Are we really making much progress in unsupervised graph outlier detection? Revisiting the problem with new insight and superior method

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Abstract—A large number of studies on Graph Outlier Detection (GOD) have emerged in recent years due to its wide applications, in which Unsupervised Node Outlier Detection (UNOD) on attributed networks is an important area. UNOD focuses on detecting two kinds of typical outliers in graphs: the structural outlier and the contextual outlier. Most existing works conduct the experiments based on the datasets with injected outliers. However, we find that the most widely-used outlier injection approach has a serious data leakage issue. By only utilizing such data leakage, a simple approach can achieve the state-of-the-art performance in detecting outliers. In addition, we observe that most existing algorithms have performance drops with varied injection settings. The other major issue is on balanced detection performance between the two types of outliers, which has not been considered by existing studies. In this paper, we analyze the cause of the data leakage issue in depth since the injection approach is a building block to advance UNOD. Moreover, we devise a novel variance-based model to detect structural outliers, which is more robust to different injection settings. On top of this, we propose a new framework, Variance-based Graph Outlier Detection (VGOD), which combines our variance-based model and attribute reconstruction model to detect outliers in a balanced way. Finally, we conduct extensive experiments to demonstrate the effectiveness and the efficiency of VGOD. The results on 5 real-world datasets validate that VGOD achieves not only the best performance in detecting outliers but also a balanced detection performance between structural and contextual outliers.

Index Terms—Graph Outlier Detection; Graph Neural Network; Unsupervised Graph learning; Attributed Networks

I. INTRODUCTION

Graph Outlier Detection (GOD, a.k.a. graph anomaly detection) is a fundamental graph mining task. It has various applications in high-impact domains and complex systems, such as spammer detection in social networks [2], sensor fault detection [3], financial fraudster identification [4], and defense on graph adversarial attacks [5]. The detection objects of GOD can be classified into different levels like node, edge, community and graph [6]. For example, detecting abnormal users in social network is the node-level outlier detection task while detecting abnormal molecule can be regarded as graph-level outlier detection task.

Due to the high cost or unavailability of manually labeling the ground truth outliers, a large number of existing GOD approaches are carried out in an unsupervised manner [7], [8], which aims to detect the instances that significantly deviate from the majority of instances in the graph [9]. Attributed network (a.k.a. attributed graph) is a powerful data representation for many real-world complex systems (e.g. a social network with user profiles) in which entities can be represented as nodes with their attribute information; the interaction or relationship between entities can be represented as edges [10]. In recent years, the study of Unsupervised Node Outlier Detection (UNOD) on attributed networks has been blooming due to its wide applications [11], [6], [12]. Different from traditional global outlier detection and time series outlier detection, it defines two new typical types of outliers on attributed networks, namely, structural outlier and contextual outlier [7].

In Fig 1 there is a toy example for these two kinds of basic outliers. Particularly, structural outliers are those nodes structurally connected to different communities, i.e., its structural neighborhood is inconsistent. In other word, a structural outlier has normal attributes while it may have several abnormal links. For example, those people from different communities but have strong connection with each other can be regarded as structural outliers. As shown in Fig 1(a), there are two communities outlined with orange circles and structural outliers are those nodes with abnormal link to other communities. On the other hand, a contextual outlier has consistent neighborhood structure while its attributes are
corrupted, noisy or significantly different from its neighbor nodes’ attributes. For example, in Fig 1(b), suppose that the node in red is a football player while nodes in green are music teachers. In this case, the node in red is regarded as a contextual outliers since it has a vast difference from its neighbors. In the real world, datasets are much more complicated than this toy example and it is difficult to measure the degree of inconsistency among nodes.

There have been various methods proposed to solve UNOD [12]. They can be roughly divided into two categories, namely, non-deep methods and deep-learning based methods. Non-deep methods, including SCAN [13], Radar [14] and ANOMALOUS [15], usually leverage traditional machine learning methods such as matrix factorization [16], density-based clustering [17] and relational learning [18] to encode the graph information and detect outliers. However, these methods fail to address the computational challenge with high-dimension data [19]. With the success of deep learning [20] and rapid prevalence of Graph Neural Networks (GNNs) [21], more and more methods are based on deep learning and GNNs nowadays [6]. For example, DOMINANT [7] employs two GNN autoencoders to reconstruct the attribute information and structure information of graph. According to the results reported in PyGOD [12], most deep-learning based methods have a much better performance than non-deep methods in detecting injected outliers. In order to unify outlier injection process, PyGOD adopts the outlier injection approach from [7] as the standard injection method.

**Challenge.** Although the recent deep-learning based methods have achieved quite excellent performance in UNOD, we find that the most widely-used outlier injection method [7], [22], [23], [24], [25], [12], [26], [27] has a serious data leakage issue. Concretely, structural outliers will have larger node degree than the average while attribute vectors of contextual outliers will have larger L2-norm (a.k.a. Euclidean norm) than the expected. As a result, simply utilizing node degree or L2-norm of attribute vectors as the outlier score to detect the corresponding type of outliers can acquire a quite satisfying performance as shown in Fig 2. The score of Area Under receiver operating characteristic Curve (AUC) [28] is adopted here to measure the performance of detecting outliers. In addition, we also find that most existing algorithms have a heavy rely on the current injection setting, especially for structural outliers. When the injection setting is changed, their performance drops quickly. Therefore, it is necessary to exploit a new model to detect structural outliers, which can have better robust ability to kinds of injection settings. Moreover, the balance between structural and contextual outliers detection performance is little considered in existing works [12]. An algorithm with unbalanced detection may only have detection ability for a certain type of outliers. To gain more feasible algorithms, comprehensive metrics for balance evaluation should be devised.

**Our Solution.** In this paper, we are devoted to analyzing the cause of data leakage to guide the future design of outlier injection approach, and devise superior outlier detection method for UNOD which can have much better performance both in current injection setting and varied injection settings.

In particular, we propose a novel variance-based model to detect the structural outliers, which adopts the variance of attribute vectors of neighbor nodes to detect structural outliers. To the best of our knowledge, it is the first time to employ the neighbor variance to detect outliers. Existing algorithms are based on reconstruction or contrastive learning to detect structure outliers which have neighbors from different communities. However, such methods cannot directly learn the consistency of neighbor nodes. In contrast, neighbor variance measures the consistency of neighbor nodes in direct, which achieves better effectiveness in the varied injection settings. On top of this, a new framework, Variance-based Graph Outlier Detection (VGOD), is also proposed to detect two types of outliers with variance-based model and attribute reconstruction model. To address the balance issue, we separately train two models to avoid the overtraining and normalize two types of outlier scores to eliminate the scale difference. To evaluate the balanced detection performance on two outlier types, we introduce a new metric to measure the gap of performance score. The experiment are conducted on 5 real-world datasets and the results demonstrate that VGOD achieves the best detection performance over each dataset.

**Contribution.** Our major contributions are as follows.

1) To the best of our knowledge, we are the first to identify the data leakage issue in the most widely-used outlier injection approach.
2) We analyze the cause of data leakage issue in depth and present a guide for future design of the outlier injection approach.
3) We propose a novel variance-based model and a new VGOD framework, which is more robust to the varied injection settings and the issue of balanced detection is alleviated.
4) Extensive experiments are conducted to demonstrate that our approach achieves both the best detection performance and a balanced detection performance.
II. RELATED WORK

A. Graph Neural Network

Due to the success of deep neural networks, a mass of effort has been devoted to developing deep neural networks for graph-structured data [21]. GNNs are a group of neural network models which utilize the graph structure for network representation learning and various tasks. Among GNNs, GCN [29] is one of the most influential models, which extends the convolutional operation in sequence or grid data to graph-structured data. Furthermore, in order to aggregate messages from neighbors more flexibly, GAT [30] introduces an attention mechanism to learn the importance of each neighbor node. On the other hand, GraphSage [31] adopts the sampling based method to aggregate the neighbor information in order to work in large-scale graph. In topological learning perspective, GIN [32] is a more expressive model than GCN and can achieve the same discriminativeness as 1-WL graph isomorphism test [33]. In our proposed framework, GNN plays a vital role in the network embedding representation of nodes. Flexibly, the GNN module in our framework can be set to any type of above mentioned GNNs.

B. Unsupervised Node Outlier Detection on Attributed Networks

UNOD on attributed networks has attracted considerable research interest in recent years due to its wide application in complex system. AMEN [34] detects abnormal nodes by leveraging neighborhood information of each node on attributed networks. Radar [14] utilizes the residuals of attribute information and its coherence graph structure for outlier detection. ANOMALOUS [15] conducts attribute selection and outlier detection jointly based on CUR decomposition and residual analysis. All the above methods have the computation limitation in high-dimension attributes and complex structure due to their shadow mechanisms.

Quite a few studies based on deep-learning technique have emerged recently [6]. Dominant [7] builds deep autoencoders on top of GCN layers to reconstruct the adjacency and attribute matrices in order to detect structural and contextual outliers. AnomalyDAE [24] employs dual autoencoders architecture with cross-modality interactions and attention mechanism to reconstruct the adjacency and attribute matrices. CoLA [22] performs the UNOD task via contrastive self-supervised learning and random walk with restart to embed nodes. AEGIS [23] studies UNOD in inductive setting by utilizing generative adversarial ideas to generate potential outliers. DONE [35] employs deep unsupervised autoencoders to generate the network embedding which eliminates the effects of outliers at the same time. CONAD [25] adopts four data augmentation strategies and contrastive learning for outlier detection. GUIDE [27] replaces adjacency reconstruction with higher-order structure reconstruction to detect structural outliers. Under the manner of outlier injection, all these above deep methods show superior performance than non-deep methods in detecting these two types of outliers. In order to evaluate UNOD algorithms, PyGOD adopts the most widely-used outlier injection approach from [7] as the standard injection method and provides unified benchmarks for UNOD, which facilitates the fairness for comparing different methods.

Although current UNOD methods have achieved excellent performance. However, as demonstrated in Fig 2 the widely-used outlier injection approach exists serious data leakage issue. To our surprise, simply using the combination of L2-norm and node degree to detect outliers can achieve the state-of-the-art performance. Therefore, our work focuses on analyzing the cause of data leakage issue and designing new method which has better detection performance than current UNOD methods and is more robust to varied injection settings. In addition, as mentioned in PyGOD [12] that no current method has a balanced detection performance on two outlier types, we also consider the balanced performance issue in our method.

III. PRELIMINARY

In this section, we formally present some concepts which are used throughout this paper and define the problem. We use lowercase letters (e.g. v), bold lowercase letters (e.g. x), uppercase letters (e.g. X) and calligraphic fonts (e.g. V) to denote scalars, vectors, matrices and sets, respectively.

A. Graph Neural Network

GNNs stack L layers of message passing layers. Each layer performs message passing through the given graph structure. After the initial node feature \(h_0 \in \mathbb{R}^{d_0}\) is transformed by L layers, the vector representation \(h_L \in \mathbb{R}^{d_L}\) is learned for each node \(v\). Most message passing layer can be expressed using the following rule:

\[
h_v^{(l)} = \sigma(\Psi^{(l)}(AGG(\{\Phi^{(l)}(h_u^{(l-1)}), u \in N_v \cup \{v\})))\quad (1)
\]

where \(\sigma(\cdot)\) is the active function, \(\Psi^{(l)}(\cdot)\) and \(\Phi^{(l)}(\cdot)\) denote differentiable functions such as Multi Layer Perceptrons (MLP). \(AGG(\cdot)\) denotes a differentiable, permutation invariant function (e.g. sum, mean, max) and \(N_v\) denotes node \(v\) ’s direct linked neighbors.

Here, we introduce three commonly used GNNs, namely GCN, GAT, and GIN.

**Graph Convolution Network (GCN)** [29] is the most widely-used GNN module, which adopts the propagation rule:

\[
H^{(l)} = \sigma(AH^{(l)}W^{(l)})
\]

where \(A\) is the symmetric normalized adjacency matrix, \(H^{(l)}\) is the \(l^{th}\) hidden layer node representation, \(W^{(l)}\) is the parameters in the \(l^{th}\) hidden layer.

**Graph Attention Network (GAT)** [30] flexibly aggregates messages from neighbors with importance \(\alpha_{ij}\) of each edge \(\langle i, j \rangle\) as

\[
\alpha_{ij} = \frac{\exp(\text{LeakyReLU}(\alpha^T[W_h_i][W_h_j]))}{\sum_{k \in N_i} \exp(\text{LeakyReLU}(\alpha^T[W_h_i][W_h_k]))}
\]

where \(\alpha\) and \(W\) are the learnable weights. Layer mask \(l\) is omitted for simplicity.
Graph Isomorphism Network (GIN) \[^{12}\] is the expressively more powerful GNN model, which follows the rule to propagate message as

\[
H^{(l)} = \sigma(\Psi^{(l)}(A + (1 + \epsilon) \cdot I)H^{(l-1)})
\]

(4)

where \(\epsilon\) can be fixed or learnable scalar parameter, \(I\) and \(A\) is the identity matrix and adjacency matrix, respectively.

B. Unsupervised Node Outlier Detection on Attributed Networks

**Definition 1** (Attributed Network). An attributed network can be denoted as \(\mathcal{G} = (\mathcal{V}, \mathcal{E}, X)\), where \(\mathcal{V} = \{v_1, v_2, \ldots, v_n\}\) is the set of nodes (\(|\mathcal{V}| = n\)), \(\mathcal{E}\) is the set of edges (\(|\mathcal{E}| = m\)) and \(X \in \mathbb{R}^{n \times d}\) is the attribute matrix. The \(i^{th}\) row vector \(x_i \in \mathbb{R}^d\) of the attribute matrix denotes the attribute information of the \(i^{th}\) node. Node \(i\)’s direct linked neighbors can be denoted as \(\mathcal{N}_i\).

With the aforementioned notations, the outlier detection problem on attributed network can be formally stated as a ranking problem.

**Definition 2** (Outlier Detection on Attributed Networks). Given an attributed network \(\mathcal{G} = (\mathcal{V}, \mathcal{E}, X)\), the goal is to learn a outlier score function \(f(\cdot)\) to calculate the outlier score \(o_i = f(v_i)\) for each node. The higher outlier score \(o_i\) is, the \(i^{th}\) node is more likely to be a structural outlier or a contextual outlier. By ranking all the nodes with their outlier scores, the abnormal nodes can be detected according to their ranking.

In this paper, we consider the setting of unsupervised node outlier detection (UNOD), which is generally adopted by the previous works. In this setting, none of the outlier label of the nodes is given in the training phase.

IV. DATA LEAKAGE ISSUE ANALYSIS

As shown in Fig. 2, the current widely-used outlier injection approach exists serious data leakage issue. In this section, we analyze the data leakage issue in detail. For these two types of outliers, we first introduce the outlier injection approach from \[^{12}\]. Next, we theoretically analyze the cause of data leakage issue and give our suggestion for future better design of outlier injection approach.

A. Structural Outlier

1) Injection Approach: The structural outliers are acquired by disturbing the topological structure of graph. In a clique, nodes are fully connected to each other. The intuition is that nodes in full connected clique should have strong correlation with each other. Based on this, the outlier assumption is that a clique composed of originally unrelated nodes is structural abnormal. The process of structural outlier injection is as followed. The first step is to specify the clique size \(q\) and the number of cliques \(p\). Next, for each clique, \(q\) random nodes are chosen from the set of normal nodes and made fully connected as structural outliers. Therefore, totally \(p \times q\) structural outliers will be injected to the dataset. In previous works, the clique size \(q\) is fixed to 15 for all datasets, and the value of \(p\) is set according to the size of dataset.

2) Cause Analysis: Since above injection approach only adds edges for the chosen structural outliers, all structural outliers’ node degrees have been increased due to such approach. Table I in section IV shows us the information of four datasets (Cora, Citeseer, PubMed, Flickr). The first three are citation networks and the last one Flickr is the social networks. We can find that the average node degree for citation networks are quite small. None of these citation networks has an average node degree greater than 3. However, due to the above injection approach, all the outlier will have node degree at least more than 15. In this case, the node degree can be utilized to detect the structural outliers. For Flickr, since it has a greater average node degree, therefore the data leakage issue is not as serious as these citation networks. From Fig. 2, AUC scores of node degree verify our analysis.

**Suggestion.** Therefore, we suggest that improvements of current structural outlier injection approach can be considered from the following aspects. Firstly, the clique size \(q\) should be changed to other value according to the dataset or specify multiple values in order to evaluate the performance of UNOD algorithm. Secondly, more various structural perturbation, like removing or replacing edges, should be considered as the way to disturb the topological structure of graph. Thirdly, if the approach will incur the data leakage, like node degree, the leakage information should be also evaluated as baseline for comparison.

B. Contextual Outlier

1) Injection Approach: The contextual outliers are acquired by disturbing the attributes of nodes. The outlier assumption is that a normal node’s attributes are consistent with its neighborhood’s attributes and inconsistent with unrelated nodes. The injection process is as followed. Firstly, totally \(p \times q\) normal nodes will be chosen as contextual outliers, which has the same number as structural outliers. Next, for each chosen outlier node \(v_i\), another \(k\) nodes \(\{v_{i_1}, v_{i_2}, \ldots, v_{i_k}\}\) are randomly sampled from \(\mathcal{V}\) as a candidate set \(\mathcal{V}_c\). For each \(v_{i_c}\) in \(\mathcal{V}_c\), the euclidean distance between the attribute vector \(x_{ci}\) of \(v_{ic}\) and \(x_i\) of \(v_i\) will be calculated. The attribute vector \(x_{ci}\) with the largest \(\|x_{ci} - x_i\|_2\) will be used to replace \(x_i\) as the new attribute vector of \(v_i\). The size of candidate set \(k\) is set to 50, ensuring that disturbance amplitude is large enough.

2) Cause Analysis: In order to ensure large enough disturbance of attributes, above injection approach changes the \(x_i\) to \(x_{ci}\) with the largest \(\|x_{ci} - x_i\|_2\). However, such strategy will lead to that the L2-norm of the final chosen \(x_{ci}\) (i.e. \(\|x_{ci}\|_2\)) is more likely to be large. We make the following assumptions.

**Assumption 1.** Suppose both \(x_{ci} \in \mathbb{R}^d\) and \(x_i \in \mathbb{R}^d\) are independently sampled from attribute matrix \(X\). The rank of matrix \(X\) is greater than 1.

**Assumption 2.** For \(x_{ci} \sim X\), \(x_{ci} = \|x_{ci}\|_2 \cdot e_{ci}\), where \(\|x_{ci}\|_2\) and \(e_{ci}\) are the modulo and direction of \(x_{ci}\), respectively. We assumed that \(\|x_{ci}\|_2\) and \(e_{ci}\) are independently distributed.
We use $P_r(x)$ to denote the possibility of $x$, then we have following theorem.

**Theorem 1.** \( P_r(\|x_{ci} - x_i\|_2 > \|x_{cj} - x_i\|_2 \Rightarrow \|x_{ci}\|_2 > \|x_{cj}\|_2) > 0.5 \)

**Proof.** We define \( D(x_{ci}, x_i) = \|x_{ci} - x_i\|_2 \). For notational convenience, we use \( s \) to refer to \( x_{ci} \) and \( t \) to refer to \( x_i \). Please note that both \( s \) and \( t \) are independently sampled from \( X \in \mathbb{R}^{n \times d} \).

\[
D^2(s, t) = \sum_{i=1}^{d} (s_i - t_i)^2 \\
= \sum_{i=1}^{d} s_i^2 - 2 \sum_{i=1}^{d} s_i t_i + \sum_{i=1}^{d} t_i^2 \\
= \|s\|_2^2 - 2\|s\|_2\|t\|_2 \cos \alpha + \|t\|_2^2 \\
= f(\|s\|_2)
\]

where \( \alpha \) is the angle between vector \( s \) and \( t \), \( \|s\|_2 \) is the mod of \( s \). From the above Equation, and we can regard \( D^2(s, t) \) as a quadratic function \( f(\cdot) \) of \( \|s\|_2 \). Particularly, \( \|s\|_2 = \|t\|_2 \cos \alpha \) is the symmetry axis for \( f(\|s\|_2) \). According to the properties of quadratic function in one variable, the function is monotonic on both sides of the symmetry axis. Therefore,

\[
if \ \|s\|_2 > \|t\|_2 \cos \alpha \Rightarrow f(\|s\|_2) \uparrow \Rightarrow \|s\|_2 \uparrow \\
if \ \|s\|_2 < \|t\|_2 \cos \alpha \Rightarrow f(\|s\|_2) \downarrow \Rightarrow \|s\|_2 \downarrow
\]

where \( \uparrow \) means increase and \( \downarrow \) means decrease. In this case, we can draw the following conclusions.

\[
P_r(\|s\|_2 > \|t\|_2 \cos \alpha) = P_r(f(\|s\|_2) \uparrow \Rightarrow \|s\|_2 \uparrow) \\
= P_r(D^2(s, t) \uparrow \Rightarrow \|s\|_2 \uparrow) \\
= P_r(\|x_{ci} - x_i\|_2 > \|x_{cj} - x_i\|_2 \Rightarrow \|x_{ci}\|_2 > \|x_{cj}\|_2)
\]

Since \( s \) and \( t \) are independently sampled from attribute matrix \( X \), we can draw

\[
P_r(\|s\|_2 > \|t\|_2) = 0.5.
\]

Due to the assumption that rank of \( X \) is greater than 1, the angle between \( s \) and \( t \) do not always equal to zero. Therefore, \( P_r(\cos \alpha \equiv 1) < 1 \). Note that \( \cos \alpha \leq 1 \). Finally, we draw the following

\[
P_r(\|s\|_2 > \|t\|_2 \cos \alpha) > 0.5
\]

which means

\[
P_r(\|x_{ci} - x_i\|_2 > \|x_{cj} - x_i\|_2 \Rightarrow \|x_{ci}\|_2 > \|x_{cj}\|_2) > 0.5
\]

The Fig[2] verifies our analysis that only utilizing the L2-norm of attribute vectors of nodes can achieve nearly 0.98 AUC score for all these four datasets when \( k = 50 \). Due to data leakage issue, it is hard to figure out whether the outlier detection algorithm plays a vital role or potentially exploits the information of data leakage. As \( k \) is set smaller, the data leakage issue turns out better as the left part of Fig[3] shown. In the right part of Fig[3] we replace the euclidean distance of above injection approach with cosine distance. At this time, not all datasets have data leakage issue that becomes serious as \( k \) becomes larger. Therefore, euclidean distance is a key factor which leads to the data leakage issue. It is observed that current UNOD algorithms in different datasets have significantly different performance when the data leakage issue is eased. For example, attributes reconstruction-based method is the dominant model in detecting contextual outliers. We observe that such method will have a significant drop of performance for Cora while only have a slight drop of effectiveness for Citeseer when we set smaller \( k \) during the injection process. Therefore, current injection approach cannot verify the effectiveness of algorithm. Under the current injection approach, outlier assumption is that the nodes whose attribute vector with the larger L2-norm is more likely to be an outlier. Simply replacing the euclidean distance by cosine distance may be regarded as a possible improvement for injection approach. In this case, the bias of L2-norm of attribute vectors will be eliminated. However, it is still not the best solution. We find that some real-world datasets like Weibo [36], which contains labelled node outliers, also exhibits the bias on the larger L2-norm of attribute vectors of nodes. Simply utilizing the L2-norm to predict outliers can achieve the AUC score of 0.92 for Weibo. Therefore, the larger L2-norm of attribute vector may indeed indicate the deviance of a node.

**Suggestion.** Based on above cause analysis, we give our suggestion on designing better outlier injection approach for contextual outliers in the future. First, the larger L2-norm of node attribute vectors indeed implies abnormality. Meanwhile, other characteristics of outliers should also be explored and considered. Secondly, other disturbance approach, like adding noise to attribute vectors or only replacing part of attribute vector with the other, can be considered. Finally, similar to suggestion for structural outlier injection, the data leakage information (e.g., L2-norm) should be also evaluated as baseline for comparison.
C. Summary

In summary, the current most widely-used outlier injection approach exists a serious data leakage issue, both on structural outlier and contextual outlier. In this case, experiments on datasets with varied injection settings are necessary to be conducted to evaluate the performance of current SOTA algorithms. In addition, only utilizing the data leakage information (i.e. L2-norm and node degree) as a simple baseline should also be evaluated for comparison. Our experiment results demonstrate that current SOTA algorithms cannot outperform such simple baseline. Thus, new algorithm which can outperform such simple baseline is necessary to be proposed.

V. METHODOLOGY

In this section, we are going to illustrate our proposed framework VGOD in detail. Since current UNOD method cannot outperform simple baseline which only utilizing data leakage information, we propose our new framework VGOD which combines a novel variance-based model and attribute reconstruction model. Specifically, the former model is for detecting structural outliers and the latter model is for detecting contextual outliers. Then we standardize the outlier scores outputted by two models and add them to get the final score. Fig 4 presents the whole architecture of VGOD framework.

A. Variance-based Model

In order to effectively detect structural outliers, we propose a novel variance-based model (VBM). To the best of our knowledge, this is the first time to utilize neighbor variance to detect outliers. Neighbor variance is a direct measurement of consistency of neighbor nodes. The bigger the variance, the less normal the node is. In addition, our VBM has no bias on nodes with larger node degree. In this case, VBM is more robust to the injection setting when we shrink the clique size of structural outlier injection setting.

Feature Transformation. Before calculation of neighbor variance, we conduct the feature transformation \( f_\theta(\cdot) \) for original attribute matrix \( X \) and get the low-dimension hidden representation matrix \( H \) of nodes:

\[
H = f_\theta(X)
\]

where \( f_\theta(\cdot) \) denotes a neural network, such as MLP(\( \cdot \)). The \( i^{th} \) row vector \( h_i \) of the hidden representation matrix \( H \) denotes the latent representation of the \( i^{th} \) node. In our experiment, we implement it with a linear transformation and L2-normalization as:

\[
\tilde{h}_i = XW + b
\]

\[
h_i = \frac{\tilde{h}_i}{\|\tilde{h}_i\|_2}
\]

where \( W \in \mathbb{R}^{d_h \times d_i} \) and \( b \in \mathbb{R}^{d_h} \) are the learnable parameters, \( d_i \) and \( d_h \) is the input dimension and hidden dimension of representation, respectively.

Neighbor Variance. In order to capture the consistency of neighbor nodes of a given node \( v_i \), we calculate the variance of attribute vectors of neighbor nodes for \( v_i \):

\[
\mathcal{N}_i = \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} h_j
\]

\[
\text{var}(v_i) = \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} (h_j - \mathcal{N}_i)^2
\]

\[
\sigma_{\text{str}}^2 = \text{loss}_\text{var}(v_i) = \|\text{var}(v_i)\|_1
\]

where \( \mathcal{N}_i \) is the average of hidden representations of neighbor nodes of \( v_i \). The L1-norm of \( \text{var}(v_i) \) is applied as structural outlier score \( \sigma_{\text{str}} \) for node \( v_i \). Since all components of the vector \( \text{var}(v_i) \) are greater than 0, the L1 norm calculation is to simply sum components of the \( \text{var}(v_i) \). In order to efficiently calculate variance for each node, we implement the calculation of variance based on message passing scheme [37] and design two message passing layers without parameters, namely MeanConv and MinusConv, as illustrated in Fig 5. Concretely, MeanConv is employed to calculate Eq. (7) and MinusConv is used to calculate Eq. (8) as well as Eq. (9).

Train. In order to train VBM to learn the representation that a normal node has a low variance while a structural outlier has a high variance, the train objection for VBM can be formally defined as follows:

\[
\min_\theta \mathbb{E}_{v_i \sim \mathcal{V}}[\text{loss}_\text{var}(v_i) - \frac{1}{|\mathcal{V} - \mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} (h_j - \frac{1}{|\mathcal{V} - \mathcal{N}_i|} \sum_{u \in \mathcal{N}_i} h_u)^2]
\]

where \( \mathcal{V} - \mathcal{N}_i = \mathcal{V} \setminus \mathcal{N}_i \) is the non-neighbor nodes set of \( v_i \).

We minimize the neighbor variance of a node while maximize the variance of hidden representations of all the non-neighbor nodes. In this case, the model will avoid to generate the same hidden representations for all nodes. However, it is too expensive to maximize the variance of all non-neighbor nodes every time. In this case, we apply negative edge sampling each epoch to generate a network \( \mathcal{G}(-\mathcal{E}) \) whose edge set \( \mathcal{E}(-\mathcal{E}) \) has the same number of edges as \( \mathcal{E} \).

Definition 3 (negative edge set). For a give attibuted network \( \mathcal{G} = \{\mathcal{V}, \mathcal{E}, X\} \), if \( \mathcal{E}(-\mathcal{E}) \) is the negative edge set of \( \mathcal{G} \), then if \( \langle u, v \rangle \in \mathcal{E}(-\mathcal{E}) \Rightarrow \langle u, v \rangle \notin \mathcal{E}, u, v \in \mathcal{V} \).

Definition 4 (negative network). For a give attibuted network \( \mathcal{G} = \{\mathcal{V}, \mathcal{E}, X\} \), we define the negative network \( \mathcal{G}(-\mathcal{E}) \) as \( \{\mathcal{V}, \mathcal{E}(-\mathcal{E}), X\} \), where \( \mathcal{E}(-\mathcal{E}) \) is the negative edge set of \( \mathcal{G} \).

Therefore, we can utilize such negative graph to maximize the variance of unrelated nodes. In other words, we randomly sample the same number of negative neighbors for each node \( v_i \) and maximize the neighbor variance calculated by these negative neighbors. Instead of maximizing the variance of all non-neighbor nodes, fewer nodes are required for computation by using negative sampling techniques, which greatly saves time and space.

Therefore, for each node \( v_i \), it has the “related vs unrelated” neighbor nodes pair and corresponding \( \text{loss}_\text{var}(v_i)(+ \) and
Learning of neighbor nodes pair can be formalized as:

\[
\text{loss}_{\text{var}}(v_i) = \left\| \text{var}(v_i, G) \right\|_1
\]

\[
\text{loss}_{\text{var}}^+(v_i) = \left\| \text{var}(v_i, G^+) \right\|_1
\]

\[
\text{loss}_{\text{var}}^-(v_i) = \left\| \text{var}(v_i, G^-) \right\|_1
\]

\[
\text{loss}_{\text{str}}^+(v_i) = \text{loss}_{\text{var}}^+(v_i) - \text{loss}_{\text{var}}^-(v_i)
\]

where \(\text{var}(v_i, G)\) and \(\text{var}(v_i, G^-)\) means we calculate the neighbor variance based on network \(G\) and \((G^-)\), respectively.

Finally, we minimize the above \(\text{loss}_{\text{str}}\) for all nodes in \(\mathcal{V}\) as:

\[
\min_\theta \mathbb{E}_{v \sim \mathcal{V}} \text{loss}_{\text{str}}(v)
\]

Thus, trained VBM can output a larger neighbor variance score for nodes with unrelated neighbor nodes and a relatively small score for nodes with related neighbor nodes. Consequently, we can utilize VBM to detect structural outliers.

**B. Attribute Reconstruction Model**

We employ attribute reconstruction on detection of contextual outliers. The key observation is that since there is a greater difference between a contextual outlier and its neighbor nodes, aggregating neighborhood information to reconstruct the original features will result in a relatively large reconstruction error for contextual outliers. Although there are some works based on attribute reconstruction approach, previous work [7], [24], [25] are based on a specific GNN backbone to reconstruct the attributes, which limits the flexibility of model design. Our attribute reconstruction model (ARM) is more flexible that any popular GNN model can be used as backbone to reconstruct the attributes of nodes.

**Feature Transformation.** Similar to VBM, we first transform the original attribute matrix \(X\) to the low-dimension feature representation matrix \(Z^{(0)}\) as:

\[
\hat{Z} = XW' + b'
\]

\[
z_i^{(0)} = \frac{\hat{z}_i}{\|\hat{z}_i\|_2}
\]

where \(W'\) and \(b'\) are the learning parameters, \(z_i^{(0)}\) is the \(i^{th}\) row vector of \(Z^{(0)}\).

**GNN Layers.** Then we employ \(L\) GNN layers to transform \(Z^{(0)}\) to \(Z^{(L)}\) to fully absorb the message from neighbor nodes. The \(l^{th}\) GNN Layer can be formalized as:

\[
Z^{(l)} = GNN^{(l)}(Z^{(l-1)}, G)
\]
Feature Retransformation. Finally, we retransform the $Z^{(L)}$ to $\hat{X}$, where $\hat{X} \in \mathbb{R}^{||V|| \times d}$ has the same shape as original attributes matrix $X$.

$$\hat{X} = Z^{(L)}\hat{W} + \hat{b}$$

(15)

where $\hat{X}$ is the reconstruction of the attribute matrix, $\hat{W}$ and $\hat{b}$ are the weight and bias parameters learned by model. Thus we can use the reconstruction attribute matrix $\hat{X}$ to calculate the reconstruction error, which is denoted as

$$\hat{o}_{i}^{\text{context}} = \text{loss}^{\text{recon}}(v_i) = ||\hat{x}_i - x_i||^2$$

(16)

$$\min_{\theta} \mathbb{E}_{v \sim V} \text{loss}^{\text{recon}}(v)$$

(17)

By minimizing the above objective, trained ARM can learn how to aggregate neighborhood information to reconstruct the original attributes. The contextual outlier score $o_i^{\text{context}}$ of node $v_i$ is defined as its reconstruction error.

C. Outlier Detection

As mentioned in [12], current UNOD algorithms fail to have a balanced performance on two outlier types. The previous practice that combines the contextual loss and structural loss with a fixed weight during the training stage fails to balance the optimization of model parameters. Similarly, combing the contextual score and structural score with a fixed weight during the inference stage fails to achieve a balanced detection performance. Therefore, we separately train our VBM and ARM with different epochs to avoid the unbalanced optimization. After both VBM and ARM are well-trained, we employ the mean-std normalization on two types of outlier scores outputted by two models and sum scores to get the final score, which can be formalized as:

$$\hat{o}_{i}^{\text{str}} = \frac{o_{i}^{\text{str}} - \mu(O^{\text{str}})}{std(O^{\text{str}})}$$

$$\hat{o}_{i}^{\text{context}} = \frac{o_{i}^{\text{context}} - \mu(O^{\text{context}})}{std(O^{\text{context}})}$$

$$o_i = \hat{o}_{i}^{\text{str}} + \hat{o}_{i}^{\text{context}}$$

(18)

where $O^{\text{str}}$ and $O^{\text{context}}$ denotes the set of structural outlier scores and contextual outlier scores, respectively. $\mu(\cdot)$ denotes the mean function, $std(\cdot)$ denotes standard deviation function.

Other score combination method like “sum-to-unit” can be formalized as:

$$\hat{o}_{i}^{(k)} = \frac{o_{i}^{(k)}}{\sum_{j \in |V|} o_{j}^{(k)}}$$

$$o_i = \sum_{k \in K} o_{i}^{(k)}$$

(19)

where $o_{i}^{(k)}$ means the $k^{\text{th}}$ outlier score of node $v_i$ outputted by model and $o_{i}^{(k)}$ in Eq. (19) should be greater than 0.

By adopting Eq. (18) as final outlier score, our model can have a more balanced performance in detecting two types of outliers during the inference stage. The overall procedure of our VGOD framework is described in Algorithm 1.

Algorithm 1 The overall procedure of VGOD framework

Input: Attributed Network: $G = (V, E, X)$. Training epochs for VBM: $Epoch_{\text{VBM}}$, Training epochs for ARM: $Epoch_{\text{ARM}}$

Output: Well-trained VBM and ARM, outlier scores $O$

1: // Training phase
2: for $i \in 1, 2, ..., Epoch_{VBM}$ do
3: Generate the negative netowork $G^{(-)} = (V, E^{(-)}, X)$ by negative edge sampling.
4: Compute the neighbor variance of nodes in $G^{(+)}$ and $G^{(-)}$ via Eq. (6)-(9).
5: Update VBM with the loss function via Eq. (11).
6: end for
7: for $i \in 1, 2, ..., Epoch_{ARM}$ do
8: Compute the reconstruction node attributes via Eq. (13)-(15).
9: Update ARM with the loss function via Eq. (16).
10: end for
11: // Inference phase
12: Compute the $O^{\text{str}}$ and $O^{\text{context}}$ via VBM and ARM respectively.
13: Compute the final outlier scores $O$ via Eq. (18).
14: return VBM, ARM, $O$

D. Complexity Analysis

The complexity is mainly bounded by message passing layers. For simplicity, the number of layers and the number of dimensions are considered as constant. The space and time complexity both are $O(|E| + |V|)$. In addition, we are only using GNN layers and two linear layers to build our model. Since there are a large number of researches on extending GNNs to larger networks, we can make use of various mini-batch training techniques such as [31], [38], [39] to extend our model in large-scale network without much effort.

VI. Experiment

In this section, we conduct the experiments to illustrate the effectiveness of our proposed framework VGOD. Firstly, we describe the experiment settings including datasets, baselines for comparison, evaluation metrics and computing infrastructures. Then, we conduct the Unsupervised Node Outlier Detection (UNOD) experiment to validate the effectiveness of our framework. Next, we vary the setting of structural outlier injection, and analyze the robustness of algorithm. Finally, we make the further analysis for our approach, including efficiency and ablation study. Our code is available from https://github.com/goldenNormal/vgod-github.

A. Experiment settings

1) Datasets: We evaluate the proposed framework on five real-world datasets, including four widely-used benchmark datasets with injected outliers and one dataset with labelled
outliers, for UNOD on attributed networks. These datasets, shown in Table I include three citation networks and two social networks. The detailed descriptions are given as follows:

- **Citation Networks**: Cora, Citeseer, PubMed are three available public citation networks. In these networks, nodes denote the published papers while links represent the citation relationships between papers. For these datasets, the attribute vector of each node is the bag-of-word representation whose dimension is determined by the dictionary size.

- **Flickr** is a typical social network datasets acquired from the image hosting and sharing website Flickr. Users can follow each other and form a social network. Node attributes of users are defined by their specified tags that reflect their interests.

- **Weibo** is a user-posts-hashtag graph from [40]. The nodes are users in the social platform where a link connects a pair of two users denoting that they have posted the same hashtag. If two messages are posted within a specific number of seconds, it will be regarded as suspicious event. The outliers are those users who made at least 5 suspicious events.

2) Baselines: We compare our proposed framework VGOD with the following five recent deep-learning based SOTA models. These baselines are summarized in Table III Column Time Complexity indicates the time complexity of inference for these models. For simplicity, the number of layers and the number of dimensions are considered as constant. We also list here whether the baseline is based on contrastive learning or reconstruction. If model outputs more than one score for outliers, then we consider it has the feature of score combination. If a trained model can be directly deployed for outlier detection on new graphs, then it has the feature of inductive inference.

- **Dominant** [7] is based on GNNs and employs two autoencoders to reconstruct the adjacency and attribute matrices. Then the structure matrix is reconstructed via GAE [41], and the attribute matrix is reconstructed via another GCN layer.

- **AnomalyDAE** [24] employs dual autoencoders architecture with cross-modality interactions and attention mechanism to reconstruct the attribute and adjacency matrices.

- **DONE** [35] employs two deep unsupervised autoencoders to reconstruct the structure information and attribute information. The way of “sum to uni” is applied to normalize the score for combination.

- **CoLA** [22] adopts the method of contrastive learning and employs GNN for embedding, sampling a node and its random walk local structure as a positive pair, the node and the local structure of other node as a negative pair. Then the model outputs a score, representing the probability of whether current input is a negative pair as the outlier score.

- **CONAD** [23] employs reconstruction approach, which is similar to Dominant. In addition, CONAD adopts four prior human knowledge to inject outliers into the dataset for contrastive learning. It introduces an additional loss to train the model to generate different representation for original network and outlier-injected network.

Since current outlier injection approach exists data leakage issue, we also design a simple model as a new baseline for comparison and evaluation, which only utilizes the data leakage information (i.e. node degree and L2-norm of attribute vectors). We name it DegNorm. DegNorm adopts node degree as structural outlier score while L2-norm of attribute vectors of nodes are adopted as contextual outlier score. The mean-std normalization is applied to two scores. The final outlier score is the sum of these two score which have been normalized. The calculation of $o_{str}^{i}$ and $o_{context}^{i}$ can be formalized as:

$$o_{str}^{i} = |N_i|$$

$$o_{context}^{i} = \|x_i\|_2$$

where $N_i$ is the neighbor nodes of node $v_i$, $x_i$ is the attribute vector of node $v_i$.

3) Evaluation Metrics: Since all methods return a list of outlier scores, the higher the score is, the higher the probability of being an outlier. Therefore, we use Area Under receiver operating characteristic Curve (AUC) to measure. In specific, AUC evaluates the degree of alignment between the outlier score and the ground truth label under varying thresholds:

$$AUC = \frac{1}{|V^+||V^-|} \sum_{v_i^+ \in V^+} \sum_{v_j^- \in V^-} (\mathbb{I}(f(v_i^+) < f(v_j^-)))$$

where $V$, $V^-$, and $V^+ = V \setminus V^-$ are the set of all nodes, the set of all outlier nodes and the set of all normal nodes respectively. $\mathbb{I}(\cdot)$ is the indicator function and $f(v_i)$ is the outlier score of node $v_i$ given by one outlier detector. In practice, we use roc_auc_score in sklearn.metrics to calculate AUC. Generally, $AUC(V_L)$ means using $V_L$ as the outlier label to calculate the AUC score. Particularly, $AUC = AUC(V^-)$.

We also propose AucGap for evaluate the balanced detection performance for different types of outliers, which can be formalized as below:

$$AucGap = \max\left\{ \frac{AUC(V^+)}{AUC(V^-)}, \frac{AUC(V^-)}{AUC(V^+)} \right\}$$

where $AUC(V_i)$ is the AUC score of the dataset $V_i$. In this paper, we use the following conventions for datasets:

| Dataset | #nodes | #edges | #attrs | #avg_deg | #outliers | % outlier |
|---------|--------|--------|--------|----------|-----------|-----------|
| Cora    | 2,706  | 5,429  | 1,433  | 2.01     | 150       | 5.5%      |
| Citeseer| 3,327  | 4,732  | 3,703  | 1.42     | 150       | 4.5%      |
| PubMed  | 19,717 | 44,338 | 500    | 2.25     | 600       | 3.0%      |
| Flickr  | 7,575  | 239,738| 12,407 | 31.65    | 450       | 5.9%      |
| Weibo   | 8,405  | 407,963| 64     | 48.5     | 868       | 10.3%     |

*#outlier and %outlier is only for UNOD Experiments.
where $V^{str}$ and $V^{context}$ are structural outliers set and contextual outliers set respectively. $AUC(V^{str})$ denotes the AUC score of structural outliers and $AUC(V^{context})$ denotes the AUC score of contextual outliers. AucGap aims to calculate the gap of model’s AUC score for two types of outliers. The lower the AucGap is, the more balanced detection performance it indicates.

4) Computing Infrastructures: Our proposed learning framework is implemented using PyTorch 1.11.1 and PyTorch Geometric 2.1.0. All experiments are conducted on a computer with Ubuntu 16.04 OS, i7-9750H CPU, an Tesla V100 (32GB memory) GPU.

### B. Result of Unsupervised Node Outlier Detection

We first conduct the UNOD experiment to verify the effectiveness of our proposed framework. UNOD experiment hereinafter refers to this experiment.

1) Injection Setting: We adopt the most widely-used outlier injection approach as mentioned in Section [IV-A1] and Section [IV-B1]. The statistics of these datasets are demonstrated in Table I. Only Weibo contains the labelled outliers while other datasets contain injected outliers. Noted that AucGap can only be calculated on these injected datasets.

2) Parameter Setting: For each algorithm, we run 5 times and calculate the average score to list here. For our proposed framework VGOD, we fix the embedding dimension to 128 for both Variance-Based Model (VBM) and Attribute Reconstruction Model (ARM). We set learning rate to 0.01 for all injected datasets and 0.005 for Weibo. Two layers of GAT is adopted as the GNN module in ARM for all datasets and the row-normalization to the attribute vectors is applied in Weibo. We directly run the code in [22] to inject outliers. For all baselines, we adopt the default parameter setting in their code except the number of training epoch. We find the number of training epoch is the most influential parameter for baselines. We stop training their model as long as their AUC score reaches its peak. In this case, the performance can be promised to better or equal to performance of their default parameter setting. For our approach, we train ARM 100 epochs and VBM 10 epochs for all datasets since it has already significantly outperformed baselines in fixed number of training epoch. In fact, our two models require fewer epochs to converge for these datasets. Adam optimizer is employed to train all baselines and our model. We adopt the AUC score (marked with *) of Weibo published in [12] for the baseline Dominant, AnomalyDAE, DONE and CONAD.

### 3) Result Analysis:

The AUC scores and AucGap scores are shown in Table III and Table IV. The best score is in bold while the second best score is underlined. According to results, we have following observations:

- Our proposed framework VGOD achieves highest AUC score for all datasets while achieves the overall highest AucGap among all datasets. There are several reasons for such performance. Firstly, our variance-based model significantly improves the ability to detect structural outliers. Secondly, we separately train the model to prevent each component from being over-trained. Thirdly, we adopt mean-std normalization to eliminate the scale difference between two score which gives more balanced detection performance.
- DegNorm also achieves SOTA performance compared to other baseline, which indicates the importance to eliminate the data leakage issue in outlier injection.
C. Result of Structural Outliers Detection Robustness

Further, we conduct the robustness experiment for structural outlier detection to explore the effectiveness of our variance-based model (VBM). Robustness experiment hereinafter refers to this experiment.

1) Injection Setting: In order to explore the robustness of algorithm to detect structural outliers, we vary the parameter $q$ of injected clique size of structural outliers to $Q = \{3, 5, 10, 15\}$. For each dataset $D_i$, we inject 4 groups of structural outliers $\{V_q=3, V_q=5, V_q=10, V_q=15\}$ into $D_i$. Each group has the same number of outliers, which is set to 2% of total number of nodes, i.e. $|V_q=Q_i| = 2% \cdot |V|$. The outlier set $V^-$ is the union of 4 group of structural outliers set. We report the $AUC(V^-)$ in Table V and the AUC score of each group $AUC(V_q=Q_i)$ is shown in Fig 6.

2) Parameter Setting: We keep the same parameter setting for VBM and other baselines as UNOD experiment except that we train all baselines and VBM until its AUC score reaches the peak. Since we fail to get a reasonable result for CONAD, we do not list result of CONAD. We also evaluate the performance of simple baseline which only utilizes the node degree as structural score for comparison. We named it Deg, whose outlier score function can be formulated as

$$o_i = |\mathcal{N}_i|$$

For all other baselines, if their model outputs multiple scores (e.g., $o_i$, $o_i^{str}$, $o_i^{context}$), we adopt the score with highest $AUC(V^-)$ as its structural score.

| Model       | Cora   | Citeseer | PubMed | Flickr |
|-------------|--------|----------|--------|--------|
| Dominant    | 0.9277 | 0.9467   | 0.8878 | 0.5715 |
| AnomalyDAE  | 0.9127 | 0.9219   | 0.8968 | 0.6253 |
| DONE        | 0.9034 | 0.8985   | 0.8868 | 0.5516 |
| CoLA        | 0.8073 | 0.8919   | 0.8698 | 0.5712 |
| Deg         | 0.9467 | 0.9541   | 0.9333 | 0.5671 |
| VBM         | 0.9815 | 0.9816   | 0.9893 | 0.8003 |

3) Result Analysis: According to results in Table V and Fig 6, we have the following observations:

- VBM achieves the best $AUC(V^-)$ score for all datasets. In addition, VBM has a huge performance gain in Flickr. Thus the correctness of adopting neighbor variance to measure structural consistency is verified.
- As shown in Fig 6 when the clique size is reduced, which means that it is more difficult to directly employ node degree to detect structural outlier, we find that the performance of VBM declines the least compared to other baselines. Therefore, the performance of VBM is the most robust to varied injection settings.
- We find that the simple model Deg that directly utilizes a node’s degree outperforms most other baselines at most cases. It reveals that these baselines are not as effective as we previously thought.

D. Further Analysis

In this subsection, we make further analysis on our proposed framework.
Fig. 8. AUC variation trend of variance-based model during the training of VBM. Each polyline represents the group of structural outliers with different clique size.

| TABLE VII | AUC VALUES COMPARISON FOR DIFFERENT GNN LAYERS. |
|-----------|--------------------------------------------------|
| Model     | Cora     | Citeseer | PubMed | Flickr | weibo  |
| VGOD (GIN) | 0.9503   | 0.9845   | 0.9801 | 0.8773 | 0.9093 |
| VGOD (GCN) | 0.9566   | 0.9867   | 0.9802 | 0.8735 | 0.9154 |
| VGOD (GAT) | 0.9560   | 0.9868   | 0.9813 | 0.8835 | 0.9765 |

| TABLE VIII | AUCGAP VALUES COMPARISON FOR DIFFERENT GNN LAYERS. |
|-------------|---------------------------------------------------|
| Model       | Cora     | Citeseer | PubMed | Flickr |
| VGOD (GIN)  | 1.0716   | 1.0261   | 1.0215 | 1.0655 |
| VGOD (GCN)  | 1.0637   | 1.0278   | 1.0214 | 1.0713 |
| VGOD (GAT)  | 1.0680   | 1.0268   | 1.0211 | 1.0672 |

1) Efficiency of model inference: We keep the settings of the UNOD experiment and calculate the time for each model to use CPU for training and inference. The training time per epoch of all models (in second) are shown in Fig 7. In Table VII, we list the inference time in seconds. The inference time of model is roughly the same as the training time per epoch except CoLA. For all datasets, our VGOD framework completes inference in a relatively short time. For datasets with a large number of nodes, such as PubMed, our model takes significantly less time than other models due to the linear relationship to the number of nodes. Since CoLA requires multiple rounds of sampling for inference, its computational cost is much higher than other models.

2) Effect of the number of epochs for VBM: Next, we investigate the AUC variation trend of VBM during training. As shown in Fig 8, VBM shows a high AUC score at the beginning, and the AUC score reaches the peak after only a few epochs of training. Afterwards, as the training progresses, the AUC score slowly decreases due to the overfitting. Different group of structural outliers in Robustness experiment shows the similar trend while the group of smaller clique size shows a later overfitting time point.

3) Effect of different GNN Layers for ARM: Then, we investigate the effect of different GNN layers in ARM. We replace different GNN layers in UNOD experiment for research. Table VIII and Table VII show the AUC and AucGap repectively on four datasets. It is observed that GAT outperforms other GNNs significantly on Weibo. For other datasets, their AUC and AUCGAP scores are comparable.

4) Effect of score combination Strategy: Finally, we study the effectiveness of mean-std normalization employed in VGOD. We replace the score combination strategy with weighted sum and “sum-to-unit” normalization on UNOD experiment. In Table IX and Table X, both the AUC and AucGap scores of VGOD with mean-std normalization are significantly superior to others on Cora, Citeseer, Flickr and only slightly inferior to the highest score on PubMed.

VII. CONCLUSION

In this paper, we revisit the problem of unsupervised node outlier detection. Firstly, we find that current outlier injection approach exists serious data leakage issue and make a theoretical analysis in depth. Secondly, we propose a new framework, which consists of a novel variance-based model and a more general attribute reconstruction model to detect two types of outliers. Our model successfully outperforms all previous SOTA models with the best outlier detection performance and balanced detection ability.

We believe our insight into data leakage issue will lead to better outlier injection approaches and algorithms for UNOD in the future. Moreover, the concept of neighbor variance may also exhibits great potential in other research area such as graph mining and graph representation learning in the future.
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