Supplementary Material for "Towards Self-Interpretable Graph-Level Anomaly Detection"

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A Definitions of "Explainability" and "Interpretability"

Since explainable artificial intelligence is an emerging area of research, how to specifically discriminate similar concepts "explainability" and "interpretability" is not yet completely standardized. Following the recent survey paper [1], we distinguish them with definite principles rather than using them interchangeably.

Specifically, we define the term "explainability" as a more general and high-level concept that includes all learning scenarios, models, and strategies related to providing understandable knowledge for the predictions. The major reason is that "explainable artificial intelligence" and "explainable machine learning" are well-known concepts in the community. For instance, we denote the ability to explain GNNs' predictions as "explainability of GNNs", and the related learning tasks include explainable node classification, explainable graph classification, etc. Following this way, we denote our proposed learning problem as "explainable graph-level anomaly detection (GLAD)".

Differently, we denote "interpretability" as the ability of a model to intrinsically provide explanations for itself. To well emphasis the characteristic of interpreting itself, we sometimes use the concept "self-interpretability" interchangeably with the concept "interpretability". For instance, the GNNs that can jointly generate predictions and explanations are denoted as "interpretable GNNs" or "self-interpretable GNNs". Under such a definition, the models that provide post-hoc explanations for trained GNNs are not interpretable. In this paper, we aim to propose a "self-interpretable GLAD model" that is able to yield explanations for the anomaly detection results by itself.

B Related Work in Detail

Graph Neural Networks (GNNs). GNNs are the extension of the convolution-based neural networks onto graph data [2, 3, 4, 5, 6, 7, 8, 9]. Early GNNs define graph convolution based on spectral theory [8, 10]. Recently, the mainstream GNNs usually follow the paradigm of message passing for spatial graph convolution, i.e., executing graph convolution by aggregating the information for adjacent nodes [3, 4, 5, 6]. For instance, GCN [4] uses an average-based aggregation function for message passing. GIN [3], differently, employs a summation-based aggregation function to ensure its expressive ability. Apart from normal GNNs designed for simple graphs where each edge connects exactly two nodes, some recent studies apply GNNs to hypergraphs, a generalization of graphs where an edge can connect more than two nodes [11, 12, 13]. Among them, Hyper-Conv [12] is a representative HGNN that applies a GCN-like aggregation function to the graph convolution for hypergraphs. Thanks to their strong expressive power, GNNs are effective in various graph learning tasks, such as node classification [4, 14, 15, 16], graph classification [3], and also graph anomaly detection [17, 18]. Besides, GNNs can also be widely applied to diverse real-world learning

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scenarios, such as federated learning [19, 20], knowledge graph reasoning [21, 22, 23], adversarial attack [24, 25], and molecule analysis [26, 27].

Explainability of GNNs. To make the predictions of GNNs transparent and understandable, a line of studies proposes to uncover the explanation, i.e., the critical subgraphs and/or features that highly correlate to the prediction, for GNN models [1, 28, 29, 30, 31, 32]. Existing methods can be divided into two types: post-hoc GNN explainer and self-interpretable GNN [30, 32]. The post-hoc GNN explainers use specialized models or strategies to explain the behavior of a trained GNN, such as input perturbation [28, 29], surrogate model [31], and prediction decomposition [33]. For instance, PGExplainer [29] uses an edge embedding-based neural module to modify the input graph, and the learning objective is to optimize the cross-entropy between the original prediction and the modified input. Differently, the self-interpretable GNNs can intrinsically provide explanations for the predictions using the interpretable designs in GNN architectures [34, 30, 35]. GSAT [35] is one of the self-interpretable GNNs that uses a parameterized attention module to pick the graph rationale along with the training of the GNN backbone. Theoretically, the post-hoc explainers can be used to explain the well-trained GLAD models; however, the post-hoc explainers can potentially provide sub-optimal solutions since they are not directly learned with the detection models. On the other hand, most self-interpretable GNNs are designed to explain the prediction of supervised tasks, especially graph/node classification tasks. In this case, it is non-trivial to directly apply them to unsupervised graph anomaly detection tasks, since their inherent supervised learning objective cannot work without ground-truth labels.

Graph Anomaly Detection. The objective of graph anomaly detection is to identify anomalies that deviate from the majority of samples in graph-structured data [36, 17, 37]. Most efforts mainly focus on node-level anomaly detection, i.e., detecting the abnormal nodes from one or more graphs [17, 18, 38, 39]. In this paper, we mainly investigate graph-level anomaly detection (GLAD) that aims to recognize anomalous graphs from a set of graphs [36, 40, 41, 42]. A few recent studies try to address the GLAD problem with various advanced techniques. For example, OCGIN [36] combines the objective of one-class classification and a GIN encoder into the first GLAD model. GLocalKD [40] uses the knowledge distillation error between a random network and a trainable network to evaluate the abnormality of graph samples. OCGTL [41] introduces a graph transformation learning-based learning objective to identify the anomalous samples in a graph set. However, these methods can only predict the scores to indicate the degree of abnormality of each sample, but cannot provide the behind explanations, i.e., the substructure causes the abnormality. To boost the reliability and explainability of GAD methods, in this paper, we propose a self-interpretable GAD framework to generate both anomaly prediction and its explanation.

Learning by Information-Bottleneck (IB). IB is an information theory-based approach for representation learning that trains the encoder by preserving the information that is relevant to label prediction while minimizing the amount of superfluous information [43, 44, 45]. Formally, the objective of IB principle is to maximize the mutual information (MI) between representation Z and label Y, and minimize the MI between representation Z and original data X [45]. Some pioneering efforts [46, 47] extend IB principle to multi-view learning scenarios, and some of them enable the application of IB principle for unsupervised learning [46]. Recent efforts also attempt to apply IB principle to graph learning tasks [48, 35, 49, 50, 51, 52, 53, 54]. One feasible idea is to borrow the representation-based IB principle for graph representation learning [50, 53]; another line of work regards a vital bottleneck subgraph $G^{(s)}$ rather than the representation Z as the bottleneck and tries to maximize the MI between $G^{(s)}$ and label Y while minimizing the MI between $G^{(s)}$ and original graph G [48, 51, 52].

Explainable anomaly detection. Anomaly detection is an essential machine learning task that aims to detect unusual or rare patterns or instances within a dataset [55, 56]. In order to improve the trustworthiness and comprehensibility of anomaly detection systems, a brunch of research termed explainable anomaly detection focuses on generating valid explanations for the results given by anomaly detection models [57, 58, 59]. For example, to provide explanations for one-class image anomaly detection models, FCDD [57] uses a fully convolutional module to generate pixel-level explanation. ATON [58] utilizes an attention-guided triplet deviation mechanism to provide explanations for any black-box outlier detector on tabular data. Cho et al. [59] introduce an auxiliary prototypical classifier to learn explanations of anomaly detection models for medical images. Despite their success, these techniques cannot be directly applied to graph-structured data.

C Formulations of GNN and HGNN

In this section, we provide detailed definitions of message passing-based graph neural network (GNN) and hypergraph neural network (HGNN). Given a simple graph G, the target of a GNN is to learn the node-level representation following the message passing scheme:

$$\mathbf{h}_v^{(l+1)} = \mathrm{UPDATE}\left(\mathbf{h}_v^{(l)}, \mathrm{AGGREGATE}\left(\left\{\mathbf{h}_u^{(l)} : \forall u \in \mathcal{N}(v; \mathbf{A})\right\}\right)\right), \tag{A.1}$$

where $\mathbf{h}_v^{(l)}$ is the latent representation vector for node $v \in \mathcal{V}$ at the l-th layer (with $\mathbf{h}_v^{(0)} = \mathbf{x}_v = \mathbf{X}_{[v]}$), $\mathcal{N}(v; \mathbf{A})$ is the neighboring node set of v obtained from $\mathbf{A}$, $\mathrm{AGGREGATE}(\cdot)$ is is the function that aggregates messages from neighboring nodes, and $\mathrm{UPDATE}(\cdot)$ is the function that updates the node representation. With similar notations, we can formulate a HGNN as:

$$\mathbf{h}_{v^*}^{(l+1)} = \mathrm{UPDATE}\left(\mathbf{h}_{v^*}^{(l)}, \mathrm{AGGREGATE}\left(\left\{\mathbf{h}_{u^*}^{(l)} : \forall u^* \in \mathcal{N}(v^*; \mathbf{M}^*)\right\}\right)\right), \tag{A.2}$$

where $\mathcal{N}(v^*; \mathbf{M}^*)$ is the neighboring node set of $v^* \in \mathcal{V}^*$ obtained from incidence matrix $\mathbf{M}^*$.

In GNNs, a pooling operation $\mathrm{POOL}(\cdot)$ can be applied to obtain a graph-level representation vector with $\mathbf{h}_G = \mathrm{POOL}\left(\{\mathbf{h}_v^{(L)} : \forall v \in \mathcal{V}\}\right)$ by summarizing the representations of all nodes at the final layer L. A similar pooling layer can be used to obtain hypergraph-level representation $\mathbf{h}_G^*$.

D MSIB Loss Computation

Starting from Eq. (2), we can first rewrite the objective of the first graph view G^1 as a loss function into:

$$\mathcal{L}_1 = I(G^1; G^{1(s)}|G^2) - \frac{1}{\beta_1} I(G^2; G^{1(s)}), \tag{A.3}$$

which we aim to minimize during model training. Similar to Eq. (A.3), the corresponding loss function for the second graph view G^2 can be written by:

$$\mathcal{L}_2 = I(G^2; G^{2(s)}|G^1) - \frac{1}{\beta_2} I(G^1; G^{2(s)}), \tag{A.4}$$

where β_2 is the trade-off parameter for $\mathcal{L}_2$. Then, by computing the average of $\mathcal{L}_1$ and $\mathcal{L}_2$, we have a joint loss function to optimize both $G^{1(s)}$ and $G^{2(s)}$:

$$\mathcal{L}_{joint} = \frac{I(G^1; G^{1(s)}|G^2) + I(G^2; G^{2(s)}|G^1)}{2} - \frac{\frac{1}{\beta_1} I(G^2; G^{1(s)}) + \frac{1}{\beta_2} I(G^1; G^{2(s)})}{2}. \tag{A.5}$$

For term $I(G^1; G^{1(s)}|G^2)$, we can derive its upper bound by:

$$\begin{aligned}
&I_\theta\left(G^1; G^{1(s)}|G^2\right) = \mathbb{E}_{\boldsymbol{G}^1,\boldsymbol{G}^2 \sim p\left(G^1,G^2\right)} \mathbb{E}_{\boldsymbol{G}^{(s)} \sim p_\theta\left(G^{1(s)}|G^1\right)} \left[\log \frac{p_\theta\left(G^{1(s)} = \boldsymbol{G}^{(s)}|G^1 = \boldsymbol{G}^1\right)}{p_\theta\left(G^{1(s)} = \boldsymbol{G}^{(s)}|G^2 = \boldsymbol{G}^2\right)}\right] \\
&= \mathbb{E}_{\boldsymbol{G}^1,\boldsymbol{G}^2 \sim p\left(G^1,G^2\right)} \mathbb{E}_{\boldsymbol{G}^{(s)} \sim p_\theta\left(G^{1(s)}|G^1\right)} \left[\log \frac{p_\theta\left(G^{1(s)} = \boldsymbol{G}^{(s)}|G^1 = \boldsymbol{G}^1\right)}{p_\psi\left(G^{2(s)} = \boldsymbol{G}^{(s)}|G^2 = \boldsymbol{G}^2\right)} \frac{p_\psi\left(G^{2(s)} = \boldsymbol{G}^{(s)}|G^2 = \boldsymbol{G}^2\right)}{p_\theta\left(G^{1(s)} = \boldsymbol{G}^{(s)}|G^2 = \boldsymbol{G}^2\right)}\right] \\
&= D_{KL}\left(p_\theta(G^{1(s)}|G^1) \| p_\psi(G^{2(s)}|G^2)\right) - D_{KL}\left(p_\theta(G^{2(s)}|G^1) || p_\psi(G^{2(s)}|G^2)\right) \\
&\leq D_{KL}\left(p_\theta(G^{1(s)}|G^1) \| p_\psi(G^{2(s)}|G^2)\right).
\end{aligned} \tag{A.6}$$

where $D_{KL}(\cdot)$ is the Kullback–Leibler (KL) divergence. Analogously, we can acquire the upper bound of $I(G^2; G^{2(s)}|G^1)$ as $D_{KL}\left(p_\theta(G^{2(s)}|G^2)\|p_\psi(G^{1(s)}|G^1)\right)$. In this way, the first term in Eq. (A.5) can be upperbound by:

$$\frac{I(G^1; G^{1(s)}|G^2) + I(G^2; G^{2(s)}|G^1)}{2} \leq D_{SKL}\left(p_\theta(G^{1(s)}|G^1)\|p_\psi(G^{2(s)}|G^2)\right), \tag{A.7}$$

where $D_{SKL}\left(p_\theta(G^{1(s)}|G^1)\|p_\psi(G^{2(s)}|G^2)\right) = \frac{1}{2}D_{KL}\left(p_\theta(G^{1(s)}|G^1)\|p_\psi(G^{2(s)}|G^2)\right) + \frac{1}{2}D_{KL}\left(p_\theta(G^{2(s)}|G^2)\|p_\psi(G^{1(s)}|G^1)\right)$.

Then, according to the chain rule of mutual information, i.e., $I(xy; z) = I(y; z) + I(x; z|y)$, we can reform the term $I(G^2; G^{1(s)})$ by:

$$\begin{aligned} I(G^{1(s)}; G^2) &= I(G^{1(s)}; G^{2(s)}G^2) - I(G^{1(s)}; G^{2(s)}|G^2) \\ &\overset{(H)}{=} I(G^{1(s)}; G^{2(s)}G^2) \\ &= I(G^{1(s)}; G^{2(s)}) + I(G^{1(s)}; G^2|G^{2(s)}) \\ &\geq I(G^{1(s)}; G^{2(s)}), \end{aligned} \tag{A.8}$$

where (H) indicates the hypothesis that $G^{2(s)}$ is sufficient for G^1, i.e., $I(G^{1(s)}; G^{2(s)}|G^1) = 0$. Symmetrically, we can also have $I(G^{2(s)}; G^1) \geq I(G^{1(s)}; G^{2(s)})$. In this case, the second term in Eq. (A.5) has the lower bound with:

$$\frac{\frac{1}{\beta_1}I(G^2; G^{1(s)}) + \frac{1}{\beta_2}I(G^1; G^{2(s)})}{2} \geq \frac{(\beta_1 + \beta_2)}{2\beta_1\beta_2} I(G^{1(s)}; G^{2(s)}). \tag{A.9}$$

By jointly considering Eq. (A.7) and Eq. (A.9), the joint loss function (Eq. (A.5)) can be bounded by:

$$\mathcal{L}_{joint} \leq D_{SKL}\left(p_\theta(G^{1(s)}|G^1)\|p_\psi(G^{2(s)}|G^2)\right) - \frac{(\beta_1 + \beta_2)}{2\beta_1\beta_2} I(G^{1(s)}; G^{2(s)}). \tag{A.10}$$

Finally, by multiplying both terms with $\beta = \frac{2\beta_1\beta_2}{(\beta_1+\beta_2)}$ and re-parametrizing the objective, we have a tractable loss function for MSIB framework:

$$\mathcal{L}_{MSIB} = -I(G^{1(s)}; G^{2(s)}) + \beta D_{SKL}\left(p_\theta(G^{1(s)}|G^1)\|p_\psi(G^{2(s)}|G^2)\right). \tag{A.11}$$

E Methodology Discussion

E.1 Algorithm

The overall algorithm of `SIGNET` is summarized in Algo. 1.

E.2 Discussion of `SIGNET` v.s. GSAT

In this paragraph, we discuss the connections and differences between `SIGNET` and the representative self-interpretable GNNs, GSAT.

Connections between `SIGNET` and GSAT:

- Theoretical foundation. Both GSAT and `SIGNET` are based on the well-known information theory criteria, the information bottleneck, serving as their theoretical foundation for their explanation target.
- Explanation goal. As an explainable method for graphs, they have a common objective of identifying the key subgraph within the input graph sample that holds the highest relevance to the final prediction.

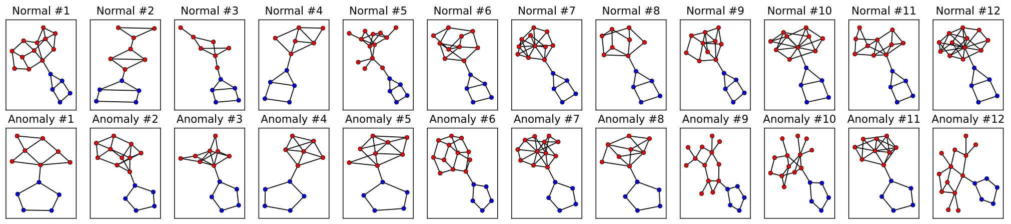
Algorithm 1: The overall algorithm of SIGNET

```
Input: Training Set $\mathcal{G}_{tr}$; Test Set $\mathcal{G}_{te}$.
Parameters : Number of epoch $E$.
Output: Anomaly Score Set $\mathcal{S}$; Explanation Subgraph Set $\mathcal{G}^{(es)}$.
/* Training                                                              */
1  Initialize model parameters
2  for $e = 1, 2, \cdots, E$ do
3      $\mathcal{B}_1, \cdots, \mathcal{B}_{n_b} \leftarrow$ Randomly split $\mathcal{G}_{tr}$ into batches
4      for $\mathcal{B} = \mathcal{B}_1, \cdots, \mathcal{B}_{n_b}$ do
5          for $G_i \in \mathcal{B}$ do
6              $G_i^* \leftarrow$ Obtain the dual hypergraph of $G_i$ by DHT
7              $\mathbf{p}_i, \mathbf{p}_i^* \leftarrow$ Calculate probability vectors by neural extractor
8              $G_i^{(s)}, G_i^{*(s)} \leftarrow$ Extract bottleneck subgraphs by Eq. (4)
9              $\mathbf{h}_i^{(s)}, \mathbf{h}_i^{*(s)} \leftarrow$ Calculate graph-level representations by GNN/HGNN encoders
10         end
11         $\mathcal{L} \leftarrow$ Calculate Info-NCE loss by Eq. (5)
12         Update model parameters via gradient descent w.r.t. $\mathcal{L}$
13     end
14 end
/* Inference                                                             */
15 for $G_i \in \mathcal{G}_{te}$ do
16     $G_i^* \leftarrow$ Obtain the dual hypergraph of $G_i$ by DHT
17     $\mathbf{p}_i, \mathbf{p}_i^* \leftarrow$ Calculate probability vectors by neural extractor
18     $G_i^{(s)}, G_i^{*(s)} \leftarrow$ Extract bottleneck subgraphs by Eq. (4)
19     $\mathbf{h}_i^{(s)}, \mathbf{h}_i^{*(s)} \leftarrow$ Calculate graph-level representations by GNN/HGNN encoders
20     $s_i = -I(\mathbf{h}_i^{(s)}, \mathbf{h}_i^{*(s)}) \leftarrow$ Calculate the anomaly score of $G_i$ by Info-NCE MI estimator
21     $G_i^{(es)} \leftarrow$ Extract explanation subgraph according to $\mathbf{p}_i$ and $\mathbf{p}_i^*$ using top-k/threshold strategy
22 end
23 $\mathcal{S}, \mathcal{G}^{(es)} \leftarrow$ Collect all the anomaly scores $s_i$ and explanations $G_i^{(es)}$ into sets
```

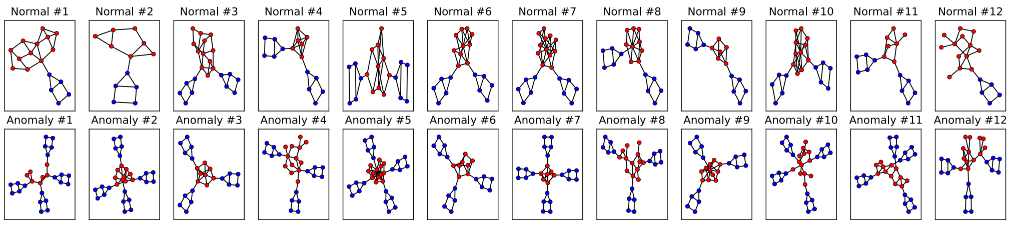
- Architecture. Both GSAT and SIGNET adopt learnable neural networks to parameterize the graph data and make the explanation differentiable, which is a common design among explainable GNNs. However, GSAT only conducts the relaxation at the edge level, while SIGNET can provide explanation scores at both node and edge levels.

Differences between SIGNET and GSAT:

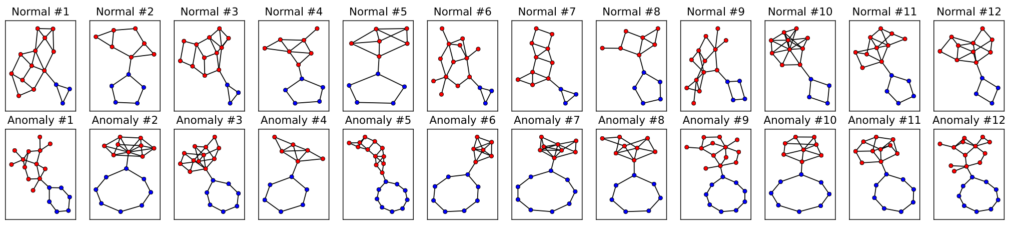
- Targeted tasks. GSAT focuses on a supervised graph-level classification task where categorical labels are available for training the self-interpretation module. On the other hand, SIGNET targets unsupervised graph-level anomaly detection, a more challenging task with unavailable labels during training.
- Theoretical framework. GSAT is designed based on the original information bottleneck framework with subgraph bottleneck, tailored to its targeted supervised setting. In contrast, SIGNET is based on the multi-view subgraph information bottleneck (MSIB) framework derived in this paper, specifically designed for unsupervised anomaly detection tasks.
- Learning objectives. GSAT is trained using cross-entropy loss, a commonly used classification loss. In contrast, SIGNET is optimized using an Info-NCE loss, aiming to maximize the mutual information between each graph and its rational subgraph.
- Graph view for learning. GSAT only considers the original view for graph learning, while SIGNET takes both the original and DHT views into account for self-interpretable graph learning.



(a) BM-MT



(b) BM-MN



(c) BM-MS

Figure 1: Examples of three synthetic datasets, where subgraphs in blue are the ground-truth explanations.

E.3 Complexity analysis

Within this paragraph, we denote the average numbers of nodes and edges as n and m respectively, and denote the number of graphs and batch size as N and B respectively. At each training iteration, we first conduct DHT to obtain the dual hypergraph, which requires $\mathcal{O}(N(m+n))$. Then, the GNN-based extractor that calculates probability consumes $\mathcal{O}(NL_1md_1+NL_1nd_1^2+Nnd_1d_f)$ complexity, where L_1 and d_1 are the layer number and latent dimension of the extractor, respectively. The bottleneck subgraph extraction for two views requires $\mathcal{O}(N(m+n))$ in total. For the GNN and HGNN encoders, their time complexities are $\mathcal{O}(NL_2md_2 + NL_2nd_2^2 + Nnd_2d_f)$ and $\mathcal{O}(NL_2nd_2 + NL_2md_2^2 + Nnd_2d_{f*})$ respectively, where L_2 and d_2 denote their layer number and latent dimension. Finally, the Info-NCE loss requires $\mathcal{O}(NBd_2)$ complexity. To simplify the overall complexity, we denote the larger terms within L_1 and L_2 as L, and the larger terms between d_1 and d_2 as d. After ignoring the smaller terms, the overall complexity of SIGNET is $\mathcal{O}(NLd^2(m+n) + Nnd(d_f + d_{f*}) + NBd)$.

F Supplement of Experimental Setup

F.1 Datasets

We consider 16 benchmark datasets in total. The statistic of the datasets is provided in Table 1. In this paper, we take “PROTEINS-F”, “IMDB-B”, and “REDDIT-B” as the abbreviations of “PROTEIN-full”, “IMDB-BINARY”, and “REDDIT-BINARY”, respectively. For our synthetic datasets, we provide some examples in Fig. 1.

Table 1: Statistics of datasets.

Dataset	# Graphs (Train/Test)	# Nodes (avg.)	# Edges (avg.)
BM-MT	500/200	14.3	44.5
BM-MN	500/200	18.4	56.7
BM-MS	500/200	14.0	42.8
MNIST-0	1000/500	69.4	572.2
MNIST-1	1000/500	57.9	419.6
MUTAG	1742/295	30.1	60.9
PROTEINS-F	360/223	39.1	72.8
ENZYMES	400/120	32.6	62.1
AIDS	1280/400	15.7	16.2
DHFR	368/152	42.4	44.5
BZR	69/81	35.8	38.4
COX2	81/94	41.2	43.5
DD	390/236	284.3	715.7
NCI1	1646/822	29.8	32.3
IMDB-B	400/200	19.8	96.5
REDDIT-B	800/400	429.6	497.8

F.2 Hyper-parameters

We select the key hyper-parameters of `SIGNET` through a group-level grid search. Specifically, the hyper-parameters for each benchmark dataset are demonstrated in Table 2. Note that for the dataset without ground-truth explanations, we would not tune the hyper-parameters for the subgraph extractor but use the default ones. The grid search is carried out on the following search space:

- Number of epochs E: {10, 50, 100, 200, 500, 800, 1000}
- Learning rate lr: {1e-2, 1e-3, 1e-4}
- Layer number of encoders L_{enc}: {2,3,4,5}
- Hidden dimension of encoders D_{enc}: {16,32,64,128}
- Model type of subgraph extractor EXT: {MLP,GIN}
- Layer number of subgraph extractor L_{ext}: {2,3,4,5}
- Hidden dimension of subgraph extractor D_{ext}: {4,8,16,32}

To ensure robust and reliable results, we also conducted a comprehensive grid search to obtain the best hyperparameter configurations for the baselines. Specifically, for deep GLAD methods (i.e., OCGIN, GLocalKD, and OCGTL), we performed grid searches on both general hyperparameters (e.g., layer number and hidden dimensions) and model-specific hyperparameters (e.g., the number of transformations in OCGTL). Similarly, for post-hoc explainers, we conducted grid searches on their post-hoc training iterations and learning rates. As for shallow GLAD methods, we focused on searching for key hyperparameters such as the training iterations of detectors and kernel-specific parameters.

F.3 Metrics for explanation performance evaluation

We tackle the explanation problem by framing it as a binary classification task for nodes and edges. We designate nodes and edges inside the explanation subgraph as positive instances and the rest as negative. The importance weights generated by the explanation methods serve as prediction scores. An effective explanation method should assign higher weights to nodes and edges within the ground truth subgraphs compared to those outside. To quantitatively evaluate the performance, we use the AUC as the metric for this binary classification problem. A higher AUC indicates better performance in providing meaningful explanations.

Table 2: Details of the hyper-parameters tuned by grid search.

Dataset	E	lr	L_{enc}	D_{enc}	EXT	L_{ext}	D_{ext}
BM-MT	1000	1e-2	5	16	GNN	2	16
BM-MN	500	1e-2	5	16	GNN	3	8
BM-MS	200	1e-2	5	16	GNN	2	32
MNIST-0	50	1e-2	2	16	MLP	2	16
MNIST-1	50	1e-2	2	16	MLP	2	16
MUTAG	50	1e-2	5	16	GNN	5	4
PROTEINS-F	800	1e-3	5	16	GNN	5	8
ENZYMES	1000	1e-3	5	128	GNN	5	8
AIDS	1000	1e-4	5	16	GNN	5	8
DHFR	1000	1e-4	5	128	GNN	5	8
BZR	1000	1e-4	5	128	GNN	5	8
COX2	1000	1e-4	5	64	GNN	5	8
DD	100	1e-4	5	128	GNN	5	8
NCI1	1000	1e-4	5	128	GNN	5	8
IMDB-B	10	1e-4	5	64	GNN	5	8
REDDIT-B	1000	1e-4	5	128	GNN	5	8

F.4 Implementation of GLAD methods with post-hoc explainers

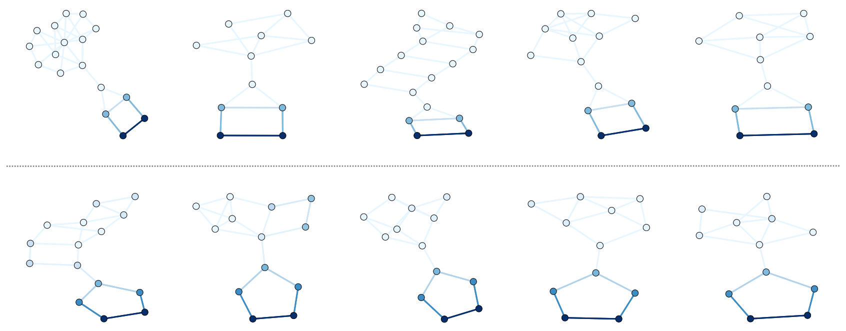
Given a GLAD model and post-hoc explainer, at first, we train the GLAD model independently on the training set. After sufficient training, the GLAD model is able to map each input graph into a scalar, i.e., its anomaly score. To address the uncertainty of the anomaly score boundaries, we apply a linear scaling function to map the scores into the [0,1] range and then use a sigmoid function to convert each score into a probability for binary classification. Subsequently, we integrate the post-hoc explainer with the probabilized output of the GLAD model and optimize the explainer accordingly.

F.5 Computing infrastructures

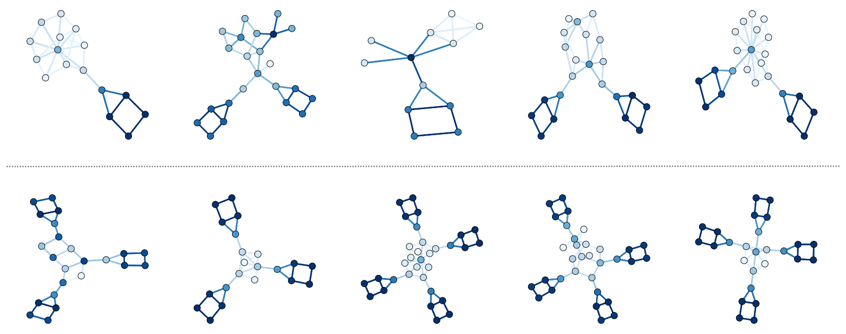
We implement the proposed `SIGNET` with PyTorch 1.12.0 [60] and PyTorch Geometric (PyG) 2.3.0 [61]. The experiments are conducted on a Linux server with an Intel Xeon E-2288G CPU and two Quadro RTX 6000 GPUs.

G Further Supplementary of Qualitative Experiments

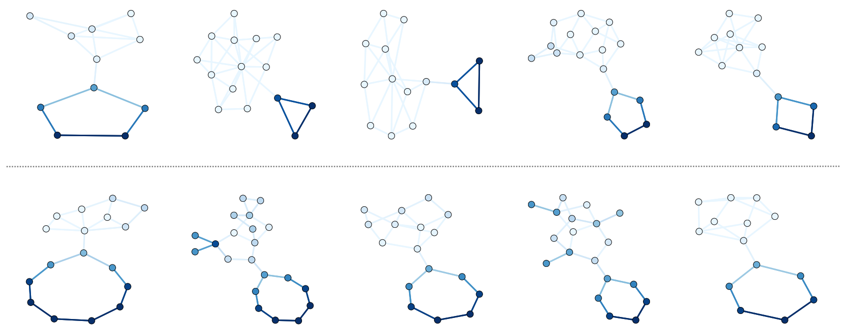
More visualization of explanation results by `SIGNET` are given in Fig. 2. In specific, we visualize the node-level and edge-level probabilities on four datasets, i.e., BM-MT, BM-MN, BM-MS, and MUTAG. For each dataset, the top row includes 5 normal examples, and the bottom row includes 5 anomalous examples. For MUTAG dataset, the normal examples do not have a specific rationale, while the rationales for anomalies are -NO2 or -NH2.



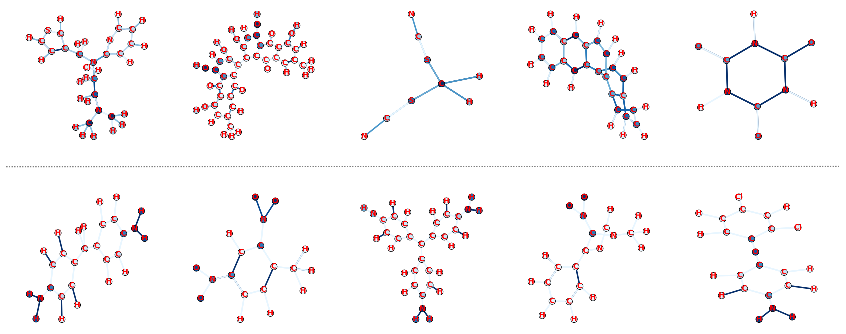
(a) BM-MT



(b) BM-MN



(c) BM-MS



(d) MUTAG

Figure 2: Visualization of explanation results w.r.t. node and edge probabilities. For each dataset, the top row includes 5 normal examples, and the bottom row includes 5 anomalous examples.

References

[1] Hao Yuan, Haiyang Yu, Shurui Gui, and Shuiwang Ji. Explainability in graph neural networks: A taxonomic survey. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2022.

[2] Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and S Yu Philip. A comprehensive survey on graph neural networks. *IEEE transactions on neural networks and learning systems*, 32(1):4–24, 2020.

[3] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? In *International Conference on Learning Representations*, 2019.

[4] Thomas N. Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. In *International Conference on Learning Representations*, 2017.

[5] Will Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs. In *Advances in neural information processing systems*, volume 30, 2017.

[6] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. Graph attention networks. In *International Conference on Learning Representations*, 2018.

[7] Kaize Ding, Zhe Xu, Hanghang Tong, and Huan Liu. Data augmentation for deep graph learning: A survey. *ACM SIGKDD Explorations Newsletter*, 24(2):61–77, 2022.

[8] Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on graphs with fast localized spectral filtering. In *Advances in neural information processing systems*, volume 29, 2016.

[9] Xin Zheng, Yixin Liu, Shirui Pan, Miao Zhang, Di Jin, and Philip S Yu. Graph neural networks for graphs with heterophily: A survey. *arXiv preprint arXiv:2202.07082*, 2022.

[10] Joan Bruna Estrach, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. Spectral networks and deep locally connected networks on graphs. In *2nd international conference on learning representations, ICLR*, 2014.

[11] Yifan Feng, Haoxuan You, Zizhao Zhang, Rongrong Ji, and Yue Gao. Hypergraph neural networks. In *Proceedings of the AAAI conference on artificial intelligence*, volume 33, pages 3558–3565, 2019.

[12] Song Bai, Feihu Zhang, and Philip HS Torr. Hypergraph convolution and hypergraph attention. *Pattern Recognition*, 110:107637, 2021.

[13] Naganand Yadati, Madhav Nimishakavi, Prateek Yadav, Vikram Nitin, Anand Louis, and Partha Talukdar. Hypergcn: A new method for training graph convolutional networks on hypergraphs. *Advances in neural information processing systems*, 32, 2019.

[14] Xin Zheng, Miao Zhang, Chunyang Chen, Qin Zhang, Chuan Zhou, and Shirui Pan. Auto-heg: Automated graph neural network on heterophilic graphs. In *Proceedings of the ACM Web Conference 2023*, page 611–620, 2023.

[15] Yizhen Zheng, He Zhang, Vincent Lee, Yu Zheng, Xiao Wang, and Shirui Pan. Finding the missing-half: Graph complementary learning for homophily-prone and heterophily-prone graphs. In *ICML*, 2023.

[16] Xin Zheng, Miao Zhang, Chunyang Chen, Quoc Viet Hung Nguyen, Xingquan Zhu, and Shirui Pan. Structure-free graph condensation: From large-scale graphs to condensed graph-free data. In *Advances in Neural Information Processing Systems*, 2023.

[17] Kaize Ding, Jundong Li, Rohit Bhanushali, and Huan Liu. Deep anomaly detection on attributed networks. In *Proceedings of the 2019 SIAM International Conference on Data Mining*, pages 594–602. SIAM, 2019.

[18] Yixin Liu, Zhao Li, Shirui Pan, Chen Gong, Chuan Zhou, and George Karypis. Anomaly detection on attributed networks via contrastive self-supervised learning. *IEEE transactions on neural networks and learning systems*, 33(6):2378–2392, 2021.

[19] Yue Tan, Guodong Long, Jie Ma, Lu Liu, Tianyi Zhou, and Jing Jiang. Federated learning from pre-trained models: A contrastive learning approach. In *Advances in Neural Information Processing Systems*, volume 35, pages 19332–19344, 2022.

[20] Yue Tan, Yixin Liu, Guodong Long, Jing Jiang, Qinghua Lu, and Chengqi Zhang. Federated learning on non-iid graphs via structural knowledge sharing. In *Proceedings of the AAAI conference on artificial intelligence*, volume 37, pages 9953–9961, 2023.

[21] Linhao Luo, Jiaxin Ju, Bo Xiong, Yuan-Fang Li, Gholamreza Haffari, and Shirui Pan. Chatrule: Mining logical rules with large language models for knowledge graph reasoning. *arXiv preprint arXiv:2309.01538*, 2023.

[22] Shirui Pan, Linhao Luo, Yufei Wang, Chen Chen, Jiapu Wang, and Xindong Wu. Unifying large language models and knowledge graphs: A roadmap. *arXiv preprint arxiv:2306.08302*, 2023.

[23] Linhao Luo, Yuan-Fang Li, Gholamreza Haffari, and Shirui Pan. Reasoning on graphs: Faithful and interpretable large language model reasoning. *arXiv preprint arxiv:2310.01061*, 2023.

[24] He Zhang, Bang Wu, Shuo Wang, Xiangwen Yang, Minhui Xue, Shirui Pan, and Xingliang Yuan. Demystifying uneven vulnerability of link stealing attacks against graph neural networks. In *ICML*, volume 202, pages 41737–41752. PMLR, 2023.

[25] He Zhang, Xingliang Yuan, Chuan Zhou, and Shirui Pan. Projective ranking-based GNN evasion attacks. *IEEE Trans. Knowl. Data Eng.*, 35(8):8402–8416, 2023.

[26] Yuning You, Tianlong Chen, Yongduo Sui, Ting Chen, Zhangyang Wang, and Yang Shen. Graph contrastive learning with augmentations. In *Advances in Neural Information Processing Systems*, volume 33, pages 5812–5823, 2020.

[27] Yizhen Zheng, Huan Yee Koh, Jiaxin Ju, Anh TN Nguyen, Lauren T May, Geoffrey I Webb, and Shirui Pan. Large language models for scientific synthesis, inference and explanation. *arXiv preprint arXiv:2310.07984*, 2023.

[28] Zhitao Ying, Dylan Bourgeois, Jiaxuan You, Marinka Zitnik, and Jure Leskovec. Gnnexplainer: Generating explanations for graph neural networks. *Advances in neural information processing systems*, 32, 2019.

[29] Dongsheng Luo, Wei Cheng, Dongkuan Xu, Wenchao Yu, Bo Zong, Haifeng Chen, and Xiang Zhang. Parameterized explainer for graph neural network. *Advances in neural information processing systems*, 33:19620–19631, 2020.

[30] Enyan Dai and Suhang Wang. Towards self-explainable graph neural network. In *Proceedings of the 30th ACM International Conference on Information & Knowledge Management*, pages 302–311, 2021.

[31] Minh Vu and My T Thai. Pgm-explainer: Probabilistic graphical model explanations for graph neural networks. *Advances in neural information processing systems*, 33:12225–12235, 2020.

[32] He Zhang, Bang Wu, Xingliang Yuan, Shirui Pan, Hanghang Tong, and Jian Pei. Trustworthy graph neural networks: Aspects, methods and trends. *arXiv preprint arXiv:2205.07424*, 2022.

[33] Thomas Schnake, Oliver Eberle, Jonas Lederer, Shinichi Nakajima, Kristof T Schütt, Klaus-Robert Müller, and Grégoire Montavon. Higher-order explanations of graph neural networks via relevant walks. *IEEE transactions on pattern analysis and machine intelligence*, 44(11):7581–7596, 2021.

[34] Yingxin Wu, Xiang Wang, An Zhang, Xiangnan He, and Tat-Seng Chua. Discovering invariant rationales for graph neural networks. In *International Conference on Learning Representations*, 2022.

[35] Siqi Miao, Mia Liu, and Pan Li. Interpretable and generalizable graph learning via stochastic attention mechanism. In *International Conference on Machine Learning*, pages 15524–15543. PMLR, 2022.

[36] Lingxiao Zhao and Leman Akoglu. On using classification datasets to evaluate graph outlier detection: Peculiar observations and new insights. *Big Data*, 2021.

[37] Xiaoxiao Ma, Jia Wu, Shan Xue, Jian Yang, Chuan Zhou, Quan Z Sheng, Hui Xiong, and Leman Akoglu. A comprehensive survey on graph anomaly detection with deep learning. *IEEE Transactions on Knowledge and Data Engineering*, 2021.

[38] Xuexiong Luo, Jia Wu, Amin Beheshti, Jian Yang, Xiankun Zhang, Yuan Wang, and Shan Xue. Comga: Community-aware attributed graph anomaly detection. In *Proceedings of the Fifteenth ACM International Conference on Web Search and Data Mining*, pages 657–665, 2022.

[39] Kaize Ding, Jundong Li, and Huan Liu. Interactive anomaly detection on attributed networks. In *Proceedings of the twelfth ACM international conference on web search and data mining*, pages 357–365, 2019.

[40] Rongrong Ma, Guansong Pang, Ling Chen, and Anton van den Hengel. Deep graph-level anomaly detection by glocal knowledge distillation. In *Proceedings of the Fifteenth ACM International Conference on Web Search and Data Mining*, pages 704–714, 2022.

[41] Chen Qiu, Marius Kloft, Stephan Mandt, and Maja Rudolph. Raising the bar in graph-level anomaly detection. In *Proceedings of the Thirty-First International Joint Conference on Artificial Intelligence, IJCAI-22*, pages 2196–2203, 7 2022.

[42] Xuexiong Luo, Jia Wu, Jian Yang, Shan Xue, Hao Peng, Chuan Zhou, Hongyang Chen, Zhao Li, and Quan Z Sheng. Deep graph level anomaly detection with contrastive learning. *Scientific Reports*, 12(1):19867, 2022.

[43] N TISHBY. The information bottleneck method. In *Proceedings of the 37-thAnnual Allerton Conference on Communication, 2000*, 2000.

[44] Naftali Tishby and Noga Zaslavsky. Deep learning and the information bottleneck principle. In *2015 ieee information theory workshop (itw)*, pages 1–5. IEEE, 2015.

[45] Alexander A Alemi, Ian Fischer, Joshua V Dillon, and Kevin Murphy. Deep variational information bottleneck. In *International Conference on Learning Representations*, 2017.

[46] Marco Federici, Anjan Dutta, Patrick Forré, Nate Kushman, and Zeynep Akata. Learning robust representations via multi-view information bottleneck. In *International Conference on Learning Representations*, 2020.

[47] Chang Xu, Dacheng Tao, and Chao Xu. Large-margin multi-view information bottleneck. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 36(8):1559–1572, 2014.

[48] Junchi Yu, Tingyang Xu, Yu Rong, Yatao Bian, Junzhou Huang, and Ran He. Graph information bottleneck for subgraph recognition. In *International Conference on Learning Representations*, 2021.

[49] Susheel Suresh, Pan Li, Cong Hao, and Jennifer Neville. Adversarial graph augmentation to improve graph contrastive learning. *Advances in Neural Information Processing Systems*, 34:15920–15933, 2021.

[50] Dongkuan Xu, Wei Cheng, Dongsheng Luo, Haifeng Chen, and Xiang Zhang. Infogcl: Information-aware graph contrastive learning. *Advances in Neural Information Processing Systems*, 34:30414–30425, 2021.

[51] Junchi Yu, Jie Cao, and Ran He. Improving subgraph recognition with variational graph information bottleneck. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 19396–19405, 2022.

[52] Chunyu Wei, Jian Liang, Di Liu, and Fei Wang. Contrastive graph structure learning via information bottleneck for recommendation. *Advances in Neural Information Processing Systems*, 35:20407–20420, 2022.

[53] Tailin Wu, Hongyu Ren, Pan Li, and Jure Leskovec. Graph information bottleneck. *Advances in Neural Information Processing Systems*, 33:20437–20448, 2020.

[54] Qingyun Sun, Jianxin Li, Hao Peng, Jia Wu, Xingcheng Fu, Cheng Ji, and S Yu Philip. Graph structure learning with variational information bottleneck. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 36, pages 4165–4174, 2022.

[55] Suseela T Sarasamma, Qiuming A Zhu, and Julie Huff. Hierarchical kohonenen net for anomaly detection in network security. *IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics)*, 35(2):302–312, 2005.

[56] Guansong Pang, Chunhua Shen, Longbing Cao, and Anton Van Den Hengel. Deep learning for anomaly detection: A review. *ACM computing surveys (CSUR)*, 54(2):1–38, 2021.

[57] Philipp Liznerski, Lukas Ruff, Robert A Vandermeulen, Billy Joe Franks, Marius Kloft, and Klaus Robert Muller. Explainable deep one-class classification. In *International Conference on Learning Representations*, 2021.

[58] Hongzuo Xu, Yijie Wang, Songlei Jian, Zhenyu Huang, Yongjun Wang, Ning Liu, and Fei Li. Beyond outlier detection: Outlier interpretation by attention-guided triplet deviation network. In *Proceedings of the Web Conference 2021*, pages 1328–1339, 2021.

[59] Wonwoo Cho, Jeonghoon Park, and Jaegul Choo. Training auxiliary prototypical classifiers for explainable anomaly detection in medical image segmentation. In *Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision*, pages 2624–2633, 2023.

[60] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, et al. Pytorch: An imperative style, high-performance deep learning library. *Advances in Neural Information Processing Systems*, 32:8026–8037, 2019.

[61] Matthias Fey and Jan Eric Lenssen. Fast graph representation learning with pytorch geometric. *arXiv preprint arXiv:1903.02428*, 2019.