Abstract
Subgraph recognition aims at discovering a compressed substructure of a graph that is most informative to the graph property. It can be formulated by optimizing Graph Information Bottleneck (GIB) with a mutual information estimator. However, GIB suffers from training instability since the mutual information of graph data is intrinsically difficult to estimate. This paper introduces a noise injection method to compress the information in the subgraphs, which leads to a novel Variational Graph Information Bottleneck (VGIB) framework. VGIB allows a tractable variational approximation to its objective under mild assumptions. Therefore, VGIB enjoys more stable and efficient training process – we find that VGIB converges 10 times faster than GIB with improved performances in practice. Extensive experiments on graph interpretation, explainability of Graph Neural Networks, and graph classification show that VGIB finds better subgraphs than existing methods.

1 Introduction
Graph classification, which aims to identify labels of graph-structured data, has attracted much attention in diverse fields such as biochemistry [11, 19, 20, 35], social network analysis [23, 14, 45], and computer vision [8, 25, 24, 28]. Recently, there has been a surge of interest in its reverse problem. That is, to recognize a compressed subgraph of the input, which is most predictive to the graph label [52]. Such a subgraph enjoys superior property since it drops noisy and redundant information and only preserves label-relevant information. Hence, recognizing a compressed yet predictive subgraph, namely the subgraph recognition, is the fundamental problem of many tasks. For example, biochemists are interested in discovering the substructure of the molecule which most affects the molecule properties [53, 20]. In the explainability of Graph Neural Networks (GNNs), it is vital to generate the explanatory subgraph of the input, which faithfully interprets the predicted results [50, 29]. In graph classification, researchers aim to emphasize the significant substructures, such as nodes, edges, and subgraphs, to improve the predictive performances [41, 3, 27]. The Graph Information Bottleneck (GIB) first formulates the subgraph recognition problem as an information-theoretic objective. Specifically, it masks the unimportant nodes with an uninformative reference value to generate a subgraph. Then GIB maximizes the mutual information between the
subgraph distribution and the graph labels and minimizes the mutual information between the subgraph distribution and the input graphs. Although the GIB permits theoretical analysis of the subgraph recognition problem, its objective is notoriously hard to optimize due to the intractability of mutual information. It introduces a bi-level optimization scheme to estimate the mutual information in the inner loop and optimize the discovered subgraph in the outer loop, which is time-consuming and suffers from an unstable training process. The above issues motivate us to advance the existing framework for improved subgraph recognition.

In this work, we propose the Variational Graph Information Bottleneck (VGIB) method for efficient subgraph recognition. Specifically, we present a noise injection method, which selectively injects noises into the node features of an input graph. The amount of injected noise controls the information transmitted from the input to the perturbed graph, which refers to the compression level. The informativeness is measured by the extent to which the perturbed graph reflects the properties of the input graph. Intuitively, perturbing the label-irrelevant subgraph causes less information loss in the perturbed graph compared with the significant subgraph. Based on this intuition, we formulate VGIB as maximizing the mutual information between the perturbed graph and graph label while minimizing that between the perturbed graph and input graph. The VGIB objective enables a tractable variational upper bound under mild assumptions and renders an efficient and stable training process compared with GIB in Figure 1. After training VGIB, one can obtain the found subgraph by selecting the nodes with less probability of injecting noise.

We evaluate the proposed VGIB framework on various tasks, including explainability of GNNs, graph interpretation, and graph classification. The experimental results show that VGIB enjoys significant efficiency in optimization and outperforms the baseline methods with better found subgraphs.

![Figure 1: Training dynamics of VGIB and GIB. $L_{\text{cls}}$ and $L_{\text{MI}}$ refer to the prediction and compression term of two methods. (a). The training dynamic of VGIB is stable. (b). GIB suffers from an unstable training process and inaccurate estimation of mutual information in the red circle (mutual information is non-negative).](image)

2 Related Work

**Information Bottleneck.** The information bottleneck (IB) principle attempts to juice out a compressed but predictive code of the input signal [44]. Alemi et al. [2] first empowers deep learning with a variational information bottleneck (VIB). Currently, the applications of IB and VIB in deep learning are mainly attributed to representation learning and feature selection. In the representation learning scenario, researchers employ a deterministic or stochastic encoder to learn a compressed yet meaningful representation of the input data, to facilitate various downstream tasks, such as computer vision [31, 30], reinforcement learning [13, 16], natural language processing [46], speech and acoustics [33], and node representation learning [47]. For the feature selection, IB is used to select a subset of input features such as pixels in images or dimensions in vectors, which are maximally predictive to the label of input data [1, 40, 22]. [1, 40] inject noises into the intermediate representations of a pretrained network and select the areas with maximal information per dimension. [22] learns the drop rates for each dimension of the vector-structured features. Unlike the prior work on the regular data, Yu et al. [52] first recognize a predictive yet compressed subgraph from the irregular
Graph Classification. The goal of graph classification is to infer the label or property of an input graph. Recently, there is a surge of interest in applying the Graph Neural Network (GNN) for graph classification [56, 34]. It first aggregates the messages in the neighborhoods for node representations, which are pooled for the graph representations for prediction by a readout function. The typical implementations of readout are mean and sum functions [23, 45, 15, 48]. Besides, it is popular to leverage the hierarchical and more complex information in the graph, which leads to the graph-pooling methods [56, 26, 34, 5, 51]. These methods generally leverage all the information in graphs for prediction. Yu et al. point out that graph classification can be enhanced by only leveraging the label-relevant information in the graphs [52], and propose the subgraph recognition problem. The difference between graph classification and subgraph recognition is in Fig. 2.

Subgraph Discovery. Subgraph discovery in the literature of traditional data mining refers to discovering subgraphs with specific topology [9, 12, 49, 21, 55]. Recently, there is a trend to leverage the importance of subgraphs in graph learning. At node-level tasks, researchers focus on passing the message of a neighborhood subgraph to the central node [7, 14, 15]. FastGCN [7] and ASGCN [15] accelerate the training of GCN with node sampling. GraphSAGE [14] samples a subset of the neighborhood for inductive node representation learning. DropEdge [36] drops a portion of edges to relieve the oversmoothing phenomenon in GCN. NeuralSparse [57] chooses the most relevant K neighborhoods of a central node for robust node classification. At the graph level, it is popular to discover the information in subgraphs for learning graph representations. Infograph [41] maximize the mutual information between representations of graphs and the corresponding local patches. VIPool [27] pools the nodes, which maximally reflect the neighborhood information for graph representations. Emily et al [3] learns subgraph representations given explicit subgraph-level annotations. Another direction closely related to subgraph recognition is to interpret a pretrained GCN with interpretable subgraphs. GNNExplainer [50] discover the neighborhood subgraph, which maximally affects the prediction of the central node. SubgraphX [54] explains the prediction of GCN with a subgraph found by Monte Carlo Tree Search.

3 Notations and Backgrounds
In this section, we introduce our notations and preliminaries. Let $G = \{A, X\} \in \mathbb{G}$ be a graph with $n$ nodes, with $A \in \mathbb{R}^{n \times n}$ and $X \in \mathbb{R}^{n \times d}$ being its adjacent matrix and node feature matrix. We denote $\{(G_1, Y_1), (G_2, Y_2), \cdots, (G_n, Y_n)\}$ as the set of $n$ graphs with its corresponding categorical labels or real-value properties. We use $G_{\text{sub}}$ to denote the subgraph in $G$. We denote $I(X,Y)$ as the mutual information between the random variables $X$ and $Y$, which takes the form:

$$I(X,Y) = \int_X \int_Y p(x,y) \log \frac{p(x,y)}{p(x)p(y)} \, dx \, dy$$

3.1 Graph Information Bottleneck
Given the input data $X$ and its label $Y$, the information bottleneck (IB) [44] principle learns the minimal sufficient representation $Z$ by optimizing the IB objective: $\min_Z -I(Z,Y) + \beta I(Z,X)$. Here $\beta$ is the
Lagrangian parameter to balance the two terms. Inspired by it, Yu et al. propose Graph Information Bottleneck (GIB) principle to recognize an informative yet compressed subgraph from the original graph [52]. The GIB objective is as follows:

$$\min_{G_{sub}} -I(G_{sub}, Y) + \beta I(G_{sub}, G). \quad (1)$$

The first term in Eq. 1 is the prediction term, which encourages $G_{sub}$ to be informative to the graph label $Y$. And the second term is the compression term. It minimizes the mutual information of $G$ and $G_{sub}$ so that $G_{sub}$ only receives limited information from the input graph $G$. The subgraph found by GIB is denoted as the IB-subgraph: $G^*_{sub} = \arg \min_{G_{sub}} -I(G_{sub}, Y) + \beta I(G_{sub}, G)$. IB-subgraph drops the label-irrelevant information in $G$ and only preserves the actionable information for predicting $Y$, which facilitates many graph-level tasks. The GIB objective cannot be directly optimized since the mutual information is intractable to compute. Yu et al. first estimate the mutual information with MINE [4], and use the estimated value as a proxy in the optimization of GIB. This process is inefficient in optimization since it is time-consuming to estimate the mutual information. Meanwhile, inaccurate estimation also leads to an unstable training process and degenerated results.

4 Method

4.1 Compression with Noise Injection

Rather than directly evaluate the compression quality of $G_{sub}$ with $I(G, G_{sub})$, we inject noise into the node representations of $G$ for an alternative as shown in Fig. 3.

For an input graph $G \in \mathbb{G}$ with node feature matrix $X$, adjacent matrix $A$ and degree matrix $D$, we first generate the node representations with a $l$-layer GNN:

$$H = \text{GNN}(A, X; W^1, \cdots, W^l)$$
$$= \sigma(D^{-1/2}AD^{-1/2} \cdots \sigma(D^{-1/2}AD^{-1/2}XW^1) \cdots W^l)$$

(2)

where $H = [h_1, h_2, \cdots, h_n]^T$ is the node representation matrix. $W^1, \cdots, W^l$ are the parameters at different layers.

Then we damp the information in $G$ by injecting noises into node representations with a learned probability. Let $\epsilon$ be the noise sampled from a parametric noise distribution. We assign each node a probability of being replaced by $\epsilon$. Specifically, for the $i$-th node, we learn the probability $p_i$ with a Multi-layer Perceptron (MLP). Then, we add a Sigmoid function on the output of MLP to ensure $p_i \in [0,1]$

$$p_i = \text{Sigmoid}(\text{MLP}(h_i)). \quad (3)$$

We then replace the node representation $h_i$ by $\epsilon$ with probability $p_i$:

$$z_i = \lambda_i h_i + (1 - \lambda_i) \epsilon, \quad (4)$$

where $\lambda_i \sim \text{Bernoulli}(p_i)$. The transmission probability $p_i$ controls the information sent from $h_i$ to $z_i$. If $p_i = 1$, then all the information in $h_i$ are transferred to $z_i$ without loss. On the contrary, when $p_i = 0$, then $z_i$ contains no information from $h_i$ but only noise. Compared with dropping nodes for compression in GIB, this method allows to flexibly adjust the amount of information from $h_i$ to $z_i$ by changing $p_i$. We denote the $G_N = \{A, Z\}$ as the perturbed graph. At graph level, the transmission probability of each node determines the information sent from $G$ to $G_N$ in a similar way. Therefore, we can compress the information of $G$ into $G_N$ with a set of $p_i$. We hope $p_i$ is learnable so that we can selectively preserve the information in $G_N$. However, $\lambda_i$ is a discrete random variable and we can not directly calculate the gradient of $p_i$. Therefore, we employ the concrete relaxation [18, 10] for $\lambda_i$:

$$\hat{\lambda}_i = \text{Sigmoid}(\frac{1}{t} \log \frac{p_i}{1-p_i} + \log \frac{u}{1-u}), \quad (5)$$

where $t$ is the temperature parameter and $u \sim \text{Uniform}(0,1)$. Our noise injection method shares similar intuitions with IB-Attribution [40] and IB-ActorCritic [16]. IB-Attribution injects noise into an intermediate layer of a pretrained network and selects the activated area for image attribution. IB-
Figure 3: (a) Illustration of the proposed Variational Graph Information Bottleneck (VGIB) framework. VGIB employs the noise injection method to generate a perturbed graph $G_N$, which is used as a "bottleneck" to distill the actionable information for predicting the graph label. The objective of VGIB has a tractable upper bound that is easy to optimize. (b) Intuition of the noise injection method. Perturbing a significant subgraph is more harmful to the graph label than perturbing a label-irrelevant subgraph.

ActorCritic continuously adds noises into the gradient to achieve better generalization performance in reinforcement learning. Our noise injection method focuses on discrete and irregular graph-structured data, which is more challenging. Moreover, our method is more adaptive since we need no pretrained model.

4.2 Variational Graph Information Bottleneck

The perturbed graph $G_N$ is employed to distill the actionable information of $G$ for predicting its label $Y$. Specifically, we compress the information of $G$ via noise injection to obtain $G_N$. Meanwhile, we hope that $G_N$ is maximally informative to $Y$, which leads to a novel Variational Graph Information Bottleneck (VGIB) framework:

$$\min_{G_N} -I(G_N,Y) + \beta I(G_N,G).$$

The first term encourages $G_N$ to be sufficient for predicting the graph label $Y$, and the second term constrains the information that $G_N$ receives from $G$. These two terms require us to inject noise into $G$ selectively so that $G_N$ receives actionable information as much as possible. The intuition is that injecting noises into the IB-subgraph of $G$ is more harmful to the functionality of $G$ than that into the label-irrelevant substructures. In that sense, the nodes in the IB-subgraph are less likely to be injected with noise. Therefore, we can select the IB-subgraph from $G_N$ by this criterion after training VGIB. We introduce the following lemma before justifying the above formulation.

**Lemma 1** Let $G \in \mathbb{G}$ and $Y \in \mathbb{R}$ be the graph and its label. $G_n \in \mathbb{G}$ is the label-irrelevant substructure, which is independent to $Y$. Denote $G_{sub}$ as the arbitrary subgraph. Suppose $G_n$ influences $G_{sub}$ only through $G$, the following inequality holds:

$$I(G_{sub},G_n) \leq I(G_{sub},G) - I(G_{sub},Y),$$

(7)

Lemma 1 indicates when setting $\beta = 1$ in Eq. 1, the GIB objective upper bounds the mutual information of $G_{sub}$ and $G_n$. That is to say, optimizing the GIB objective encourages $G_{sub}$ to be less related to the label-irrelevant substructure $G_n$. $I(G_n,G_{sub})$ is minimal when $G_{sub}$ is the IB-subgraph. The proof of
Lemma 1 is in the Supplementary Materials. We next give the theorem that minimization of VGIB objective in Eq. 6 also leads to the irrelevance of \( G_{\text{sub}} \) and \( G_n \).

**Theorem 1** Let \( G \in \mathbb{G} \) and \( Y \in \mathbb{R} \) be the graph and its label. \( G_n \in \mathbb{G} \) is the label-irrelevant substructure in \( G \), which is independent to \( Y \). Denote \( G_c \in \mathbb{G} \) as the subgraph formed by injected noise. Then, if we choose the subgraph \( G_{\text{sub}} \) by dropping \( G_c \) in \( G_N \), the following inequality holds:

\[
I(G_{\text{sub}}, G_n) \leq I(G_N, G_n) \leq I(G_N, G) - I(G_N, Y)
\]

(8)

Please refer to the Supplementary Materials for the proof of Theorem 1. VGIB differs from GIB mainly in noise injection. In the next section, we will show that this process leads to convenience in optimization.

### 4.3 Optimization of Variational Graph Information Bottleneck

We first examine the first term \( I(G_N, Y) \) in Eq. 6, which encourages \( G_N \) is informative of graph label \( Y \).

\[
-I(G_N, Y) \leq E_{Y,G_N} - \log q_\theta(Y|G_N) \\
:= \mathcal{L}_{\text{cls}}(G_N, Y),
\]

(9)

where \( q_\theta(Y|G_N) \) is the variational approximation to \( p(Y|G_N) \). \( q_\theta(Y|G_N) \) outputs the label distribution of \( G_N \) and can be modeled as a classifier. \( \mathcal{L}_{\text{cls}} \) is the classification loss. We choose the cross-entropy loss and mean square loss for categorical \( Y \) and continuous \( Y \), respectively.

For the second term \( I(G_N, G) \) in Eq. 6, we first obtain the graph representation \( z_N \) of \( G_N \) via a readout function. We employ the sufficient encoder assumption [43] that the information of \( z_N \) is lossless in the encoding process, leading to \( I(z_N, G) \approx I(G_N, G) \). By choosing the distribution of noise and the readout function as the Gaussian distribution, \( I(G_N, G) \) has a tractable variational upper bound.

**Proposition 1 (Variational upper bound of \( I(G_N, G) \))**

Let \( m_G \) be the number of nodes in \( G \). \( \epsilon_j \) is the

| Method     | QED   | HLM-CLint | MLM-CLint | RLM-CLint |
|------------|-------|-----------|-----------|-----------|
| GCN+Att05  | 0.48±0.07 | 0.90±0.89 | 0.92±0.61 | 1.17±0.63 |
| GCN+Att07  | 0.41±0.07 | 1.18±0.60 | 1.69±0.88 | 1.22±0.85 |
| GCN+GIB    | 0.38±0.12 | 0.37±0.30 | 0.72±0.55 | 1.15±0.68 |
| GCN+VGIB   | **0.32±0.12** | **0.34±0.28** | **0.69±0.58** | **1.02±0.64** |

Table 1: Mean and standard deviation of absolute property divergence between the input molecules and the found subgraphs. The results of the baselines are copied from the existing literature [52]. The lower the better.

Table 2: Training time of different methods on QED dataset.

| Method     | Time   |
|------------|--------|
| GCN+Att05  | 142.01s|
| GCN+Att07  | 141.18s|
| GCN+GIB    | 1712.93s|
| GCN+VGIB   | 146.53s|

5 Experiments

We evaluate the proposed method on two tasks, i.e., graph interpretation and graph classification. For the first task, we aim to verify whether VGIB can recognize the substructures that interpret the properties of the input molecules [52] or not. For the second
We evaluate QED values of molecules with the toolkit on https://www.rdkit.org/. Moreover, we obtain HLM-CLint, MLM-CLint, and RLM-CLint value of molecules on https://drug.ai.tencent.com/.

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5.1 Graph Interpretation

In this experiment, we extract the substructures which have the most similar properties to the original molecules. We consider four properties: QED, HLM-CLint, MLM-CLint, and RLM-CLint. QED measures the probability of a molecule being a drug within the range of [0, 1]. HLM-CLint, MLM-CLint, and RLM-CLint are estimated values of in vitro human, mouse and rat liver microsome metabolic stability, respectively (base 10 logarithm of mL/min/g)1. We collect molecules with QED ≥ 0.85, HLM-CLint ≥ 2, MLM-CLint ≥ 2, and RLM-CLint ≥ 2 from ZINC250K [17], and we individually build datasets with the selected molecules for the four properties. For each property, we use 85%, 5%, and 10% of the molecules for training, validating, and testing, respectively. Please refer to the Supplementary Materials for the statistics of datasets.

We compare the proposed VGIB with GIB [52] and the attention-based method [26]. For VGIB, we first learn the node representation with a GCN and inject noise into each node as shown in Eq. 4 and Eq. 3. Then we obtain the perturbed graph representation by pooling the noisy node representations with a readout function. We thereafter optimize the loss function in Eq. 11 and collect the nodes with $p_i \geq 0.5$ in Eq. 3 to obtain the IB-subgraph. We simultaneously supervise the classifier in Eq. 9 with the representation of the input graph and its label to enhance the informativeness of the subgraph. For GIB, we follow the existing method [52] and optimize the model in a bilevel optimization scheme. As for the attention-based method, we attentively pool the node representations with the attention scores for la-
Table 3: Performance of different methods on explaining the predictions of GCN in terms of fidelity scores. We set the sparsity score of the explanatory subgraphs as 0.5 for a fair comparison.

| Metric        | Fidelity+↑ | Fidelity-↓ |
|---------------|------------|------------|
| **Property**  | RLM-Clint  | HLM-Clint  | QED     | DRD2     | RLM-Clint  | HLM-Clint  | QED     | DRD2     |
| GNNExplainer  | 0.694      | 0.778      | 0.602   | 0.74     | 0.478      | 0.616      | 0.498   | 0.433    |
| PGExplainer   | 0.632      | 0.692      | 0.598   | 0.686    | 0.502      | 0.62       | 0.56    | 0.54     |
| GraphMask     | 0.632      | 0.706      | 0.602   | 0.673    | 0.516      | 0.592      | 0.574   | 0.4866   |
| IGExplainer   | 0.684      | 0.758      | 0.592   | 0.693    | 0.602      | 0.686      | 0.584   | 0.58     |
| GraphGrad-CAM | 0.67       | 0.782      | 0.586   | 0.659    | 0.56       | 0.668      | 0.564   | 0.566    |
| GIB           | 0.684      | 0.781      | 0.601   | 0.724    | 0.483      | 0.643      | 0.525   | 0.428    |
| VGIB          | **0.765**  | **0.792**  | **0.627** | **0.756** | **0.463**  | **0.579**  | **0.487** | **0.424** |

We then compare the training time of different methods on the QED dataset. We train different methods 3 times and report the average training time in Fig. 2. It is shown that the attention-based methods achieve the fastest training due to their simple architectures. Although VGIB is slower than the attention-based methods, it achieves significant performance gain in finding subgraphs with more similar properties to the input molecules. Compared with GIB, VGIB trains over ten times faster than GIB with better performance. The reason is that estimating the mutual information in GIB is time-consuming. However, VGIB a enjoys tractable upper bound of its objective, which is easy to optimize.

5.2 Explainability of GCN

In this section, we employ the proposed VGIB to explain the prediction of GCN for molecule classification on ZINC250K dataset. We consider four properties: QED, HLM-Clint, RLM-Clint and DRD2 construct the dataset for each property. For QED, we label the molecules with $\text{QED} \geq 0.85$ / $< 0.85$ as 1/0. For DRD2, we label the molecules with $\text{DRD2} \geq 0.50$ / $< 0.50$ as 1/0. For HLM-Clint and RLM-Clint, we label the molecules with the property value greater than 2.0 as 1 or 0 otherwise. For each property, we train the GCN on the training set and employ VGIB to generate post-hot explanation on the test set. Please refer to Supplementary Materials for more details on the dataset splits and the training process.

We compare VGIB with various explanation model including GNNExplainer [50], PGExplainer [29], GraphMask [39], IGExplainer [42], GraphGrad-CAM [32] and GIB [52]. These methods interpret the prediction of GCN with the node importance score ranging in $[0, 1]$, where 1 indicates the node is the most important to the molecule classification and 0 otherwise. Please refer to Supplementary Materials for more details on the baseline methods. We employ the fidelity score to evaluate how the explanation is faithful to the GCN model [54]. Specifically, let $y_i$ and $\hat{y}_i$ be the ground-truth and the prediction of the i-th input molecule. Define $k$ as the sparsity score of the explanatory subgraph. The explanatory subgraph is
Figure 5: Performance of different methods on explaining the predictions of GCN in terms of fidelity scores (Fidelity+ ↑ and Fidelity− ↓). VGIB generates the most faithful explanations to the predictions of GCN by identifying the most important nodes under different sparsity scores.

Table 3 shows the fidelity scores of the explanations produced by different methods. The sparsity score is set to be $k = 0.5$ for all the explanatory subgraphs. As shown in table 3, VGIB achieves best fidelity scores on all the properties. This shows that VGIB generate faithful explanation to the predictions of the GCN. Moreover, to comprehensively evaluate different methods, we set $k \in \{0.30, 0.35, 0.40, 0.45, 0.50, 0.55, 0.60\}$ and compare the performance under different sparsity scores. As shown in Figure 5, VGIB generate most faithful explanations to the predictions of GCN in terms of fidelity scores by under different sparsity scores. This shows that VGIB can identify most important nodes to the predictions of GCN.

### 5.3 Graph Classification

In this subsection, we aim to find out whether the found subgraph can improve the performance of baselines on graph classification or not. We evaluate different methods on MUTAG [38], PROTEINS [6], DD, IMDB-BINARY, REDDIT-BINARY, and COLLAB [37] datasets, which are wildly used for graph classi-
We consider four GNN baselines including GCN [23], GAT [45], GraphSAGE [14] and GIN [48]. We use the mean and sum pooling as a read-out function for the baseline methods to obtain the graph representation for prediction. Then, similar to GIB [52], we plug VGIB into these baselines. Specifically, we adopt the baseline models to extract node representation. Then, we recognize the IB-subgraph by optimizing the VGIB objective. We pool the node representations in the IB-subgraph for classification with the same readout function as the baselines. For a fair comparison, we adopt a 2-layer network architecture and 16 hidden dimensions for different methods. We train these methods for 100 epochs and test the models with the smallest validation loss. We report the mean and standard deviation of accuracy across 10 folds.

The experimental results are summarized in Table 4. Compared with the baselines, VGIB can discover an informative yet compressed subgraph of the input. Therefore, it relieves the perturbation of noise structures and redundant information and boosts the performance of the baselines. VGIB also outperforms the GIB-based methods on most of the datasets.

6 Discussions

Potential Negative Impacts: Our method aims to discover a predictive yet compressed subgraph of the input graph, and can be deployed in social network analysis and biochemistry. The concern is that if not adequately used under administration, our method potentially leads to the leakage in privacy and intellectual property.

Limitations: We assume the encoding process from \( G_N \) to \( z_N \) is lossless following the sufficient encoder assumption \([43]\). Hence we approximate the compression term \( I(G_N, G) \) with \( I(z_N, G) \) and obtain a tractable variational upper bound for optimization. In fact, the encoding process is not lossless due to the data processing inequality. Thus, we actually approach \( I(G_N, G) \) with \( I(z_N, G) \) in practice. We leave the in-depth analysis in our future work.

7 Conclusion

We propose a novel Variational Graph Information Bottleneck framework for improved and efficient subgraph recognition. The proposed noise injection method serves as an alternative to compress the information in the discovered subgraph and allows a tractable objective of VGIB for efficient and stable training. Using the proposed method, we make the practical training more than 10 times faster than the existing methods. The experimental results show that the proposed method performs favorably against the existing methods on various tasks.

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| Method         | MUTAG  | PROTEINS | IMDB-B | DD    | COLLAB | REDDIT-B |
|----------------|--------|----------|--------|-------|--------|----------|
| Sum pooling    |        |          |        |       |        |          |
| GCN            | 0.76±0.09 | 0.72±0.05 | 0.71±0.04 | 0.74±0.03 | 0.78±0.03 | 0.75±0.05 |
| GIB+GCN        | 0.77±0.07 | 0.74±0.04 | 0.72±0.04 | 0.75±0.05 | 0.78±0.02 | 0.77±0.04 |
| VGIB+GCN       | 0.79±0.09 | 0.74±0.04 | 0.74±0.04 | 0.77±0.09 | 0.80±0.02 | 0.82±0.02 |
| GraphSAGE      | 0.74±0.08 | 0.73±0.05 | 0.71±0.05 | 0.75±0.03 | 0.78±0.02 | 0.78±0.10 |
| GIB+GraphSAGE  | 0.75±0.07 | 0.73±0.04 | 0.72±0.05 | 0.76±0.04 | 0.79±0.02 | 0.80±0.03 |
| VGIB+GraphSAGE | 0.77±0.07 | 0.74±0.04 | 0.73±0.03 | 0.78±0.05 | 0.80±0.03 | 0.80±0.09 |
| Mean pooling   |        |          |        |       |        |          |
| GIB+GIN        | 0.84±0.07 | 0.74±0.05 | 0.71±0.05 | 0.71±0.03 | 0.78±0.02 | 0.81±0.10 |
| GIB+GIN        | 0.84±0.06 | 0.74±0.05 | 0.74±0.07 | 0.74±0.04 | 0.78±0.03 | 0.84±0.03 |
| VGIB+GIN       | **0.86±0.08** | **0.75±0.04** | **0.74±0.05** | **0.75±0.04** | **0.79±0.03** | **0.86±0.03** |
| GIB+GAT        | 0.75±0.08 | 0.72±0.04 | 0.72±0.03 | 0.75±0.04 | 0.76±0.04 | 0.71±0.08 |
| GIB+GAT        | 0.75±0.09 | 0.73±0.04 | 0.72±0.05 | 0.76±0.04 | 0.77±0.03 | 0.73±0.04 |
| VGIB+GAT       | 0.76±0.07 | 0.73±0.04 | 0.73±0.07 | 0.77±0.04 | 0.79±0.03 | 0.76±0.05 |
| GAT            | 0.75±0.08 | 0.72±0.04 | 0.72±0.03 | 0.75±0.04 | 0.76±0.02 | 0.79±0.02 |
| GIB+GAT        | 0.75±0.09 | 0.73±0.04 | 0.72±0.05 | 0.74±0.04 | 0.78±0.03 | 0.79±0.03 |
| VGIB+GAT       | **0.84±0.09** | **0.72±0.05** | **0.74±0.05** | **0.75±0.04** | **0.79±0.03** | **0.85±0.03** |

Table 4: Classification accuracy of graphs with **sum pooling** and **mean pooling** as the readout function. We report the mean and standard deviation of the testing accuracy in 10-fold cross-validation for each method. The bold results are the overall best performances and the underlining results are the best performances of certain backbones.