Towards Explanation for Unsupervised Graph-Level Representation Learning

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Abstract

Due to the superior performance of Graph Neural Networks (GNNs) in various domains, there is an increasing interest in the GNN explanation problem "which fraction of the input graph is the most crucial to decide the model’s decision?" Existing explanation methods focus on the supervised settings, e.g., node classification and graph classification, while the explanation for unsupervised graph representation learning is still unexplored. The opaqueness of the graph representations may lead to unexpected risks when deployed for high-stake decision-making scenarios. In this paper, we advance the Information Bottleneck principle (IB) to tackle the proposed explanation problem for unsupervised graph representations, which leads to a novel principle, Unsupervised Subgraph Information Bottleneck (USIB). We also theoretically analyze the connection between graph representations and explanatory subgraphs on the label space, which reveals that the expressiveness and robustness of representations benefit the fidelity of explanatory subgraphs. Experimental results on both synthetic and real-world datasets demonstrate the superiority of our developed explainer and the validity of our theoretical analysis.

1 Introduction

Graph Neural Networks (GNNs) have emerged as a promising learning paradigm and demonstrated superior learning performance on different graph learning tasks, such as node classification [1][2][3][4], graph classification [5][6], and link prediction [7][8]. Despite their strengths, GNNs are usually treated as black boxes and thus cannot provide human-intelligible explanations [9][10]. Such opaqueness impedes their broad adoption in many decision-critical applications pertaining to fairness, privacy, and safety [11]. To better understand the working mechanisms of GNNs, researchers focus on the GNN explanation problem recently: what knowledge does the GNN model extract to make the specific decision? Specifically, given a graph and a GNN model, explanation methods try to find the intrinsic graph components that are crucial in the procedure of prediction for the target instance. To the best of our knowledge, all existing works [12][13][9][14] only consider explanations in supervised settings, such as graph classification and node classification. More specifically, these works aim to provide trustworthy explanations on why graphs and nodes are classified into a specific category by GNN models. However, the explanation problem for unsupervised graph representation learning is still unexplored. Different from supervised GNNs, unsupervised graph representation learning methods [15][16][17][18] embed graph data into low-dimensional representations without any supervision.
signals. Because of their opaqueness, it is hazardous to employ these representations for high-stake
decision-making problems directly. In consequence, it is imperative to lift the veil of unsupervised
graph representations by answering the following question: what knowledge do unsupervised GNNs
incorporate to generate the graph representations?

To provide a universal perspective, in this paper, we focus on the explanation for unsupervised
graph-level representations\(^1\). Specifically, we aim to find explanatory subgraphs most relevant to the
representations while incorporating superfluous information as little as possible. There are mainly
two challenges in the unexplored explanation problem: (1) Different from supervised GNNs which
are designed for specific tasks, unsupervised graph representations are usually task-agnostic. Thus,
existing explanation methods based on specific learning tasks cannot be directly grafted to explain
unsupervised graph representations. (2) It is computational intractably to evaluate the relevance
between the subgraphs and the representation vectors since they are located in different spaces, i.e.,
the non-Euclidean space and Euclidean space, respectively. As a result, an effective and efficient
measurement is urgently needed.

To address the above challenges, we propose a novel method named Unsupervised Subgraph Infor-
mation Bottleneck (USIB) in light of the Information Bottleneck (IB) principle \([19, 20]\) that learns
compressed representations from the input data while keeping the most predictive information of
labels. Specifically, USIB adopts the mutual information to formalize the relevance. It maximizes
the mutual information between explanatory subgraphs and graph representations while minimizing
the mutual information between explanatory subgraphs and given graph instances, simultaneously.
Moreover, we theoretically analyze the connection between representations and explanatory sub-
graphs on the label space, which reveals that the expressiveness and robustness of representations
benefit the fidelity of explanatory subgraphs. Intuitively, as shown in Fig. 1 when the graphs have
different motifs, expressive and robust representations extract the motif-related information exactly
while uninformative and fragile representations focus more on noises. Thus, explanations generated
for powerful representations can explore the essential structure, while the fidelity of explanation
for powerless representations is not guaranteed. The contributions of this paper are summarized as
follows.

- We consider an unexplored explanation problem. To the best of our knowledge, this is the first
  work to explore the explanation for unsupervised graph representation learning with GNNs.
- We propose a novel explanation method USIB based on the IB principle, which aims to find the most
  informative yet compressed explanation. We also theoretically analyze the connection between
  representations and explanatory subgraphs on the label space, revealing that representations’
  expressiveness and robustness benefit the explanatory subgraphs.
- Extensive experiments show that our method achieves the state-of-the-art performance on several
  benchmark datasets and also demonstrate the validity of our theoretical analysis.

\(^1\)The explanation for node-level representations can be seen as a particular case by considering the corre-
sponding \(k\)-hop neighbor subgraphs of each node as a graph instance.
2 Related works

Instance-level explanation. Instance-level explanation aims to give explanations for specific instances. In general, there are mainly two lines of works: (1) Non-parametric explanation methods [21, 22, 23] usually involve gradient-like scores as heuristics to quantify the importance of edges and nodes. The gradient-like scores can be easily obtained by conducting backpropagation from the target model prediction to the input, e.g., adjacency matrix. For example, SA [21] directly employs the squared values of gradients as the importance scores of different input features. However, these methods can only reflect the sensitivity between input and output, which cannot accurately show the importance. (2) Parametric explanation methods [9, 24, 10, 25, 14] generate the explanatory subgraphs with a parametrized explainer model. To name a few, GNNExplainer [9] learns soft masks with a local view and applies the masks on the adjacency matrix. To provide a global understanding, GNNExplainer focuses on the explanation for supervised GNNs, and formalizes the relevance measures the relevance between subgraph $S$, i.e., $S$ explanation aims to learn explanatory subgraphs $G$ that are most relevant with GNN’s computation results, so as to provide human-intelligible explanations. Specifically, given a graph $G$ and a GNN model $\psi$ that learns a conditional distribution $P_{\psi}(Z|G)$, GNN explanation aims to learn explanatory subgraphs $S$ that are most relevant with GNN’s computation results, i.e.,

$$S = \arg \max_{S \in \hat{S}} \text{Score}(S, \hat{Z}) \quad (2)$$

where $S$ denotes the universe set consisting of all possible subgraphs of graph $G$; $\text{Score}(S, \hat{Z})$ measures the relevance between subgraph $S$ and GNN’s computation results $\hat{Z}$. For example, GNNExplainer [9] focuses on the explanation for supervised GNNs, and formalizes the relevance $\text{Score}(S, \hat{Z})$ as mutual information, i.e., $S = \arg \max_{S \in \hat{S}} I(S; \hat{Y})$, where random variable $\hat{Y} = \hat{Z}$ refers to the classification probabilities.

3 Notations and preliminaries

Notations. In most cases, we denote random variables with upper-case letters (e.g., $G$ and $Z$), and represent its support set by calligraphic letters (e.g., $\mathcal{G}$ and $\mathcal{Z}$). Upper-case letters with superscript (e.g., $G^{(b)}$ and $Z^{(m)}$) refers to the instances of random variables correspondingly. Suppose the graph data is given as $G = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V}$ and $\mathcal{E}$ are the nodes and edges respectively. The representations of graph $G$, denoted as $Z$, is learned by an unsupervised GNN model $f_t : \mathcal{G} \rightarrow \mathcal{Z}$, such as the state-of-the-arts Infograph [27], GCL [28], and ADGCL [29]. Moreover, we denote the ground-truth labels of graphs as $Y$ which are unreachable in the unsupervised setting.

Information Bottleneck [30, 31]. Given input data $X$ and its label $Y$, Information Bottleneck aims to discover a compressed latent representation $Z$ that is maximally informative in terms of $Y$. Formally, one can learn the latent representation $Z$ by optimizing the following optimization problem

$$\max_Z L_{IB} = I(Z; Y) - \beta I(X; Z) \quad (1)$$

where $\beta$ denotes a hyper-parameter trading-off the informativeness and compression. Mutual information (MI) $I(X; Z)$ measures the relevance of two random variables, formulated as $I(X; Z) = \int_x \int_z p(x, z) \log \frac{p(x, z)}{p(x)p(z)} dx dz$.

GNN explanation. GNN explanation aims to understand the intrinsic information of the graphs that are crucial for GNN’s computation process, so as to provide human-intelligible explanations. Specifically, given a graph $G$ and a GNN model $\psi$ that learns a conditional distribution $P_{\psi}(Z|G)$, GNN explanation aims to learn explanatory subgraphs $S$ that are most relevant with GNN’s computation results, i.e.,

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4 Methodology

In this section, we first introduce our proposed explanation method for unsupervised graph representation learning, i.e., USIB. Then, we elaborate on the mutual information estimation methods for USIB. Finally, the reparameterization trick is presented for the optimization of USIB objective.

4.1 Unsupervised Subgraph Information Bottleneck

In this paper, we study the unexplored explanation problem for unsupervised graph-level representation learning. Given a graph $G$ and its corresponding representation $Z$ extracted by unsupervised GNNs, our goal is to identify the explanatory subgraph $S$ that is most relevant to the representations. Following the previous explanation works [2,10], we leverage mutual information to measure the relevance and therefore formulate the explanation problem as $\arg \max_S I(S; Z)$. Unfortunately, it has been proved that there is a trivial solution $S = G$ since $I(Z; S) \leq I(Z; G)$ (The proof is shown in the Appendix B). The trivial solution indicates that the explanatory subgraph $S$ may incorporate superfluous information, e.g., noise and irrelevant information with representations $Z$. Inspired by the success of IB principle in explanation for supervised GNNs [19], we generalize the IB principle to the unsupervised setting to avoid the trivial solution and exploit a novel principle.

Definition. (Unsupervised Subgraph Information Bottleneck: USIB). Given a graph $G$ and its representation $Z$, the USIB seeks for the most informative yet compressed explanation $S$ through optimization problem

$$\max_S \mathcal{L}_{USIB} = I(Z; S) - \beta I(G; S).$$

By optimizing the USIB objective, one can make a trade-off between the informativeness and compression of explanatory subgraphs. However, it is notoriously intractable to optimize the USIB objective because the mutual information involves integral on high-dimensional data, i.e., $Z$, $S$, and $G$. As a result, a mutual information estimation method is necessary to be exploited.

4.2 Optimization for USIB

We tackle the two terms $I(Z; S)$ and $I(G; S)$ in the objective of USIB separately.

Maximizing $I(Z; S)$. We adopt Jensen-Shannon MI estimator [32,33] to assign an approximate lower bound for $I(Z; S)$, i.e.,

$$J_{JSD}^{Z}(Z; S) := \sup_{f_{\phi}} \mathbb{E}_{p(S, Z)} \left[ -sp \left( -f_{\phi}(S, Z) \right) \right] - \mathbb{E}_{p(S), p(Z)} \left[ sp \left( f_{\phi}(S, Z) \right) \right] \quad (4)$$

where $sp(x) = \log(1 + e^x)$ is the softplus function; Function $f_{\phi} : S \times Z \rightarrow \mathbb{R}$ with parameters $\phi$ is learned to discriminate whether an instance of $S$ and an instance of $Z$ are sampled from the joint distribution or not. It is implemented with function composite of MLP$_{\phi_1}$ and GNN$_{\phi_2}$, i.e.,

$$f_{\phi} \left( S^{(k)}, Z^{(k)} \right) = \text{MLP}_{\phi_1} \left( \text{GNN}_{\phi_2} \left( S^{(k)} \right) \right) \quad \| \cdot \| \quad (5)$$

where $\phi = \{\phi_1, \phi_2\}; \| \cdot \| \text{ refers to the concatenation operator}. Note that the prior distributions $p(S, Z)$ and $p(Z)$ are usually unreachable in practice. In conjunction with Monte Carlo sampling to approximate the prior distributions, we reach an approximate lower bound of Eq. (4) by

$$\max_{\phi} \mathcal{L}_1(\phi, S) = \frac{1}{K} \sum_{k=1}^{K} -sp \left( -f_{\phi} \left( S^{(k)}, Z^{(k)} \right) \right) - \frac{1}{K} \sum_{k=1, m \neq k}^{K} sp \left( f_{\phi} \left( S^{(k)}, Z^{(m)} \right) \right) \quad (6)$$

where $K$ is the number of samples. $(S^{(k)}, Z^{(k)})$ is sampled form joint distribution $p(S, Z)$ while $(S^{(k)}, Z^{(m)})$ is independently sampled from the marginal distributions $p(S)$ and $p(Z)$, respectively.

In practice, we sample $(S^{(k)}, Z^{(m)})$ by randomly permutating $(S^{(k)}, Z^{(k)})$ pairs sampled from the joint distribution.
Minimizing $I(G; S)$. Note that the entropy of explanatory subgraph $H(S) = \mathbb{E}_{p(S)}[-\log p(S)]$ provides an upper bound for $I(G; S)$ since the inequality $I(G; S) = H(S) - H(S|G) \leq H(S)$ holds. However, it is intractable to calculate the entropy because the prior distribution of $S$ is unknown in practice. To address this issue, we consider a relaxation and assume that the explanatory graph is a Gilbert random graph \[^{[34]}\] where edges are conditionally independent to each other. Specifically, let $(i, j) \in \mathcal{E}$ denote the edge of graph $G$, and $e_{i,j} \sim \text{Bernoulli}(\mu_{i,j})$ be a binary variable indicating whether the edge $(i, j)$ is selected for subgraph $S$. Thus, the probability of subgraph $S$ is factorized as $p(S) = \prod_{(i, j) \in \mathcal{E}} p(e_{i,j})$, where $p(e_{i,j}) = \mu_{i,j} (1 - \mu_{i,j})^{1-e_{i,j}}$. In this way, we can arrive at an approximate upper bound for $I(G; S)$ with Monte Carlo sampling, which is denoted by

$$
\mathcal{L}_{2}(S) = -\frac{1}{K} \sum_{k=1}^{K} \sum_{(i, j) \in \mathcal{E}} e_{i,j}^{(k)} \log \mu_{i,j}^{(k)} + (1 - e_{i,j}^{(k)}) \log (1 - \mu_{i,j}^{(k)})
$$  

(7)

The reparametrization trick. Gradients-based optimization methods may fail to optimize Eq. (6) and Eq. (7) because of the non-differentiable sampling process and the discrete nature of subgraph structure. On this account, we follow the Gumbel-Softmax reparametrization trick \[^{[35, 36]}\] and relax the binary variables $e_{i,j}$ to a continuous edge weight variables $\hat{e}_{i,j} = \sigma((\log \epsilon - \log (1 - \epsilon) + w_{i,j})/\tau) \in [0, 1]$, where $\sigma(\cdot)$ is the sigmoid function; $\epsilon \sim \text{Uniform}(0, 1)$; $\tau$ is the temperature hyper-parameter such that $\lim_{\tau\rightarrow 0} p(\hat{e}_{i,j} = 1) = \sigma(w_{i,j})$; $w_{i,j}$ is the latent variables which is calculated by a neural network following previous work \[^{[10]}\].

$$
w_{i,j}^{(k)} = \text{MLP}_{\theta_1}(z_{i}^{(k)}||z_{j}^{(k)}) \text{ with } z_{i}^{(k)} = \text{GNN}_{\theta_2}(G^{(k)}, i), i = 1, 2, \ldots
$$  

(8)

where $z_{i}^{(k)}$ denotes the node representations of node $i$. For better representation, we denote $\theta = \{\theta_1, \theta_2\}$, and generate the relaxed subgraph $S$ by $\hat{S}^{(k)} = g_{\theta}(G^{(k)}) \[^{[1]}\]$. Let $\mu_{i,j}^{(k)} = \sigma(w_{i,j}^{(k)})$, the objective in Eq. (7) can be rewritten as

$$
\mathcal{L}_{2} \left( g_{\theta} \left( G^{(k)} \right) \right) = -\frac{1}{K} \sum_{k=1}^{K} \sum_{(i, j) \in \mathcal{E}} \hat{e}_{i,j}^{(k)} \log \sigma \left( w_{i,j}^{(k)} \right) + (1 - \hat{e}_{i,j}^{(k)}) \log (1 - \sigma \left( w_{i,j}^{(k)} \right)).
$$  

(9)

In summary, we rewrite the USIB optimization problem Eq. (5) as

$$
\max_{\phi, \theta} \mathcal{L}_{\text{USIB}}(\phi, \theta, G) = \mathcal{L}_{1} \left( \phi, g_{\theta} \left( G^{(k)} \right) \right) - \beta \cdot \mathcal{L}_{2} \left( g_{\theta} \left( G^{(k)} \right) \right).
$$  

(10)

An overview of our method is shown in Fig. 2. We first generate the explanatory subgraphs by a neural network, then another network is involved to estimate the mutual information between explanatory subgraphs and graph representations. Finally, the subgraph generator and the mutual information estimator are optimized collaboratively. The final explanatory subgraphs can be achieved by selecting edges with the top-$n$ edge weights (i.e., $\hat{e}_{i,j}^{(k)}$). Detailed algorithms can be found in the Appendix.

5 Theoretical analysis

In this section, we theoretically analyze the connection between representations and explanatory subgraphs on the label space. Before analyzing the connection, we first introduce two definitions to evaluate the expressiveness and robustness of representations.

Definition. Sufficiency: Considering a specific downstream task with label $Y$, the representation $Z$ of graph $G$ is sufficient for $Y$ if and only if $I(G; Y|Z) = 0$.

A sufficient representation $Z$ indicates that it is capable of predicting $Y$ at least as accurately as the original graph $G$. Based on this definition, Proposition holds (see proof in Appendix B).

Proposition 1. Let $G$ and $Y$ be random variables with joint distribution $p(G, Y)$, and $Z$ be a representation of $G$. Considering a Markov Chain $Y \rightarrow G \rightarrow Z$, we assume that $Z$ is conditionally independent from $Y$ once $G$ is given. Then, $Z$ is sufficient for $Y$ if and only if $I(Z; Y|G) = I(G; Y)$.

$^{3}$ $g_{\theta}$ computes $w_{i,j}$ first and then generates the subgraph $\hat{S}^{(k)}$ by combining the relaxed edge weights and $G^{(k)}$ into a weighted graph.
The sufficiency of representations evaluates the expressiveness of unsupervised representations, i.e., for graph representations that are sufficient for a specific task, no information regarding the task is lost in the embedding procedure. Thus the unsupervised representations are expressive enough for the task.

Definition. Necessity: Considering a specific downstream task with label \( Y \), the representation \( Z \) of graph \( G \) is necessary for \( Y \) if and only if \( I(G; Z|Y) = 0 \).

A necessary representation indicates that \( Z \) only extracts information relevant to \( Y \) from the graph \( G \).

Proposition 2. Let \( G \) and \( Y \) be random variables with joint distribution \( p(G,Y) \), and \( Z \) be a representation of \( G \). Considering a Markov Chain: \((G_N, Y) \rightarrow G \rightarrow Z \) where \( G_N \) collects all label-irrelevant information in \( G \), \( Z \) is necessary for \( Y \) if and only if \( I(G_N; Z) = 0 \).

The necessity of representations evaluates the robustness of unsupervised representations, i.e., graph representations are unacted on label-irrelevant information, and thus the representations can be robust against noise information.

Given the definition of sufficiency and necessity, we have the following Theorem that provides a theoretical connection between the graph representations and explanatory subgraphs on the label space (see proof in Appendix B).

Theorem 1. Let \( G \) and \( Y \) be random variables with joint distribution \( p(G,Y) \). Given unsupervised graph representation \( Z \) and its explanations \( S \) in graph \( G \), we assume that \( S \) is conditionally independent from \( Y \) and \( Z \) when \( G \) is observed. We have,

1. if \( Z \) is sufficient for \( Y \), then \( I(S; Z) \geq I(S; Y) \);
2. if \( Z \) is necessary for \( Y \), then \( I(S; Z) \leq I(S; Y) \);
3. if \( Z \) is sufficient and necessary for \( Y \), then \( I(S; Z) = I(S; Y) \);

Theorem provides theoretical support for our USIB explanation method, i.e., for representations that are expressive and robust enough, one can explore explanatory subgraphs that are highly relevant to the ground-truth labels by maximizing the mutual information between representations and explanatory subgraphs. In contrast, if representations are uninformative and fragile, the fidelity of explanatory subgraphs is not guaranteed. We experimentally analyze the influence of representations’ expressiveness and robustness in the next section.

6 Experiments

In this section, we empirically evaluate the effectiveness and superiority of our proposed method by answering the following questions.

- RQ1 How does our proposed method perform compared to other baseline explainers?
- RQ2 Does expressiveness and robustness of representations affect the fidelity of explanatory subgraphs in agreement with the theoretical analysis?
6.1 Experimental settings

Datasets. We take four benchmark datasets for experiments, including Mutagenicity, NCI1, PROTEINS [37], and BA3 [25]. The first two are molecule graph datasets, while PROTEINS is a bioinformatics graph dataset. BA3 is a synthetic dataset created by Wang et al. [25]. Specifically, the Barabasi-Albert (BA) graphs are adopted as the base and attach each base with one of three motifs: house, cycle, and grid. The statistical details for these datasets can be found in Appendix D.

Target models. We consider three state-of-the-art target models to generate graph representations for explanation: Infograph [28], GCL [28], and ADGCL [29]. Note that all these target models adopt the same GNN encoder architecture for a fair comparison. The details of implementation can be found in Appendix D.

Baselines. To our best knowledge, there is no previous work focusing on the explanation for unsupervised graph representation learning. We train an MLP classifier based on representations generated by the target models and then compose the target models and the classifiers as end-to-end graph classifiers. Following this strategy, previous explanation methods for supervised setting, such as GNNExplainer [9], PGExplainer [10], PGM-Explainer [14], and Refine [25], could be adopted as baselines. Moreover, to provide a fair comparison without the involvement of label information, we also adapt several typical explanation methods for CNNs to our unsupervised graph representation explanation setting. Specifically, we adopt three methods which involve gradient-like scores by conducting backpropagation from the representations’ $l_2$ norm to the input, such as IG [23], GradCam [12], and SA [21].

Evaluation metrics. It is challenging to evaluate explanatory subgraphs quantitatively because the ground-truth explanations in practice are usually unreachable. Following previous works [9] [25] [38] [39], we adopt the following two metrics: (1) Predictive Accuracy (ACC@$r$). For the explanatory subgraphs, which are crucial for the target GNN encoders, the corresponding subgraph representations should behave similarly to representations of the original graph on downstream tasks, e.g., graph classification. To evaluate the fidelity of explanatory subgraphs, we feed the subgraphs to the target models first and get the subgraph representations. Then we train logistic classifiers on the subgraph representations and report the 10-fold cross-validation accuracy as ACC@$r$ for explanatory subgraphs with edge selection ratio $r$. Moreover we further denote ACC-AUC as the area under the ACC curve over different selection ratios $r \in \{0.1, 0.2, \cdots , 0.9\}$. (2) Recall@$n$. Ground-truth explanations for the synthetic dataset BA3 are reachable. Thus we adopt the recall metric to evaluate explanatory subgraphs. It is formulated as Recall@$n = \frac{|S \cap S^*|}{|S^*|}$, where $n$ is the number of edges involved in the explanatory subgraphs; $S^*$ denotes the ground-truth explanations. Note that each experiment is repeated 10 times to reduce randomness.

6.2 Quantitative evaluations

Effectiveness of USIB. To investigate the effectiveness of our proposed USIB explanation method, we present the ACC curve over different selection ratios in Fig. 3 and report the results on ACC-AUC and Recall@$n$ in Table 1. We only present the results on Infograph because of page limitation and present the results on other target models in Appendix D. The experimental results show that our proposed USIB achieves superior performance in the unsupervised setting and is comparable to baseline methods in the supervised setting. Specifically, USIB achieves the best performance on
We can clearly observe that the untrained Infograph focuses more on the random base graph. This is because there is only a slight gap of expressiveness over clean graphs.

The qualitative results on the synthetic dataset BA3 in Fig. 5. Specifically, we compare the explanation results of our USIB on untrained Infograph and fine-tuned Infograph qualitatively. We can clearly observe that the untrained Infograph focuses more on the random base graph. This can be attributed to the untrained Infograph recursively incorporates node’s information with a significant relative improvement is achieved (i.e., 14.8% on ACC-AUC and 10.44% on Recall@5) on the synthetic dataset BA3. It indicates that the performance of USIB is related to the expressiveness of target models (three target models achieve more than 90% ACC on BA3, which is much better than other datasets).

**Influence of representations’ expressiveness and robustness.** We quantitatively evaluate the expressiveness and robustness by the downstream graph classification accuracy (i.e., ACC) on representations extracted respectively from the clean graphs and noisy graphs. The noisy graphs are generated by randomly adding $|E|$ noise edges to the clean graphs. To investigate how representations’ expressiveness and robustness affect the fidelity of explanatory subgraphs, we show a scatter diagram in Fig. 4, where each point denotes a target model on a specific dataset. From Fig. 4 we can observe that: (1) There is a positive correlation between representations’ expressiveness/robustness and explanatory subgraphs’ fidelity. Representations achieving higher ACC on clean and noisy graphs usually lead to explanatory subgraphs with higher ACC-AUC. This observation is consistent with our theoretical analysis. (2) Expressiveness matters more than robustness when there is a significant gap on expressiveness. For example, we can observe that the fidelity of explanatory subgraphs on BA3 is positively related to the expressiveness while robustness makes less influence. (3) Robustness matters when there is only a slight gap on expressiveness. Specifically, the fidelity of explanatory subgraphs on Mutagenicity, NCI1, and PROTEINS is positively related to representations’ robustness since there is only a slight gap of expressiveness over clean graphs.

### Table 1: Comparison of our USIB and other baseline explainers. **Bold** indicates the best results.

| Target Model | Setting   | Method       | Mutagenicity | NCI1 | PROTEINS | BA3 |
|--------------|-----------|--------------|--------------|------|----------|-----|
|              |           | ACC-AUC      | ACC-AUC      | ACC-AUC | ACC-AUC  | Recall@5 | Relative Improvement |
| Infograph    | Supervised| PG-Explainer | 69.29 ± 2.10 | 59.93 ± 1.42 | 65.50 ± 2.32 | 89.99 ± 3.81 | 44.93% |
|              |           | GNNExplainer | 68.99 ± 2.08 | 54.68 ± 1.34 | 62.16 ± 2.20 | 74.76 ± 3.94 | 18.80 ± 0.92 |
|              |           | PGM-Explainer| 66.93 ± 0.42 | 54.80 ± 1.26 | 64.64 ± 1.97 | 83.70 ± 1.85 | 24.76 ± 0.07 |
|              |           | ReFine       | 67.45 ± 0.97 | 57.88 ± 1.30 | 66.28 ± 1.06 | 84.78 ± 6.59 | 17.88 ± 8.79 |
|              | Unsupervised| IG          | 68.87 ± 1.52 | 54.65 ± 0.94 | 63.30 ± 2.25 | 79.52 ± 2.18 | 16.22 ± 5.11 |
|              |           | GraCam       | 67.60 ± 0.93 | 54.79 ± 0.71 | 63.12 ± 2.36 | 80.62 ± 3.84 | 18.74 ± 1.74 |
|              |           | SA           | 68.24 ± 0.97 | 53.94 ± 0.65 | 62.71 ± 2.16 | 76.02 ± 3.07 | 16.53 ± 3.01 |
|              |           | USIB         | 69.55 ± 0.96 | 56.70 ± 1.65 | 64.46 ± 2.75 | 92.55 ± 3.28 | 27.16 ± 4.46 |

**Figure 4:** Influence of target models’ expressiveness and robustness. We distinguish different target models and datasets with different colors and markers separately.

Mutagenicity and BA3 among all baseline methods and outperforms other unsupervised methods on NCI1 and PROTEINS. However, there is still a gap between our USIB and supervised baseline methods on NCI1 and PROTEINS because of the involvement of label information. It is noteworthy that a significant relative improvement is achieved (i.e., 14.8% on ACC-AUC and 10.44% on Recall@5) on the synthetic dataset BA3. It indicates that the performance of USIB is related to the expressiveness of target models (three target models achieve more than 90% ACC on BA3, which is much better than other datasets).

**6.3 Qualitative analysis.**

We present the qualitative results on the synthetic dataset BA3 in Fig. 5. Specifically, we compare the explanation results of our USIB on untrained Infograph and fine-tuned Infograph qualitatively. We can clearly observe that the untrained Infograph focuses more on the random base graph. This can be attributed to the untrained Infograph recursively incorporates node’s information with...
random weights, and thus pays more attention to the central nodes in the graph, i.e., the base graph. In contrast, the second row shows that the fine-tuned Infograph transfers its attention to the house motifs after the unsupervised training, which reveals why representations perform well on the downstream tasks. Moreover, we surprisingly find that Infograph’s performance does not rely on the completeness of motifs, e.g., Infograph performs well even with only 30% edges according to Fig.3. A rational explanation is the redundancy of graph information, i.e., node features may preserve redundant information that is also contained in structural features. The redundancy may jeopardize the evaluation of explanation methods [40]. We consider it a future direction to construct datasets carefully designed for unsupervised graph representation explanation. We can also observe a limitation of USIB that it considers edges independently but ignores the substructures of graphs whose importance is emphasized in previous work [41].

7 Conclusion and future work

We study an unexplored explanation problem: the explanation for unsupervised graph representation learning. We advance the IB principle to tackle the explanation problem, which leads to a novel explanation method USIB. Moreover, we theoretically analyze the connection between representations and explanatory subgraphs on the label space, which reveals that expressiveness and robustness benefit the fidelity of explanatory subgraphs. Extensive results on four datasets and three target models demonstrate the superiority of our methods and the validity of our theoretical analysis. As a future direction, we consider the counterfactual explanation [42] for unsupervised representation learning and explore whether there is a connection between explanation and adversarial examples [43] [44] [45].

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A PROPERTIES OF MUTUAL INFORMATION

In this section we enumerate some properties \cite{46} of mutual information that are used to prove the theorems reported in this work. For any random variables \(G, Y, Z\) and \(S\):

\begin{align}
(P_1) \text{ Positivity:} & \quad I(G; Y) \geq 0, I(G; Y|Z) \geq 0 \\
(P_2) \text{ Chain rule:} & \quad I(G, Y; Z) = I(G; Z) + I(Y; Z|G) \\
(P_3) \text{ Chain rule (Multivariate Mutual Information):} & \quad I(G; Y; Z) = I(Y; Z) - I(Y; Z|G) \\
& \quad I(G; Y; Z|S) = I(Y; Z|S) - I(Y; Z|G, S)
\end{align}

B THEOREMS AND PROOFS

In the following section we prove the statements reported in the main body of the paper. We consider the following graphical model \(G\):

\[
Y \rightarrow G \rightarrow Z \\
\downarrow \\
S
\]

Following Federici \textit{et al.} \cite{46}, we state that \(Z\) and \(S\) are conditionally independent from any other variables in the system once \(G\) is observed. As a result, whenever \(Z\) is the representation of \(G\) and \(S\) is an explanation of \(G\), we have

\[
I(Z; A|G, B) = 0, \quad I(S; A|G, B) = 0
\]

for any variable (or groups of variables) \(A\) and \(B\) in the system.

**Lemma B.1.** \textit{Let \(G\) be a random variable which denotes a graph, \(Z\) is the representation of \(G\) and \(S\) denotes the regarding explanatory subgraph, we have}

\[
I(Z; S) \leq I(Z; G)
\]

**Hypothesis:**

\((H_1) Z\) is an explanation of \(G\): 

\[I(S; Z|G) = 0\]

**Thesis:**

\((T_1) I(Z; S) \leq I(Z; G)\)

**Proof.**

\[
I(Z; S) \overset{P_3}{=} I(Z; S; G) + I(Z; S|G) \\
\overset{H_1}{=} I(Z; S; G) \\
\overset{P_3}{=} I(Z; G) - I(Z; G|S) \\
\leq I(Z; G)
\]

\(\square\)

**Proposition B.1.** \textit{Let \(G\) and \(Y\) be random variables with joint distribution \(p(G, Y)\), and \(Z\) be a representation of \(G\). Considering a Markov Chain \(Y \rightarrow G \rightarrow Z\), we assume that \(Z\) is conditionally independent from \(Y\) once \(G\) is given. Then, \(Z\) is sufficient for \(Y\) if and only if } \(I(Z; Y) = I(G; Y)\).

**Hypothesis:**

\((H_1) Z\) is a representation of \(G\): 

\[I(Z; Y|G) = 0\]

**Thesis:**

\((T_1) I(G; Y|Z) = 0 \iff I(Z; Y) = I(G; Y)\)
Proof.

\[ I(G; Y|Z) \overset{p}{=} I(G; Y) - I(G; Y; Z) \]
\[ \overset{p}{=} I(G; Y) - I(Y; Z) + I(Y; Z|G) \]
\[ \overset{H}{=} I(G; Y) - I(Y; Z) \]

Thus we can have \( I(G; Y|Z) = 0 \iff I(Z; Y) = I(G; Y) \). \( \square \)

**Proposition B.2.** Let \( G \) and \( Y \) be random variables with joint distribution \( p(G, Y) \), and \( Z \) be a representation of \( G \). Considering a Markov Chain: \( (G_N, Y) \to G \to Z \) where \( G_N \) collects all label-irrelevant information in \( G \), \( Z \) is necessary for \( Y \) if and only if \( I(G_N; Z) = 0 \).

**Hypothesis:**

\( H_1 \) \( Z \) is a representation of \( G \): \( I(Z; G_N|G) = 0 \);
\( H_2 \) \( G_N \) is label-irrelevant: \( I(G_N; Y) = 0 \);
\( H_3 \) \( G_N \) collects all label-irrelevant information in \( G \): \( I(G; Z|Y, G_N) = 0 \)

**Thesis:**

\( T_1 \) \( I(Z; G|Y) = 0 \iff I(Z; G_N) = 0 \)

**Proof.**

\[ I(Z; G|Y) \overset{p}{=} I(Z; G) - I(Z; G; Y) \]
\[ = I(Z; G) - I(Y; G_N; G; Z) + I(Y; G_N; G; Z) - I(Z; G; Y) \]
\[ \overset{p}{=} I(Z; G|Y, G_N) + I(Y; G_N; G; Z) - I(Z; G; Y) \]
\[ \overset{H}{=} I(Y; G_N; G; Z) - I(Z; G; Y) \]
\[ \overset{p}{=} I(G_N; G; Z|Y) \]
\[ \overset{p}{=} I(G_N; G; Z) - I(G_N; G; Z; Y) \]
\[ \overset{H}{=} I(G_N; G; Z) \quad \text{(Note that} \ I(G_N; G; Z; Y) \leq I(G_N; Y)) \]
\[ \overset{p}{=} I(G_N; Z) - I(G_N; Z|G) \]
\[ \overset{H}{=} I(Z; G_N) \]

Thus we can have \( I(Z; G|Y) = 0 \iff I(Z; G_N) = 0 \). \( \square \)

**Lemma B.2.** \( (L_1) \) Let \( G \) and \( Y \) be random variables with joint distribution \( p(G, Y) \), \( Z \) is a representation of graph \( G \), \( S \) denotes the explanatory subgraph, if \( Z \) is sufficient for \( Y \), then

\[
I(S; Y|Z) = 0
\]

**Hypothesis:**

\( H_1 \) \( S \) is an explanation of \( G \): \( I(S; Y|Z, G) = 0 \)

**Thesis:**

\( T_1 \) \( I(G; Y|Z) = 0 \Rightarrow I(S; Y|Z) = 0 \)

**Proof.**

\[ I(S; Y|Z) \overset{p}{=} I(S; Y|Z, G) + I(S; Y; G|Z) \]
\[ \overset{H}{=} I(S; Y; G|Z) \]
\[ \overset{p}{=} I(G; Y|Z) - I(G; Y|Z; S) \leq I(G; Y|Z) \]

Since \( I(S; Y|Z) \) is non-negative, \( I(G; Y|Z) = 0 \Rightarrow I(S; Y|Z) = 0 \). \( \square \)
Lemma B.3. (L2) Let $G$ and $Y$ be random variables with joint distribution $p(G, Y)$, $Z$ is a representation of graph $G$, $S$ denotes the explanatory subgraph, if $Z$ is necessary for $Y$, then
\[ I(S; Z|Y) = 0 \] (23)

Hypothesis:

$(H_1)$ $S$ is an explanation of $G$: $I(S; Z|G, Y) = 0$

Thesis:

$(T_1)$ $I(Z; G|Y) = 0 \Rightarrow I(S; Z|Y) = 0$

Proof. \[
I(S; Z|Y) \overset{H_1}{=} I(S; Z; G|Y) + I(S; Z|G, Y) \\
\overset{P_3}{=} I(Z; G|Y) - I(Z; G|S, Y) \\
\leq I(Z; G|Y)
\] (24)

Since $I(S; Z|Y)$ is non-negative, $I(Z; G|Y) = 0 \Rightarrow I(S; Z|Y) = 0$. \hfill \Box

Theorem B.1. Let $G$ and $Y$ be random variables with joint distribution $p(G, Y)$. Given unsupervised graph representation $Z$ and its explanations $S$ in graph $G$. Assume that $S$ is conditionally independent from $Y$ and $Z$ when $G$ is observed, then

1. if $Z$ is sufficient for $Y$, then $I(S; Z) \geq I(S; Y)$;
2. if $Z$ is necessary for $Y$, then $I(S; Z) \leq I(S; Y)$;
3. if $Z$ is sufficient and necessary for $Y$, then $I(S; Z) = I(S; Y)$;

Thesis:

$(T_1)$ $I(G; Y|Z) = 0 \Rightarrow I(S; Z) \geq I(S; Y)$
$(T_2)$ $I(Z; G|Y) = 0 \Rightarrow I(S; Z) \leq I(S; Y)$
$(T_3)$ $I(G; Y|Z) = 0$ and $I(Z; G|Y) = 0 \Rightarrow I(S; Z) = I(S; Y)$

Proof. We prove the thesis $T_1$ first:
\[
I(S; Y) \overset{P_3}{=} I(S; Z; Y) + I(S; Y|Z) \\
\overset{L_3}{=} I(S; Z|Y) \quad \text{(see proof in Lemma B.2)} \\
\overset{P_3}{=} I(S; Z) - I(S; Z|Y) \\
\leq I(S; Z)
\] (25)

Then, for thesis $T_2$, we have:
\[
I(S; Y) \overset{P_3}{=} I(S; Z; Y) + I(S; Y|Z) \\
\geq I(S; Z; Y) \\
\overset{P_3}{=} I(S; Z) - I(S; Z|Y) \\
\overset{L_3}{=} I(S; Z) \quad \text{(see proof in Lemma B.3)}
\] (26)

Finally, having thesis $T_1$ and $T_2$, thesis $T_3$ can be proved simply. \hfill \Box
C Explanation algorithms

The algorithm of USIB is shown in Algorithm 1. We first get the unsupervised graph representations by feeding the graph instances into the target model (line 1-2). Then relaxed explanatory subgraphs \( \hat{S} \) is generated by the subgraph generator for each batch (line 6-7). After that, we estimate the mutual information and optimize the subgraph generator at the same time (line 8-9). Finally, we get the explanatory subgraph \( S \) by selecting edges with top-n edge weights on \( \hat{S} \).

**Algorithm 1 Pseudo-code for USIB**

**Input:** A set of graphs where \( k \)-th graph is denoted by \( G^{(k)} \), the trade-off parameter \( \beta \), the temperature parameter \( \tau \), batch size \( K \), selection ratio \( r \), the target model \( f_t \);

**Output:** The explanatory subgraphs \( S^{(k)} \);

1. for each graph \( G^{(k)} \) do
2. \( Z^{(k)} = f_t(G^{(k)}) \);
3. \( B_1, B_2, \ldots, B_b \leftarrow \text{Batch sample with batch size } K \);
4. for each epoch do
5. for each batch \( B_i \) do
6. for \( k \in B_i \) do
7. \( \hat{S}^{(k)} = g_\theta(G^{(k)}) \);
8. Calculate loss with Eq.(10);
9. Update parameters with Adam optimizer;
10. for each graph \( G^{(k)} \) do
11. \( \hat{S}^{(k)} = g_\theta(G^{(k)}) \);
12. \( S^{(k)} \leftarrow \text{Select top-n edges with selection ratio } r \text{ on } \hat{S}^{(k)} \);
return The explanatory subgraphs \( S^{(k)} \);

D Experiments

D.1 Datasets

We summarize the statistics of the datasets in Table 2. The first three datasets are obtained from Pytorch Geometric Library\(^4\) while the last one can be found in work \([25]\).

| Dataset    | Graphs# | Classes# | Avg.Nodes# | Avg.Edges# |
|------------|---------|----------|------------|------------|
| Mutagenicity | 4337    | 2        | 30.32      | 61.54      |
| NCI1       | 4110    | 2        | 29.87      | 64.6       |
| PROTEINS   | 1113    | 2        | 39.06      | 145.63     |
| BA3        | 3000    | 3        | 21.92      | 29.51      |

D.2 Implementation details.

**Target models.** We follow the official implementations of target models\(^5\). For comparison fairness, we adopt the same encoder architecture for three target models. Specifically, a 3-layer GIN with hidden dimension as 64 is adopted. Output from every GIN layer is concatenated as node representations and the graph-level representations is extracted by conducting add pooling on node representations. Following each linear layer is a ReLU activation function.

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\(^4\)https://pytorch-geometric.readthedocs.io/en/latest/modules/datasets.html
\(^5\)https://github.com/fanyun-sun/InfoGraph
\(^6\)https://github.com/Shen-Lab/GraphCL
\(^7\)https://github.com/susheels/adgcl
Baselines. Here we introduce more details of baseline methods:

- **GNNExplainer** [9] optimizes soft masks for edges in the graph, where each mask indicates an edge weight. The soft masks are trained individually for each graph instance.
- **PG-Explainer** [10] adopts a parameterized neural network to generate explanations for GNNs. The neural network is trained on multiple instances and thus provides a global view for explanations.
- **PGM-Explainer** [14] observes the prediction change when the nodes are randomly perturbed, and then a Bayesian network is trained on these observations to capture the dependency among the nodes and the prediction.
- **Refine** [25] follows a pre-training and fine-tuning strategy to generate explanations incorporating multi-granularity information.
- **IG** [23] adopts the integrated gradients as heuristic scores to evaluate the importance of graph edges. Specifically, the integrated gradients are calculated by accumulating gradients with respect to edge weights while interpolating between a baseline and the current instance.
- **SA** [21] calculates the gradients of the output with respect to edge weights and use the gradients as heuristic scores.
- **GradCam** [12] calculates the gradients of the output with respect to edge weights first and then multiply the gradients and the edge weights as heuristic scores.

To adapt the gradient-based explanation methods, i.e., IG, SA and GradCam to explain unsupervised graph representations, we redesign the heuristic scores to be gradients of $l_2$ norm of graph representations instead of classification probabilities.

**USIB.** There are mainly two components in USIB: subgraph generator and mutual information estimator. Specifically,

- **Subgraph generator:** GNN Type = ARMAConv, hidden dim = 32, num layers = 2, batch normalization = True, pooling = add, activation = Relu(), num layers of mlp = 2, activation of mlp = Tanh(), hidden dim of mlp = 32, $\tau = 0.1$
- **Mutual information estimator:** GNN Type = GCN, hidden dim = 32, num layers = 3, batch normalization = True, pooling = add, activation = Relu(), num layers of mlp = 2, activation of mlp = Relu(), hidden dim of mlp = 32

Moreover, the optimization of USIB is performed using Adam and the learning rates is fixed as 0.001. Batch size of all datasets is set as 64, and number of epochs is 10. The implementation of USIB is based on the Pytorch Geometric library.

**Hardware settings.** All experiments are conducted on a Linux machine with an Nvidia GeForce RTX 3080 GPU with 24GB memory. CUDA version is 11.1 and Driver Version is 460.67.

**D.3 Experimental results on other target models**

To show the explanation results on GCL and ADGCL, we summarize the ACC-AUC score in Table 3 and ACC curves in Fig. 6 and Fig. 7. We can observe similar conclusions from results on GCL.
Table 3: Comparison of our USIB and other baseline explainers. The relative improvement is calculated on unsupervised setting methods. **Bold** indicates the best results.

| Target Model | Setting | Method  | Mutagenicity | NCI1 | PROTEINS | BA3 |
|--------------|---------|---------|--------------|------|----------|-----|
|              |         | ACC-AUC | ACC-AUC | ACC-AUC | ACC-AUC | ACC-AUC | Recall@5 |
| GCL          | Supervised | PG-Explainer | 69.43 ± 2.12 | 63.39 ± 2.00 | 67.08 ± 1.00 | 88.53 ± 2.01 | 27.08 ± 1.98 |
|              |         | GNN-Explainer | 71.94 ± 2.20 | 63.87 ± 2.02 | 63.98 ± 1.07 | 77.29 ± 1.80 | 18.63 ± 0.30 |
|              |         | PGM-Explainer | 68.77 ± 0.29 | 62.07 ± 0.52 | 66.97 ± 1.24 | 84.53 ± 1.15 | 24.73 ± 0.07 |
|              |         | ReFine | 70.19 ± 0.76 | 64.25 ± 0.69 | 67.25 ± 1.46 | 83.37 ± 2.75 | 20.37 ± 0.10 |
|              | Unsupervised | IG | 71.20 ± 0.73 | 63.98 ± 1.14 | 64.99 ± 1.23 | 79.90 ± 2.11 | 10.50 ± 0.29 |
|              |         | GradCam | 69.57 ± 0.98 | 62.52 ± 0.72 | 64.99 ± 0.78 | 79.10 ± 1.21 | 10.90 ± 1.39 |
|              |         | SA | 70.59 ± 0.66 | 62.84 ± 0.78 | 64.27 ± 1.44 | 77.17 ± 1.06 | 16.95 ± 1.92 |
|              |         | USIB | 72.01 ± 0.89 | 64.79 ± 1.50 | 63.62 ± 2.09 | 90.37 ± 2.95 | 20.50 ± 1.13 |

Relative Improvement | 1.47% | 1.27% | 0.97% | 13.09% | 51.36% |

| ADGCL         | Supervised | PG-Explainer | 69.85 ± 0.41 | 59.20 ± 0.70 | 66.60 ± 1.29 | 85.53 ± 2.80 | 26.63 ± 1.36 |
|              |         | GNN-Explainer | 66.06 ± 0.31 | 54.80 ± 0.57 | 62.93 ± 1.16 | 75.73 ± 2.22 | 18.46 ± 0.09 |
|              |         | PGM-Explainer | 67.26 ± 0.40 | 57.73 ± 0.99 | 64.51 ± 0.98 | 81.97 ± 2.37 | 24.76 ± 0.07 |
|              |         | ReFine | 69.19 ± 0.68 | **60.58 ± 1.59** | **66.84 ± 1.12** | 84.54 ± 5.77 | 17.30 ± 7.02 |
|              | Unsupervised | IG | 69.48 ± 0.96 | 57.91 ± 0.93 | 63.82 ± 0.70 | 77.72 ± 3.02 | 9.76 ± 3.65 |
|              |         | GradCam | 67.87 ± 1.10 | 57.13 ± 1.05 | 63.03 ± 1.05 | 77.51 ± 3.10 | 15.67 ± 1.99 |
|              |         | SA | 69.24 ± 0.93 | 56.49 ± 1.23 | 62.65 ± 1.40 | 76.38 ± 2.85 | 10.68 ± 1.99 |
|              |         | USIB | **70.33 ± 1.31** | **59.99 ± 1.65** | **64.93 ± 1.95** | **89.11 ± 3.71** | **29.55 ± 0.88** |

Relative Improvement | 1.22% | 3.59% | 1.92% | 14% | 88.58% |

Figure 7: ACC curve for of different explainers on ADGCL.

and ADGCL: USIB outperforms other explanation methods in unsupervised settings and can be comparable to baseline explanation methods in supervised settings, which is consistent with our analysis on Infograph.

Figure 8: Influence of hyper-parameter $\beta$.

D.4 Parameter Study

To investigate the influence of hyper-parameter $\beta$ in our USIB objective, we show the ACC-AUC score with different value of $\beta$ in Fig. 8. We can observe a similar tendency for different target models on various datasets, i.e., either a too low or too high value of $\beta$ degrades the performance of USIB. The observation indicates a trade-off between informativeness and compression of explanatory subgraphs. Specifically, a higher value of $\beta$ leads to higher compressibility, while the informativeness of explanatory subgraphs is not guaranteed. Additionally, the USIB will lead to a trivial solution when the value of $\beta$ is too small, while the edge weights learned for the graph instances will be less informative.
Table 4: Time costs (in second).

| Method       | Mutagenicity | NCI1 | PROTEINS | BA3  |
|--------------|--------------|------|----------|------|
| PG-Explainer | 8.06         | 6.38 | 1.74     | 4.74 |
| GNNExplainer | 41.97        | 43.38| 11.35    | 26.87|
| PGM-Explainer| 570.16       | 605.76| 151.77  | 287.75|
| Refine       | 7.28         | 6.81 | 1.79     | 4.87 |
| IG           | 7.36         | 6.48 | 2.23     | 5.50 |
| GradCam      | 0.55         | 0.49 | 0.13     | 0.54 |
| SA           | 0.63         | 0.47 | 0.15     | 0.40 |
| USIB         | 7.27         | 6.37 | 1.82     | 4.88 |

D.5 Time complexity

The main time cost during the inference procedure is the calculation of the relaxed edge weights by the neural network. We summarize the time costs in Table 4. The time cost of our methods is similar to PG-Explainer as we adopt the same architecture to generate the edge weights. GradCam and SA are the most efficient methods since they only conduct backpropagation for one time. However, the effectiveness of GradCam and SA is not guaranteed according to our above experimental results.