Robust Hierarchical Graph Classification with Subgraph Attention

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ABSTRACT

Graph neural networks get significant attention for graph representation and classification in machine learning community. Attention mechanism applied on the neighborhood of a node improves the performance of graph neural networks. Typically, it helps to identify a neighbor node which plays more important role to determine the label of the node under consideration. But in real world scenarios, a particular subset of nodes together, but not the individual pairs in the subset, may be important to determine the label of the graph. To address this problem, we introduce the concept of subgraph attention for graphs. On the other hand, hierarchical graph pooling has been shown to be promising in recent literature. But due to noisy hierarchical structure of real world graphs, not all the hierarchies of a graph play equal role for graph classification. Towards this end, we propose a graph classification algorithm called SubGattPool which jointly learns the subgraph attention and employs two different types of hierarchical attention mechanisms to find the important nodes in a hierarchy and the importance of individual hierarchies in a graph. Experimental evaluation with different types of graph classification algorithms shows that SubGattPool is able to improve the state-of-the-art or remains competitive on multiple publicly available graph classification datasets. We conduct further experiments on both synthetic and real world graph datasets to justify the usefulness of different components of SubGattPool and to show its consistent performance on other downstream tasks.

CCS CONCEPTS
- • Computer systems organization → Embedded systems; Redundancy; Robotics; • Networks → Network reliability.

KEYWORDS
datasets, neural networks, gaze detection, text tagging

1 INTRODUCTION

Graphs are the most suitable way to represent different types of relational data such as social networks, protein interactions and molecular structures. Typically, a graph is represented by $G = (V, E)$, where $V$ is the set of nodes and $E$ is the set of edges. Further, each node $v_i \in V$ is also associated with an attribute (or feature) vector $x_i \in \mathbb{R}^D$. Recent advent of deep representation learning has heavily influenced the field of graphs. Graph neural networks (GNNs) [10, 41] are developed to use the underlying graph as a computational graph and aggregate node attributes from the neighbors of a node to generate the node embeddings [17]. A simplistic message passing framework [12] for graph neural networks can be presented by the following equations.

$$h'_v = \text{COMBINE} \left( \text{AGGREGATE} \left( \{h'^{-1}_{v' \in N_G(v)} \} \right) \right)$$

$$x^G = \text{READOUT} \left( \left\{ h^L_v : v \in V(G) \right\} \right)$$ (1)

Here, $h'_v$ is the representation of node $v$ of graph $G$ in $l$-th layer of the GNN. The function AGGREGATE considers representation of the neighboring nodes of $v$ from the $(l - 1)$th layer of the GNN and maps them into a single vector representation. As neighbors of a node do not have any ordering in a graph and the number of neighbors can vary for different nodes, AGGREGATE function needs to be permutation invariant and should be able to handle different number of nodes as input. Then, COMBINE function uses the node representation of $v$th node from $(l - 1)$th layer of GNN and the aggregated information from the neighbors to obtain an updated representation of the node $v$. Finally for the graph level tasks, READOUT function (also known as graph pooling) generates a summary representation $x^G$ for the whole graph $G$ from all the node representations $h^L_v$ for $v \in V(G)$ from the final layer of the GNN. Similar to AGGREGATE, the function READOUT also needs to be invariant to different node permutations of the input graph, and should be able to handle graphs with different number of nodes.

In the existing literature, different types of neural architectures are proposed to implement each of the three functions mentioned in Equation 1. For example, GraphSAGE [14] implements 3 different variants of the AGGREGATE function with mean, maxpool and LSTM respectively. For a graph level task such as graph classification [11, 41], GNNs jointly derive the node embeddings and use different pooling mechanisms [19, 45] to obtain a representation of the entire graph. Recently, attention mechanisms on graphs show promising results for both node classification [38] and graph classification [19, 20] tasks. There are different ways to compute
attention mechanisms on graph. [38] compute attention between a pair of nodes in the immediate neighborhood to capture the importance of a node on the embedding of the other node by learning an attention vector. [20] compute attention between a pair of nodes in the neighborhood to guide the direction of a random walk in the graph for graph classification. [19] propose self attention pooling of the nodes which is then used to capture the importance of the node to generate the label of the entire graph.

Most of the attention mechanisms developed in graph literature use attention to derive the importance of a node or a pair of nodes for different tasks. But in real world situation, calculating importance up to a pair of nodes is not adequate. In molecular biology or in social networks, the presence of particular sub-structures (a subset of nodes with their connections and features), potentially of varying sizes, in a graph often determines its label. Hence, all the nodes collectively in such a substructure are important, and they may not be important individually or in pairs to classify the graph. In Figure 1, each node (indexed from a to g) in the small synthetic graph can be considered as an agent whose attributes determine its opinion (1-positive, 0: neutral, -1: negative) about 4 products. Suppose the graph can be labelled +1 only if there is a subset of connected (by edges) agents who jointly have positive opinion about the entire product. In this case, the blue shaded connected subgraph (a, b, c) is important to determine the label of the graph. Please note, attention over the pairs [38] is not enough as (a, b) cannot make the label of the graph +1 by itself. Also, multiple layers of graph convolution [17] with pair-wise attention may not work as the aggregated features of a node get corrupted after the feature aggregation by the first few convolution layers. Besides, recent literature also shows that higher order GNNs that directly aggregate features from higher order neighborhood of a node are theoretically more powerful than 1st order GNNs [24]. With these motivations, we develop a novel higher order attention mechanism in the graph which operates in the subgraph level in the vicinity of a node. We call it subgraph attention mechanism and use it for graph classification1.

On the other hand, different types of graph pooling (i.e., READOUT function in Equation 1) mechanisms [11, 12, 24] have been proposed in the recent GNN literature. Simple functions such as taking sum or mean of all the node representations to compute the graph-level representation are studied in [11]. Recently, hierarchical graph pooling [24, 45] gains significant interest as it is able to capture the intrinsic hierarchical structure of several real-world graphs. For e.g., in a social network, one must model both the ego-networks around individual nodes, as well as the coarse-grained relationships between entire communities [28]. Instead of directly obtaining a graph level summary vector, hierarchical pooling mechanisms recursively converts the input graph to graphs with smaller sizes. But hierarchical representation [45] often fails to perform well in practice mainly due to two major shortcomings. First, there is significant loss of information in learning the sequential hierarchies of a graph when the data is limited. Second, it treats all the nodes within a hierarchy, and all the hierarchies equally while computing the entire graph representation. But for some real-world graphs, the structure between the sub-communities may be more important than that between the nodes or the communities to determine the label of the entire graph [28]. Moreover, due to presence of noise, some of the discovered hierarchies may not follow the actual hierarchical structure of the graph [34], and can negatively impact the overall graph representation. To address these issues, we again use attention to differentiate different units of a hierarchical graph representation in a GNN framework. Thus, our contributions in this paper are manifold, as follows:

- We propose a novel higher order attention mechanism (called subgraph attention) for graph neural networks, which is based on the importance of a subgraph of dynamic size to determine the label of the graph.
- We also propose hierarchical attentions in graph representation. More precisely, we propose intra-level and inter level attention which respectively find important nodes within a hierarchy and important hierarchies of the hierarchical representation of the graph. This enables the overall architecture to minimize the loss of information in the hierarchical learning and to achieve robust performance on real world noisy graph datasets.
- We propose a novel neural network architecture SubGatPool (Sub-Graph attention network with hierarchically attentive graph Pooling) to combine the above two ideas for graph classification. Thorough experimentation on both real world and synthetic graphs shows the merit of the proposed algorithms over the state-of-the-arts.

2 RELATED WORK AND THE RESEARCH GAPS

A survey on network representation [5, 13] learning and graph neural networks can be found in [40]. For the interest of space, we briefly discuss some more prominent approaches for graph classification and representation. Graph kernel based approaches [39], which map the graphs to Hilbert space implicitly or explicitly, remain to be the state-of-the-art for graph classification for long time. There are different types of graph kernels present in the literature, such as random walk based kernel [16], shortest path based kernels [8], graphlet counting based kernel [31], Weisfeiler-Lehman subtree kernel [30] and Deep graph kernel [43]. But most of the existing graph kernels use hand-crafted features and they often fail to adapt the data distribution of the graph. Significant progress happened in the domain of node representation and node level tasks via graph neural networks. Spectral graph

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1Subgraph attention can easily be applied for node classification as well. But we focus only on graph classification in this paper.
convolutional neural networks with fast localized convolutions [10, 17], graph attention (GAT) over a pair of connected node in the graph convolution framework [38], attention over different layers of convolution [42], position aware graph neural networks [46] and hyperbolic graph convolution networks [9] are some notable examples of GNN for node representation. To go from node embeddings to a single representation for the whole graph, simple aggregation technique such as taking the average of node embeddings in the final layer of a GCN [11] and more advanced deep learning architectures that operate over the sets [12] have been used. Attention based graph classification technique GAM [20] is proposed, which processes only a portion of the graph by adaptively selecting a sequence of informative nodes. DIFFPOOL [45] is a recently proposed hierarchical GNN which uses a GCN based pooling to create a set of hierarchical graphs in each level. [19] propose a self attention based pooling strategy which determines the importance of a node to find the label of the graph. Different extensions of GNNs, such as Ego-CNN [35] and ChebyGIN [18] are proposed for graph classification. Theoretical frameworks to analyze the representational power of GNNs are proposed in [22, 41]. [18] study the ability of attention GNNs to generalize to larger and complex graphs.

Higher order GNNs which operate beyond immediate neighborhood are proposed recently. Based on higher dimensional Weisfeiler-Leeman algorithm, k-GNN [24] is proposed which derive the representation of all the subgraphs of size $k$ through convolution. Mixhop GNN for node classification is proposed in [1] which aggregates node features according to the higher order adjacency matrices. Though these higher order GNNs are more powerful representation of graphs, they do not employ attention in the higher order neighborhood. To the best of our knowledge, [44] is the only work to propose an attention mechanism on the shortest paths starting from a node to generate the node embedding. However, their computation of shortest path depends on the pairwise node attention and this may fail in the cases when a collection of nodes together is important, but not the individual pairs. Our proposed subgraph attention addresses this gap in the literature. Further, hierarchical pooling as proposed in DIFFPOOL [45] has become a popular pooling strategy in GNNs [24]. But it suffers because of the loss of information and its nature to represent the whole graph by the last level (containing only a single node) of the hierarchy. As discussed in Section 1, some intermediate levels may play more important role to determine the label of the entire graph than the last one [28]. The intra-level and inter level attention mechanisms proposed in this work precisely address this research gap in hierarchical graph representation.

### 3 PROPOSED APPROACH: SUBGATTPOOL

We formally define the problem of graph classification first. Given a set of $M$ graphs $\mathcal{G} = \{G_1, G_2, \ldots, G_M\}$, and a subset of graphs $\mathcal{G}_s \subset \mathcal{G}$ with each graph $G_i \in \mathcal{G}_s$ is labelled with $Y_i \in \mathcal{L}_g$ (the subscript $g$ stands for ‘graphs’), the task is to predict the label of a graph $G_i \in \mathcal{G}_s = \mathcal{G} \setminus \mathcal{G}_g$ using the structure of the graphs and the node attributes, and the graph labels from $\mathcal{G}_g$. Again, this leads to learning a function $f_g : \mathcal{G} \mapsto \mathcal{L}_g$. Here, $\mathcal{L}_g$ is the set of discrete labels for the graphs.

| Notations | Explanations |
|-----------|--------------|
| $\mathcal{G} = \{G_1, \ldots, G_M\}$ | Set of graphs in a graph dataset |
| $G = (V, E, X)$ | One single graph |
| $\mathcal{L}_g$ | Set of discrete labels for graphs |
| $x_j \in \mathbb{R}^D$ | Attribute vector for $j$th node |
| $S_i = \{S_{i1}, \ldots, S_{iL}\}$ | Multiset of sampled subgraph for the node $v_i$. |
| $x_{i1}$ | Derived feature vector of a subgraph |
| $L$ | Maximum size (i.e., number of nodes) of a subtree |
| $\mathcal{T}$ | Number of subgraphs to sample for each node |
| $\mathcal{x}^G \in \mathbb{R}^K$ | Final representation of the graph $G$ |
| $G^1, \ldots, G^R$ | Level graphs of some input graph $G$ |
| $Z_r \in \mathbb{R}^{N_r \times k}$ | Embedding matrix of $G^r$ |
| $P_r \in \mathbb{R}^{N_r \times N_{r+1}}$ | Node assignment matrix from $G^r$ to $G^{r+1}$ |

Table 1: Different notations used in the paper

Figure 2 shows the high-level architecture of SubGattPool. One major component of SubGattPool is the generation of node representations through SubGraph attention (referred as SubGatt) layer. Below, we describe the building blocks of SubGat for any arbitrary graph. For the ease of reading, we summarize all the important notations used in this paper in Table 1.

#### 3.1 Subgraph Attention Mechanism

The input to the subgraph attention network is an attributed graph $G = (V, E)$, where $V = \{v_1, v_2, \ldots, v_N\}$ is the set of $N$ nodes and $x_j \in \mathbb{R}^D$ is the attribute vector of the node $v_i \in V$. The output of the model is a set of node features (or embeddings) $h_j \in \mathbb{R}^K$, $\forall i \in [N]$ ($K$ is potentially different from $D$). We use $[N]$ to denote the set $\{1, 2, \ldots, N\}$ for any positive integer $N$. We define the immediate (or first order) neighborhood of a node $v_i$ as $N^i \{v_i/v_j \mid (v_i, v_j) \in E\}$. For the simplicity of notations, we assume an input graph $G$ to be undirected for the rest of the paper, but extending it for directed graph is straightforward.

**3.1.1 Subgraph selection and Sampling.** For each node in the graph, we aim to find the importance of the nearby subgraphs to that node. In general, subgraphs can be of any shape or size. Motivated by the prior works on graph kernels [30], we choose to consider only a set of rooted subtrees as the set of candidate subgraphs. So for a node $v_i$, any tree of the form $(v_i)$, or $(v_i, v_j)$ where $(v_i, v_j) \in E$, or $(v_i, v_j, v_k)$ where $(v_i, v_j, v_k) \in E$ and so on will form the set of candidate subgraphs of $v_i$. We restrict that maximum size (i.e., number of nodes) of a subtree is $T$. Also note that, the node $v_i$ is always a part of any candidate subgraph for the node $v_i$ according to our design. For example, all possible subgraphs of maximum size 3 for the node $v$ in Figure 1 are: (a), (a,b), (a,d), (a,f), (a,b,c), (a,b,f), (a,b,g), (a,d,e), (a,f,e) and (a,f,b).

Depending on the maximum size $T$ of a rooted subtree, the number of candidate subgraphs for a node can be very large. For example, the number of rooted subgraphs for the node $v_i$ is $d_i^* \times \sum_{v_j \in N(v_i)} (d_{v_j} - 1) \times \sum_{v_k \notin \{v_i, v_j\}} \left| N(v_k) \setminus \{v_i, v_j\} \right|$, where $d_i^*$ is the degree of a node $v$ and $T = 4$. Clearly, computing attention over these many subgraphs for each node is computationally difficult. So we employ a subgraph subsampling technique, inspired by the node subsampling techniques for network embedding [14]. First, we fix
the number of subgraphs to sample for each node. Let the number be \( L \). For each node in the input graph, if the total number of rooted subtrees of size \( T \) is more than (or equal to) \( L \), we randomly sample \( L \) number of subtrees without replacement. If the total number of rooted subtrees of size \( T \) is less than \( L \), we use round robin sampling (i.e., permute all the subtrees, picking up samples from the beginning of the list; after consuming all the trees, again start from the beginning till we complete picking \( L \) subtrees). For each node, sample of subtrees remains same for one epoch of the algorithm (explained in the next subsection) and new samples are taken in each epoch. In any epoch, let us use the notation \( S_l = \{S_{l1}, \ldots, S_{lL}\} \) to denote the set (more precisely it is a multiset as subgraphs can repeat) of sampled subgraph for the node \( v_i \).

### 3.1.2 Subgraph Attention Network

This subsection describes the attention mechanism on the set of rooted subtrees selected for each epoch of the algorithm. As mentioned, the node of interest is always positioned as the root of each subgraph generated for that node. Next step is to generate a feature for the subgraph. We tried different simple feature aggregations (for e.g., mean) of the nodes that belong to the subgraph as the feature of the subgraph. It turns out that concatenation of the features of nodes gives better performance. But for the attention to work, we need equal length feature vectors (the length is \( TD \)) for all the subgraphs. So if a subgraph has less than \( T \) nodes, we append zeros at the end to assign equal length feature vector for all the subgraphs. For example, if the maximum size of a subgraph is \( T = 4 \), then the feature of the subgraph \((v_i, v_j, v_k)\) is \([x_i|x_j|x_k]|0| \in \mathbb{R}^{4D}\), where \(|\) is the concatenation operation and \( 0 \) is the zero vector in \( \mathbb{R}^D \). Let us denote this derived feature vector of any subgraph \( S_l \) as \( \hat{x}_{il} \in \mathbb{R}^{TD} \), \( \forall i \in [N] \) and \( \forall l \in [L] \).

Next, we use self-attention on the features for the sampled subgraphs for each node as described here. As the first step, we use a shared linear transformation, parameterized by a trainable weight matrix \( W \in \mathbb{R}^{K \times TD} \), to the feature of all the sampled subgraphs \( S_l, \forall i \in [N] \) and \( \forall l \in [L] \) selected in an epoch. Next we introduce a trainable self attention vector \( a \in \mathbb{R}^K \) to compute the attention coefficient \( a_{il} \) which captures the importance of the subgraph \( S_l \) on the node \( v_i \), as follows:

\[
a_{il} = \frac{\exp(\sigma(a^T W \hat{x}_{il}))}{\sum_{i' \in [L]} \exp(\sigma(a^T W \hat{x}_{i'l}))},
\]

\[
h_l = \sigma \left( \sum_{i=1}^{L} a_{il} W \hat{x}_{il} \right) \in \mathbb{R}^K, \quad \forall i \in [N]
\]

Here \( \sigma() \) is a non-linear activation function. We have used Leaky ReLU as the activation function for all the experiments. \( a_{il} \) gives normalized attention scores over the set of sampled subgraphs for each node. We use them to compute the representation \( h_l \) of a node \( v_i \) as shown in Eq. 2. Please note, the attention mechanism described in [38] operates only over the immediate neighboring nodes, whereas the higher order attention mechanism proposed in this work operates over the subgraphs. Needless to say, one can easily extend the above subgraph attention by multi-head attention by employing few independent attention mechanisms of Eq. 2 and concatenating the resulting representations [37]. This completes one full subgraph attention layer. We can stack such multiple layers to design a full SubGatt network.

### 3.2 Hierarchically Attentive Graph Pooling

This subsection discusses all the components of SubGattPool architecture. As shown in Figure 2, there are \( R = 4 \) different levels of the graphs in the hierarchical architecture. The first level is the input graph. Let us denote these level graphs (i.e., graphs at different levels) by \( G^1, \ldots, G^R \). There is a GNN layer between the level graph \( G^r \) (i.e., the graph at level \( r \)) and the level graph \( G^{r+1} \). This GNN layer comprises of an embedding layer which generates the embedding of the nodes of \( G^r \) and a pooling layer which maps the nodes of \( G^r \) to the nodes of \( G^{r+1} \). We refer the GNN layer between the level graph \( G^r \) and \( G^{r+1} \) by \( r \)th layer of GNN, \( \forall r = 1, 2, \ldots, R - 1 \).

Let us assume that any level graph \( G^r \) is defined by its adjacency matrix \( A_r \in \mathbb{R}^{N_r \times N_r} \) and the feature matrix \( X_r \in \mathbb{R}^{N_r \times D} \) (except for \( G^1 \), which is the input graph and its feature matrix \( X_1 \in \mathbb{R}^{N \times D} \)). The \( r \)th embedding layer and the pooling layer are defined by:

\[
Z_r = \begin{cases} 
\text{SubGatt}_{\text{emb}}(A_r, X_r), & r = 1 \\
\text{GIN}_{r, \text{emb}}(A_r, X_r), & r > 1 
\end{cases}
\]

\[
P_r = \begin{cases} 
\text{softmax}(\text{SubGatt}_{\text{pool}}(A_r, X_r)), & r = 1 \\
\text{softmax}(\text{GIN}_{r, \text{pool}}(A_r, X_r)), 1 < r \leq R - 1 
\end{cases}
\]

Here, \( Z_r \in \mathbb{R}^{N_r \times K} \) is the embedding matrix of the nodes of \( G^r \). The softmax after the pooling is applied row-wise. \((i, j)\)th element of \( P_r \in \mathbb{R}^{N_r \times N_{r+1}} \) gives the probability of assigning node \( v'_r \) in \( G^r \) to node \( v_{r+1} \) in \( G^{r+1} \). Based on these, the graph \( G^{r+1} \) is constructed as follows,

\[
A_{r+1} = P_r A_r P_r \quad \text{and} \quad X_{r+1} = P_r^T Z_r
\]

The matrix \( P_r \) contains information about how nodes in \( G^r \) are mapped to the nodes of \( G^{r+1} \), and the adjacency matrix \( A_r \) contains information about the connection of nodes in \( G^r \). Eq. 4 combines them to generate the connections between the nodes (i.e., the adjacency matrix \( A_{r+1} \)) of \( G^{r+1} \). Node feature matrix \( X_{r+1} \) of \( G^{r+1} \) is also generated similarly. As the embedding and pooling GNNs, we use SubGatt networks (Section 3.1) only after the level graph 1. This is because other level graphs \( G^r \) (\( r > 1 \)) have more number of soft edges (i.e., with probabilistic edge weights) due to use of softmax at the end of pooling layers. Hence, the number of neighboring rooted subtrees will be high in those level graphs and the chance of having discrete patterns will be less. We use GIN [41] as the embedding and pooling GNNs for \( G^r, r > 1 \). GIN has been shown to be the most powerful 1st order GNN and the \( l \)th layer of GIN can be defined as:

\[
h_{i+1}^{l+1} = MLP^l \left( (1 + e^l)h_i^l + \sum_{u \in N(i)} h_u^l \right)
\]
Here, $h^{l+1}_v \in \mathbb{R}^K$ is the hidden representation of the node $v$ in $l+1$ th layer of GIN and $\epsilon$ is a learnable parameter.

**Intra-level attention layer:** As observed in [19], hierarchical GNNs often suffer because of the loss of information in various embedding and pooling layers, from the input graph to the last level graph summarizing the entire graph. Moreover, the learned hierarchy is often not perfect due to noisy structure of the real world graphs. To alleviate these problems, we propose to use attention mechanisms again, to combine features from different level graphs of our hierarchical architecture. We consider level graphs $G^2$ to $G^K$ for this, as their respective numbers of nodes are same across all the graphs in a dataset. We introduce *intra-level attention layer* to obtain a global feature for each level graphs $G^r$, $\forall r = 2, \cdots, R$. More precisely, we use the convolution based self attention within the level graph $G^r$ as:

$$e_r = \text{softmax}(\tilde{D}_r^{-1/2} \tilde{A}_r \tilde{D}_r^{-1/2} x_r) \in \mathbb{R}^{N_r} \quad \text{and} \quad x' = x_r^T e_r \in \mathbb{R}^K$$ (6)

Here, the softmax to compute $e_r$ is taken so that a component of $e_r$ becomes the normalized (i.e., probabilistic) importance of the corresponding node in $G^r$. $\tilde{A}_r = A_r + I_{N_r}$ is the adjacency matrix with added self loops of $G^r$. $\tilde{D}$ is the diagonal matrix of dimension $N_r \times N_r$ with $\tilde{D}(i,i) = \sum_{j=1}^{N_r} \tilde{A}_{ij}$. $\theta \in \mathbb{R}^K$ is the trainable vector of parameters of intra-level attention, which is shared across all the level graphs $G^r$, $\forall r = 2, \cdots, R$. Intuitively, $\theta$ contains the importance of individual attributes and the components of $N_r$ dimensional $X_r \theta$ gives the same for each node. Finally, multiplying with $\tilde{D}_r^{-1/2} \tilde{A}_r \tilde{D}_r^{-1/2}$ produces the (normalized) importance of a node based on its own features and the features of immediate neighbors (for one layer of intra-level attention). Hence, $x'$, which is a $K$ dimensional representation of the level graph $G^r$, is a sum of the features of the nodes weighted by the respective normalized node importance. Please note, the impact from the first few level graphs becomes noisy due to too many subsequent operations in a hierarchical pooling method. But representing level graphs separately by the proposed intra-level attention makes their impact more prominent.

**Inter-level attention layer:** This layer aims to get the final representation, referred as $x^G \in \mathbb{R}^K$, of the input graph from $x_2, \cdots, x_R$; as obtained from the intra-level attention layers. It is fed to a neural classifier. As different level graphs of the hierarchical representation have different importance to determine the label of the input graph, we propose to use the following self-attention mechanism.

$$\bar{\epsilon} = \text{softmax}(X_{\text{inter}} \theta) \in \mathbb{R}^{R-1} \quad \text{and} \quad x^G = X_{\text{inter}}^T \bar{\epsilon} \in \mathbb{R}^K$$ (7)

$X_{\text{inter}}$ is the $(R-1) \times K$ dimensional matrix whose rows correspond to $x'$ (the output of intra-level attention layer for $G^r$), $r = 2, \cdots, R$. $\theta \in \mathbb{R}^K$ is a trainable self attention vector. Similar to Eq. 6, softmax is taken to convert $\bar{\epsilon}$ to a probability distribution of importance of different graph levels. Finally, the vector representation $x^G$ of the input graph is computed as a weighted sum of representations of different level graphs $G^r, \cdots, G^K$. $x^G$ is fed to a classification layer of the GNN, which is a dense layer followed by a softmax to classify the entire input graph in an end-to-end fashion. This completes the construction of SubGattPool architecture.

### 3.3 Key Insights of SubGattPool

First layer of SubGattPool consists of an embedding SubGatt network and a pooling SubGatt network, which have a total of $O(KTD)$ trainable parameters. Consequent layers of SubGattPool have GIN as embedding and pooling layers, which have a total of $O(RKD)$ parameters. Total number of parameters for $R-1$ intra-level attention layers is $O(K)$, as $\theta \in \mathbb{R}^K$ is shared across the level graphs. Finally the inter-level attention layer has $O(K)$ parameters. Hence, total number of parameters to train in SubGattPool network is $O(KTD + RKD)$, which is independent of both the average number of nodes and the number of graphs in the dataset. We use ADAM (with learning rate set to 0.001) on the cross-entropy loss of graph classification to train these parameters.
We use 5 bioinformatics graph datasets (MUTAG, PTC, PROTEINS, IMDB-MULTI) to evaluate the performance for graph classification. The details of these datasets can be found at (https://bit.ly/39T079X). Table 2 contains a high-level summary of these datasets. To compare the performance of SubGattPool, we choose twenty state-of-the-art baseline algorithms from the domains of graph kernels, unsupervised graph representation and graph neural networks (Table 3). The reported accuracy numbers of the baseline algorithms are collected from [22, 25, 33] where the same experimental setup is adopted. Thus, we avoid any degradation of the performance of the baseline algorithms due to insufficient parameter tuning and validation.

We adopt the same experimental setup as there in [41]. We perform 10-fold cross validation and report the averaged accuracy and corresponding standard deviation for graph classification. We keep the values of the hyperparameters to be the same across all the datasets, based on the averaged validation accuracy. We set the pooling ratio (defined as $\gamma = \frac{N_r}{N}-1$, $\forall r \leq R-1$) at 0.5, the number of levels $R=3$ and the maximum subgraph size ($T$) to be 3. We sample $L=12$ subgraphs for each node in each epoch of SubGatt. Following most of the literature, we set the embedding dimension $K$ to be 128. We use L2 normalization and dropout in SubGattPool architecture to make the training stable.

4.2 Performance on Graph Classification

Table 3 shows the performance of SubGattPool along with the diverse set of baseline algorithms for graph classification on multiple real-world datasets. From the results, we can observe that SubGattPool is able to improve the state-of-the-art on MUTAG, PTC, IMDB-B and IMDB-M for graph classification. On PROTEINS, the performance gap with the best performing baseline (which is 3WL-GNN [22] for both) is less than 1%. But on NCI1 and NCI109, WL kernel turns out to be the best performing algorithm with a good margin (> 1%) from all the GNN based algorithms. It is interesting to note that SubGattPool is able to outperform existing hierarchical GNN algorithms DIFFPOOL and 1-2-3GNN consistently on all the datasets. This is because of the use of (i) attention over subgraphs in SubGatt embedding and pooling layers, and (ii) use of intra-level and inter-level attention mechanisms over different level graphs which makes the overall architecture more robust and reduces information loss. In terms of standard deviation, SubGattPool is highly competitive and often better than most of the better performing GNNs (specially GIN and 3WL-GNN).

4 EXPERIMENTAL EVALUATION

This section describes the details of the experiments conducted on both real-life and synthetic datasets.

4.1 Experimental Setup for Graph Classification

We use 5 bioinformatics graph datasets (MUTAG, PTC, PROTEINS, NCI1 and NCI109) and 2 social network datasets (IMDB-BINARY and IMDB-MULTI) to evaluate the performance for graph classification. The details of these datasets can be found at (https://bit.ly/39T079X). Table 2 contains a high-level summary of these datasets. To compare the performance of SubGattPool, we choose twenty state-of-the-art baseline algorithms from the domains of graph kernels, unsupervised graph representation and graph neural networks (Table 3). The reported accuracy numbers of the baseline algorithms
which determines the label of a graph.

Table 3: Classification accuracy (%) of different algorithms (21 in total) for graph classification. NA denotes the case when the result of a baseline algorithm could not be found on that particular dataset from the existing literature. The last row 'Rank' is the rank (1 being the highest position) of our proposed algorithm SubGattPool among all the algorithms present in the table.

| Algorithms  | MUTAG   | PTC   | PROTEINS | NCI1  | NCI109 | IMDB-B   | IMDB-M   |
|-------------|---------|-------|----------|-------|--------|----------|----------|
| GK [31]     | 81.39±1.7 | 55.65±0.5 | 71.39±0.3 | 62.49±0.3 | 62.35±0.3 | NA       | NA       |
| RW [39]     | 79.17±2.1 | 55.91±0.3 | 59.57±0.1 | NA    | NA     | NA       | NA       |
| FK [27]     | 76±2.7   | 59.5±2.4 | 73.68±0.7 | 82.54±0.5 | NA     | NA       | NA       |
| WL [30]     | 84.11±1.9 | 57.97±2.5 | 74.68±0.5 | 84.46±0.5 | 85.12±0.3 | NA       | NA       |
| AWE-DD [15] | NA      | NA    | NA       | 74.45±5.8 | 51.54±3.6 | NA       | NA       |
| AWE-FB [15] | 87.87±9.7 | NA    | NA       | 73.13±3.2 | 51.58±4.6 | NA       | NA       |

Table 2: Statistics of different datasets used in our experiments

| Algorithms | MUTAG | PTC  | PROTEINS | NCI1 | NCI109 | IMDB-B | IMDB-M |
|------------|-------|------|----------|------|--------|--------|--------|
| DGCNN [47] | 85.83±1.7 | 58.59±2.5 | 75.54±0.9 | 74.44±0.5 | NA     | 70.03±0.9 | 47.83±0.9 |
| FSCN [29]  | 88.95±4.4 | 62.29±5.7 | 75±2.5   | 76.34±1.7 | NA     | 71±2.3  | 45.23±2.8 |
| DCNN [4]   | NA    | 61.29±1.6 | 56.61±1.0 | NA    | 49.06±1.4 | 33.49±1.4 |        |
| ECC [32]   | 76.11  | NA   | 76.82    | 75.03 | NA     | NA      |        |
| DGK [43]   | 87.44±2.7 | 60.08±2.6 | 75.68±0.5 | 80.31±0.3 | 66.96±0.6 | 44.55±0.5 |        |
| DIFFPPOO [45] | 83.56  | NA   | 76.25    | NA    | NA     | 47.91   |        |
| IGN [23]   | 83.89±12.95 | 58.53±6.86 | 76.58±5.49 | 74.33±2.71 | 72.82±1.45 | 72.0±5.54 | 48.73±3.41 |
| GIN [41]   | 89.4±5.6 | 64.6±7.0 | 76.2±2.8 | 82.7±1.7 | NA     | 75.1±5.1 | 52.3±2.8 |
| 1-3GNN [24] | 86.1±   | 60.9±   | 75.5±    | 76.2± | NA     | 47.2±   | 49.5±   |
| 3WL-GNN [22] | 90.55±8.7 | 66.17±6.54 | 77.2±4.73 | 83.19±1.11 | 81.84±1.85 | 72.6±4.9 | 50±3.15 |

4.3 Interpretation of Subgraph Attention via Synthetic Experiment

Subgraph attention is a key component of SubGattPool. Here, we validate the learned attention values on different subgraphs by conducting an experiment on a small synthetic dataset containing 50 graphs, and each graph having 8 nodes. Each graph has 2 balanced communities and exactly for 50% of the graphs, one community consists of a clique of size 4. We label a graph with +1 if the clique of size 4 is present, otherwise the label is -1. The goal of this experiment is to see if SubGattPool is able to learn this simple rule of graph classification by paying proper attention to the substructure which determines the label of a graph.

We run SubGattPool on this synthetic dataset, with $K = 16$, $T = 4$, $L = 12$, #SubGatt layers=1, $γ = 0.75$ and $R = 3$. Once the training is complete, we randomly select a graph from the positive class and a node in it and plot the attention values of all the subgraphs selected in the last epoch for that node, in Figure 3. Clearly, the attention value corresponding to the clique (containing the nodes 7, 6, 5 and 4) is much higher than that to the other subgraphs. We have manually verified the same observation on multiple graphs in this synthetic dataset. Thus, SubGattPool is able to pay more attention to the correct substructure (i.e., subgraph) and pay less attention to other irrelevant substructures. This also explains the robust behavior of SubGattPool.

4.4 Graph Clustering

Though our proposed algorithm SubGattPool is for graph classification, we also want to check the quality of the graph representations
Figure 4: t-SNE visualization of the graphs from MUTAG (different colors show different labels of the graphs) by the representations generated by: (a) DIFFPOOL; (b) SubGattPool, but the SubGatt embedding and pooling layers being replaced by GIN; (c) SubGattPool without intra and inter layer attention; (d) the complete SubGattPool network. Compared to (a), there is improvement of performances for both the SubGatt layer and the intra/inter-level attention individually. Finally different classes are separated most by SubGattPool which again shows the merit of the proposed algorithm.

Figure 5: t-SNE visualization of the graphs from PTC (different colors show different labels of the graphs) by the representations generated by different GNN algorithms. The description of each variant of SubGattPool is exactly the same as in Figure 4. Again for PTC also, we can see the performances of different variants of SubGattPool are better than that of DIFFPOOL and the overall performance of SubGattPool in visualizing PTC is better than the other variants which are obtained by removing one or more components from SubGattPool.

$x^G, \forall G \in \mathcal{G}$ obtained in SubGattPool through graph clustering. We use only a subset of recently proposed GNN based algorithm as baselines in this experiment. We use similar hyperparameter values (discussed in Section 4) as applicable and adopt same hyperparameter tuning strategy to obtain the graph representation for all the algorithms considered. The vector representations obtained for all the graphs by a GNN are given to K-Means++ [3] algorithm to get the clusters. To evaluate the quality of clustering, we use unsupervised clustering accuracy [6, 7] which uses different permutations of the labels and chooses the label ordering which gives the best possible accuracy $\text{Acc} = \max_{P} \frac{\sum_{i=1}^{N} \mathbb{1}(P(\hat{C}_i) = C_i)}{N}$. Here $C$ is the ground truth labeling of the dataset such that $C_i$ gives the ground truth label of $i$th data point. Similarly $\hat{C}$ is the clustering assignments discovered by some algorithm, and $P$ is a permutation of the set of labels. We assume $\mathbb{1}$ to be a logical operator which returns 1 when the argument is true, otherwise returns 0. Table 4 shows that SubGattPool is able to outperform all the baselines we used for graph clustering on all the three datasets. Please note that DGI and InfoGraph derive the graph embeddings in an unsupervised way, whereas DIFFPOOL and SubGattPool use supervision. Naturally, the performance of the later two are better on all the datasets. Further, the use of subgraph attention along with the hierarchical attention layers helps SubGattPool to perform consistently better than DIFFPOOL which is also hierarchical in nature.

### 4.5 Model Ablation Study
SubGattPool has mainly two novel components. They are the SubGatt layer, and the intra-level and inter-level attention layers which makes SubGattPool a mixture of both global and hierarchical pooling strategy. To see the usefulness of each component, we show the performance after removing that component from SubGattPool. We chose graph visualization of MUTAG in Figure 4 and graph visualization of PTC in Figure 5 as the downstream tasks for this experiment. We use t-SNE [36] to convert the graph embeddings into two dimensional plane. Different colors represent different labels of the graphs and the performance is better when different colors form different clusters in the plot. We choose DIFFPOOL as

| Algorithms | MUTAG | PROTEINS | IMDB-M |
|------------|-------|----------|--------|
| DGI        | 74.73 | 59.20    | 36.83  |
| InfoGraph  | 77.65 | 59.93    | 35.93  |
| DIFFPOOL   | 82.08 | 60.81    | 41.72  |
| SubGattPool| 90.68 | 65.45    | 50.23  |

Table 4: Clustering accuracy(%)
We have shown both average graph classification accuracy and we aim to conduct sensitivity analysis of the proposed algorithm which combines all these components into a single network. Clearly, the performances in Figure 4b and 4c are better than in Figure 4a, but the best performance is achieved in Figure 4d which uses the complete SubGattPool network on MUTAG. The same observation of improved performance of the variants of SubGattPool over DIFFPOOL and the performance of SubGattPool over its variants is also prominent in Figure 5 on PTC dataset. This clearly shows the individual and combined usefulness of various components of SubGattPool for graph representation.

4.6 Sensitivity Analysis

We aim to conduct sensitivity analysis of the proposed algorithm in this section. SubGatt network has four important hyperparameters. They are: (i) Maximum size of a subgraph (T), (ii) Number of subgraphs sampled per node in each epoch (L) and (iii) Dimension of the final node representation or embedding (K) (See Eq. 2) and (iv) Number of SubGatt layers used in the network. We conduct graph classification experiment on MUTAG to see the sensitivity of SubGattPool with respect to each of these hyperparameters. Figure 6 shows the variation of the performance of SubGattPool network for graph classification with respect to all these hyper-parameters. We have shown both average graph classification accuracy and standard deviation over 10 repetitions for each experiment. From Figure 6, we can see that the performance of SubGattPool on MUTAG improves when maximum length of subgraph is set to 3. As the average size of a graph in MUTAG is quite small, a subgraph of size more than 3 does not help. Similarly, Figure shows that with increasing number of samples (L) for each node in an epoch, the performance of SubGattPool improves first, and then saturates. The same observation can be made in Figure for embedding dimension of the graphs. We use SubGatt as the embedding and pooling layers of the GNN after level graph 1. Figure shows that best performance on MUTAG is obtained with 2 layers of SubGatt.

Adding more number of layers actually deteriorates the performance because of oversmoothing which is a well-known problem of graph neural networks [21]. Overall, the variation is as expected and often less with respect to each hyper-parameter and hence it shows the robustness of SubGattPool. Please note, when we are varying one hyper-parameter of SubGattPool, the values of all other hyper-parameters are fixed to the values mentioned in Section 4.1.

5 CONCLUSION

We have proposed a novel GNN based robust graph classification algorithm called SubGattPool which uses higher order attention over the subgraphs of a graph and also addresses some shortcomings of the existing hierarchical graph representation techniques. We conduct experiments with both real world and synthetic graph datasets on multiple graph-level downstream tasks to show the robustness of our algorithm. We are also able to improve the state-of-the-art graph classification performance on four popularly used graph datasets. In future, we would like to theoretically examine the expressiveness power of SubGatt and SubGattPool for node and graph representations respectively. We will also analyze and see the recovery of communities in a graph in the hierarchical structure of SubGattPool. Overall, we believe that this work would encourage further development in the area of hierarchical graph representation and classification.

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