 | 64.8±2.1 | 89.9±0.5 |
| 0 0  | 90.1±0.6 | 95.3±0.6 | 95.7±0.3 |
| 5 0  | 70.1±0.6 | 73.8±0.9 | 93.4±0.3 |
| 10 0 | 69.8±0.8 | 72.8±0.4 | 90.8±0.2 |
| 15 0 | 66.5±0.5 | 70.1±1.2 | 88.7±0.3 |
| 20 0 | 64.4±0.9 | 68.5±1.0 | 88.0±0.3 |
| 25 0 | 57.9±0.6 | 64.8±2.1 | 89.9±0.5 |

**Table 5: Efficacy comparison between GaSoliNe and GaSoliNe-LR**

Given graphs. Arts such as NE [36], E-net [42], Mask-GVAE [23] study this problem under various scenarios. For network connectivity analysis, Chen et al. [5, 6] modify the underlying topology in order to manipulate the graph connectivity. Another relevant line is adversarial defense, which is as a response for the attack on graph mining models. Wu et al. [41] claim that deleting edges connecting two dissimilar nodes is an effective defense strategy; Entezari et al. [9] utilize the low-rank approximation of given graphs to retain the performance of downstream GCNs; Jin et al. [17] merge the topology sparsity and feature smoothness into the optimization goal and jointly learn the downstream classifiers. In addition, supervised PageRank [2, 24] and constrained spectral clustering [38] also encode extra supervision to guide the modification of graphs.

### B - Bilevel Optimization

Bilevel optimization problem is a powerful mathematical tool with broad applications. For instance, Finn et al. [10] formulate the learning to initialization problem in the bilevel optimization context; Li et al. [22] propose a bilevel optimization-based poisoning attack method for factorization-based systems. There are effective solutions such as the forward and reverse gradients [11], truncated back-propagation [29] and so on. In addition, Colson et al. [8] provide a detailed review about this topic. The most related arts to our work are [7] and [12]. Both of them aim to modify (or generate from scratch) the given data in a bilevel optimization context. The former studies a data debugging problem under the collaborative filtering scenario whose lower-level problem has a closed-form solution. The latter models every edge with a Bernoulli random variable. As a comparison, the lower-level problem of graph sanitation may not necessarily have a closed-form solution and we modify the initially provided graphs deterministically with versatile variants and broader applications.

### 6 CONCLUSION

In this paper, we introduce the graph sanitation problem, which aims to improve an initially-provided graph for a given graph mining model. We formulate the graph sanitation problem as a bilevel optimization problem and show that it can be instantiated by a
variety of graph mining models such as supervised PageRank, supervised clustering and node classification. We further propose an effective solver named GaSoLiNE for the graph sanitation problem with semi-supervised node classification. GaSoLiNE adopts an efficient approximation of hyper-gradient to guide the modification over the initially-provided graph. GaSoLiNE is versatile, and equipped with multiple variants. The extensive experimental evaluations demonstrate the broad applicability and effectiveness of the proposed GaSoLiNE.
### A REPRODUCIBILITY

We will release the source code upon the publication of the paper. Three public graph datasets, Cora\(^1\), Citeseer\(^1\), and Polblogs\(^2\), are used in our paper with following detailed statistics in Table 6.

| Data     | Nodes | Edges | Classes | Features |
|----------|-------|-------|---------|----------|
| Cora     | 2,485 | 5,069 | 7       | 1,433    |
| Citeseer | 2,110 | 3,668 | 6       | 3,703    |
| Polblogs | 1,222 | 16,714| 2       | N/A      |

Table 6: Statistics of Datasets

#### A.1 Hyper-Parameter Settings

We summarize the hyper-parameter settings of models implemented in our experiments including baseline methods, backbone and downstream classifiers of GASOLiNE:

- **GCN**\(^{[20]}\)/GAT\(^{[34]}\)/RGCN\(^{[45]}\): We follow the default settings of publicly available implementation of GCN\(^5\), GAT\(^3\), RGCN\(^9\).
- **SGC**\(^{[40]}\): The implementation of SGC is the same as GCN\(^{[20]}\) but we remove the activation function of the hidden layers.
- **APPNP**\(^{[21]}\): We follow the recommended hyper-parameter settings of APPNP \(^{[21]}\) in the original paper.
- **Jaccard**\(^{[41]}\): We search the edge removing threshold of Jaccard similarity from \([0.01, 0.03, 0.05, 0.1, 0.3, 0.5]\) and report the best.
- **SVD**\(^{[9]}\): We search the rank of SVD from \([10, 30, 50, 100\), \(200, 300]\) and report the best results from the above settings.
- **DE**\(^{[28]}\): We search the dropout rate of DE over existing edges from \([0.05, 0.1, 0.15, 0.2, 0.25]\) and report the best results from the above settings.
- **LDS**\(^{[12]}\): We implement LDS with the same modification budget as GASOLiNE-CT.

The detailed settings of GASOLiNE are as follows: (1) for all the modification strategies (discretized vs. continuous and topology vs. feature), the modification budget towards topology \(B_{\text{topo}}\) and the modification budget towards feature \(B_{\text{feat}}\) are introduced in the Section 4.1. Specifically, the modification rate \(r_{\text{topo}} = 0.1\) and modification rate \(r_{\text{feat}} = 0.001\). We modify the graph in 10 steps so the budget \(b\) in every modification step is \([\frac{b}{10}]\) (i.e., \(B_{\text{topo}} = \lceil \frac{B_{\text{topo}}}{10} \rceil\) and \(B_{\text{feat}} = \lceil \frac{B_{\text{feat}}}{10} \rceil\)). (2) The settings of backbone classifiers and downstream classifiers (GCN\(^{[20]}\), SGC\(^{[40]}\), APPNP\(^{[21]}\)) used in our experiments follow the aforementioned settings. (3) The number of iterations for the optimization of lower-level problem \(T\) is set as 200 and the truncating iteration \(P\) is set as 196. The number of folds \(K\) is set as 8.

For the attacking methods, their attacking perturbation rates are introduced in the Section 4.3, and here we present the detailed implementation of them. (1) We follow the publicly-available implementation\(^5\) of metattack\(^{[47]}\) and adopt the 'Meta-Self' variant to attack the provided graphs; (2) we follow \([17]\) to select nodes with degree larger than 10 as the target nodes and implement NETTACK with the publicly-available implementation\(^6\); (3) we implement random attack by symmetrically flipping \(B_{\text{attack}}\) entries of the adjacency matrix \(A\) of provided graphs.

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\(^{[1]}\)https://github.com/stkip/gcn
\(^{[2]}\)https://github.com/ChandlerBang/Pro-GNN
\(^{[3]}\)https://github.com/PetarV-/GAT
\(^{[4]}\)https://github.com/ZW-ZHANG/RobustGCN
\(^{[5]}\)https://github.com/danielzuegner/gnn-meta-attack
\(^{[6]}\)https://github.com/danielzuegner/nettack

### B PROOF OF LEMMA 1

Our complexity analysis is mainly based on the propagation formula of matrix multiplication-based GNNs and only focuses on a single-layered GNN with first order approximation of the hyper-gradient. However, it can be easily generalized into a wide range of scenarios (e.g., multi-layered GNNs) with similar analysis and conclusions. For brevity, we only analyze the complexity of computing \(\nabla_U \mathcal{L}\). The analysis w.r.t. computing \(\nabla_Y \mathcal{L}\) is similar and we omit here.

**Proof.** For typical matrix multiplication-based GNNs (e.g., \([20]\)), their propagation formula can be represented as \(X \leftarrow \sigma(AXW)\) (or even simplified by removing the nonlinear activation function \(\sigma\) and feature transformation matrix \(W\) between several layers \([21, 40]\)). If we do not consider the gradient across the model parameter (i.e., \(W\)) updating trajectory (i.e., first order approximation), and assume that our GNN contains only one layer, the hyper-gradient with respect to the vector \(U\) can be computed as follows,

\[
\nabla_U \mathcal{L} = \frac{\partial \mathcal{L}}{\partial \sigma((A + UV')XW)} \circ \sigma'((A + UV')XW) W'X'V. \tag{15}
\]

The computation of \((A + UV')XW\) can be rewritten as \(AXW + UV'XW\). Note that \(A\) is a sparse matrix and the space cost is \(O(m)\) for computing \(AXW\). The space cost is \(O(nd)\) for \(UV'XW\). For \(W'X'V\) the space cost is \(O(nd)\). Put everything together the space cost for computing \(\nabla_U \mathcal{L}\) is \(O(m + nd)\).

The time complexity of the part within \([\cdot]\) in Eq.(15) is \(O(nd^2 + md)\). The time complexity of computing \(W'X'V\) is \(O(ndr)\). The time complexity about the multiplication between \([\cdot]\) and \(W'X'V\) is \(O(ndr)\). Hence, put everything together the total time complexity for computing \(\nabla_U \mathcal{L}\) is \(O(nd^2 + md)\) given \(r << d\). \(\square\)

### C CASE STUDY ABOUT THE BEHAVIOUR OF GASOLINE

Here, we further study the potential reasons behind the success of GASOLiNE. To this end, we conduct a case study whose core idea is to label malicious modifications (from adversaries) and test if GASOLiNE is able to detect them. The specific procedure is that we utilize different kinds of attackers (i.e., metattack\(^{[47]}\), NETTACK\(^{[46]}\), and random attack) to modify the graph structure of a benign graph \(G\) (with adjacency matrix \(A\)) into a poisoned graph \(G_{\text{adv}}\) (with adjacency matrix \(A_{\text{adv}}\)). Then, we utilize the score matrix \(S\) from Eq. (12) to assign a score to every entry of the poisoned adjacency matrix \(A_{\text{adv}}\). As we mentioned in Section 3, the higher score an entry obtains, the more likely GASOLiNE will modify it. We compute the average score of three groups of entries from \(A_{\text{adv}}\): the poisoned entries after adding/deleting perturbations from adversaries, the benign existing edges without perturbation, and the benign non-existing edges without perturbation. Remark that both the benign graphs and the poisoned graphs are unweighted and we define following auxiliary matrices. \(A_{\text{diff}} = |A_{\text{adv}} - A|\) is a difference matrix whose entries with value 1 indicate poisoned entries. \(A_{\text{benign-E}} = A \odot (1 - A_{\text{diff}})\) is a benign edge indicator matrix whose entries with value 1 indicate the benign existing edges without perturbation. \(\odot\) indicates element-wise multiplication. \(A_{\text{benign-NE}} = (1 - A) \odot (1 - A_{\text{diff}})\) is a benign non-existing edge indicator matrix whose entries with value 1 indicate the benign non-existing edges without perturbation. Based on that, we have the following three statistics:
D EFFECT OF MODIFICATION BUDGET

In this section we study the relationships between the budget of GaSoliNe and the corresponding performance of the downstream classifier. Here, we instantiate two variants of GaSoliNe: discretized modification towards topology (GaSoliNe-DT) and continuous modification towards feature (GaSoliNe-CF). The provided graph is Cora [20] which is heavily-poisoned by metattack [47] with perturbation rate $= 25\%$ (i.e., $B$). The perturbation budget per modification step $b$ is set to be $B/b$. Both the backbone classifier and the downstream classifier of GaSoliNe are the APPNP [21] models with the aforementioned settings. From Figure 5 we observe that with the increase of the modification budget ($\text{modification rate}_\text{topo}$ and modification rate$_\text{fea}$), GaSoliNe enjoys great potential to further improve the performance of the downstream classifiers. At the same time, ‘economic’ choices are strong enough to benefit downstream classifiers so we set modification rate$_\text{topo}$ as 0.1 and modification rate$_\text{fea}$ as 0.001 throughout our experiment settings.

Figure 4: Score of various entries under metattack (a), Nettack (b), and random attack (c). Best viewed in color.

$$S_{\text{adv}} = \frac{\sum_{i,j} (S \odot A_{\text{diff}})[i,j]}{\sum_{i,j} A_{\text{diff}}[i,j]},$$

$$S_{\text{benign-E}} = \frac{\sum_{i,j} (S \odot A_{\text{benign-E}})[i,j]}{\sum_{i,j} A_{\text{benign-E}}[i,j]},$$

$$S_{\text{benign-NE}} = \frac{\sum_{i,j} (S \odot A_{\text{benign-NE}})[i,j]}{\sum_{i,j} A_{\text{benign-NE}}[i,j]}$$

which denote the average score obtained by poisoned entries, benign existing edges, and benign non-existing edges.

Detailed results are presented in Figure 4. We observe that GaSoliNe tends to modify poisoned entries more (with higher scores) than to modify benign unperturbed entries in the adjacency matrix of poisoned graphs, which is consistent with our expectation and enables the algorithm to partially recover the benign graphs and to boost the performance of downstream classifiers.

Figure 5: Performance of downstream classifier vs. the modification budget of GaSoliNe-DT (a) and GaSoliNe-CF (b)

Figure 6: Performance of GaSoliNe-DTCF vs. the update steps (a) and the number of folds $K$ (b)

E EFFECTS OF MODIFICATION STEPS AND NUMBER OF FOLDS

As we claimed in the main content, in implementation we set the budget in every iteration as $b$ and update the given graph multiple iterations till we run out of total budget $B$. Hence, the update steps equals to $\lfloor B/b \rfloor$. Intuitively less budget per iteration can provide finer update towards the given graphs. To validate that we test the performance of an instantiation of GaSoliNe with discretized modification towards topology and continuous modification towards feature (GaSoliNe-DTCF) on the Cora [20] graph which is poisoned by metattack [47] with perturbation rate $= 25\%$. Both the backbone classifier and the downstream classifier of GaSoliNe are the APPNP [21] with the aforementioned settings. From Figure 6a we observe that with more update steps downstream classifiers can get better performance. However, when the number of steps is larger than 20, the improvement of performance is minor.

In addition, the number of training/validation split fold $K$ is another important hyper-parameter in our model. Intuitively larger $K$ leads into better usage of the given data. To study the relationships between $K$ and the corresponding performance of the downstream classifier, we implement GaSoliNe-DTCF on the original Cora graph to verify that. Note that the modification rate$_\text{topo} = 0.1$, modification rate$_\text{fea} = 0.001$, and the number of modification steps is set as 10. From Figure 6b we observe that performance of the downstream classifier is improved with the increase of the number of folds. However, such performance gaining stops when $K = 6$. Hence, $K = 6$ is enough to make full use of the given graph by GaSoliNe.