CommPOOL: An Interpretable Graph Pooling Framework for Hierarchical Graph Representation Learning

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Abstract

Recent years have witnessed the emergence and flourishing of hierarchical graph pooling neural networks (HGPNNs) which are effective graph representation learning approaches for graph level tasks such as graph classification. However, current HGPNNs do not take full advantage of the graph’s intrinsic structures (e.g., community structure). Moreover, the pool operations in existing HGPNNs are difficult to be interpreted. In this paper, we propose a new interpretable graph pooling framework - CommPOOL, that can capture and preserve the hierarchical community structure of graphs in the graph representation learning process. Specifically, the proposed community pooling mechanism in CommPOOL utilizes an unsupervised approach for capturing the inherent community structure of graphs in an interpretable manner. CommPOOL is a general and flexible framework for hierarchical graph representation learning that can further facilitate various graph-level tasks. Evaluations on five public benchmark datasets and one synthetic dataset demonstrate the superior performance of CommPOOL in graph representation learning for graph classification compared to the state-of-the-art baseline methods, and its effectiveness in capturing and preserving the community structure of graphs.

Introduction

In recent years, Graph Neural Network (GNN) has emerged and been broadly used as a generalized deep learning architecture for graph representation learning in many fields, such as social network analysis (Chen, Ma, and Xiao 2018, Huang et al. 2018), chemical molecule studies (Dai, Dai, and Song 2016, Duvenaud et al. 2015, Gilmer et al. 2017) and brain network analysis (Ma et al. 2019a, Liu et al. 2019). Generally, GNN models learn node embeddings by passing, transforming and aggregating node features across the graph. The generated node representations can then be forwarded to further layers for specific learning tasks, such as node classification (Kipf and Welling 2016a, Veličković et al. 2017) and link prediction (Kipf and Welling 2016b).

Most of the existing GNN models (e.g., GCN (Kipf and Welling 2016a), GAT (Veličković et al. 2017), GraphSage (Hamilton, Ying, and Leskovec 2017)) focus on node-level representation learning and only propagate information across edges of the graph in a flat way. When applying these GNNs for graph-level tasks such as graph classifications, existing works usually apply simple global pooling strategies (i.e., a summation over the learned node representations) to obtain the graph-level embedding and use it for graph label prediction (Li et al. 2015, Vinyals, Bengio, and Kudlur 2015, Zhang et al. 2018) or graph similarity learning (Ma et al. 2019b). One main drawback in these GNNs is that the hierarchical structure, often existing in graphs, is ignored during the global pooling process, which makes the models less effective for graph-level tasks. Hierarchical structure is a very important structure for many graphs in various domains. For example, the hierarchical community structure shown in Figure 1 is a typical pattern that often appears in social networks (Girvan and Newman 2002, Long et al. 2019), chemical molecule networks (Spirin and Mirny 2003) and brain networks (Kong and Yu 2014, Meunier et al. 2009). Therefore, preserving these community structures is critical for better understanding and analyzing these graphs.

![Figure 1: An example of hierarchical community structures in graphs](image)

Some recent works proposed hierarchical graph pooling neural networks (HGPNNs) to address the hierarchical pooling operations. (Ying et al. 2018, Lee et al. 2019, Gao and Ji 2019, Zhang et al. 2019). Generally, these HGPNNs consist of two components: the GNN backbone which is used to embed the graph nodes and local structures, and the pooling operation which represents graph structure in a hierarchical way. These HGPNNs have demonstrated the necessity of adding hierarchical pooling operations in GNNs to better preserve the graph hierarchical structure.

However, a critical limitation of the existing hierarchical graph pooling (HGP) strategies is that few of the pooling operations in the models are interpretable. In many real
applications, it is desirable to have an interpretable model, where human can understand the cause of a decision made by the model [Miller 2019; Molnar 2020]. Moreover, an interpretable model is more robust under adversarial attacks [Dai et al. 2018; Zügner, Akbarnejad, and Günnemann 2018; Zügner and Günnemann 2018; Zhang et al. 2020]. A few of recent works [Ying et al. 2019; Hou et al. 2019; Yuan et al. 2020] interpreted the node feature embedding via GNN as a neighborhood aggregation scheme. Particularly, they stated that the GNN embed the local feature of each node $v$ within two steps: (1) neighbor node features aggregation and (2) node feature transformation. However, the interpretability of pooling operations is still not well solved. (Details are discussed in the Related Work). In order to make the HGP operation interpretable, three questions should be considered:  
Q1: How to capture the graph hierarchical structures in an interpretable way?  
Q2: How to scale down the graph representation while preserving the structures via an interpretable process?  
Q3: What do we obtain after the pooling operation?  

To address these challenges, we propose a Community-Based HGP framework, COMMUNITY-POOL or CommPOOL. We aim to encode the hierarchical community structure in graphs, which is a natural structure in many graphs, where nodes within each community are more densely connected than the nodes across different communities. Specifically, we propose a community-based hierarchical pooling operation which aggregates and synthesizes the node features based on the detected communities, such that the community structure of graphs can be preserved during the pooling process. Moreover, we introduce a GNN-based framework with the proposed community-based hierarchical pooling operation for learning latent graph representations, where both local node features and the hierarchical community-structure information are encoded and preserved. Our contributions here can be summarized as:  

- We propose a community-based HGP framework (CommPOOL) for learning graph representation in a hierarchical way that can preserve both the local node features and the hierarchical community structure of graphs.  
- The proposed hierarchical community pooling strategy relies on the community structure which is explicitly detected from the graphs, therefore the pooling operation can capture the intrinsic community-level latent representation of graphs and the pooling process is inherently interpretable.  
- We evaluate our CommPOOL framework for the whole graph classification task on multiple public benchmark datasets. The results demonstrate the superior performance of our model compared to several state-of-the-art graph pooling neural networks.  
- Evaluations on synthetic graphs with community ground-truth labels show that our proposed CommPOOL can capture and preserve the intrinsic community structure of graphs during the learning process.

Related Work

Graph Pooling

Graph pooling operation is a strategy aiming to scale down the size of input graphs. It can not only help to avoid model overfitting and reduce the computational cost but also generate graph-level representations [Wu et al. 2020]. In the early works [Henaff, Bruna, and LeCun 2015; Levie et al. 2018; Dhillon, Guan, and Kulis 2007; Vinyals, Bengio, and Kudlur 2015], the graph pooling methods simply compute the mean/max/sum of all graph node features as the representation of the whole graph. Such a primitive pooling strategy is named as global pooling. Later on, a few advanced techniques (e.g. attention mechanisms [Li et al. 2015; Gilmer et al. 2017; Tran, Navarin, and Sperduti 2018], feature sorted [Zhang et al. 2018]) are proposed to improve the performance and efficiency of the global pooling. However, the global pooling methods do not learn the hierarchical representations, which are crucial for capturing the structural information of graphs. Therefore, HGPNNs are proposed.

Interpretability of HGPNNs

Most HGP operations in the current HGPNNs [Zhang et al. 2019; Ying et al. 2018; Lee, Lee, and Kang 2019; Gao and Ji 2019; Kefato and Girdzijauskas 2020; Bianchi, Grattarola, and Alippi 2020] show little interpretability and are difficult to be understood by the users. Moreover, very few studies present the interpretability of their HGP operations in the paper, which may be accounted for by the following two issues: (1) Hardly any clear definition or analysis can be found to explain what is the captured graph structure. Therefore, the model users are lack of heuristic knowledge to understand the pooling operation. (2) Although some studies [Ying et al. 2018] present the visualization of hierarchical clusters captured by the model, no quantitative analysis is provided to examine whether the captured clusters of nodes are aligned with the intrinsic clusters in the original graph. Apart from these, most recent studies unfold the HGP operation as a neural network layer with trainable parameters. The black-box nature of neural networks may also raise extra difficulties to interpret the models in a way.

Preliminaries

Graph Notation

We consider the graph classification problem on attributed graphs with different numbers of nodes. Let $G = (A, H)$ be any of the attributed graph with $N$ nodes, where $A \in \{0, 1\}^{N \times N}$ is the graph adjacency matrix and $H \in \mathbb{R}^{N \times d}$ is the node feature matrix assuming that each node has $d$ features. Also, $Z = [Z_1, ..., Z_N]^T$ is defined as the node latent feature matrix where $Z_i$ is the latent feature vector for the node $i$. Given a set of labeled data $D = \{(G_1, y_1), (G_2, y_2), (G_3, y_3), ...\}$ where $y_i \in \mathcal{Y}$ is the classification label to the corresponding graph $G_i \in \mathcal{G}$. The graph classification task can be formulated as learning a mapping, $f: \mathcal{G} \rightarrow \mathcal{Y}$. 

\[ f(G) = \arg \max_{y \in \mathcal{Y}} \mathcal{L}(D; y, f(G)) \]
Graph Neural Network

Graph Neural Network (GNN) is an effective message-passing architecture for embedding the graph nodes and their local structures. Generally, GNN can be formulated as:

$$Z^{(k)} = F(A^{(k-1)}, Z^{(k-1)}; \theta^{(k)})$$

where \(k\) denotes the layer \(k\) of GNN, \(A^{(k-1)}\) is the graph adjacency matrix computed by layer \((k - 1)\) of the GNN, \(\theta^{(k)}\) is the trainable parameters in the layer \(k\) of the GNN. Particularly, \(Z^0 = H\).

\(F(\cdot)\) is the forward function to combine and transform the messages across the nodes. Many different versions of forward functions \(F(\cdot)\) are proposed in the previous studies (Gilmer et al. 2017) such as Graph Convolutional Neural Network (GCN) (Kipf and Welling 2016a) and Graph Attention Network (GAT) (Veličković et al. 2017). The GCN linearly combines the neighborhoods as the node the representation. And the GAT computes node representations in entire neighborhoods based on attention mechanisms (Bruna et al. 2013).

The Proposed Framework

Model Architecture

Our goal is to provide a general graph pooling framework that can capture and preserve the hierarchical community structure of graphs in the representation learning process of GNNs. The framework should be interpretable and it should be able to facilitate further graph-level learning tasks, for example, graph classification. To achieve this goal, we propose a community-based hierarchical graph pooling (HGP) framework: CommPOOL, which is composed of \(k\) cascaded Embedding-Pooling (EP) modules to learn the graph representation in a hierarchical way. Each EP module consists of (1) an Embedding stage, where a GNN model is employed to get the latent node representations (i.e., node embeddings) of the input graph, and (2) a Pooling stage, where a newly proposed community pooling mechanism is conducted on the node embeddings to detect communities from the graph and obtain a scaled-down graph-level representation that encodes both the local node features and the community structure of the graph. The output of the last EP module will be the final graph-level representation that preserves the overall hierarchical community structure of the graph. Figure 2(A, B) shows an instance of the proposed framework with two cascaded EP modules. In real applications of our framework, the choice of value for \(k\) is flexible and it can be decided based on the practical needs or domain knowledge for the specific application (e.g., domain evidence about how many community hierarchies exist in the graphs). In this paper, we set \(k = 2\) and use the architecture given in Figure 2(A, B) for illustrating our framework and we use the MLP shown in Figure 2(C) for evaluating the CommPOOL in graph representation learning for facilitating graph classification task.

In the following subsections, we introduce the two main parts in the proposed EP module for CommPOOL: (1) the GNN-based Node Embedding, and (2) the Community Pooling Operation.

GNN-based Node Embedding

We aim at a general GNN-based model to embed the graph nodes into the latent feature space \(Z\) that well preserves the inherent graph structures. On the one hand, the desired node latent features should well encode the node information and the information between the node and its neighbors. On the other hand, the latent features should preserve the intrinsic structures of the graphs without task-specific influences or supervised information. On account of the above considerations, we choose the Variational Graph Auto-Encoders (VGAE) (Kipf and Welling 2016b) to embed nodes into the latent space by reconstructing the graph itself.

Encoder In the VGAE, we need to learn a Gaussian distribution \(q(Z|H, A) = \mathcal{N}(Z|\mu, \sigma^2)\) which is used to approximate the Gaussian prior \(p(Z) = \mathcal{N}(Z|0, I)\). Particularly, we utilize two GNN layers to compute the \(\mu\) and \(\sigma^2\) parameters of \(q\). In the first layer, \(\mu\) and \(\sigma^2\) share the same GNN encoder. And in the second layer, two separate GNNs are used to generate \(\mu\) and \(\sigma^2\) respectively. The approximation can be achieved by maximizing the Kullback–Leibler (KL) loss between \(p\) and \(q\):

$$\mathcal{L}_{KL} = KL(q(Z|H, A)||p(Z))$$

The latent features \(Z\) can be obtained by resampling from the optimal \(q(Z|H, A)\).

Decoder After we obtain the latent features \(Z\), we reconstruct the original graph adjacency matrix by:

$$\hat{A} = \text{sigmoid}(ZZ^T)$$

We define \(+\) and \(-\) as the edges and non-edges position index in \(A\). So we reconstruct the adjacency matrix by minimizing the \(\mathcal{L}_A\):

$$\mathcal{L}_A = \mathcal{L}_1 + \mathcal{L}_2$$

$$\mathcal{L}_1 = -\frac{1}{E_1} \sum(\text{log}(\hat{A}_1)) - \frac{1}{E_2} \sum(\text{log}(1 - \hat{A}_2))$$

where \(E_1, E_2\) is the number of edges and non-edges. The overall objective function of VGAE is:

$$\text{minimize}_{Z \in R^n} \mathcal{L}_A - \mathcal{L}_{KL}$$

In our CommPOOL, we use GCN (Kipf and Welling 2016a) to build up the basic encoder layers and use GAT (Veličković et al. 2017) as the encoder variations.

Community Pooling

Community Capturing After embedding the graph nodes into the latent space \(Z\), we adopt an unsupervised clustering method Partitioning Around Medoids (PAM) (Kaufman 1987; Lee et al. 2019) on the node latent feature vectors to group the graph nodes into \(L\) different communities, where \(L\) is a parameter denoting the number of communities in the graph. Our community partition problem can be defined as: given all the \(N\) nodes in graph \(G\) with their latent feature vectors set \(V = \{Z_1, ..., Z_N\}\), find \(L\) different nodes with their latent features \(Z_C = \{Z_{C_1}, ..., Z_{C_L}\} \subset V\) from the \(N\) nodes as the optimal community centers, and assign
the other nodes into these $L$ communities based on the distances between their latent feature vectors ($O = V \setminus Z_C$) and $Z_C$. PAM realizes the community partition problem via the following four steps.

- **Step 1.** Initialization: Randomly select $L$ nodes with their features $Z_C$ as the community medoid nodes.
- **Step 2.** Clustering: Compute the $L_1$ distances between the medoid nodes and the rest nodes based on their feature vectors, and assign each non-medoid node to its closest community; Calculate the value for the below cost function, which computes the total distance between the non-medoid node feature vectors $O_j \in O$ and their community medoid feature vectors by:
  \[
  \text{Cost} = \sum_{j=1}^{N-L} |O_j - Z_{C_z}|_{L_1},
  \]
  where $Z_{C_z} \in Z_C$ is the corresponding medoid of $O_j$.
- **Step 3.** Adjusting: Swap each medoid node by all other non-medoid and calculate the total cost for current configuration referring to Step 2. Compare the cost of current and previous configuration and keep the configuration with the smaller total cost.
- **Step 4.** Optimization: Repeat Step 2 and 3 until the configuration does not change.

Community Pooling In order to preserve the captured community structure during the pooling process for the entire-graph representation learning, we propose a new pooling mechanism called “community pooling”, which summarizes the learned node representations based on the detected community structure. Suppose $Z_{M_i} = \{Z_{M_i}^{1}, \ldots, Z_{M_i}^{W}\}$ is the set consisting of the latent feature vectors of all $W$ community member nodes except for the community center nodes $Z_{C_i} \in Z_C$ in the community $i$. Our community pooling problem can be defined as: given a community center feature $Z_{C_i} \in Z_C$, and the corresponding $W$ community member features $Z_{M_i}$, compute the community representation $Z_{Comm_i}$. The community pooling operation computes the community $i$’s representation by:

\[
Z_{Comm_i} = Z_{C_i} + \sum_{w=1}^{W} \text{Sim}(Z_{M_i}^w, Z_{C_i}) Z_{M_i}^w,
\]

where $\text{Sim}(\cdot)$ is a function to measure the similarity between each member $Z_{M_i}^w$ and the community center $Z_{C_i}$. In our model, we mainly define $\text{Sim}(\cdot)$ based on $L_1$ distance:

\[
\text{Sim}(Z_{M_i}^w, Z_{C_i}) = \frac{1}{\|Z_{M_i}^w - Z_{C_i}\|_{L_1}}
\]

When each community representation $Z_{Comm_i}$ is computed, we replace the center node feature $Z_{C_i}$ by $Z_{Comm_i}$ and remove other community member nodes. As for the graph topology structure, the preserved center nodes are connected if and only if they are connected in the original graph. To sum up, during the pooling, the community structure information and the node features are preserved onto the community center nodes. And the graph structures among the communities are presented as the topology structure of downscaled graph with $M < N$ nodes.

**CommPOOL for Graph Classification**

When the community representations $Z_{Comm}^{(K)} = [Z_{Comm_1}^{(K)}, \ldots, Z_{Comm_{K}}^{(K)}]^T$ are obtained from the last Embedding-Pooling module ($k = K$), a global readout operation is used to generate the whole graph representation $Z_{graph}$ by averaging $Z_{Comm}^{(K)}$. Finally, an Multilayer Perceptron (MLP) utilizes $Z_{graph}$ to make predictions for graph classification.

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**Figure 2: Framework of the CommPOOL for graph classification.** (A) is the 1st Embedding-Pooling (EP) module and (B) is the 2nd EP module. In each module, we embed the graph into the latent space by using VGAE. In the latent space, we scale down the graph representation based on the detected communities. (C) is the MLP for graph classification.
classification. The training procedure of CommPOOL for the graph classification task is summarized in Algorithm 1.

**Algorithm 1: Training Procedure**

**Input:** graph: \( G = (A, H) \), classification label: \( y \), \( K \)

**Output:** prediction: \( \hat{y} \)

for \( k = 1, 2, ..., K \) do

Step 1: Use \( G \) to train the V Gaines

Step 2: Obtain the latent feature using trained V Gaines

Step 3: Community Pooling on latent features and generate down-scaled graph \( G^{(k)} = (A^{(k)}, Z^{(k)}_{Comm}). \) Set \( G = G^{(k)} \).

end

Step 4: \( Z_{graph} = \text{GlobalReadout}(Z^{(K)}_{Comm}) \)

Step 5: Train MLP to generate \( \hat{y} = \text{MLP}(Z_{graph}) \)

**Experiment**

In this section, we evaluate our CommPOOL framework using graph classification tasks. We present our experiment results in the following four subsections: (1) We introduce the dataset used in the experiments. (2) We compare the graph classification performance between CommPOOL and several competing HGPPN models. (3) We provide some variations of the CommPOOL. (4) We test our model on the simulation data to evaluate whether CommPOOL can accurately preserve the community structures in the graph.

**Dataset.** Five graph dataset are selected from the public benchmark graph data collection (Kersting et al. 2016). Table 2 summarizes the statistics of all dataset.

| Models   | BZR     | Synthie | FRANKENSTEIN | PROTEINS | AIDS   |
|----------|---------|---------|--------------|----------|--------|
| Set2Set  | 80.50 ± 1.03 | 22.50 ± 0.86 | 60.62 ± 0.27 | 68.08 ± 0.56 | 88.80 ± 0.45 |
| SortPool | 77.00 ± 1.24 | 32.50 ± 1.24 | 59.86 ± 1.22 | 70.11 ± 0.04 | 86.00 ± 2.42 |
| DISFFPOOL | 80.50 ± 1.48 | 57.00 ± 2.62 | 60.60 ± 1.62 | 72.43 ± 0.26 | 93.50 ± 1.00 |
| SAG-POOL | 82.00 ± 2.13 | 45.00 ± 4.21 | 61.73 ± 0.76 | 71.86 ± 0.97 | 93.50 ± 1.00 |
| HGP-SL   | 83.00 ± 4.30 | 54.00 ± 0.04 | 59.51 ± 1.50 | 84.91 ± 1.62 | 95.50 ± 1.00 |
| CommPOOL | 86.00 ± 1.23 | 66.50 ± 0.38 | 62.15 ± 0.37 | 74.74 ± 0.06 | 98.50 ± 0.05 |

**Graph Classification**

**Baseline Methods** Our baseline methods include: two graph global pooling models (Set2Set (Vinyals, Bengio, and Kudlur 2015) and SortPool (Zhang et al. 2018), and three HGP models (DIFFPOOL (Ying et al. 2018), SAGPOOL (Lee et al. 2019) and HGP-SL (Zhang et al. 2019)). For fair comparisons, we set two embedding-pooling modules for all HGP models including three baseline HGPs and our CommPOOL. For the baselines, we follow the original hyperparameter search strategies provided in the related papers.

**Experiments Setting** Following previous works (Ma et al. 2019c, Ying et al. 2018, Zhang et al. 2019), we randomly split the whole dataset into training (80%) set, validation (10%) set and testing (10%) set. We repeat this randomly splitting process 10 times, and the average test performance with standard derivation is reported in Table 1. We optimize the model via Pytorch Adam optimizer. For the V Gaines in the first module, the learning rate (lr) and the weight decay (wd) are searched in \( \{0.0001, 0.001, 0.005, 0.01, 0.05, 0.1\} \) set. The dimension of two latent GNN layers are 32 and 16. For the V Gaines in the second module, the lr and wd are searched in \( \{0.0001, 0.001, 0.005, 0.01\} \) and the dimension of two latent GNN layers are 64 and 32. In the community pooling operation, the number of communities is searched in \( \{40\%, 50\%, 60\%\} \) of the number of graph nodes (N). The MLP consists of two fully connected layers with 64 and 32 neurons and a softmax output layer. The lr for training the MLP is searched in \( \{0.001, 0.005, 0.01\} \). We stop training if the validation loss does not decrease for 50 epochs. Our experiments are deployed on NVIDIA Tesla P100 GPUs. We implement all baselines and CommPOOL using PyTorch (Paszke et al. 2017) and the torch geometric library (Fey and Lenssen 2019).

**Summary of Results** Table 1 summarizes the classification performances of six models on five public datasets. Our CommPOOL outperforms all baselines in the graph classi-
classification task on almost all datasets, especially on the four-class data **Synthie**. For example, our CommPOOL shows about 5.11% improvement in the classification accuracy comparing to all baselines on **BZR** data. This superiority of CommPOOL may be credited to its advanced mechanism for capturing and preserving the community structure in the pooling operation. Also, these results indicate that the community is a crucial hierarchical structure for learning the whole graph representation.

Moreover, Table 1 shows that hierarchical pooling methods generally perform better than global pooling methods, which verifies that the hierarchical pooling can better capture the graph global representations. Among all baseline models, HGP-SL relatively performs better than others, which may be attributed to the structure learning (SL) operations in the model. On PROTEINS, HGP-SL performs the best among all baseline methods and even better than ours, which implies that the structural learning strategy in HGP-SL might be specifically suitable for PROTEINS data.

### Model Variations

To show the flexibility of CommPool, we compare several variations of CommPOOL on PROTEINS and FRANKENSTEIN data. As noted in the **The Proposed Framework** section, GAT (Veličković et al. 2017) is used to replace GCN as a VGAE encoder variation. Moreover, instead of using the reciprocal of $L_1$ distance, we adopt the cosine-similarity as $Sim(\cdot)$ to measure the similarity between community members $Z_M$ and the corresponding community center $Z_C$, in community $i$:

$$Sim(Z_M^i, Z_C^i) = \frac{Z_M^i \cdot Z_C^i}{\|Z_M^i\| \|Z_C^i\|}$$  \hspace{1cm} (9)

The performance of CommPool with different encoders and similarity measures are listed in Table 3, which indicates that GAT, compared to GCN, has a better performance as the encoder in CommPOOL to embed the graph nodes. In addition, Table 3 shows that $L_1$ distance is better than cosine distance when measuring the similarity between the latent features of community member nodes and the community center nodes. A possible explanation is that $L_1$ distance is used in the PAM clustering. Therefore, it may be better to use the same distance metric in the community partition process.

### Community Evaluation on Simulation Data

Since no community ground-truth is provided in any publicly graph classification datasets, we simulate a set of graphs with the known community ground-truth and evaluate how CommPOOL preserves the intrinsic community structures on these simulation graphs.

Table 4: Average graph classification accuracy ± standard deviation (%) on the simulation data.

| Models    | Classification Accuracy |
|-----------|------------------------|
| Set2Set   | 46.54 ± 3.85           |
| SortPOOL  | 51.29 ± 0.61           |
| DIFF-POOL | 67.14 ± 2.16           |
| SAG-POOL  | N/A                    |
| HGP-SL    | 72.70 ± 1.95           |
| CommPOOL  | 80.14 ± 2.15           |

**Simulation Graphs.** We create 3 classes of simulation graphs using different graph generating methods, including the Random Partition Graphs, the Relax Caveman Graphs, and the Gaussian Random Community Graphs (Brandes, Gaertler, and Wagner 2003; Fortunato 2010). Each class contains 300 graphs and each graph has 4 communities with the average size of 6 nodes. A community label is assigned to each graph node. Meanwhile, we randomly sample from the normal distribution $\mathcal{N}(0, I)$ as node features. We evaluate CommPOOL on the simulation graphs to predict their class labels. Table 4 compares the graph classification performance of CommPool with the baseline models. The results show that, on the simulation data, the CommPOOL can also outperform all the baseline models. N/A in Table 4 indicates the SAG-POOL cannot achieve an optimal point in reachable epochs.

More importantly, in order to evaluate if CommPool can capture the community structures, we compare the node community label assigned by PAM clustering in the 1st EP module to the community ground-truth labels. Specifically, we compute the **Normalized Mutual Information (NMI)** (Strehl and Ghosh 2002) between distribution of community labels predicted by the model and given by the ground-truth for each graph. Figure 3a is a histogram presenting the distribution of NMI scores for all 900 simulation graphs. Statistically, 79.44% graphs have an NMI score larger than 0.9 and the mean NMI score is 0.952 ± 0.098.

### Evaluation and Discussion

In this section, we firstly discuss the interpretability of our proposed community pooling operation. And then we analyze the importance of community structure to the graph classification task.

#### Interpretability of Community Pooling

CommPOOL is a hierarchical graph pooling framework with an interpretable pooling operation. The user can transparently understand the pooling results by monitoring the pooling operation. An interpretable pooling operation should be capable of clearly answering three questions mentioned in the **Introduction** section. Our CommPOOL provides the heuristic and knowledgeable answers for the questions in the following way:
contains the corresponding community information.

Community Effect on Graph Classification

We design a further experiment named semi-random pooling to show that a solid community preservation is important to the graph classification. Instead of randomly partitioning the graph into multiple communities, we only randomly select the community center nodes. After determining the community center nodes, we assign each other node to the closest community based on the similarity of node features. Such a semi-random partition method can generate a few node cliques in graphs. These cliques, though are not the optimal communities, can still maintain the hierarchical information to some degree. We replace the PAM clustering by the semi-random partition in the pooling operation. Table 5 indicates that the community pooling has significant improvements in the graph classification tasks comparing to the semi-random pooling, which demonstrates that the success of community capture and preservation is crucial to the graph classification. To visualize, we select two simulation graphs to show (1) a positive example of community structure captured by the CommPOOL (Figure 3b), and (2) a negative example of community structure captured by the CommPOOL, which eventually leads to the graph’s misclassification (Figure 3c). In addition, the performance of semi-random pooling does not decrease a lot comparing with the community pooling, which is beyond our expectations in a way. A reasonable explanation is that although unable to preserve the optimal community structure, the semi-random pooling method can still capture some degree of graph hierarchical structure, which again justifies that the significance of the community structure in the graph.

Table 5: Graph Classification Accuracy of Semi-random Pooling vs. Community-Based Pooling

| Dataset     | semi-rand.       | community-based |
|-------------|------------------|-----------------|
| PROTEINS    | 64.90 ± 2.45     | 74.74 ± 0.06    |
| BZR         | 81.50 ± 2.82     | 86.00 ± 1.23    |
| Synthie     | 59.00 ± 5.89     | 66.50 ± 0.38    |
| Simulation  | 70.34 ± 1.26     | 80.14 ± 2.15    |

Conclusion

In this paper, we propose CommPOOL, a new interpretable hierarchical graph pooling framework. CommPOOL is designed for being able to capture and preserve the inherent hierarchical community structures in graphs during the graph representation learning and scaling-down process. Moreover, CommPOOL is a general graph representation learning framework that can facilitate various graph-level tasks. Experiments on both real-world graph datasets from different domains and synthetic graph data have shown that CommPOOL outperforms the state-of-the-art methods in graph representation learning for the graph classification task. In future work, we will explore leveraging CommPOOL for other graph-level tasks, such as graph regression.
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